



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 12:57 AM EDT

PDB ID : 8G2B / pdb_00008g2b
Title : Crystal structure of the A2503-C2,C8-dimethylated *Thermus thermophilus* 70S ribosome in complex with iboxamycin, mRNA, deacylated A- and E-site tRNA^{phe}, and aminoacylated P-site fMet-tRNA^{met} at 2.55Å resolution
Authors : Aleksandrova, E.V.; Wu, K.J.Y.; Tresco, B.I.C.; Syroegin, E.A.; Killeavy, E.E.; Balasanyants, S.M.; Svetlov, M.S.; Gregory, S.T.; Atkinson, G.C.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2023-02-03
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

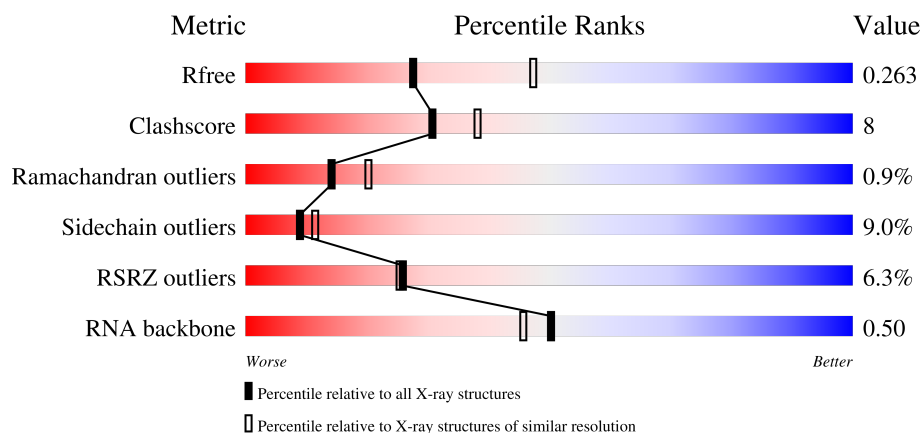
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

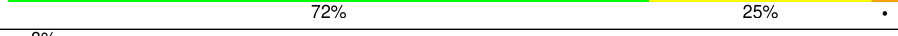
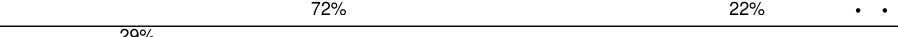
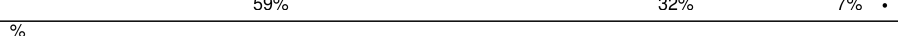
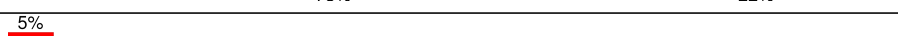
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 65% 27% 7%
1	2A	2915	3% 59% 31% 7%

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	1B	121	
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	

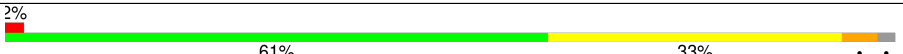
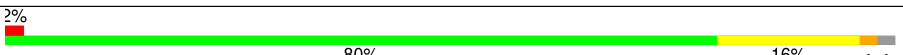
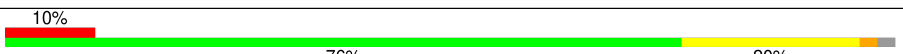
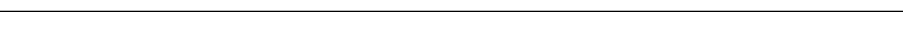
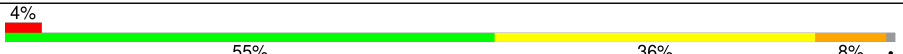
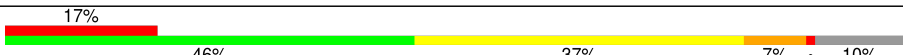
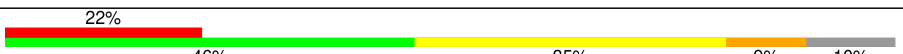
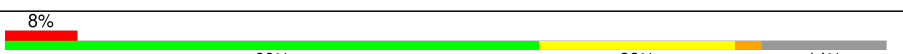
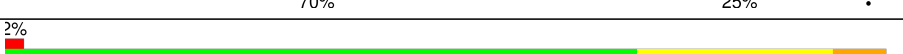
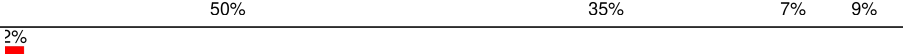
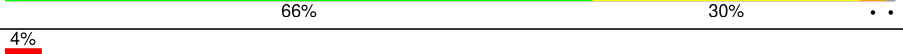
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1a	1680	-	-	-	X
59	SF4	2d	303	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299868 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61853	27532	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60323	26849	11284	19390	2800			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called MF-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site and E-site Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0	0
			1570	703	280	512	73	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	70	Total	C	N	O	P	S	0	0	0
			1502	671	270	489	70	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site Aminoacylated fMet-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1083	Total	Mg	0	0
			1083	1083		
56	1B	38	Total	Mg	0	0
			38	38		
56	1D	13	Total	Mg	0	0
			13	13		
56	1E	14	Total	Mg	0	0
			14	14		
56	1F	13	Total	Mg	0	0
			13	13		
56	1G	5	Total	Mg	0	0
			5	5		
56	1H	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1I	1	Total Mg 1 1	0	0
56	1N	6	Total Mg 6 6	0	0
56	1O	4	Total Mg 4 4	0	0
56	1P	6	Total Mg 6 6	0	0
56	1Q	6	Total Mg 6 6	0	0
56	1R	5	Total Mg 5 5	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	2	Total Mg 2 2	0	0
56	1U	11	Total Mg 11 11	0	0
56	1V	7	Total Mg 7 7	0	0
56	1W	9	Total Mg 9 9	0	0
56	1X	6	Total Mg 6 6	0	0
56	1Y	4	Total Mg 4 4	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	8	Total Mg 8 8	0	0
56	11	6	Total Mg 6 6	0	0
56	12	2	Total Mg 2 2	0	0
56	13	4	Total Mg 4 4	0	0
56	14	1	Total Mg 1 1	0	0
56	15	8	Total Mg 8 8	0	0
56	16	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	17	6	Total 6	Mg 6	0	0
56	18	5	Total 5	Mg 5	0	0
56	19	1	Total 1	Mg 1	0	0
56	1a	211	Total 211	Mg 211	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	2	Total 2	Mg 2	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1r	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	2	Total 2	Mg 2	0	0
56	1w	7	Total 7	Mg 7	0	0
56	1x	15	Total 15	Mg 15	0	0
56	1y	1	Total 1	Mg 1	0	0
56	2A	830	Total 830	Mg 830	0	0
56	2B	19	Total 19	Mg 19	0	0
56	2D	7	Total 7	Mg 7	0	0

Continued on next page...

Continued from previous page...

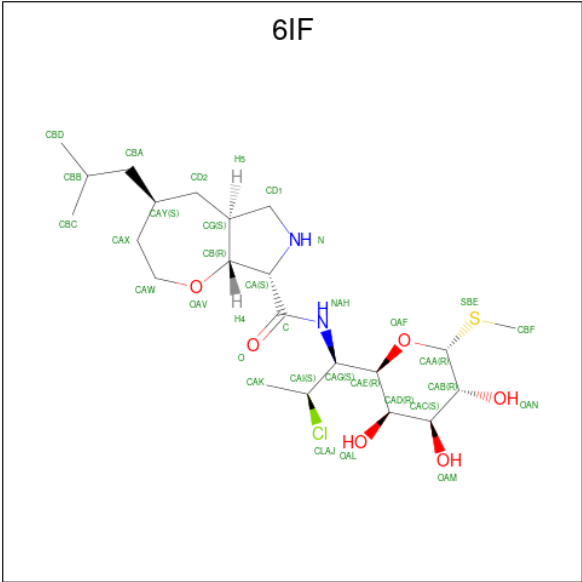
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	9	Total 9	Mg 9	0	0
56	2F	7	Total 7	Mg 7	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2P	2	Total 2	Mg 2	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	3	Total 3	Mg 3	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	1	Total 1	Mg 1	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	3	Total 3	Mg 3	0	0
56	2X	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	5	Total 5	Mg 5	0	0
56	21	2	Total 2	Mg 2	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	7	Total 7	Mg 7	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	3	Total 3	Mg 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	28	2	Total 2	Mg 2	0	0
56	29	1	Total 1	Mg 1	0	0
56	2a	211	Total 211	Mg 211	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2j	1	Total 1	Mg 1	0	0
56	2l	3	Total 3	Mg 3	0	0
56	2p	1	Total 1	Mg 1	0	0
56	2q	3	Total 3	Mg 3	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	3	Total 3	Mg 3	0	0
56	2w	4	Total 4	Mg 4	0	0
56	2x	7	Total 7	Mg 7	0	0
56	2y	5	Total 5	Mg 5	0	0

- Molecule 57 is methyl 7-chloro-6,7,8-trideoxy-6-[[[(4S,5aS,8S,8aR)-4-(2-methylpropyl)octahydro-2H-oxepino[2,3-c]pyrrole-8-carbonyl]amino]-1-thio-L-threo- α -D-galacto-octopyranoside (CCD ID: 6IF) (formula: C₂₂H₃₉ClN₂O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
57	1A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		
57	2A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

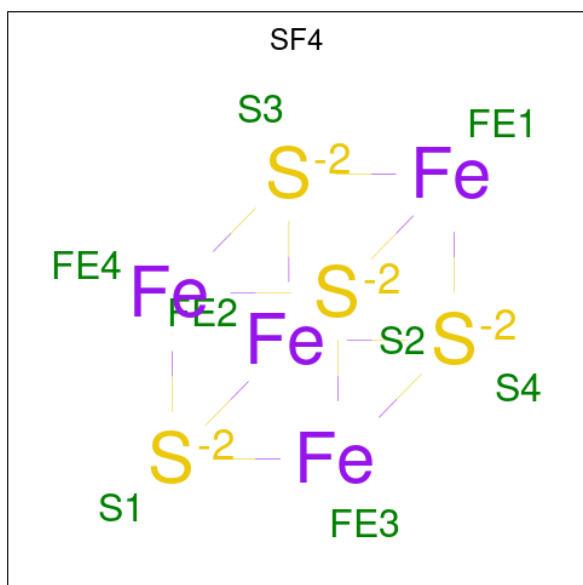
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1x	1	Total	K	0	0
			1	1		
60	2x	1	Total	K	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1971	Total	O	0	0
			1971	1971		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1B	60	Total 60	O 60	0	0
61	1D	28	Total 28	O 28	0	0
61	1E	30	Total 30	O 30	0	0
61	1F	16	Total 16	O 16	0	0
61	1G	2	Total 2	O 2	0	0
61	1H	3	Total 3	O 3	0	0
61	1N	9	Total 9	O 9	0	0
61	1O	4	Total 4	O 4	0	0
61	1P	15	Total 15	O 15	0	0
61	1Q	10	Total 10	O 10	0	0
61	1R	12	Total 12	O 12	0	0
61	1S	5	Total 5	O 5	0	0
61	1T	8	Total 8	O 8	0	0
61	1U	14	Total 14	O 14	0	0
61	1V	8	Total 8	O 8	0	0
61	1W	4	Total 4	O 4	0	0
61	1X	6	Total 6	O 6	0	0
61	1Y	2	Total 2	O 2	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	13	Total 13	O 13	0	0
61	11	9	Total 9	O 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	12	4	Total 4	O 4	0	0
61	13	3	Total 3	O 3	0	0
61	14	1	Total 1	O 1	0	0
61	15	4	Total 4	O 4	0	0
61	16	2	Total 2	O 2	0	0
61	17	9	Total 9	O 9	0	0
61	18	13	Total 13	O 13	0	0
61	1a	357	Total 357	O 357	0	0
61	1b	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1i	2	Total 2	O 2	0	0
61	1l	4	Total 4	O 4	0	0
61	1m	2	Total 2	O 2	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1t	1	Total 1	O 1	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	4	Total 4	O 4	0	0
61	1w	10	Total 10	O 10	0	0
61	1x	17	Total 17	O 17	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1y	1	Total 1	O 1	0	0
61	2A	1109	Total 1109	O 1109	0	0
61	2B	20	Total 20	O 20	0	0
61	2D	21	Total 21	O 21	0	0
61	2E	13	Total 13	O 13	0	0
61	2F	11	Total 11	O 11	0	0
61	2O	3	Total 3	O 3	0	0
61	2P	8	Total 8	O 8	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	3	Total 3	O 3	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	4	Total 4	O 4	0	0
61	2W	1	Total 1	O 1	0	0
61	2X	1	Total 1	O 1	0	0
61	2Y	1	Total 1	O 1	0	0
61	20	4	Total 4	O 4	0	0
61	21	6	Total 6	O 6	0	0
61	23	2	Total 2	O 2	0	0
61	25	2	Total 2	O 2	0	0
61	27	1	Total 1	O 1	0	0
61	28	6	Total 6	O 6	0	0

Continued on next page...

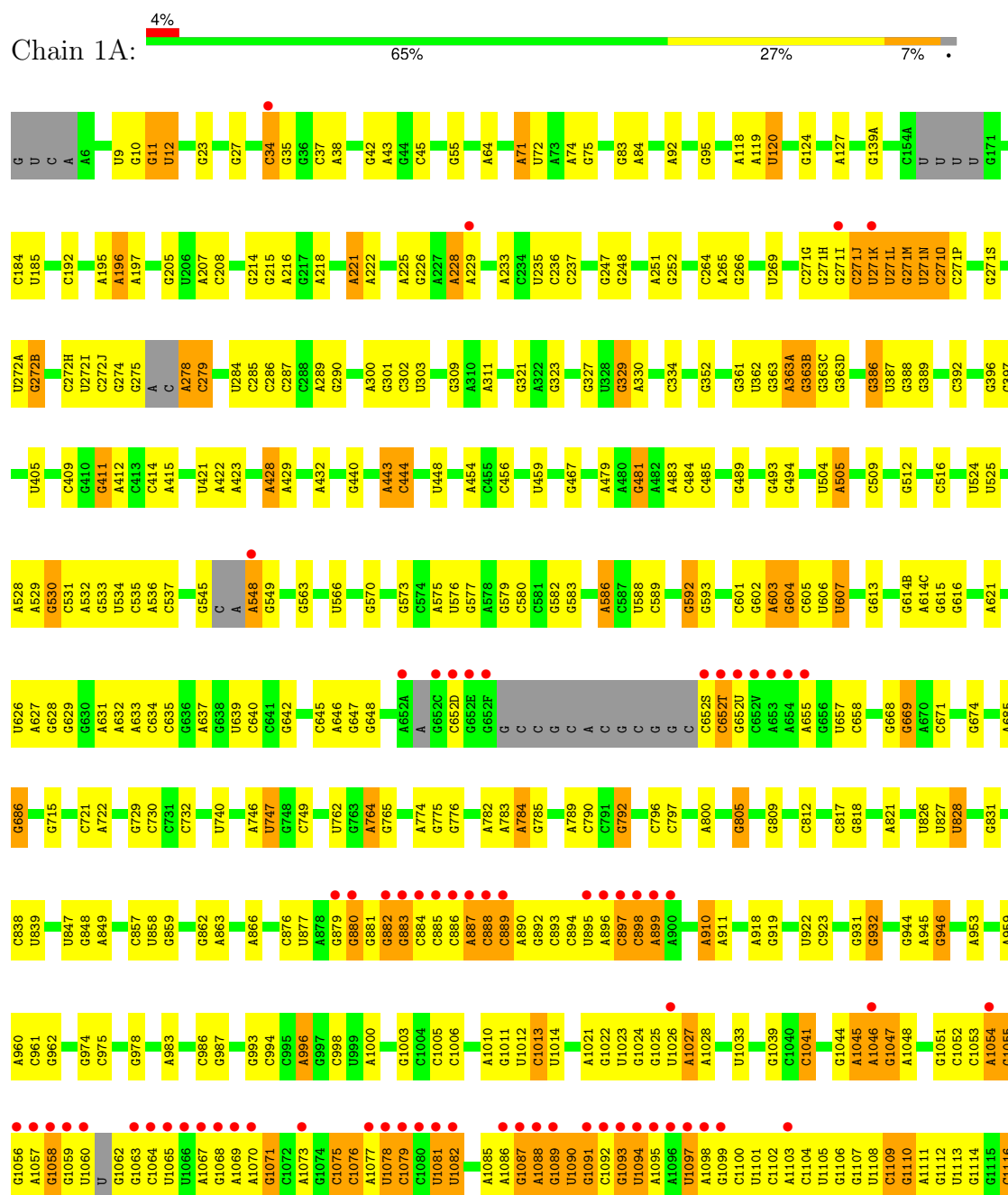
Continued from previous page...

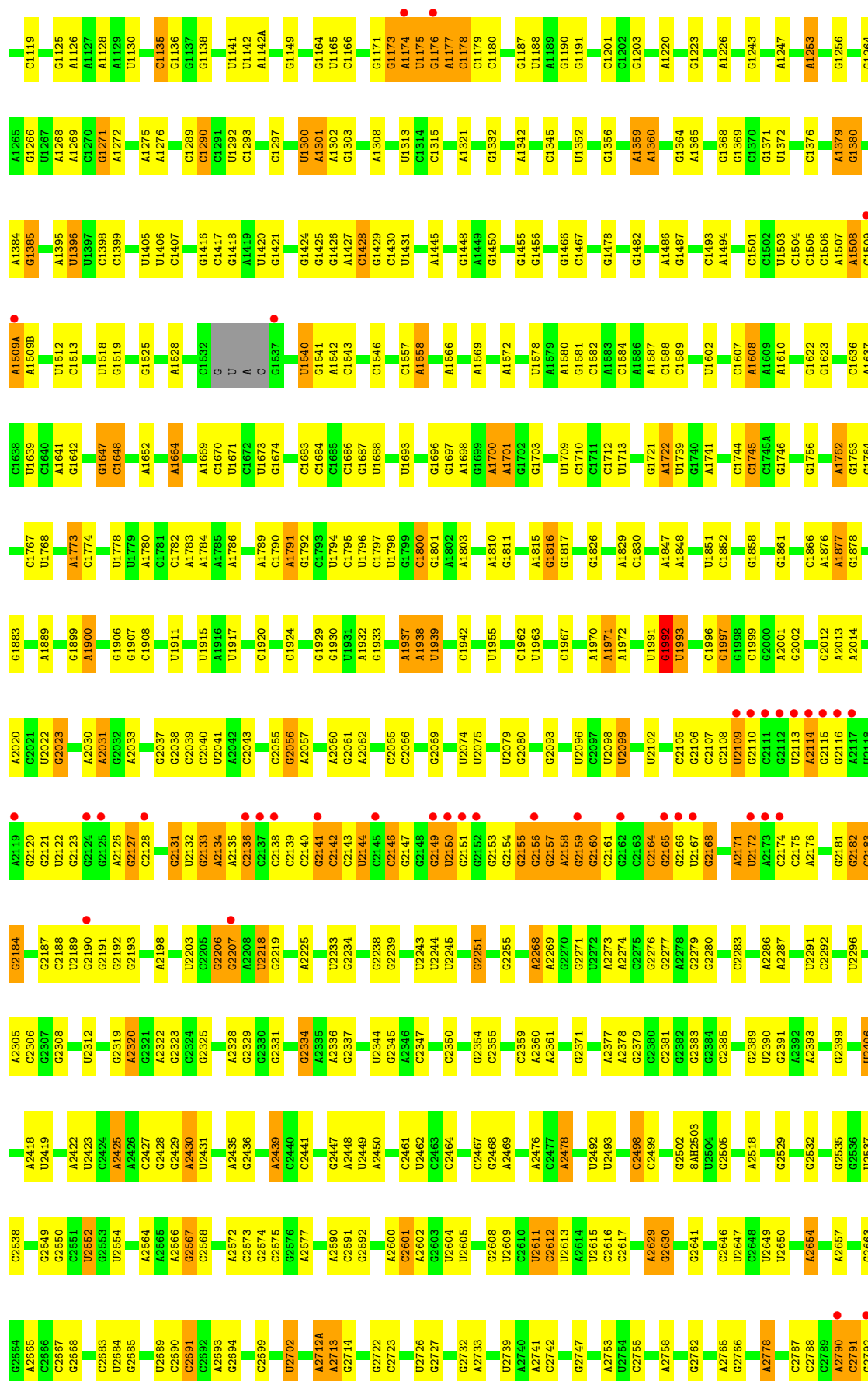
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	29	1	Total 1	O 1	0	0
61	2a	221	Total 221	O 221	0	0
61	2d	2	Total 2	O 2	0	0
61	2j	3	Total 3	O 3	0	0
61	2l	1	Total 1	O 1	0	0
61	2o	1	Total 1	O 1	0	0
61	2p	1	Total 1	O 1	0	0
61	2t	2	Total 2	O 2	0	0
61	2x	4	Total 4	O 4	0	0
61	2y	7	Total 7	O 7	0	0

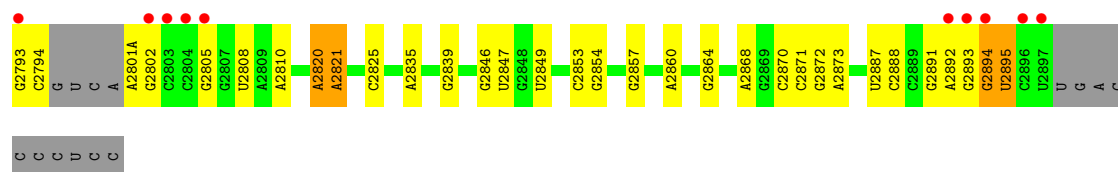
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

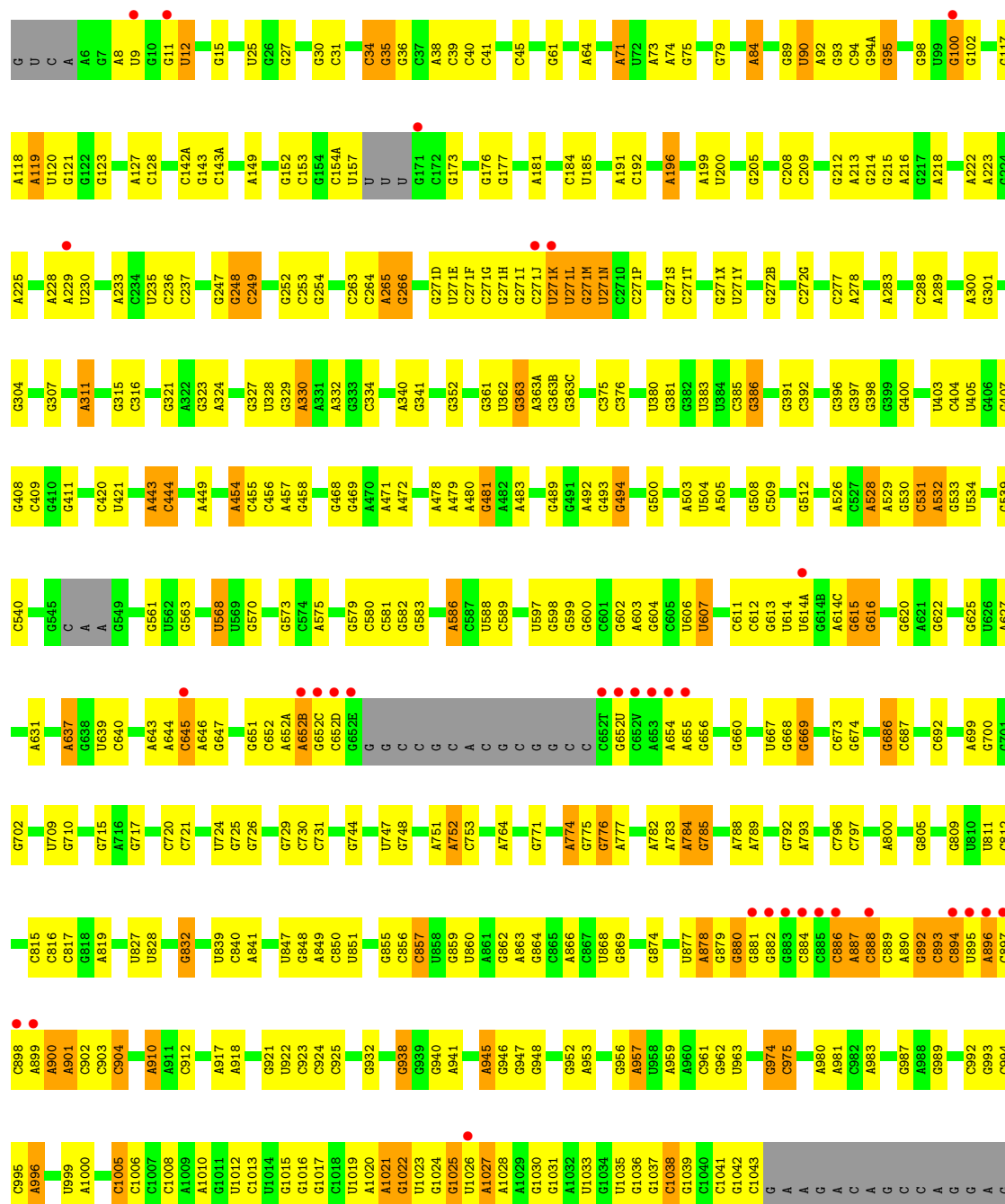
• Molecule 1: 23S Ribosomal RNA







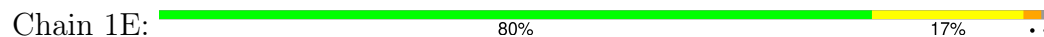
• Molecule 1: 23S Ribosomal RNA



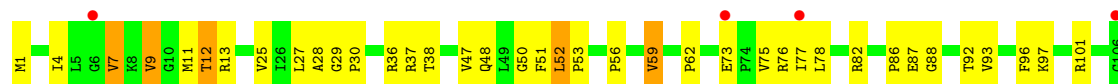
C2380	C2384	C2164	U2099	U1911	C1790	C1670	G1539	A1434	U1316	U1211	G
G2383	C2285	G2165	C2105	A1912	A1791	G1674	U1540	A1434	A1317	G1212	U
G2384	A2286	U2167	A2013	A1913	U1794	G1674	G1541	C1437	A1318	A1213	U
C2385	A2288	G2168	A2014	C1914	C1795	C1686	A1542	C1437	G1325	U1220	G
G2391	G2291	A2169	A2019	U1915	U1796	U1687	C1543	G1442	U1334	G1231	C
A2392	C2292	A2170	A2020	U1917	C1797	U1688	C1546	G1442	U1335	G1232	U
A2393	C2293	A2171	C2021	A1918	U1798	U1689	C1547	A1445	A1336	G1232	U
C2394	C2294	A2172	U2022	A1919	G1799	A1689	C1547	A1445A	A1337	A1237	A
C2395	C2295	A2173	G2023	C1920	U1799	A1690	C1547	G1446	G1337	G1238	G
G2396	U2296	C2174	A2114	C1924	G1801	U1693	A1554	G1447	U1240	G1239	A
G2400	G2299	G2175	G2115	G2027	A1802	G1696	G1555	G1448	U1345	G1240	C
G2403	G2303	C2176	G2116	A2030	A1803	G1697	G1556	G1449	U1352	U1241	C
C2404	G2304	C2177	U2118	A1927	A1810	A1697	C1557	G1450	A1354	A1242	A
C2405	A2305	G2182	A2119	A1928	G1811	A1698	C1558	G1450A	A1354	G1243	G
G2406	G2306	G2183	G2120	G1929	A1812	A1699	A1588	C1451	A1354	G1244	C
U2406	C2307	G2184	A2033	U1931	A1815	G1702	A1566	G1459	U1357	G1248	C
G2410	G2308	C2185	G2036	A1932	G1816	G1703	A1567	A1460	G1358	G1248	A
G2413	C2313	C2188	G2037	G1933	A1821	U1709	A1568	G1461	A1359	G1252	U
G2414	G2314	U2189	G2038	A1936	A1822	C1710	U1578	G1462	A1360	A1253	C
U2419	G2315	A2191	C2043	A1937	G1829	C1711	A1579	G1466	A1366	G1256	C
C2420	C2316	G2192	G2049	U1938	C1830	C1712	A1580	C1467	A1367	C1257	U
A2425	G2317	A2198	C2050	U1939	G1835	U1720	A1583	A1471	G1368	G1260	U
G2429	G2318	U2199	A2051	C1942	U1836	G1721	A1584	A1477	G1369	C1261	A
A2430	C2319	C2128	G2055	U1955	G1837	U1722	C1592	G1478	A1370	G1262	A
A2431	A2320	G2129	C2056	C1958	G1838	A1741	G1593	G1482	G1371	U1263	G
G2432	G2325	U2203	A2057	C1962	G1839	C1752	G1594	A1482	A1372	G1264	G
G2433	C2326	C2206	G2058	U1963	C1843	G1753	A1608	A1490	A1378	G1266	U
A2435	G2327	U2207	A2059	U1963	C1843	C1754	A1609	A1490	A1379	U1267	C
A2439	A2328	U2218	G2060	C1967	A1847	A1755	A1610	A1493	A1269	G1171	U
G2440	G2329	A2225	G2061	G1968	A1848	U1757	A1616	A1495	C1270	G	A
C2441	G2330	G2228	A2062	A1969	U1851	G1758	A1632	A1496	A1384	A	A
A2448	A2335	C2229	C2063	A1970	U1852	C1758	A1632	U1497	G1385	U	U
G2454	G2336	U2232	C2064	A1971	G1852	A1762	A1639	C1506	G1386	G	A
A2459	C2343	U2233	C2065	A1972	G1857	G1763	U1639	A1507	G1387	A	G
C2465	C2347	G2234	G2069	G1973	G1858	G1764	C1640	A1508	G1389	C1178	C
A2469	U2348	G2235	G2070	A1981	G1861	U1769	G1647	C1509	U1405	G1183	U
G2472	G2350	G2236	A2071	G1984	U1864	G1769	C1648	A1509A	G1406	G1184	A
C2475	G2354	U2349	U2074	U1991	U1874	A1773	A1651	G1510	U1292	C1185	C
A2476	C2355	G2239	U2075	G1992	A1876	C1774	G1652	G1510	G1293	G1186	U
G2483	G2356	G2240	C2078	U1993	G1877	U1775	G1653	U1514	U1294	U1188	G
G2484	G2357	G2241	U2079	C1996	G1878	U1778	A1654	G1515	C1295	G1191	U
G2485	A2373	A2268	U2086	G1997	A1889	U1779	C1657	G1529	G1296	G1192	C
G2489	A2376	G2273	G2087	G1998	A1890	U1780	C1658	C1530	U1300	G1195	A
	G2373	C2274	C2090	C1999	G1899	C1781	C1531	G1532	A1301	G1195	U
	A2376	G2275	G2090	G2000	A1900	A1782	A1664	G1533	A1302	U1205	G
	G2376	G2276	U2096	C2006	A1785	A1784	A1665	U	G1303		
	G2379	G2277	C2097	G2010	A1786	U1786	G1667	A	C1314	G1209	
		C2283	U2098	G2010	G1906			C1536	G1315	A1210	



• Molecule 4: 50S ribosomal protein L3



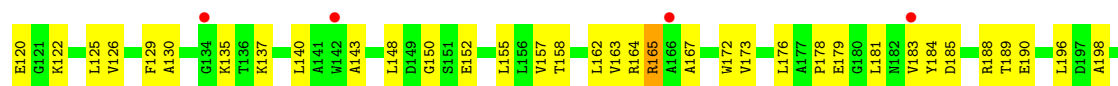
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

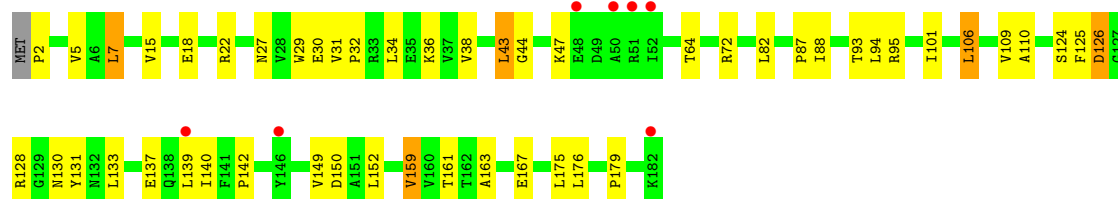


• Molecule 5: 50S ribosomal protein L4



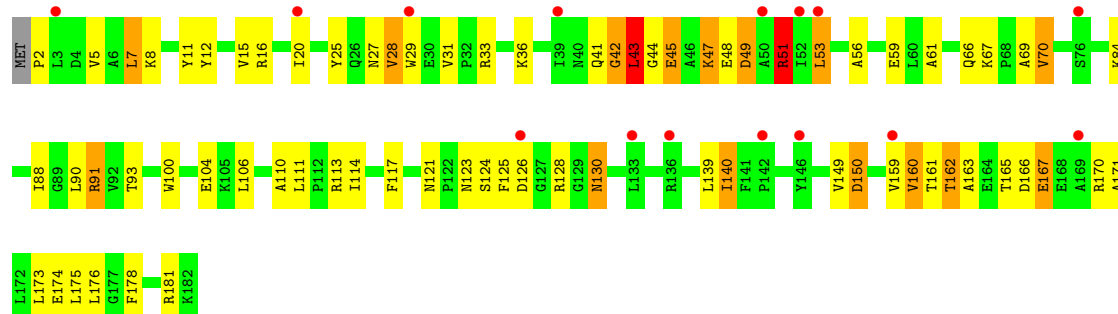
• Molecule 6: 50S ribosomal protein L5

Chain 1G: 



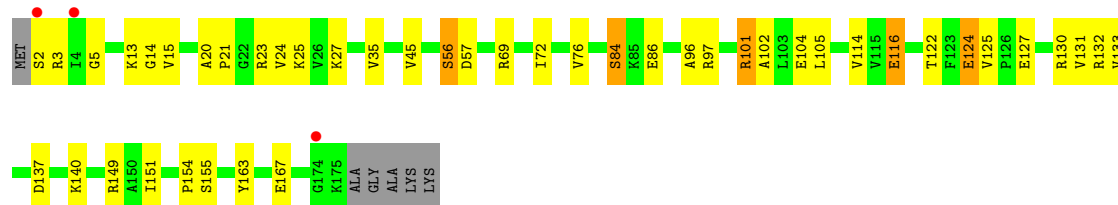
- Molecule 6: 50S ribosomal protein L5

Chain 2G: 



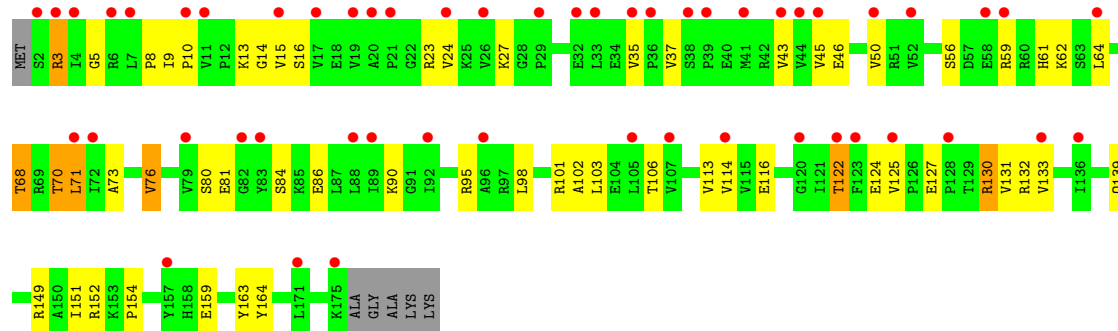
- Molecule 7: 50S ribosomal protein L6

Chain 1H: 

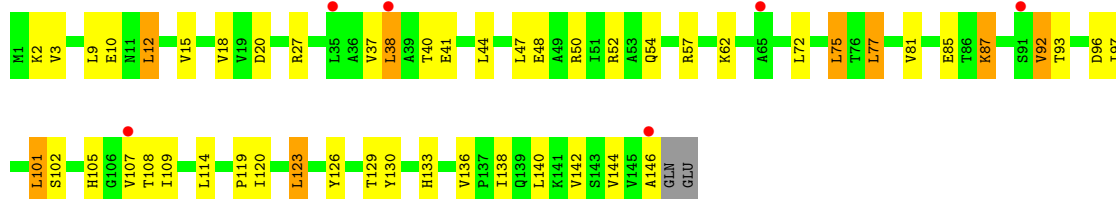


- Molecule 7: 50S ribosomal protein L6

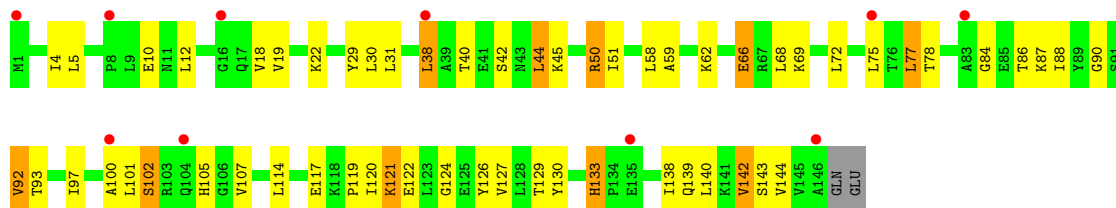
Chain 2H: 



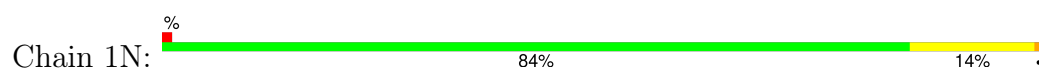
- Molecule 8: 50S ribosomal protein L9



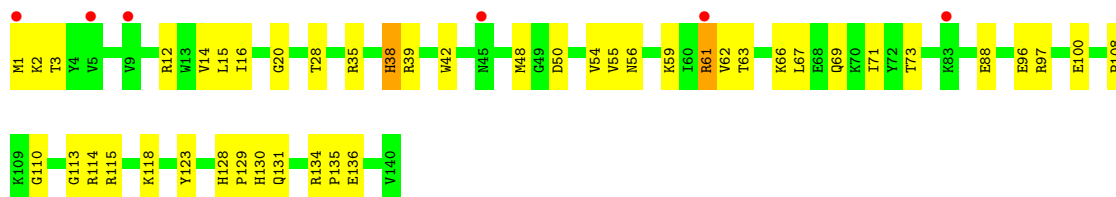
- Molecule 8: 50S ribosomal protein L9



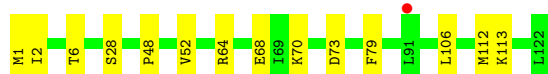
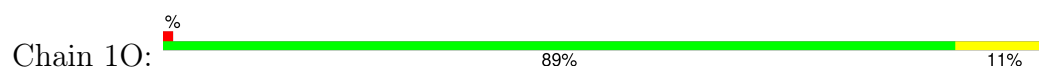
- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13

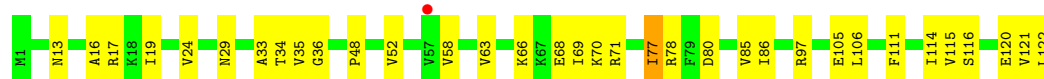


- Molecule 10: 50S ribosomal protein L14

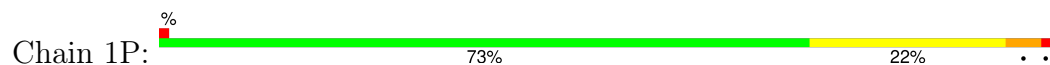


- Molecule 10: 50S ribosomal protein L14





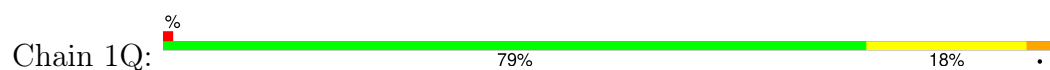
- Molecule 11: 50S ribosomal protein L15



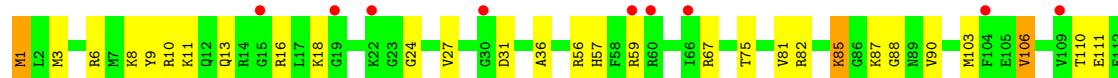
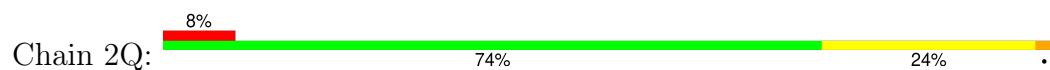
- Molecule 11: 50S ribosomal protein L15



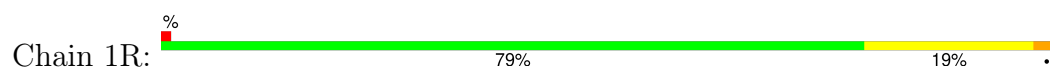
- Molecule 12: 50S ribosomal protein L16



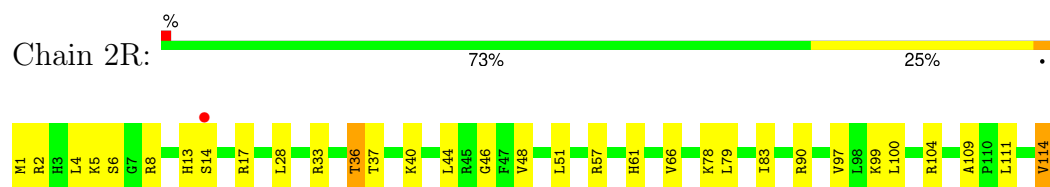
- Molecule 12: 50S ribosomal protein L16



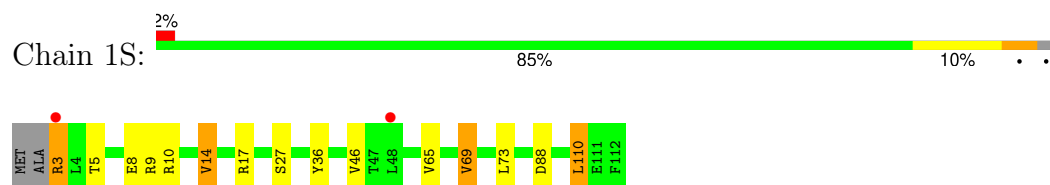
- Molecule 13: 50S ribosomal protein L17



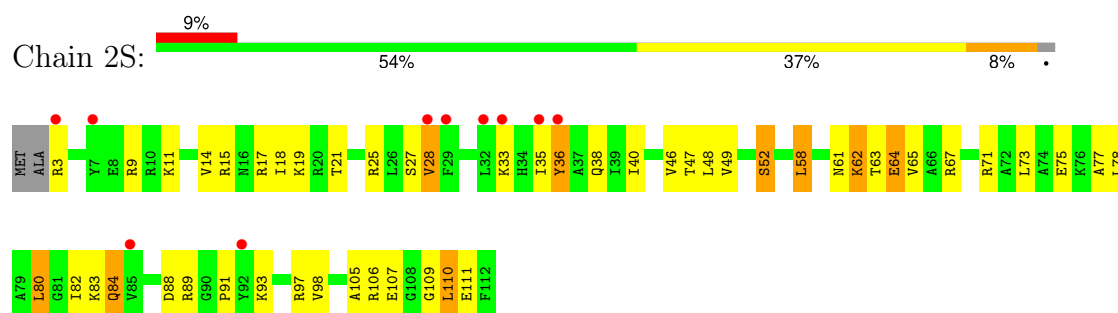
- Molecule 13: 50S ribosomal protein L17



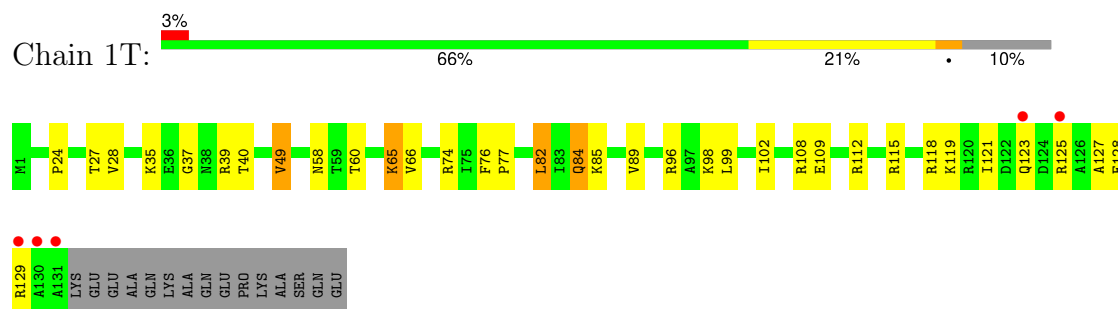
- Molecule 14: 50S ribosomal protein L18



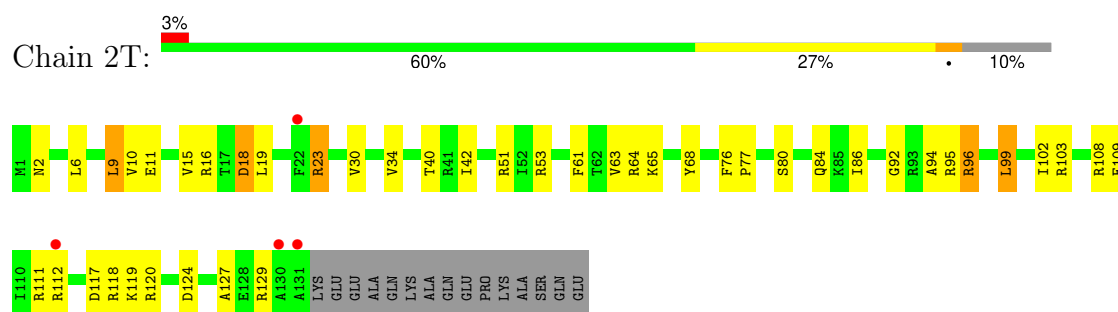
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



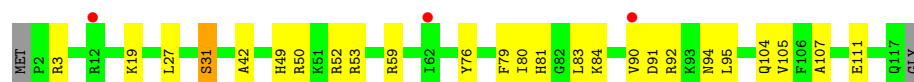
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  82% 14% ..



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  3% 77% 20% ..



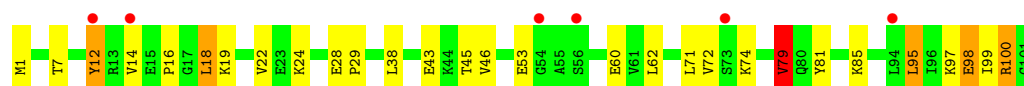
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  82% 16% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  6% 71% 23% 5% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  82% 16% ..



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  72% 26% ..

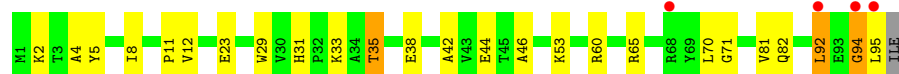
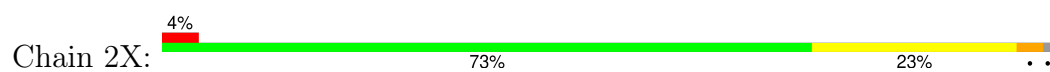


- Molecule 19: 50S ribosomal protein L23

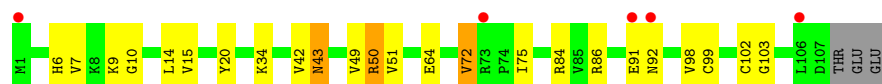
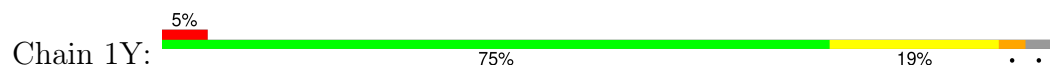
Chain 1X:  83% 15% ..



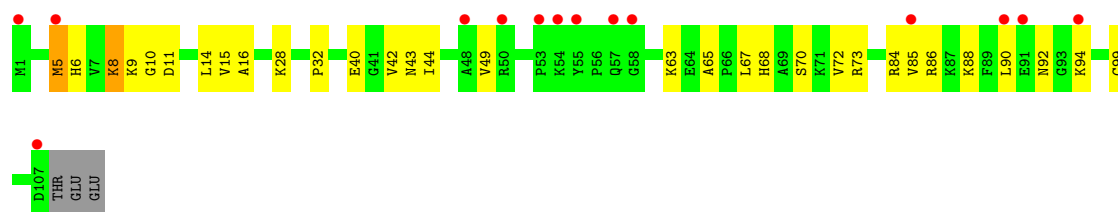
- Molecule 19: 50S ribosomal protein L23



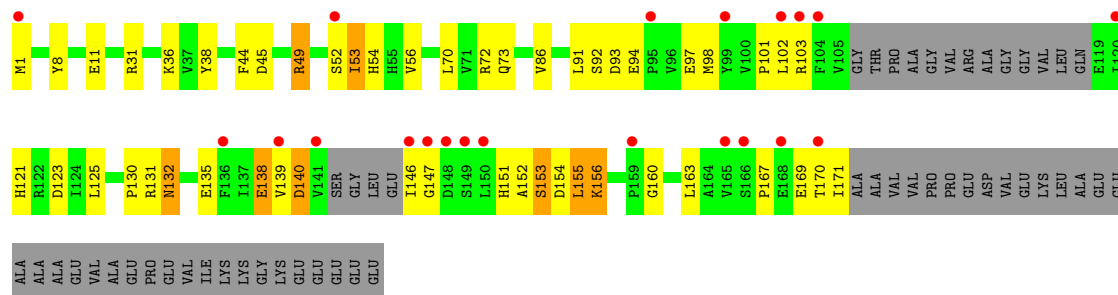
• Molecule 20: 50S ribosomal protein L24



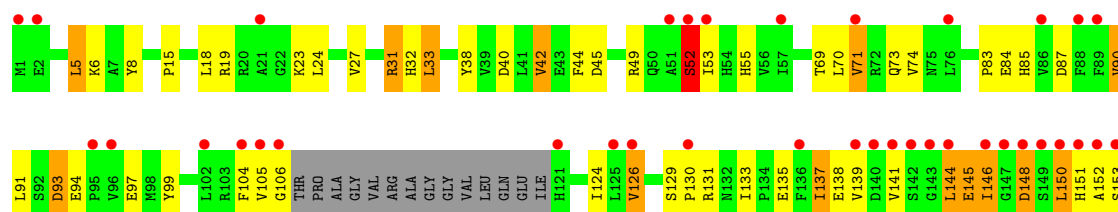
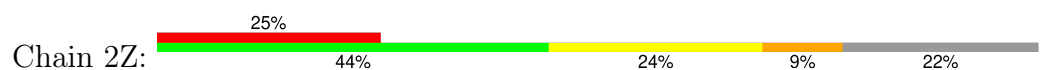
• Molecule 20: 50S ribosomal protein L24

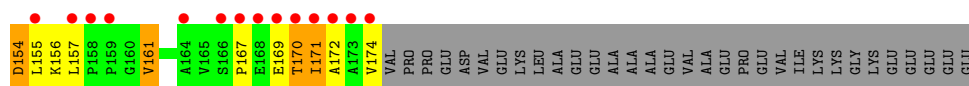


• Molecule 21: 50S ribosomal protein L25

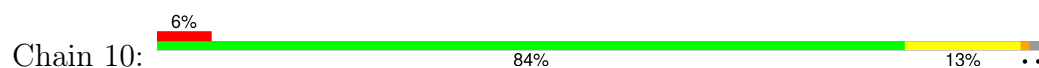


• Molecule 21: 50S ribosomal protein L25

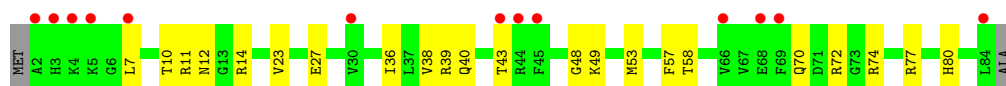




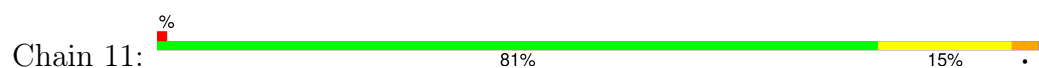
- Molecule 22: 50S ribosomal protein L27



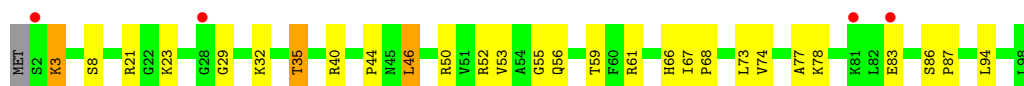
- Molecule 22: 50S ribosomal protein L27



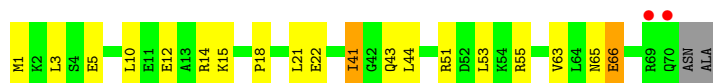
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



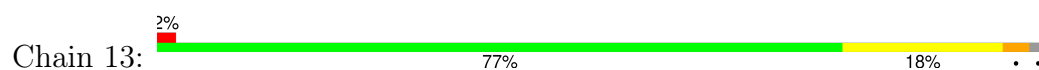
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



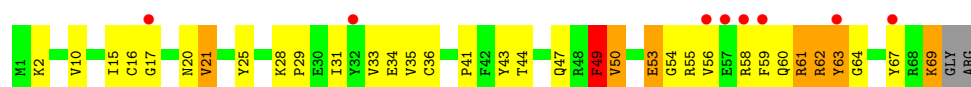
- Molecule 25: 50S ribosomal protein L30



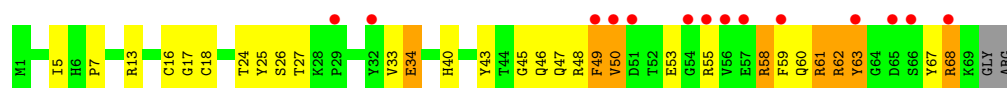
- Molecule 25: 50S ribosomal protein L30



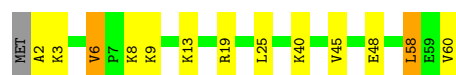
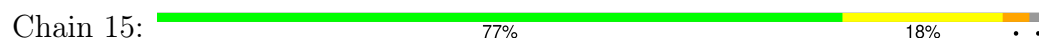
- Molecule 26: 50S ribosomal protein L31



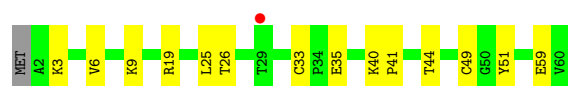
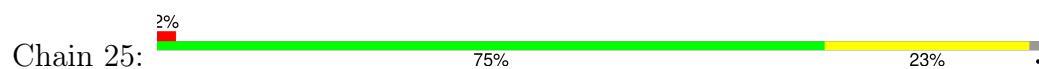
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



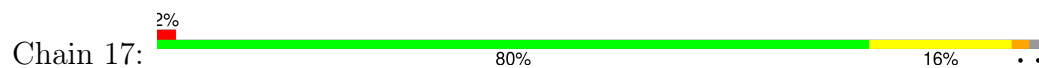
- Molecule 28: 50S ribosomal protein L33



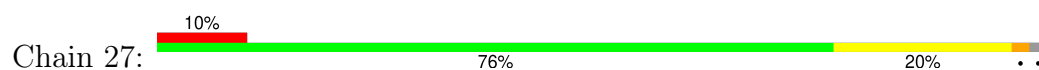
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



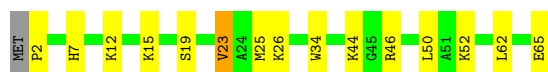
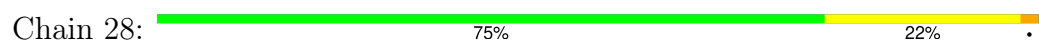
- Molecule 29: 50S ribosomal protein L34



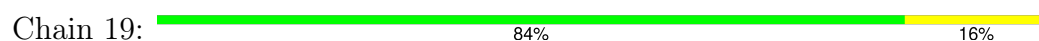
- Molecule 30: 50S ribosomal protein L35



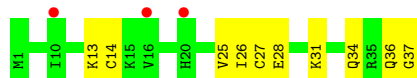
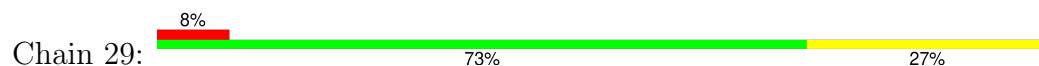
- Molecule 30: 50S ribosomal protein L35



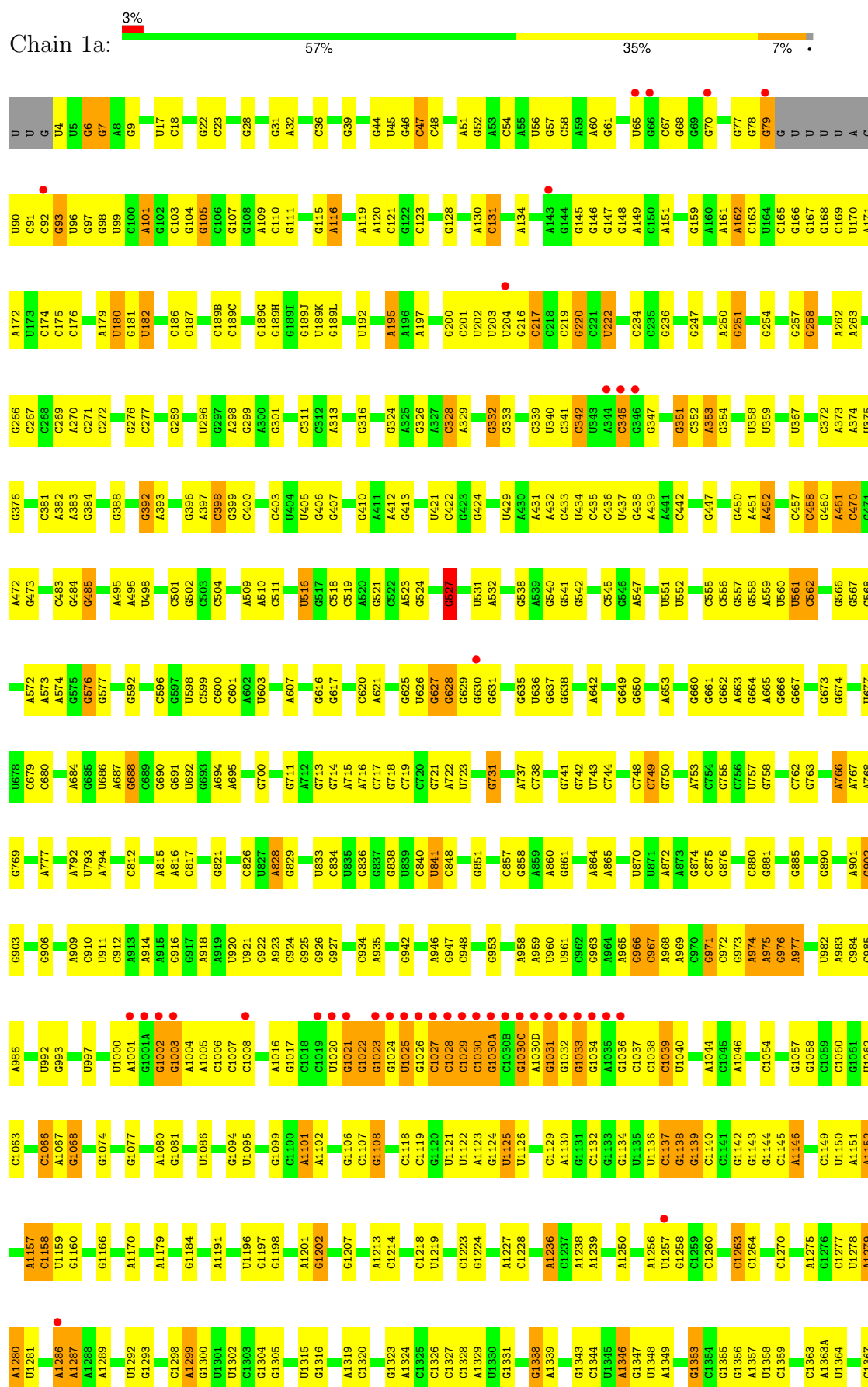
- Molecule 31: 50S ribosomal protein L36

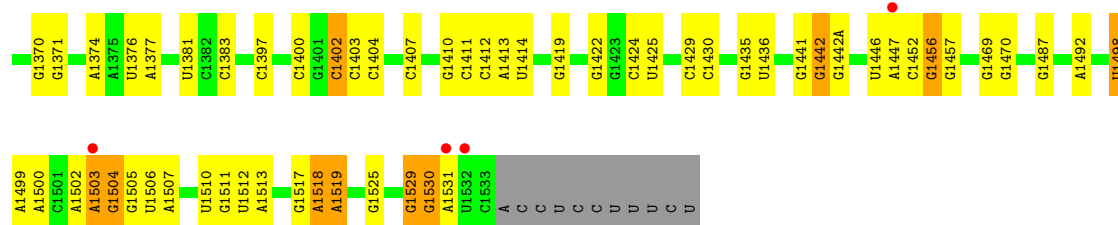


- Molecule 31: 50S ribosomal protein L36

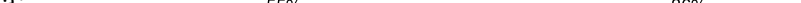


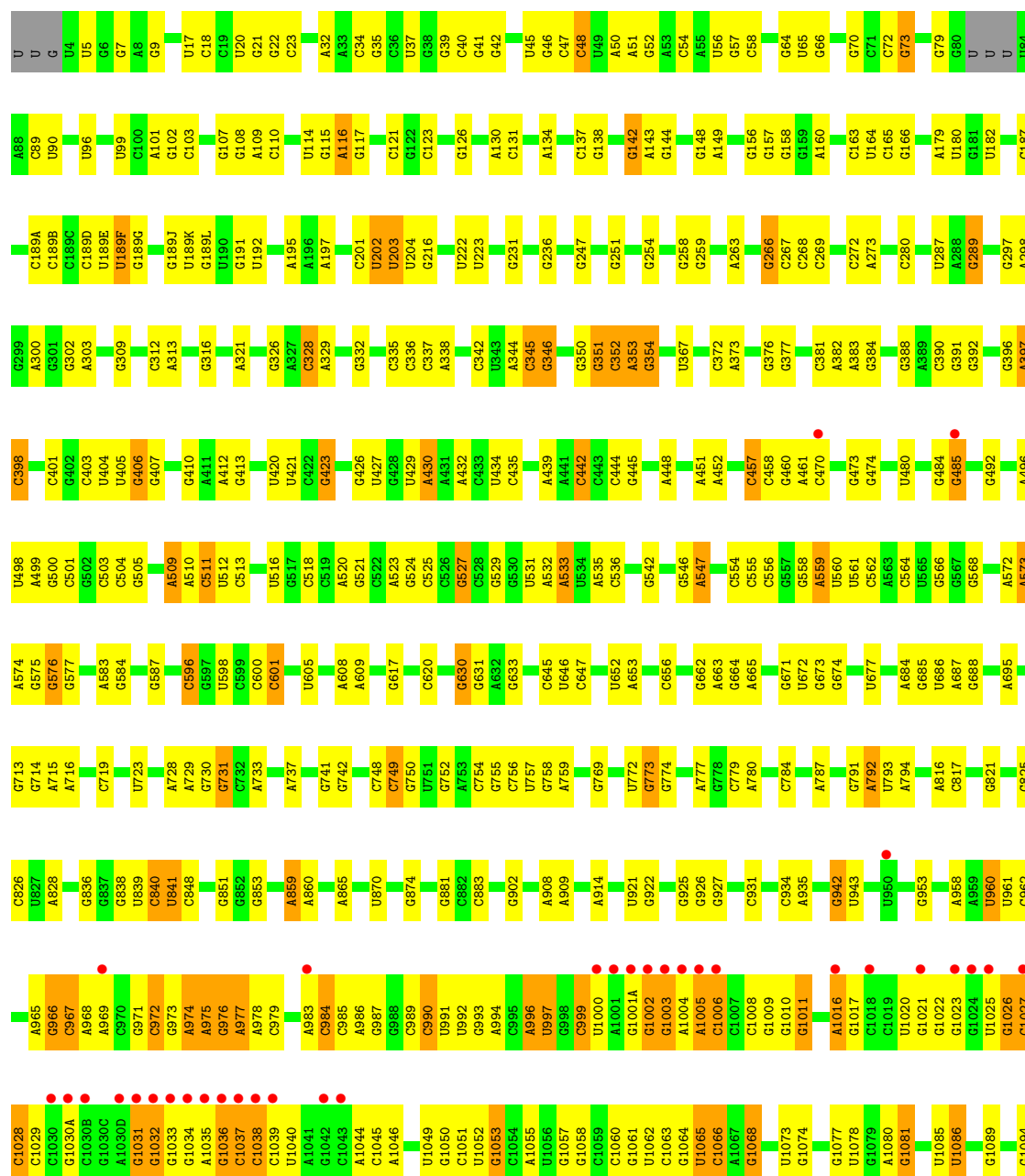
- Molecule 32: 16S Ribosomal RNA

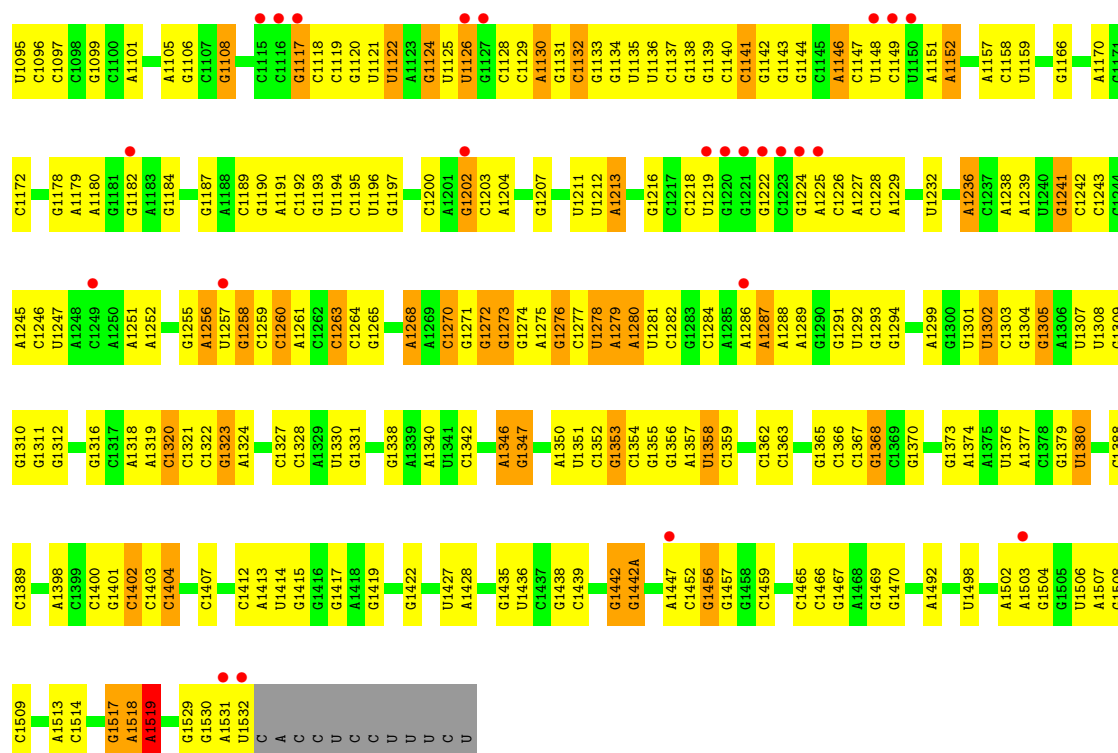




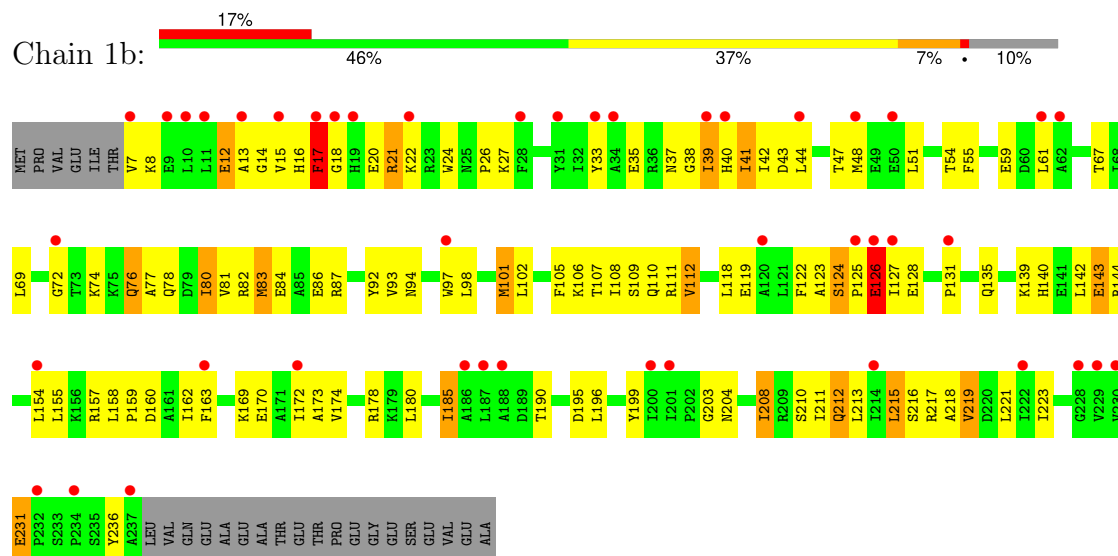
- Molecule 32: 16S Ribosomal RNA

Chain 2a: 

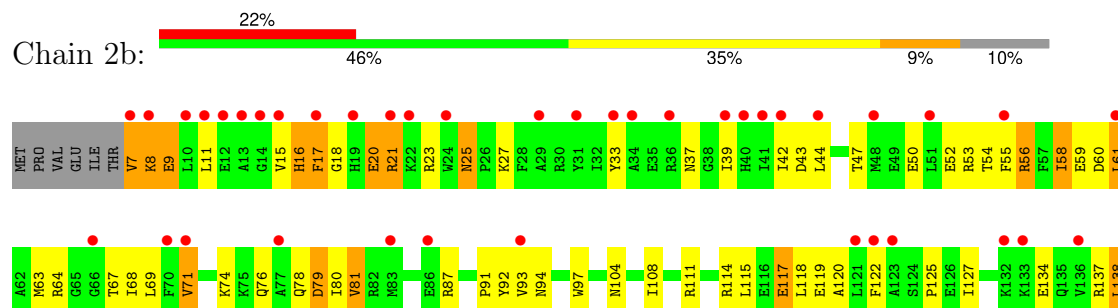


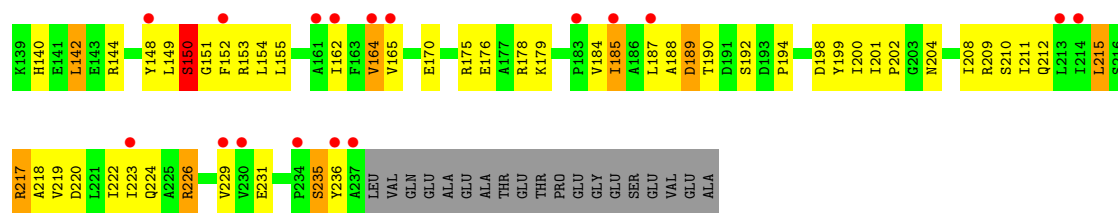


• Molecule 33: 30S ribosomal protein S2

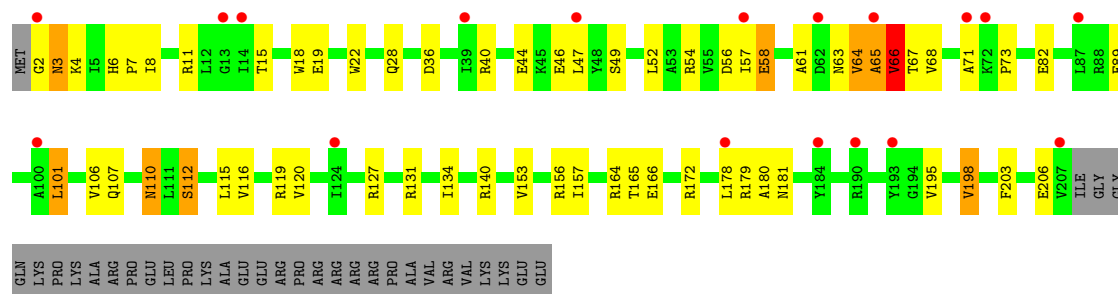


• Molecule 33: 30S ribosomal protein S2

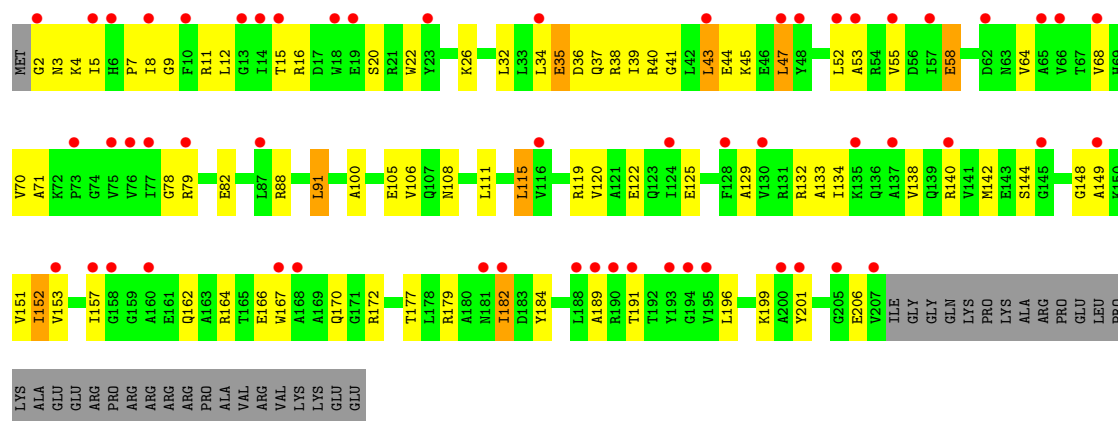




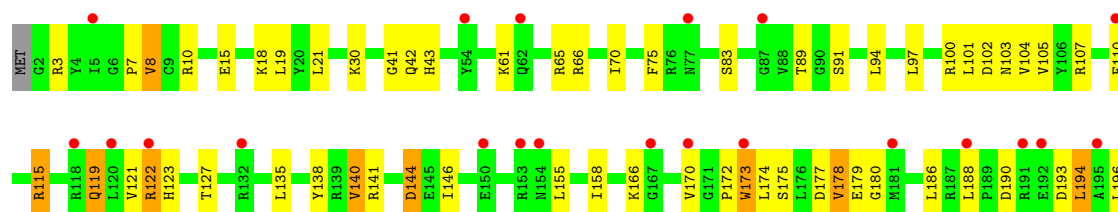
• Molecule 34: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S3

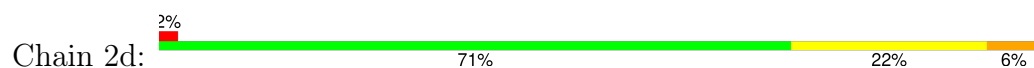


• Molecule 35: 30S ribosomal protein S4

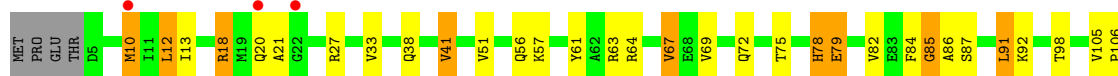




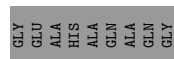
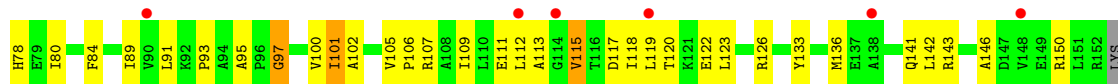
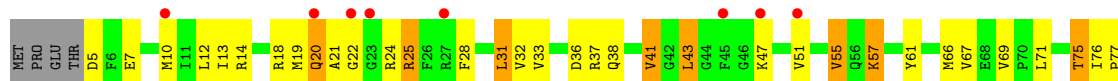
• Molecule 35: 30S ribosomal protein S4



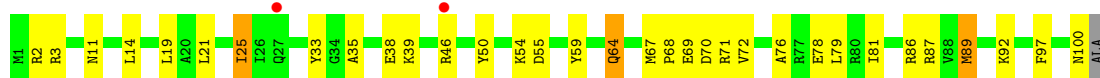
• Molecule 36: 30S ribosomal protein S5



• Molecule 36: 30S ribosomal protein S5

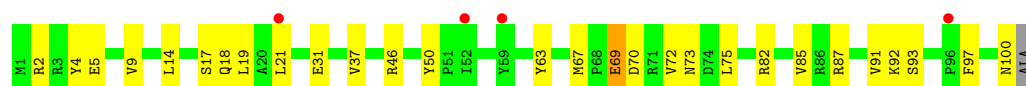


• Molecule 37: 30S ribosomal protein S6

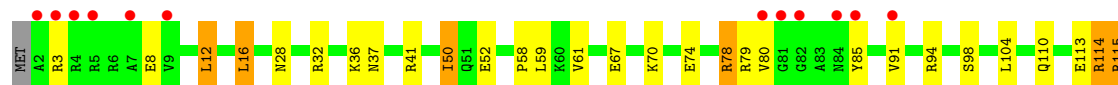
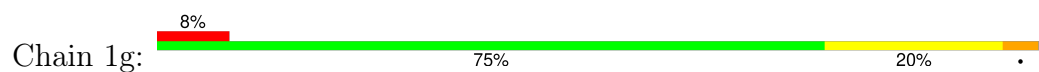


• Molecule 37: 30S ribosomal protein S6

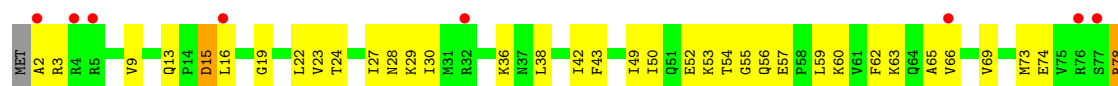




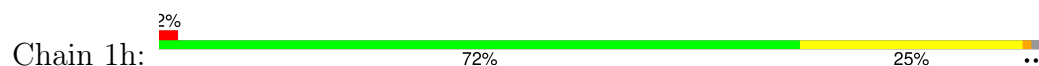
- Molecule 38: 30S ribosomal protein S7



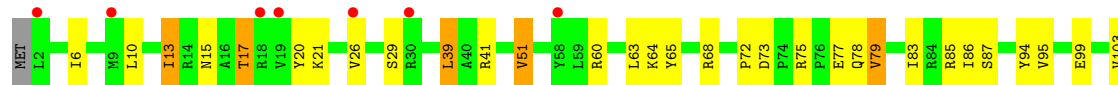
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

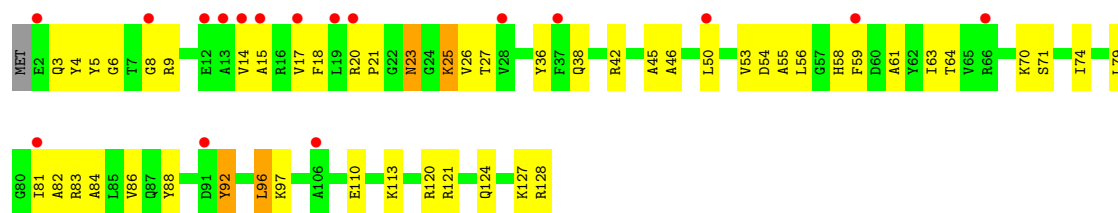


- Molecule 39: 30S ribosomal protein S8

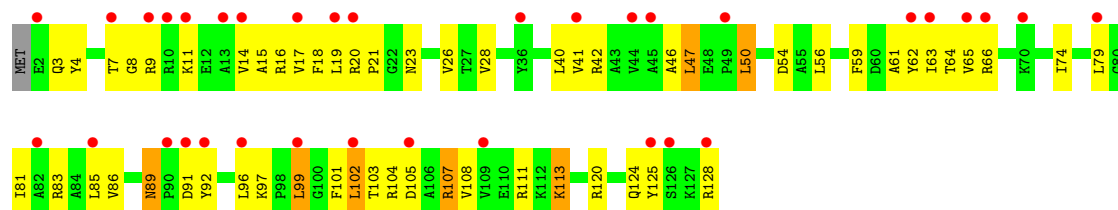


- Molecule 40: 30S ribosomal protein S9

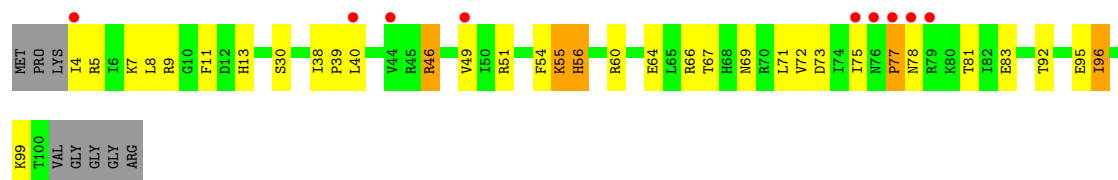




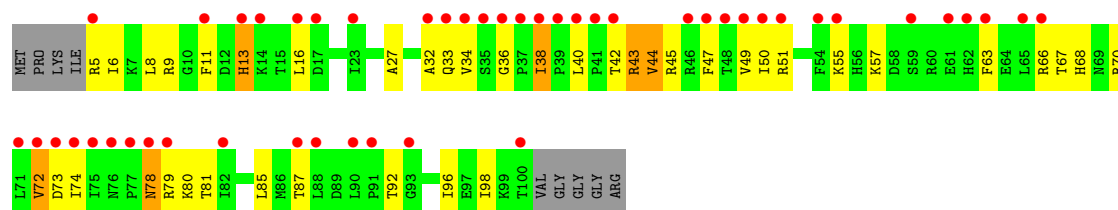
• Molecule 40: 30S ribosomal protein S9



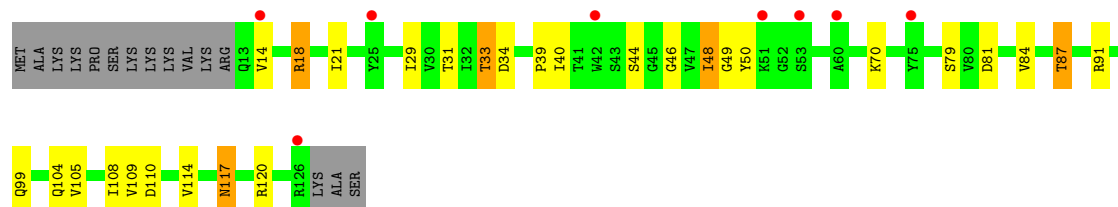
• Molecule 41: 30S ribosomal protein S10



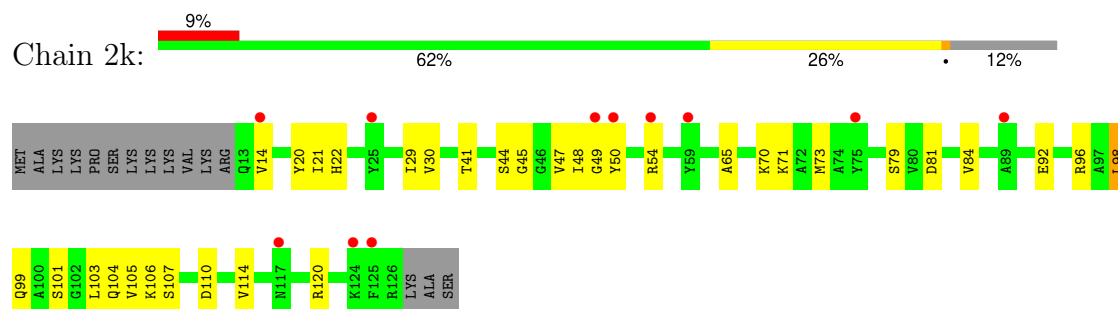
• Molecule 41: 30S ribosomal protein S10



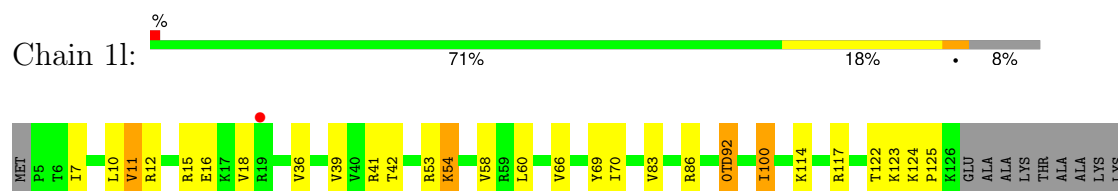
• Molecule 42: 30S ribosomal protein S11



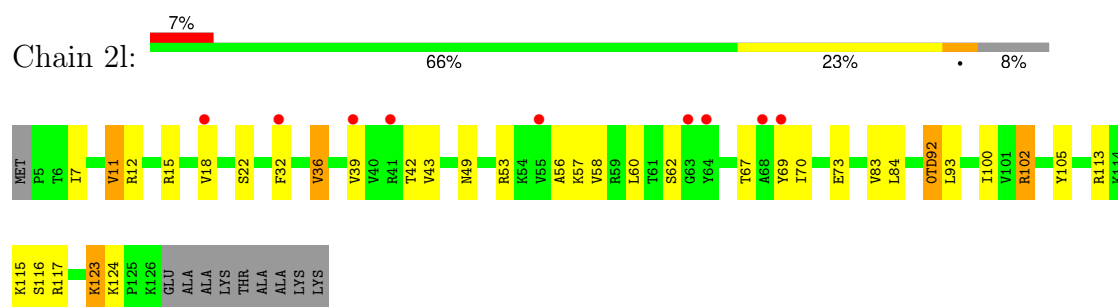
- Molecule 42: 30S ribosomal protein S11



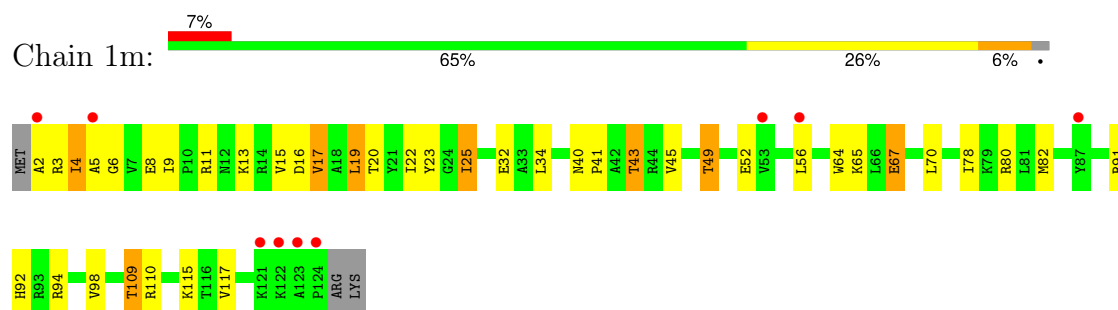
- Molecule 43: 30S ribosomal protein S12



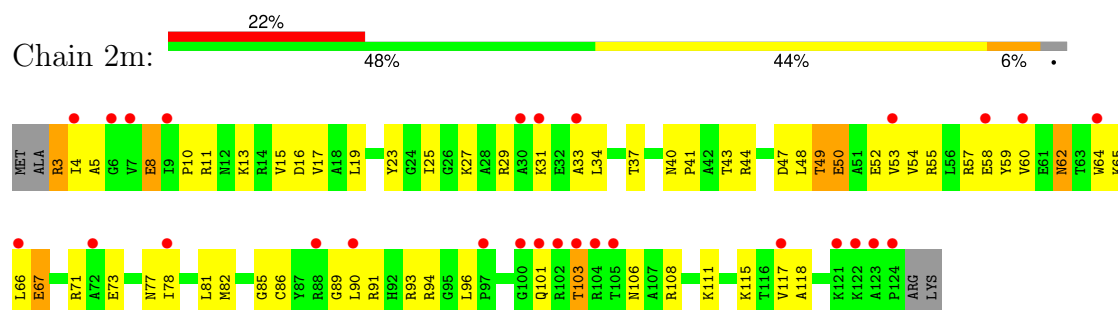
- Molecule 43: 30S ribosomal protein S12



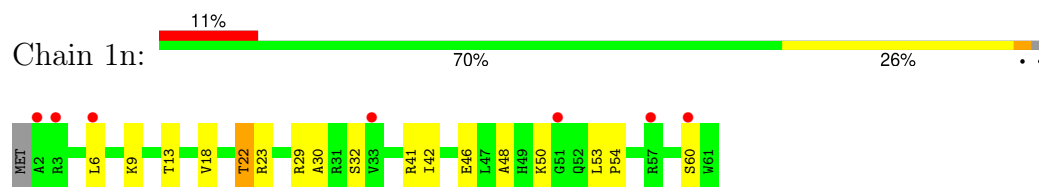
- Molecule 44: 30S ribosomal protein S13



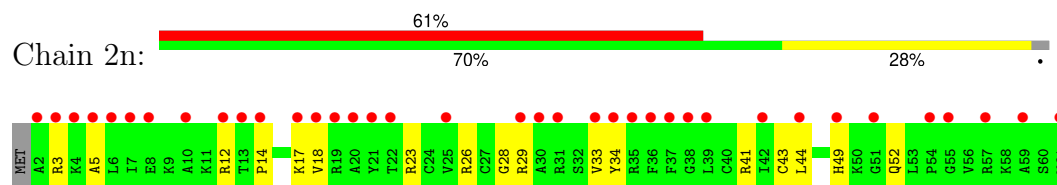
- Molecule 44: 30S ribosomal protein S13



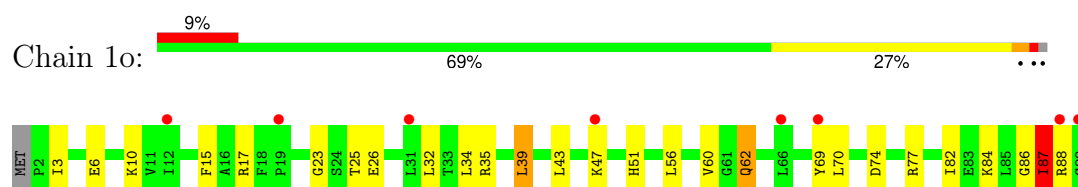
- Molecule 45: 30S ribosomal protein S14 type Z



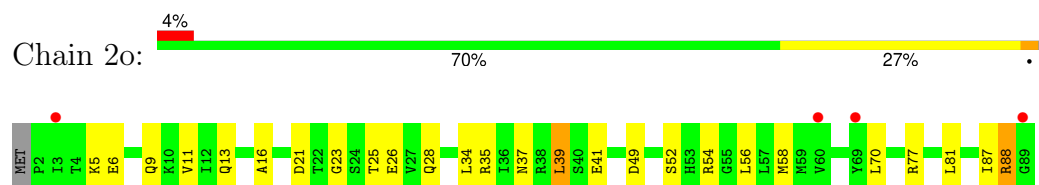
- Molecule 45: 30S ribosomal protein S14 type Z



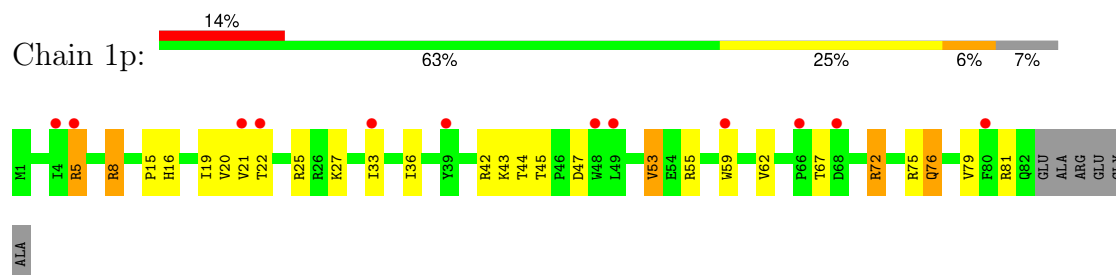
- Molecule 46: 30S ribosomal protein S15



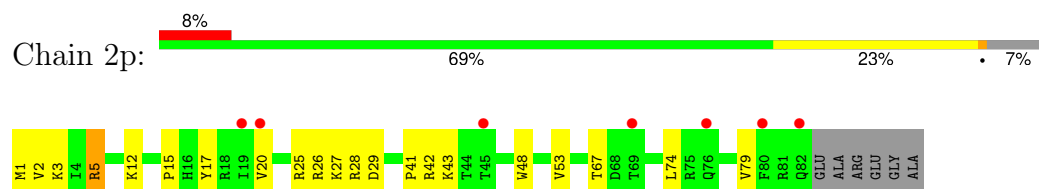
- Molecule 46: 30S ribosomal protein S15



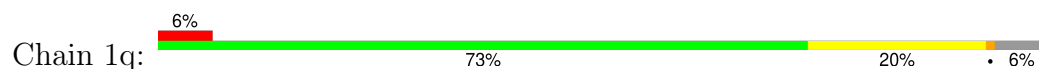
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16

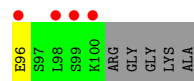
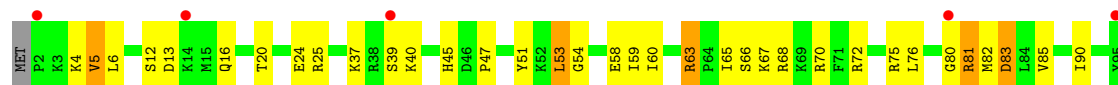


- Molecule 48: 30S ribosomal protein S17





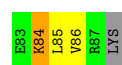
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18



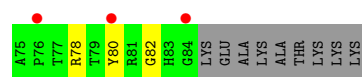
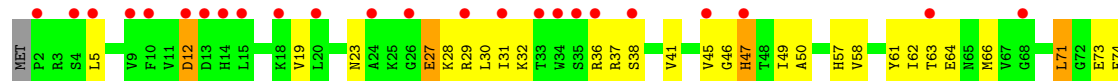
- Molecule 49: 30S ribosomal protein S18



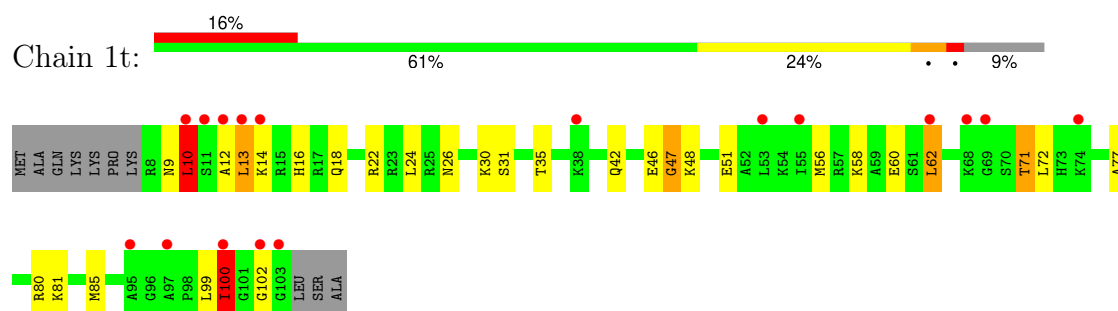
- Molecule 50: 30S ribosomal protein S19



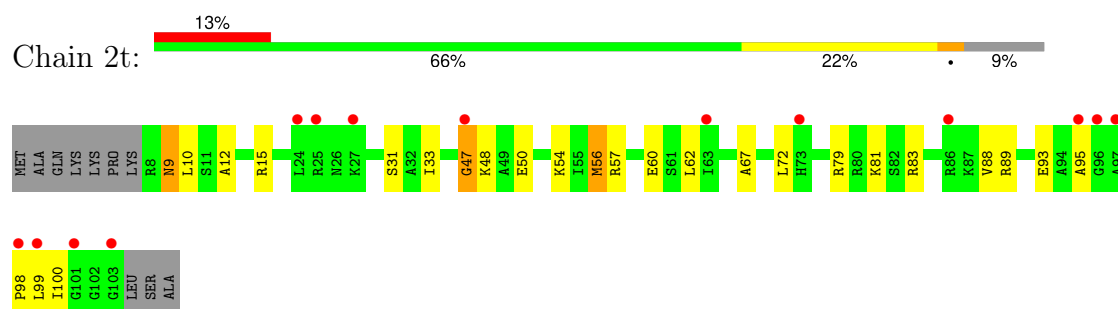
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20



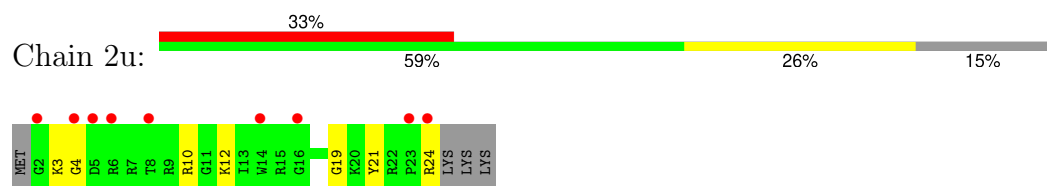
- Molecule 51: 30S ribosomal protein S20



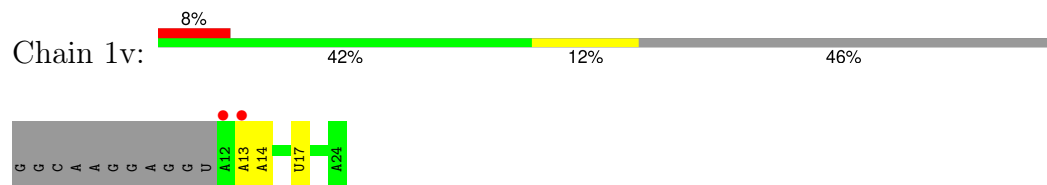
- Molecule 52: 30S ribosomal protein Thx



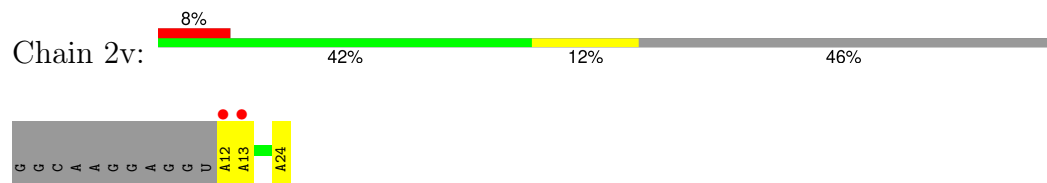
- Molecule 52: 30S ribosomal protein Thx



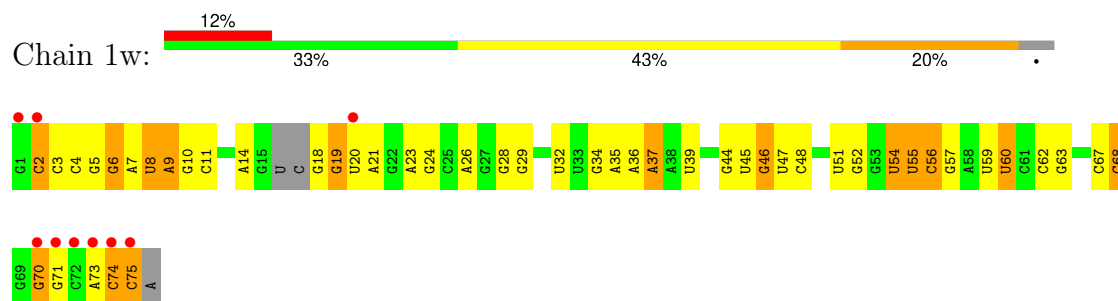
- Molecule 53: MF-mRNA



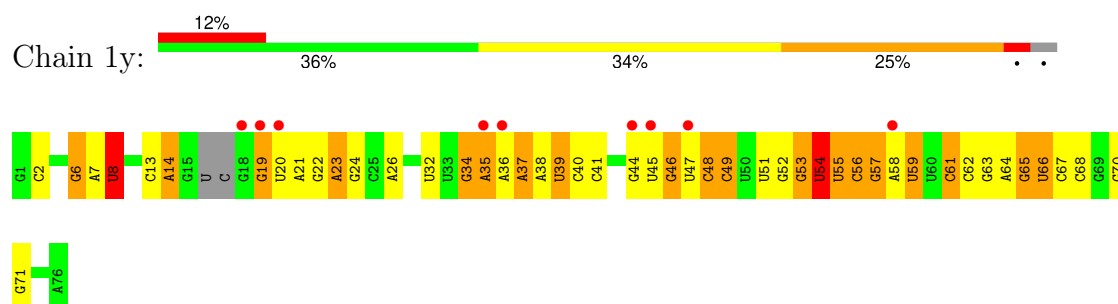
- Molecule 53: MF-mRNA



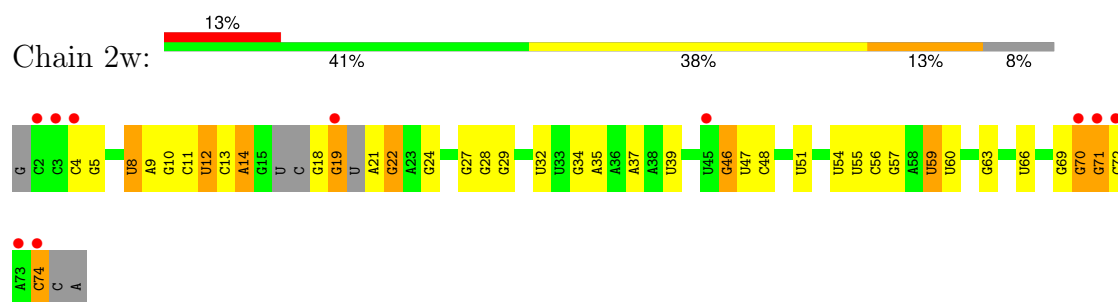
- Molecule 54: A-site and E-site Deacylated tRNA^{phe}



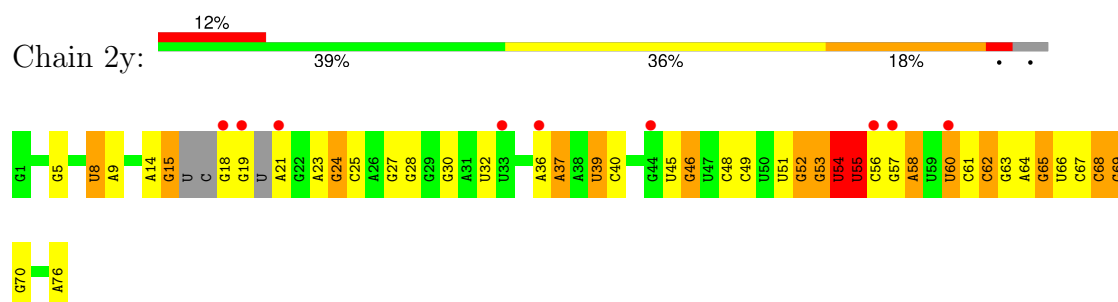
- Molecule 54: A-site and E-site Deacylated tRNA^{phe}



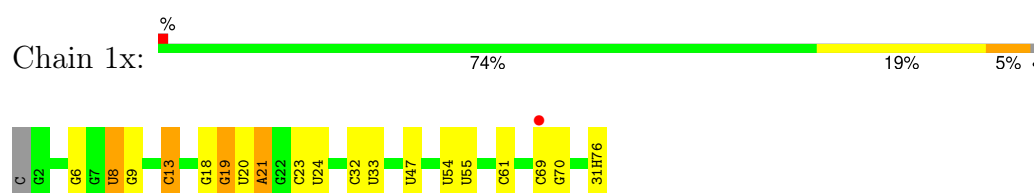
- Molecule 54: A-site and E-site Deacylated tRNA^{phe}



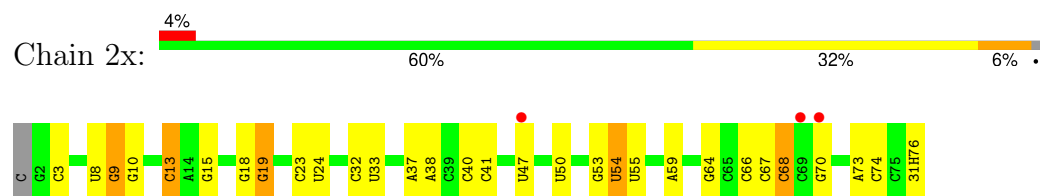
- Molecule 54: A-site and E-site Deacylated tRNA^{phe}



- Molecule 55: P-site Aminoacylated fMet-tRNA^{met}



- Molecule 55: P-site Aminoacylated fMet-tRNA^{Met}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.64Å 449.56Å 621.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.21 – 2.55 123.21 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.2 (123.21-2.55) 98.2 (123.21-2.55)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.218 , 0.262 0.220 , 0.263	Depositor DCC
R_{free} test set	92600 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	299868	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 31H, 5MC, G7M, 5MU, ZN, 2MU, 4OC, 6IF, 8AH, PSU, 0TD, UR3, OMG, MA6, MG, OMC, K, MIA, 2MG, M2G, 4SU

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	1A	0.27	0/69010	0.46	1/107716 (0.0%)
1	2A	0.21	0/67294	0.40	1/105038 (0.0%)
2	1B	0.21	0/2882	0.39	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.22	0/2186	0.44	0/2944
4	1E	0.27	0/1592	0.51	0/2149
4	2E	0.21	0/1592	0.46	0/2149
5	1F	0.25	0/1618	0.49	0/2191
5	2F	0.19	0/1614	0.44	2/2186 (0.1%)
6	1G	0.23	0/1448	0.47	0/1957
6	2G	0.19	0/1453	0.46	0/1963
7	1H	0.22	0/1356	0.46	0/1834
7	2H	0.18	0/1356	0.35	0/1834
8	1I	0.20	0/1112	0.43	0/1514
8	2I	0.19	0/1079	0.46	0/1475
9	1N	0.25	0/1144	0.48	0/1543
9	2N	0.19	0/1144	0.39	0/1543
10	1O	0.24	0/943	0.43	0/1269
10	2O	0.19	0/943	0.40	0/1269
11	1P	0.25	0/1152	0.54	0/1533
11	2P	0.21	0/1152	0.48	0/1533
12	1Q	0.26	0/1143	0.48	0/1527
12	2Q	0.20	0/1143	0.43	0/1527
13	1R	0.27	0/982	0.49	0/1312
13	2R	0.23	0/982	0.51	0/1312
14	1S	0.23	0/883	0.48	0/1176
14	2S	0.21	0/880	0.48	0/1172
15	1T	0.22	0/1105	0.45	0/1477
15	2T	0.20	0/1097	0.43	0/1468
16	1U	0.27	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.39	0/1301
17	1V	0.25	0/782	0.46	0/1049
17	2V	0.18	0/782	0.38	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.20	0/897	0.40	0/1205
19	1X	0.26	0/764	0.53	0/1025
19	2X	0.20	0/764	0.46	2/1025 (0.2%)
20	1Y	0.22	0/819	0.47	0/1095
20	2Y	0.21	0/819	0.41	0/1095
21	1Z	0.22	0/1267	0.46	0/1717
21	2Z	0.21	0/1299	0.45	0/1763
22	10	0.28	0/662	0.52	0/881
22	20	0.20	0/662	0.45	0/881
23	11	0.24	0/762	0.42	0/1014
23	21	0.23	0/762	0.43	0/1014
24	12	0.24	0/590	0.52	1/781 (0.1%)
24	22	0.18	0/590	0.40	0/781
25	13	0.28	0/474	0.49	0/635
25	23	0.20	0/469	0.44	0/630
26	14	0.25	0/565	0.60	0/761
26	24	0.23	0/545	0.53	0/737
27	15	0.29	0/469	0.57	1/635 (0.2%)
27	25	0.22	0/469	0.40	0/635
28	16	0.25	0/460	0.46	0/613
28	26	0.20	0/456	0.41	0/608
29	17	0.30	0/426	0.50	0/561
29	27	0.25	0/426	0.49	0/561
30	18	0.24	0/525	0.49	0/691
30	28	0.21	0/525	0.40	0/691
31	19	0.26	0/310	0.50	0/407
31	29	0.18	0/310	0.42	0/407
32	1a	0.20	0/35795	0.39	0/55864
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.22	0/1881	0.50	1/2542 (0.0%)
33	2b	0.21	0/1860	0.49	0/2518
34	1c	0.20	0/1572	0.45	0/2126
34	2c	0.21	0/1566	0.43	0/2119
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.19	0/1704	0.43	0/2284
36	1e	0.20	0/1145	0.46	0/1543
36	2e	0.19	0/1149	0.45	0/1548
37	1f	0.20	0/823	0.39	0/1115
37	2f	0.20	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.39	0/1679
38	2g	0.17	0/1254	0.40	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.19	0/1108	0.43	0/1494
40	1i	0.20	0/1002	0.48	0/1346
40	2i	0.21	0/997	0.47	0/1343
41	1j	0.22	0/722	0.44	0/982
41	2j	0.20	0/727	0.49	0/988
42	1k	0.18	0/844	0.43	0/1145
42	2k	0.18	0/848	0.38	0/1149
43	1l	0.22	0/937	0.43	0/1260
43	2l	0.19	0/937	0.42	0/1260
44	1m	0.21	0/969	0.47	0/1302
44	2m	0.20	0/961	0.49	0/1291
45	1n	0.19	0/501	0.42	0/664
45	2n	0.22	0/501	0.43	0/664
46	1o	0.20	0/739	0.41	0/985
46	2o	0.18	0/739	0.39	0/985
47	1p	0.20	0/697	0.48	0/939
47	2p	0.20	0/693	0.49	0/935
48	1q	0.20	0/836	0.42	0/1117
48	2q	0.19	0/836	0.44	0/1117
49	1r	0.20	0/560	0.44	0/746
49	2r	0.18	0/560	0.40	0/746
50	1s	0.18	0/667	0.46	0/900
50	2s	0.24	0/661	0.58	0/893
51	1t	0.20	0/730	0.48	0/965
51	2t	0.20	0/729	0.43	0/965
52	1u	0.17	0/203	0.48	0/266
52	2u	0.21	0/203	0.45	0/266
53	1v	0.20	0/310	0.34	0/480
53	2v	0.17	0/310	0.32	0/480
54	1w	0.28	0/1581	0.42	0/2458
54	1y	0.29	2/1606 (0.1%)	0.41	0/2497
54	2w	0.30	1/1509 (0.1%)	0.42	0/2345
54	2y	0.28	1/1583 (0.1%)	0.40	0/2459
55	1x	0.28	0/1700	0.41	0/2650
55	2x	0.25	0/1700	0.40	0/2650
All	All	0.23	4/316564 (0.0%)	0.42	12/473927 (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
11	1P	0	1
11	2P	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	46	G7M	O3'-P	5.39	1.61	1.56
54	1y	8	4SU	O3'-P	5.35	1.61	1.56
54	2w	46	G7M	O3'-P	5.32	1.61	1.56
54	2y	46	G7M	O3'-P	5.04	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	12	41	ILE	N-CA-C	-7.41	105.50	112.83
1	1A	1992	G	C2'-C3'-O3'	6.31	118.96	109.50
32	2a	1272	G	N1-C2-N2	-5.78	98.85	116.20
32	2a	1263	C	N1-C2-O2	5.62	135.77	118.90
33	1b	13	ALA	N-CA-C	-5.47	106.68	113.19
1	2A	1992	G	C2'-C3'-O3'	5.36	117.54	109.50
5	2F	21	ALA	CA-C-N	5.23	131.12	121.70
5	2F	21	ALA	C-N-CA	5.23	131.12	121.70
32	2a	1272	G	N3-C2-N2	5.15	135.35	119.90
19	2X	94	GLY	CA-C-N	5.13	130.93	121.70
19	2X	94	GLY	C-N-CA	5.13	130.93	121.70
27	15	6	VAL	CB-CA-C	5.04	114.27	109.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	2P	35	HIS	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	1A	61853	0	31181	578	0
1	2A	60323	0	30413	661	0
2	1B	2577	0	1305	19	0
2	2B	2575	0	1303	41	0
3	1D	2136	0	2218	42	0
3	2D	2136	0	2218	36	0
4	1E	1559	0	1618	24	0
4	2E	1559	0	1618	38	0
5	1F	1583	0	1625	37	0
5	2F	1579	0	1619	43	0
6	1G	1423	0	1436	31	0
6	2G	1428	0	1438	58	0
7	1H	1330	0	1407	25	0
7	2H	1330	0	1407	30	0
8	1I	1097	0	1140	30	0
8	2I	1064	0	1082	39	0
9	1N	1117	0	1184	11	0
9	2N	1117	0	1184	31	0
10	1O	933	0	996	10	0
10	2O	933	0	996	20	0
11	1P	1135	0	1212	35	0
11	2P	1135	0	1212	38	0
12	1Q	1122	0	1179	18	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	15	0
13	2R	968	0	1033	23	0
14	1S	873	0	927	13	0
14	2S	870	0	923	42	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	31	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	21	0
17	1V	771	0	830	12	0
17	2V	771	0	830	18	0
18	1W	886	0	940	10	0
18	2W	886	0	940	18	0
19	1X	750	0	814	12	0
19	2X	750	0	814	19	0
20	1Y	806	0	881	15	0
20	2Y	806	0	881	16	0
21	1Z	1240	0	1240	33	0
21	2Z	1271	0	1273	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	10	653	0	673	9	0
22	20	653	0	674	16	0
23	11	755	0	826	12	0
23	21	755	0	826	20	0
24	12	588	0	643	10	0
24	22	588	0	643	15	0
25	13	469	0	518	7	0
25	23	464	0	514	17	0
26	14	552	0	533	30	0
26	24	532	0	503	25	0
27	15	455	0	465	9	0
27	25	455	0	465	9	0
28	16	453	0	473	11	0
28	26	449	0	469	12	0
29	17	418	0	467	5	0
29	27	418	0	467	9	0
30	18	517	0	582	13	0
30	28	517	0	582	12	0
31	19	307	0	335	4	0
31	29	307	0	335	7	0
32	1a	32246	0	16295	385	0
32	2a	32327	0	16337	432	0
33	1b	1846	0	1867	75	0
33	2b	1825	0	1828	78	0
34	1c	1548	0	1535	38	0
34	2c	1542	0	1517	59	0
35	1d	1655	0	1672	39	0
35	2d	1674	0	1714	45	0
36	1e	1129	0	1185	30	0
36	2e	1133	0	1191	46	0
37	1f	810	0	804	21	0
37	2f	816	0	808	18	0
38	1g	1231	0	1238	21	0
38	2g	1235	0	1249	37	0
39	1h	1088	0	1126	26	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	36	0
40	2i	978	0	966	40	0
41	1j	709	0	650	30	0
41	2j	714	0	672	36	0
42	1k	829	0	825	17	0
42	2k	833	0	836	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	1l	932	0	981	18	0
43	2l	932	0	980	20	0
44	1m	958	0	1002	25	0
44	2m	950	0	988	50	0
45	1n	492	0	529	13	0
45	2n	492	0	529	15	0
46	1o	728	0	760	19	0
46	2o	728	0	760	17	0
47	1p	681	0	697	21	0
47	2p	677	0	686	15	0
48	1q	823	0	891	16	0
48	2q	823	0	891	19	0
49	1r	555	0	618	13	0
49	2r	555	0	618	20	0
50	1s	652	0	662	14	0
50	2s	646	0	644	23	0
51	1t	728	0	798	18	0
51	2t	727	0	796	20	0
52	1u	199	0	208	6	0
52	2u	199	0	208	7	0
53	1v	277	0	140	4	0
53	2v	277	0	140	3	0
54	1w	1570	0	807	30	0
54	1y	1585	0	803	24	0
54	2w	1502	0	765	24	0
54	2y	1565	0	794	34	0
55	1x	1635	0	839	7	0
55	2x	1635	0	839	16	0
56	10	8	0	0	0	0
56	11	6	0	0	0	0
56	12	2	0	0	0	0
56	13	4	0	0	0	0
56	14	1	0	0	0	0
56	15	8	0	0	0	0
56	16	1	0	0	0	0
56	17	6	0	0	0	0
56	18	5	0	0	0	0
56	19	1	0	0	0	0
56	1A	1083	0	0	0	0
56	1B	38	0	0	0	0
56	1D	13	0	0	0	0
56	1E	14	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1F	13	0	0	0	0
56	1G	5	0	0	0	0
56	1H	1	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	4	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	5	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	11	0	0	0	0
56	1V	7	0	0	0	0
56	1W	9	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	4	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	211	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	1	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	2	0	0	0	0
56	1n	2	0	0	0	0
56	1r	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	2	0	0	0	0
56	1w	7	0	0	0	0
56	1x	15	0	0	0	0
56	1y	1	0	0	0	0
56	20	5	0	0	0	0
56	21	2	0	0	0	0
56	23	1	0	0	0	0
56	25	7	0	0	0	0
56	26	1	0	0	0	0
56	27	3	0	0	0	0
56	28	2	0	0	0	0
56	29	1	0	0	0	0
56	2A	830	0	0	0	0
56	2B	19	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2D	7	0	0	0	0
56	2E	9	0	0	0	0
56	2F	7	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	3	0	0	0	0
56	2T	3	0	0	0	0
56	2U	1	0	0	0	0
56	2V	2	0	0	0	0
56	2W	3	0	0	0	0
56	2X	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	211	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2j	1	0	0	0	0
56	2l	3	0	0	0	0
56	2p	1	0	0	0	0
56	2q	3	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	3	0	0	0	0
56	2w	4	0	0	0	0
56	2x	7	0	0	0	0
56	2y	5	0	0	0	0
57	1A	32	0	0	0	0
57	2A	32	0	0	0	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	1	0
59	2d	8	0	0	2	0
60	1x	1	0	0	0	0
60	2x	1	0	0	0	0
61	10	13	0	0	1	0
61	11	9	0	0	1	0
61	12	4	0	0	0	0
61	13	3	0	0	0	0
61	14	1	0	0	0	0
61	15	4	0	0	0	0
61	16	2	0	0	1	0
61	17	9	0	0	1	0
61	18	13	0	0	0	0
61	1A	1971	0	0	75	0
61	1B	60	0	0	1	0
61	1D	28	0	0	1	0
61	1E	30	0	0	1	0
61	1F	16	0	0	0	0
61	1G	2	0	0	1	0
61	1H	3	0	0	0	0
61	1N	9	0	0	0	0
61	1O	4	0	0	0	0
61	1P	15	0	0	1	0
61	1Q	10	0	0	0	0
61	1R	12	0	0	1	0
61	1S	5	0	0	0	0
61	1T	8	0	0	1	0
61	1U	14	0	0	0	0
61	1V	8	0	0	0	0
61	1W	4	0	0	2	0
61	1X	6	0	0	1	0
61	1Y	2	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	357	0	0	25	0
61	1b	1	0	0	0	0
61	1e	1	0	0	0	0
61	1i	2	0	0	0	0
61	1l	4	0	0	0	0
61	1m	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1o	1	0	0	0	0
61	1p	1	0	0	0	0
61	1q	2	0	0	0	0
61	1t	1	0	0	0	0
61	1u	1	0	0	1	0
61	1v	4	0	0	0	0
61	1w	10	0	0	1	0
61	1x	17	0	0	1	0
61	1y	1	0	0	0	0
61	20	4	0	0	0	0
61	21	6	0	0	1	0
61	23	2	0	0	0	0
61	25	2	0	0	0	0
61	27	1	0	0	0	0
61	28	6	0	0	0	0
61	29	1	0	0	0	0
61	2A	1109	0	0	58	0
61	2B	20	0	0	2	0
61	2D	21	0	0	0	0
61	2E	13	0	0	2	0
61	2F	11	0	0	0	0
61	2O	3	0	0	0	0
61	2P	8	0	0	2	0
61	2Q	1	0	0	0	0
61	2R	3	0	0	0	0
61	2T	6	0	0	0	0
61	2U	4	0	0	0	0
61	2W	1	0	0	0	0
61	2X	1	0	0	1	0
61	2Y	1	0	0	0	0
61	2a	221	0	0	16	0
61	2d	2	0	0	0	0
61	2j	3	0	0	2	0
61	2l	1	0	0	0	0
61	2o	1	0	0	0	0
61	2p	1	0	0	1	0
61	2t	2	0	0	0	0
61	2x	4	0	0	0	0
61	2y	7	0	0	0	0
All	All	299868	0	196647	4007	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 8.

All (4007) 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)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.44	1.14
1:1A:2136:C:N4	1:1A:2155:G:H1	1.60	1.00
1:1A:1082:U:O4	1:1A:1086:A:N1	1.95	0.99
1:1A:1082:U:N3	1:1A:1086:A:N6	2.07	0.98
21:2Z:145:GLU:HB3	21:2Z:148:ASP:HB2	1.47	0.96
29:27:24:THR:HG22	29:27:27:GLY:H	1.30	0.95
1:1A:2136:C:H42	1:1A:2155:G:H1	0.99	0.95
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.46	0.94
7:1H:101:ARG:HH22	7:1H:122:THR:HA	1.32	0.91
1:1A:2427:C:OP1	61:1A:4103:HOH:O	1.90	0.89
1:1A:2136:C:N3	1:1A:2155:G:N2	2.20	0.89
29:17:24:THR:HG22	29:17:27:GLY:H	1.35	0.89
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.20	0.88
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.23	0.87
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.57	0.87
1:1A:2499:C:OP1	61:1A:4104:HOH:O	1.93	0.87
1:1A:1602:U:O4	61:1A:4105:HOH:O	1.93	0.85
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.59	0.85
1:2A:1010:A:OP2	61:2A:3903:HOH:O	1.95	0.85
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.41	0.85
32:2a:953:G:H5'	32:2a:965:A:H61	1.38	0.84
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.10	0.84
32:2a:975:A:H4'	32:2a:976:G:H5''	1.60	0.84
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.25	0.84
1:2A:2127:G:H1	1:2A:2161:C:H42	1.27	0.82
1:2A:1689:A:H62	1:2A:1698:A:H2	1.27	0.82
1:2A:2592:G:OP1	61:2A:3904:HOH:O	1.96	0.82
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.62	0.81
7:1H:101:ARG:HH12	7:1H:122:THR:HG22	1.45	0.81
1:1A:1669:A:OP2	61:1A:4106:HOH:O	1.98	0.81
42:1k:79:SER:HA	42:1k:104:GLN:HB3	1.62	0.81
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.60	0.81
1:2A:2049:G:OP2	61:2A:3905:HOH:O	1.98	0.80
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.14	0.80
32:2a:1106:G:H5''	34:2c:172:ARG:HG2	1.64	0.80
32:1a:1108:G:O6	61:1a:1902:HOH:O	1.99	0.80
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.45	0.80
41:2j:6:ILE:HB	41:2j:72:VAL:HG13	1.64	0.79
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.61	0.79
33:2b:58:ILE:HA	33:2b:61:LEU:HB3	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1670:C:OP1	61:2A:3906:HOH:O	2.01	0.79
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.64	0.79
1:1A:826:U:OP1	61:1A:4103:HOH:O	2.01	0.79
1:1A:792:G:O6	61:1A:4107:HOH:O	2.01	0.78
1:2A:1938:A:OP2	61:2A:3907:HOH:O	2.02	0.78
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.64	0.78
21:2Z:144:LEU:HG	21:2Z:148:ASP:HB3	1.64	0.77
32:2a:117:G:OP2	61:2a:1903:HOH:O	2.01	0.77
28:16:13:CYS:SG	28:16:47:THR:HG21	2.24	0.77
1:1A:271(L):U:H4'	8:1I:50:ARG:HH22	1.50	0.77
32:2a:731:G:OP1	61:2a:1902:HOH:O	2.01	0.77
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.18	0.77
32:2a:1086:U:H3	32:2a:1099:G:H22	1.33	0.77
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.18	0.77
32:2a:1152:A:H5'	41:2j:13:HIS:HD2	1.48	0.76
32:1a:664:G:H22	32:1a:741:G:H1	1.32	0.76
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.68	0.76
5:2F:116:ASP:OD2	11:2P:1:MET:N	2.19	0.76
14:2S:67:ARG:HG2	14:2S:71:ARG:HD2	1.68	0.76
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.67	0.76
32:1a:1505:G:OP2	61:1a:1903:HOH:O	2.02	0.76
54:2w:11:C:H42	54:2w:24:G:H1	1.32	0.76
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.18	0.76
32:1a:812:C:N3	61:1a:1915:HOH:O	2.18	0.76
1:2A:1021:A:H62	1:2A:1141:U:H3	1.34	0.76
1:2A:570:G:O6	61:2A:3908:HOH:O	2.03	0.75
22:20:10:THR:HG22	22:20:12:ASN:H	1.51	0.75
1:2A:2099:U:H3	1:2A:2190:G:H1	1.34	0.75
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.66	0.75
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.20	0.75
38:2g:57:GLU:HG3	38:2g:60:LYS:H	1.52	0.75
1:1A:1014:U:OP2	61:1A:4108:HOH:O	2.03	0.75
33:2b:8:LYS:HD2	33:2b:9:GLU:H	1.51	0.75
1:2A:1568:G:N7	61:2A:3941:HOH:O	2.20	0.75
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.67	0.75
1:1A:2277:G:OP2	22:10:10:THR:HG21	1.87	0.74
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	1.68	0.74
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.21	0.74
32:1a:558:G:OP1	61:1a:1904:HOH:O	2.04	0.74
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.21	0.74
32:2a:1347:G:HO2'	32:2a:1373:G:H1	1.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:122:ARG:NH1	35:2d:134:ASP:O	2.21	0.74
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.68	0.74
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.70	0.74
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.23	0.74
44:2m:54:VAL:HG22	44:2m:57:ARG:HH12	1.52	0.74
1:1A:2447:G:OP2	61:1A:4109:HOH:O	2.05	0.74
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.51	0.74
4:2E:119:ARG:HD3	4:2E:160:TYR:HB2	1.68	0.73
32:2a:547:A:OP1	61:2a:1904:HOH:O	2.06	0.73
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.68	0.73
1:2A:123:G:OP2	61:2A:3910:HOH:O	2.06	0.73
1:1A:2550:G:OP1	61:1A:4106:HOH:O	2.06	0.73
2:1B:66:A:H61	2:1B:109:C:H5'	1.52	0.73
32:1a:975:A:H4'	32:1a:976:G:H5''	1.69	0.73
45:2n:12:ARG:HH12	45:2n:14:PRO:HA	1.52	0.73
1:1A:1648:C:OP1	61:1A:4112:HOH:O	2.07	0.73
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.71	0.73
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.33	0.73
1:2A:2576:G:OP1	61:2A:3909:HOH:O	2.05	0.73
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.34	0.73
1:1A:2276:G:N7	61:1A:4145:HOH:O	2.21	0.73
1:1A:2871:C:N3	61:1A:4144:HOH:O	2.21	0.73
1:1A:1670:C:OP1	61:1A:4110:HOH:O	2.06	0.72
2:1B:21:G:N7	61:1B:301:HOH:O	2.22	0.72
52:1u:5:ASP:OD2	61:1u:101:HOH:O	2.06	0.72
1:1A:1013:C:OP2	61:1A:4108:HOH:O	2.07	0.72
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.22	0.72
1:1A:1332:G:OP1	61:1A:4113:HOH:O	2.08	0.72
19:2X:35:THR:HG22	19:2X:38:GLU:H	1.53	0.72
32:1a:299:G:O6	61:1a:1904:HOH:O	2.07	0.72
55:1x:19:G:O2'	61:1x:201:HOH:O	2.07	0.72
1:2A:2127:G:H1	1:2A:2161:C:N4	1.87	0.72
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.72	0.72
11:2P:121:LYS:HB3	11:2P:123:LEU:HD13	1.72	0.72
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	1.72	0.72
32:1a:1025:U:O2	32:1a:1036:G:O6	2.07	0.72
32:2a:673:G:H2'	32:2a:674:G:C8	2.25	0.72
33:1b:17:PHE:HB3	33:1b:44:LEU:HD11	1.72	0.72
32:2a:558:G:OP1	61:2a:1905:HOH:O	2.08	0.72
1:2A:963:U:OP2	61:2A:3911:HOH:O	2.07	0.71
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:248:G:OP1	61:2A:3912:HOH:O	2.07	0.71
1:2A:878:A:H61	1:2A:899:A:H1'	1.54	0.71
1:2A:1204:A:H2	1:2A:1241:A:H62	1.38	0.71
22:20:11:ARG:O	22:20:14:ARG:NH2	2.23	0.71
32:1a:677:U:H3	32:1a:713:G:H22	1.39	0.71
47:1p:53:VAL:HG23	47:1p:79:VAL:HG13	1.71	0.71
1:2A:947:G:O6	61:2A:3915:HOH:O	2.08	0.71
26:24:60:GLN:O	26:24:62:ARG:NH1	2.23	0.71
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.55	0.71
1:2A:2143:C:H42	1:2A:2148:G:H1	1.39	0.71
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.72	0.71
27:25:33:CYS:HB2	27:25:40:LYS:HD3	1.72	0.71
1:1A:1054:A:H61	1:1A:1105:U:H3	1.39	0.71
3:1D:237:GLU:OE2	61:1D:401:HOH:O	2.09	0.71
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.22	0.71
26:24:53:GLU:HG2	26:24:55:ARG:H	1.56	0.71
32:1a:116:A:OP1	61:1a:1905:HOH:O	2.09	0.71
32:2a:1353:G:OP1	52:2u:10:ARG:NH1	2.23	0.71
1:1A:1041:C:H42	1:1A:1114:G:H1	1.39	0.71
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.71	0.71
61:1A:4157:HOH:O	13:1R:50:HIS:ND1	2.24	0.71
8:2I:40:THR:O	8:2I:44:LEU:HB2	1.90	0.71
15:2T:16:ARG:HE	15:2T:19:LEU:HD11	1.54	0.71
54:1y:7:A:O2'	54:1y:49:C:OP2	2.08	0.71
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.71	0.70
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.72	0.70
1:2A:1648:C:OP1	61:2A:3916:HOH:O	2.09	0.70
44:2m:3:ARG:HH22	44:2m:11:ARG:HG3	1.56	0.70
54:2y:18:G:N2	54:2y:55:PSU:N3	2.35	0.70
54:2y:55:PSU:HN1	54:2y:57:G:H5''	1.55	0.70
39:1h:95:VAL:HB	39:1h:99:GLU:HG3	1.72	0.70
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.24	0.70
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.23	0.70
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.24	0.70
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.73	0.70
1:2A:2592:G:OP2	61:2A:3914:HOH:O	2.08	0.70
1:1A:1993:U:OP2	61:1A:4115:HOH:O	2.08	0.70
1:1A:2821:A:OP2	61:1R:301:HOH:O	2.10	0.70
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.24	0.70
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.55	0.70
21:2Z:138:GLU:HB2	21:2Z:156:LYS:HD3	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.73	0.70
34:2c:119:ARG:HG2	34:2c:140:ARG:HH22	1.54	0.70
1:2A:528:A:OP1	61:2A:3913:HOH:O	2.08	0.70
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.25	0.70
1:1A:1456:G:OP2	61:1A:4114:HOH:O	2.08	0.70
41:1j:46:ARG:NH2	41:1j:64:GLU:OE1	2.25	0.70
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.74	0.70
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.73	0.70
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.57	0.70
1:1A:1056:G:H1'	1:1A:1103:A:H61	1.57	0.70
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.73	0.70
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.24	0.70
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.74	0.70
1:2A:2115:G:O2'	1:2A:2117:A:N7	2.21	0.70
35:2d:191:ARG:NH1	35:2d:191:ARG:O	2.24	0.70
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.74	0.70
1:1A:880:G:H2'	1:1A:881:G:H8	1.56	0.69
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.74	0.69
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.56	0.69
1:1A:192:C:OP1	61:1A:4116:HOH:O	2.10	0.69
1:1A:505:A:OP2	61:1A:4118:HOH:O	2.10	0.69
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.57	0.69
33:1b:59:GLU:HB2	33:1b:221:LEU:HD21	1.73	0.69
34:2c:41:GLY:O	34:2c:45:LYS:NZ	2.24	0.69
32:1a:504:C:OP1	61:1a:1906:HOH:O	2.09	0.69
32:1a:1198:G:OP1	61:1a:1907:HOH:O	2.10	0.69
1:2A:2060:A:N3	61:2A:3965:HOH:O	2.25	0.69
1:1A:1023:U:OP2	61:1A:4111:HOH:O	2.10	0.69
32:1a:700:G:N7	61:1a:1924:HOH:O	2.24	0.69
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.11	0.69
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.74	0.69
32:2a:598:U:O4	61:2a:1906:HOH:O	2.09	0.69
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.55	0.69
1:1A:2136:C:N4	1:1A:2155:G:N1	2.28	0.69
1:1A:2552:2MU:OP2	61:1A:4119:HOH:O	2.11	0.69
37:1f:38:GLU:HB2	37:1f:64:GLN:HG2	1.74	0.69
54:1w:26:A:H61	54:1w:44:G:H1	1.41	0.69
40:2i:79:LEU:HG	40:2i:83:ARG:HD2	1.74	0.69
40:2i:7:THR:O	40:2i:83:ARG:NH1	2.25	0.69
36:1e:18:ARG:HD3	36:1e:27:ARG:HH12	1.57	0.69
1:2A:400:G:N7	61:2A:3966:HOH:O	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:596:C:OP2	61:2a:1906:HOH:O	2.10	0.69
32:2a:838:G:H1	32:2a:848:C:H42	1.40	0.69
32:2a:1456:G:O6	51:2t:54:LYS:NZ	2.25	0.69
1:1A:1062:G:H1	1:1A:1077:A:H61	1.38	0.69
1:1A:1315:C:OP2	61:1A:4113:HOH:O	2.10	0.69
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.25	0.69
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.41	0.69
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.27	0.69
43:2l:57:LYS:HG2	43:2l:67:THR:HG22	1.73	0.69
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.73	0.69
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.26	0.69
1:1A:409:C:OP1	61:1A:4117:HOH:O	2.10	0.69
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	1.75	0.69
1:2A:449:A:OP2	61:2A:3919:HOH:O	2.11	0.69
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.57	0.69
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.25	0.69
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.26	0.69
32:2a:1239:A:H62	32:2a:1299:A:H62	1.41	0.69
33:2b:219:VAL:HA	33:2b:222:ILE:HG12	1.75	0.69
32:1a:165:C:H2'	32:1a:166:G:H8	1.57	0.68
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.25	0.68
44:2m:86:CYS:HB2	50:2s:73:GLU:HG2	1.74	0.68
32:1a:504:C:OP1	61:1a:1908:HOH:O	2.10	0.68
32:2a:1228:C:OP1	44:2m:115:LYS:NZ	2.24	0.68
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.74	0.68
54:2y:15:G:H22	54:2y:48:C:H42	1.40	0.68
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.58	0.68
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.73	0.68
1:2A:253:C:O2'	61:2A:3918:HOH:O	2.10	0.68
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.39	0.68
32:2a:1224:G:OP1	61:2a:1908:HOH:O	2.11	0.68
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.16	0.68
1:1A:2096:U:H3	1:1A:2193:G:H1	1.40	0.68
6:1G:125:PHE:O	61:1G:3701:HOH:O	2.12	0.68
32:1a:78:G:O6	32:1a:92:C:N4	2.26	0.68
32:2a:297:G:N2	32:2a:300:A:OP2	2.25	0.68
32:2a:1272:G:N2	32:2a:1273:G:N7	2.40	0.68
1:2A:304:G:O6	61:2A:3920:HOH:O	2.12	0.68
32:2a:576:G:OP1	61:2a:1907:HOH:O	2.10	0.68
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.27	0.68
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:67:C:H2'	32:1a:68:G:C8	2.29	0.68
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.75	0.68
32:2a:1271:G:N2	32:2a:1272:G:N7	2.40	0.68
33:2b:114:ARG:O	33:2b:118:LEU:N	2.26	0.68
32:1a:148:G:H2'	32:1a:149:A:H8	1.59	0.68
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.26	0.68
17:1V:60:GLU:HB2	17:1V:97:LYS:HE2	1.76	0.68
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.09	0.68
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.57	0.68
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.75	0.68
44:2m:25:ILE:HD11	44:2m:60:VAL:HG11	1.74	0.68
1:1A:72:U:OP1	61:1A:4120:HOH:O	2.11	0.68
1:2A:2448:A:OP1	61:2A:3908:HOH:O	2.12	0.68
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.74	0.68
9:1N:123:TYR:HH	9:1N:130:HIS:HE2	1.39	0.68
32:1a:953:G:H5'	32:1a:965:A:H61	1.57	0.68
6:2G:121:ASN:HD22	6:2G:181:ARG:HH22	1.42	0.68
1:1A:2099:U:H3	1:1A:2190:G:H1	1.40	0.67
26:14:16:CYS:SG	26:14:17:GLY:N	2.66	0.67
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.76	0.67
32:2a:148:G:H2'	32:2a:149:A:H8	1.59	0.67
32:1a:159:G:N2	32:1a:162:A:OP2	2.27	0.67
32:2a:189(F):U:O2	48:2q:63:ARG:NH2	2.27	0.67
1:1A:1094:U:N3	1:1A:1097:U:OP2	2.27	0.67
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.76	0.67
26:14:34:GLU:HG2	26:14:35:VAL:HG12	1.76	0.67
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.76	0.67
1:2A:1812:A:OP2	61:2A:3917:HOH:O	2.10	0.67
1:2A:962:G:OP1	61:2A:3911:HOH:O	2.12	0.67
1:2A:1721:G:H8	1:2A:1741:A:H62	1.42	0.67
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	1.77	0.67
7:2H:124:GLU:HG3	7:2H:132:ARG:HB3	1.77	0.67
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.26	0.67
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.25	0.67
1:1A:2337:G:OP1	61:1A:4122:HOH:O	2.11	0.67
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.13	0.67
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.77	0.67
17:2V:1:MET:HE2	17:2V:43:GLU:HB2	1.77	0.67
32:2a:1270:C:OP2	52:2u:24:ARG:NH2	2.26	0.67
1:1A:392:C:OP1	61:1A:4117:HOH:O	2.12	0.67
1:1A:1342:A:OP2	61:1A:4105:HOH:O	2.11	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.75	0.67
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.27	0.67
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.58	0.67
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.28	0.67
20:1Y:34:LYS:NZ	61:1Y:301:HOH:O	2.27	0.67
54:1y:8:4SU:H4'	54:1y:48:C:H4'	1.77	0.67
21:2Z:5:LEU:HD11	21:2Z:44:PHE:HA	1.76	0.67
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.77	0.67
1:1A:429:A:OP2	61:1A:4123:HOH:O	2.12	0.67
32:1a:567:G:N3	61:1a:1926:HOH:O	2.27	0.67
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.30	0.67
44:2m:78:ILE:HA	44:2m:81:LEU:HD12	1.75	0.67
32:1a:1414:U:O4	61:1a:1909:HOH:O	2.12	0.67
44:1m:80:ARG:NH1	50:1s:65:ASN:O	2.28	0.67
32:2a:289:G:OP2	61:2a:1903:HOH:O	2.13	0.67
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.28	0.67
32:1a:1191:A:OP1	34:1c:4:LYS:NZ	2.28	0.66
1:2A:975:C:OP1	61:2A:3927:HOH:O	2.14	0.66
1:2A:1490:A:OP2	61:2A:3926:HOH:O	2.13	0.66
1:2A:1973:G:OP1	61:2A:3924:HOH:O	2.13	0.66
24:22:38:GLN:HG3	24:22:43:GLN:HB2	1.77	0.66
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.30	0.66
19:2X:44:GLU:OE2	61:2X:201:HOH:O	2.13	0.66
1:1A:847:U:OP2	61:1A:4125:HOH:O	2.13	0.66
1:1A:1057:A:H61	1:1A:1081:U:H3	1.43	0.66
1:1A:2106:G:H1	1:1A:2183:C:H42	1.43	0.66
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.30	0.66
1:1A:2575:C:OP2	61:1A:4124:HOH:O	2.13	0.66
32:1a:1224:G:OP1	61:1a:1910:HOH:O	2.13	0.66
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.76	0.66
1:2A:89:G:H3'	1:2A:90:U:H5''	1.77	0.66
1:2A:1253:A:OP1	61:2A:3925:HOH:O	2.13	0.66
7:2H:64:LEU:O	7:2H:68:THR:OG1	2.13	0.66
7:2H:80:SER:OG	7:2H:81:GLU:OE2	2.13	0.66
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.96	0.66
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.29	0.66
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.77	0.66
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.29	0.66
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.78	0.66
42:2k:48:ILE:O	42:2k:50:TYR:N	2.27	0.66
1:2A:948:G:OP1	61:2A:3911:HOH:O	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2y:58:A:O2'	54:2y:60:U:OP2	2.13	0.66
11:1P:2:LYS:NZ	11:1P:4:SER:OG	2.22	0.66
34:1c:57:ILE:HG12	34:1c:66:VAL:HG12	1.77	0.66
1:2A:1830:C:OP2	61:2A:3921:HOH:O	2.12	0.66
1:2A:2049:G:N7	61:2A:3980:HOH:O	2.28	0.66
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.25	0.66
11:1P:126:VAL:HG12	11:1P:148:LEU:HD13	1.78	0.66
1:2A:1968:G:OP1	61:2A:3904:HOH:O	2.14	0.66
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.78	0.66
1:1A:831:G:O2'	11:1P:38:GLN:OE1	2.13	0.66
1:1A:1670:C:OP2	61:1A:4106:HOH:O	2.14	0.66
1:2A:2577:A:OP1	61:2A:3909:HOH:O	2.12	0.66
1:1A:944:G:N7	61:1A:4185:HOH:O	2.29	0.66
32:1a:769:G:N7	61:1a:1925:HOH:O	2.27	0.66
1:2A:900:A:O2'	1:2A:901:A:OP1	2.13	0.66
1:2A:1268:A:OP1	61:2A:3922:HOH:O	2.12	0.66
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.29	0.66
21:2Z:53:ILE:HA	21:2Z:71:VAL:HG23	1.77	0.66
32:2a:560:U:H5'	32:2a:566:G:N2	2.11	0.66
1:2A:1024:G:OP2	61:2A:3923:HOH:O	2.13	0.65
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.28	0.65
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH22	1.61	0.65
35:2d:155:LEU:HB3	35:2d:158:ILE:HG13	1.78	0.65
1:2A:321:G:OP1	5:2F:135:LYS:NZ	2.29	0.65
1:2A:1981:A:N7	61:2A:3984:HOH:O	2.29	0.65
32:2a:79:G:H1	32:2a:90:U:H3	1.42	0.65
32:2a:1256:A:OP1	34:2c:26:LYS:NZ	2.30	0.65
44:2m:31:LYS:HA	44:2m:34:LEU:HD12	1.78	0.65
1:1A:1418:G:OP2	61:1A:4127:HOH:O	2.14	0.65
1:1A:1652:A:OP1	13:1R:8:ARG:NH1	2.30	0.65
32:1a:557:G:OP1	61:1a:1911:HOH:O	2.14	0.65
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.78	0.65
38:1g:78:ARG:HD3	38:1g:79:ARG:H	1.62	0.65
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.26	0.65
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.31	0.65
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.78	0.65
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.20	0.65
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.78	0.65
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	1.79	0.65
12:1Q:138:ASP:N	12:1Q:138:ASP:OD1	2.28	0.65
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:533:A:OP1	61:2a:1909:HOH:O	2.14	0.65
26:14:55:ARG:N	26:14:56:VAL:HA	2.12	0.65
34:1c:71:ALA:HA	34:1c:106:VAL:HG21	1.77	0.65
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.79	0.65
7:1H:124:GLU:HG3	7:1H:132:ARG:HB3	1.79	0.65
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.62	0.65
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.29	0.65
12:2Q:10:ARG:HH11	12:2Q:11:LYS:HE2	1.60	0.65
32:2a:1226:C:H2'	44:2m:103:THR:HB	1.78	0.65
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.78	0.65
1:1A:2344:U:OP1	28:16:37:ARG:NH1	2.30	0.65
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.32	0.65
33:1b:15:VAL:HG11	33:1b:213:LEU:HD22	1.77	0.65
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.79	0.65
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.29	0.65
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.32	0.65
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.79	0.65
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.29	0.64
1:1A:1069:A:H5'	1:1A:1070:A:H8	1.62	0.64
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	1.78	0.64
32:1a:1500:A:OP1	61:1a:1912:HOH:O	2.14	0.64
1:2A:1434:A:H61	1:2A:1558:A:H62	1.44	0.64
1:1A:1176:G:H21	1:1A:1178:C:P	2.21	0.64
54:1w:35:A:OP1	61:1w:201:HOH:O	2.14	0.64
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.30	0.64
44:2m:25:ILE:HG13	44:2m:66:LEU:HD21	1.79	0.64
1:1A:483:A:H5''	20:1Y:50:ARG:HE	1.63	0.64
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.70	0.64
28:26:7:ILE:HD13	28:26:27:LYS:HD3	1.79	0.64
1:2A:2867:G:OP2	15:2T:119:LYS:NZ	2.27	0.64
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.61	0.64
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.80	0.64
1:1A:1039:G:H1	1:1A:1116:C:H42	1.46	0.64
9:1N:123:TYR:OH	9:1N:130:HIS:NE2	2.28	0.64
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.81	0.64
43:1l:117:ARG:HB3	43:1l:122:THR:HB	1.78	0.64
1:2A:1890:A:OP2	61:2A:3928:HOH:O	2.14	0.64
32:2a:1099:G:OP2	33:2b:144:ARG:NH2	2.31	0.64
1:1A:593:G:H4'	30:18:4:MET:HE2	1.80	0.64
5:1F:135:LYS:HB2	5:1F:138:GLU:HG3	1.79	0.64
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	1.77	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:162:ILE:O	33:1b:185:ILE:HG12	1.98	0.64
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.31	0.64
1:2A:2807:G:H22	1:2A:2892:A:H62	1.44	0.64
32:2a:664:G:H22	32:2a:741:G:H1	1.46	0.64
32:2a:1126:U:H3	41:2j:40:LEU:HD11	1.63	0.64
34:2c:47:LEU:HD12	34:2c:68:VAL:HG11	1.80	0.64
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.80	0.63
1:2A:1023:U:OP2	61:2A:3923:HOH:O	2.15	0.63
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.80	0.63
11:2P:54:GLY:O	61:2P:301:HOH:O	2.15	0.63
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.27	0.63
1:2A:526:A:OP1	61:2A:3929:HOH:O	2.15	0.63
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.14	0.63
32:2a:1133:G:H1	32:2a:1141:C:H42	1.46	0.63
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.12	0.63
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.80	0.63
1:2A:1345:C:OP2	61:2A:3930:HOH:O	2.15	0.63
9:2N:12:ARG:HH21	9:2N:38:HIS:HE2	1.47	0.63
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.30	0.63
1:1A:1075:C:H2'	1:1A:1076:C:H5'	1.81	0.63
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.31	0.63
1:2A:397:G:N7	61:2A:3993:HOH:O	2.30	0.63
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.64	0.63
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.30	0.63
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.63	0.63
16:2U:50:ARG:HH22	17:2V:72:VAL:HG22	1.62	0.63
33:2b:223:ILE:HA	33:2b:226:ARG:HD3	1.81	0.63
1:1A:528:A:O2'	1:1A:529:A:H5'	1.98	0.63
6:1G:72:ARG:HH12	6:1G:87:PRO:HG3	1.62	0.63
11:1P:42:SER:O	61:1P:301:HOH:O	2.16	0.63
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.32	0.63
1:2A:2430:A:OP2	61:2A:3932:HOH:O	2.16	0.63
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.80	0.63
32:2a:972:C:O2'	41:2j:55:LYS:O	2.16	0.63
34:2c:157:ILE:HD12	34:2c:164:ARG:HB3	1.79	0.63
32:1a:903:G:OP2	61:1a:1913:HOH:O	2.15	0.63
1:2A:615:G:OP1	5:2F:40:GLN:NE2	2.30	0.63
32:2a:1147:C:O2	40:2i:16:ARG:NH1	2.31	0.63
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.16	0.63
1:1A:668:G:H5'	1:1A:669:G:OP2	1.99	0.63
1:2A:2022:U:O2'	1:2A:2617:C:H5'	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:677:U:H3	32:2a:713:G:H22	1.47	0.63
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.32	0.62
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.81	0.62
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE2	1.81	0.62
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.32	0.62
1:2A:9:U:OP1	9:2N:115:ARG:NH2	2.31	0.62
32:2a:1301:U:O2'	32:2a:1302:U:H5'	1.98	0.62
39:2h:116:LYS:HG3	39:2h:129:VAL:HG11	1.81	0.62
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.63	0.62
22:10:46:LYS:NZ	22:10:75:LEU:O	2.32	0.62
32:2a:48:C:OP2	61:2a:1912:HOH:O	2.15	0.62
1:1A:2107:C:H42	1:1A:2182:G:H1	1.47	0.62
1:1A:2133:G:O2'	1:1A:2157:G:N2	2.31	0.62
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.32	0.62
32:2a:148:G:H2'	32:2a:149:A:C8	2.34	0.62
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.81	0.62
41:1j:30:SER:HB3	41:1j:81:THR:HB	1.80	0.62
13:2R:104:ARG:HD2	13:2R:109:ALA:HB3	1.80	0.62
32:2a:376:G:H5''	47:2p:5:ARG:HB2	1.80	0.62
34:2c:162:GLN:NE2	53:2v:24:A:O2'	2.33	0.62
1:1A:2128:C:N4	1:1A:2160:G:H1	1.97	0.62
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.81	0.62
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.80	0.62
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.82	0.62
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.29	0.62
32:2a:1239:A:H62	32:2a:1299:A:N6	1.97	0.62
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.15	0.62
5:2F:20:LEU:HD13	5:2F:125:LEU:HD13	1.82	0.62
6:2G:166:ASP:O	6:2G:170:ARG:N	2.28	0.62
32:2a:1060:C:C5	34:2c:2:GLY:HA3	2.35	0.62
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.35	0.62
54:2y:15:G:N2	54:2y:48:C:H42	1.98	0.62
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.32	0.62
6:2G:7:LEU:HD23	6:2G:100:TRP:HE3	1.65	0.62
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.30	0.62
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.80	0.62
18:1W:92:ARG:NH1	61:1W:302:HOH:O	2.32	0.62
33:1b:163:PHE:CD1	33:1b:185:ILE:HG13	2.34	0.62
34:1c:11:ARG:HB3	34:1c:15:THR:HB	1.82	0.62
1:2A:1778:U:OP1	61:2A:3931:HOH:O	2.15	0.62
32:2a:56:U:H2'	32:2a:57:G:C8	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2t:79:ARG:HD2	51:2t:83:ARG:HH21	1.65	0.62
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.31	0.62
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.80	0.62
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.81	0.62
42:1k:29:ILE:HG23	42:1k:44:SER:HB3	1.82	0.62
54:1w:2:C:N4	54:1w:71:G:C6	2.67	0.62
54:1y:51:U:H3	54:1y:63:G:H1	1.47	0.62
41:2j:78:ASN:O	41:2j:80:LYS:N	2.32	0.62
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.32	0.61
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.22	0.61
1:1A:2713:A:OP1	13:1R:14:SER:HB2	2.00	0.61
26:14:16:CYS:HB3	26:14:20:ASN:HB3	1.80	0.61
26:24:61:ARG:NH1	26:24:62:ARG:O	2.32	0.61
34:2c:47:LEU:HB2	34:2c:52:LEU:HD22	1.81	0.61
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.81	0.61
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.33	0.61
1:1A:642:G:OP1	61:1A:4131:HOH:O	2.16	0.61
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.30	0.61
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.30	0.61
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.49	0.61
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.48	0.61
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.46	0.61
32:2a:1379:G:O6	38:2g:2:ALA:N	2.34	0.61
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.65	0.61
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.81	0.61
32:1a:44:G:N7	61:1a:1936:HOH:O	2.31	0.61
1:2A:2116:G:N1	1:2A:2162:G:OP1	2.33	0.61
32:2a:921:U:O2	36:2e:19:MET:HB2	2.00	0.61
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.30	0.61
26:24:46:GLN:HE21	26:24:48:ARG:HD3	1.66	0.61
1:1A:1321:A:N1	61:1A:4192:HOH:O	2.31	0.61
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.65	0.61
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.82	0.61
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.36	0.61
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.18	0.61
32:1a:148:G:H2'	32:1a:149:A:C8	2.36	0.61
32:1a:1359:C:OP1	45:1n:22:THR:OG1	2.18	0.61
33:1b:178:ARG:HH22	39:1h:74:PRO:HB3	1.64	0.61
1:1A:998:C:OP1	61:1A:4130:HOH:O	2.16	0.61
5:1F:116:ASP:OD2	11:1P:1:MET:N	2.33	0.61
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1354:A:H5''	3:2D:38:LYS:HD3	1.83	0.61
11:2P:99:LEU:HD12	11:2P:102:ARG:HH21	1.66	0.61
32:2a:979:C:N4	61:2a:1927:HOH:O	2.32	0.61
33:2b:178:ARG:HH22	39:2h:68:ARG:HH22	1.48	0.61
1:1A:671:C:N4	61:1A:4216:HOH:O	2.34	0.61
1:1A:1664:A:OP1	61:1A:4132:HOH:O	2.16	0.61
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.36	0.61
1:2A:882:G:H22	1:2A:894:C:H42	1.49	0.61
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.13	0.61
7:2H:98:LEU:HD11	7:2H:124:GLU:HA	1.82	0.61
54:2y:65:G:H2'	54:2y:66:U:C6	2.36	0.61
1:1A:588:U:H2'	1:1A:589:C:C6	2.36	0.60
1:1A:602:G:O2'	1:1A:655:A:N6	2.33	0.60
1:1A:1647:G:OP1	61:1A:4112:HOH:O	2.16	0.60
1:1A:2131:G:N2	1:1A:2158:A:N1	2.49	0.60
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.83	0.60
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.81	0.60
32:2a:1002:G:H1	32:2a:1038:C:H42	1.47	0.60
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.16	0.60
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.14	0.60
32:1a:574:A:OP2	61:1a:1914:HOH:O	2.16	0.60
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.35	0.60
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.83	0.60
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.33	0.60
42:2k:54:ARG:NH1	54:2y:39:PSU:O2'	2.34	0.60
1:1A:279:C:H42	1:1A:361:G:H1	1.48	0.60
1:2A:880:G:N2	1:2A:898:C:O2	2.35	0.60
32:2a:1417:G:O6	61:2a:1910:HOH:O	2.14	0.60
41:2j:8:LEU:HG	41:2j:96:ILE:HG12	1.84	0.60
32:1a:324:G:N7	61:1a:1937:HOH:O	2.31	0.60
32:1a:757:U:H2'	32:1a:758:G:O4'	2.01	0.60
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.83	0.60
33:2b:53:ARG:HA	33:2b:56:ARG:HH11	1.66	0.60
34:2c:7:PRO:HG3	34:2c:201:TYR:HE1	1.67	0.60
1:1A:1356:G:OP2	61:1A:4133:HOH:O	2.17	0.60
1:2A:1334:G:O6	61:2A:3934:HOH:O	2.17	0.60
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.16	0.60
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.37	0.60
7:2H:16:SER:HB3	7:2H:27:LYS:HB2	1.83	0.60
21:2Z:104:PHE:HA	21:2Z:139:VAL:HB	1.83	0.60
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	1.83	0.60
48:1q:37:LYS:O	48:1q:38:ARG:NH2	2.33	0.60
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.83	0.60
21:2Z:31:ARG:HH11	21:2Z:94:GLU:HG2	1.66	0.60
32:2a:1272:G:N2	32:2a:1273:G:C5	2.70	0.60
1:1A:483:A:OP1	20:1Y:50:ARG:NH2	2.34	0.60
9:2N:123:TYR:HH	9:2N:130:HIS:CD2	2.18	0.60
32:2a:5:U:H3	35:2d:87:GLY:H	1.48	0.60
32:2a:1089:G:H1	32:2a:1096:C:H42	1.47	0.60
38:2g:80:VAL:HB	38:2g:85:TYR:HE2	1.65	0.60
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.67	0.60
32:1a:7:G:H2'	36:1e:119:LEU:HD22	1.81	0.60
1:2A:2554:U:O2	54:2w:74:C:N4	2.20	0.60
27:25:35:GLU:HG2	27:25:51:TYR:CG	2.37	0.60
32:2a:1134:G:C2	32:2a:1135:U:H1'	2.37	0.60
33:2b:91:PRO:HG3	33:2b:154:LEU:HB3	1.83	0.60
38:2g:78:ARG:HE	38:2g:79:ARG:HG3	1.67	0.60
38:2g:111:ARG:NH1	38:2g:113:GLU:OE2	2.35	0.60
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.83	0.60
33:1b:37:ASN:C	33:1b:39:ILE:H	2.10	0.60
33:1b:78:GLN:NE2	33:1b:94:ASN:O	2.34	0.60
47:1p:72:ARG:HA	47:1p:75:ARG:HB3	1.84	0.60
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.84	0.60
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.19	0.60
1:2A:2892:A:H2'	1:2A:2893:G:H5'	1.84	0.60
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.17	0.60
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.82	0.60
1:1A:2690:C:OP2	13:1R:17:ARG:NH2	2.35	0.59
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.83	0.59
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.66	0.59
55:2x:3:C:H42	55:2x:70:G:H1	1.50	0.59
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.37	0.59
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.37	0.59
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.84	0.59
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.01	0.59
12:2Q:10:ARG:HH12	12:2Q:90:VAL:H	1.50	0.59
32:2a:838:G:H1	32:2a:848:C:N4	2.00	0.59
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.66	0.59
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.33	0.59
1:1A:2128:C:N3	1:1A:2160:G:N2	2.49	0.59
1:2A:731:C:OP1	61:2A:3935:HOH:O	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:890:A:H2'	1:2A:892:G:H8	1.68	0.59
4:2E:76:ARG:NH1	61:2E:402:HOH:O	2.35	0.59
32:2a:1226:C:O2'	44:2m:111:LYS:NZ	2.35	0.59
32:2a:1228:C:H2'	32:2a:1229:A:H8	1.66	0.59
33:2b:119:GLU:HG3	33:2b:142:LEU:HD11	1.82	0.59
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.85	0.59
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.83	0.59
28:26:40:CYS:O	28:26:44:ARG:N	2.35	0.59
46:2o:26:GLU:HG3	46:2o:81:LEU:HD13	1.84	0.59
1:1A:516:C:OP1	27:15:13:LYS:NZ	2.35	0.59
1:1A:883:G:H21	1:1A:893:C:H42	1.51	0.59
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.85	0.59
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.36	0.59
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.83	0.59
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.83	0.59
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.20	0.59
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.85	0.59
1:2A:2000:G:N7	61:2A:4002:HOH:O	2.32	0.59
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.35	0.59
2:2B:82:G:N7	61:2B:301:HOH:O	2.32	0.59
6:2G:70:VAL:HA	6:2G:90:LEU:HD23	1.84	0.59
26:24:46:GLN:C	26:24:48:ARG:H	2.10	0.59
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.35	0.59
1:2A:568:U:H5'	1:2A:945:A:N1	2.17	0.59
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.35	0.59
8:2I:75:LEU:HD13	8:2I:105:HIS:CD2	2.37	0.59
18:2W:12:ILE:O	18:2W:101:SER:OG	2.21	0.59
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.34	0.59
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	1.85	0.59
54:1w:2:C:N3	54:1w:71:G:C2	2.70	0.59
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.21	0.59
5:2F:20:LEU:HD23	5:2F:21:ALA:H	1.68	0.59
6:2G:121:ASN:HD21	6:2G:123:ASN:HD22	1.51	0.59
48:2q:54:GLY:O	48:2q:81:ARG:N	2.34	0.59
1:1A:2469:A:O3'	12:1Q:56:ARG:NH1	2.35	0.59
7:1H:72:ILE:O	7:1H:76:VAL:HG23	2.03	0.59
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.03	0.59
1:2A:84:A:OP2	20:2Y:8:LYS:NZ	2.30	0.59
18:2W:19:LEU:HB3	27:25:25:LEU:HG	1.85	0.59
32:1a:1030:C:N4	32:1a:1030(A):G:N3	2.51	0.59
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2552:2MU:H2'	1:2A:2554:U:OP2	2.02	0.59
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.18	0.59
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.38	0.59
32:2a:1271:G:C2	32:2a:1272:G:N7	2.71	0.59
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.35	0.59
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.85	0.59
32:1a:396:G:O2'	32:1a:398:C:OP1	2.19	0.58
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.85	0.58
1:2A:1271:G:OP2	61:2A:3916:HOH:O	2.17	0.58
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.38	0.58
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	1.85	0.58
32:2a:1073:U:O2'	33:2b:104:ASN:OD1	2.20	0.58
32:2a:1263:C:N3	32:2a:1272:G:O6	2.35	0.58
33:2b:21:ARG:HA	33:2b:39:ILE:HA	1.83	0.58
54:2w:13:C:O2'	54:2w:14:A:O5'	2.14	0.58
1:1A:493:G:O6	61:1A:4129:HOH:O	2.15	0.58
1:1A:652(D):C:H42	1:1A:652(U):G:H1	1.50	0.58
32:2a:1060:C:H2'	32:2a:1061:G:H8	1.67	0.58
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.01	0.58
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.68	0.58
32:1a:407:G:OP1	35:1d:115:ARG:NH2	2.36	0.58
43:1l:42:THR:HG22	43:1l:54:LYS:HD2	1.85	0.58
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.68	0.58
32:2a:7:G:H5'	32:2a:298:A:O4'	2.03	0.58
32:2a:405:U:O4	35:2d:2:GLY:N	2.36	0.58
1:1A:1094:U:H1'	1:1A:1097:U:C4	2.38	0.58
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.68	0.58
16:1U:104:GLN:HE21	16:1U:105:VAL:HG23	1.67	0.58
8:2I:124:GLY:H	8:2I:144:VAL:HB	1.69	0.58
21:2Z:73:GLN:H	21:2Z:87:ASP:HB2	1.68	0.58
32:2a:1279:A:H4'	32:2a:1280:A:OP1	2.04	0.58
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.86	0.58
1:2A:236:C:H2'	1:2A:237:C:C6	2.38	0.58
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.01	0.58
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.36	0.58
8:2I:38:LEU:HB2	8:2I:40:THR:HG23	1.84	0.58
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.52	0.58
33:2b:175:ARG:HH12	33:2b:179:LYS:HD2	1.68	0.58
40:2i:9:ARG:HG2	40:2i:14:VAL:HG22	1.84	0.58
1:1A:2306:C:O2	61:1A:4126:HOH:O	2.14	0.58
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:48:MET:HA	33:1b:51:LEU:HB2	1.84	0.58
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.68	0.58
54:1y:67:C:H2'	54:1y:68:C:C6	2.39	0.58
32:2a:841:U:C5	32:2a:848:C:H1'	2.39	0.58
38:2g:16:LEU:HD22	40:2i:42:ARG:HA	1.85	0.58
45:2n:34:TYR:HD2	45:2n:44:LEU:HD13	1.68	0.58
54:2w:51:U:H3	54:2w:63:G:H1	1.51	0.58
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.19	0.58
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.03	0.58
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.84	0.58
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.37	0.58
21:2Z:154:ASP:OD1	21:2Z:154:ASP:N	2.30	0.58
32:2a:157:G:H2'	32:2a:158:G:H8	1.69	0.58
40:2i:64:THR:OG1	40:2i:66:ARG:NH2	2.33	0.58
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.19	0.58
1:1A:1119:C:N4	61:1A:4172:HOH:O	2.35	0.58
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.30	0.58
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.39	0.58
33:1b:22:LYS:HA	33:1b:40:HIS:HE1	1.68	0.58
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.68	0.58
54:1w:51:U:H2'	54:1w:52:G:C8	2.38	0.58
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.39	0.58
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.02	0.58
1:1A:467:G:OP1	29:17:33:ARG:NH1	2.37	0.58
1:2A:288:C:H2'	1:2A:289:A:C8	2.39	0.58
1:2A:2875:C:O2'	15:2T:2:ASN:OD1	2.17	0.58
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG12	1.85	0.58
6:1G:126:ASP:OD2	6:1G:130:ASN:ND2	2.29	0.58
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.39	0.58
1:2A:2666:C:O2	7:2H:152:ARG:NH1	2.32	0.58
2:2B:14:U:OP2	2:2B:70:C:O2'	2.18	0.58
8:2I:4:ILE:HD11	8:2I:44:LEU:HD13	1.85	0.58
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	1.86	0.58
32:2a:70:G:H1	32:2a:99:U:H3	1.51	0.58
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.68	0.57
35:1d:190:ASP:H	35:1d:193:ASP:HB2	1.68	0.57
21:2Z:105:VAL:N	21:2Z:139:VAL:O	2.35	0.57
35:2d:59:ARG:HH11	35:2d:59:ARG:HA	1.69	0.57
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.85	0.57
1:1A:387:U:O4	61:1A:4128:HOH:O	2.14	0.57
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.40	0.57
11:1P:121:LYS:HB3	11:1P:123:LEU:HD13	1.85	0.57
32:1a:1036:G:H5'	32:1a:1037:C:C5	2.39	0.57
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.17	0.57
18:2W:34:ASN:OD1	18:2W:37:ARG:NH1	2.33	0.57
32:2a:986:A:H2'	32:2a:987:G:O4'	2.05	0.57
6:1G:7:LEU:HD22	6:1G:176:LEU:HD22	1.85	0.57
32:1a:642:A:N3	39:1h:113:SER:OG	2.36	0.57
2:2B:3:C:H2'	2:2B:4:C:C6	2.39	0.57
14:2S:71:ARG:NH1	14:2S:107:GLU:OE1	2.36	0.57
32:2a:45:U:H2'	32:2a:46:G:C8	2.39	0.57
32:2a:1255:G:N7	41:2j:43:ARG:NH2	2.52	0.57
33:2b:69:LEU:HD13	33:2b:155:LEU:HD22	1.86	0.57
34:2c:39:ILE:HG22	34:2c:43:LEU:HD11	1.87	0.57
7:1H:101:ARG:NH2	7:1H:122:THR:HA	2.13	0.57
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.05	0.57
1:2A:288:C:H2'	1:2A:289:A:H8	1.68	0.57
1:2A:1815:A:OP2	3:2D:54:ARG:NH2	2.36	0.57
29:27:24:THR:HG22	29:27:27:GLY:N	2.10	0.57
32:2a:1212:U:H5'	32:2a:1213:A:C8	2.39	0.57
32:2a:1320:C:H42	50:2s:36:ARG:HE	1.49	0.57
40:2i:11:LYS:HA	40:2i:108:VAL:HG12	1.86	0.57
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.85	0.57
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.19	0.57
32:2a:187:C:O2'	51:2t:89:ARG:NH2	2.37	0.57
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.86	0.57
25:13:55:ARG:HH22	25:13:57:GLU:HB2	1.69	0.57
41:1j:9:ARG:HG2	41:1j:69:ASN:HD22	1.69	0.57
50:1s:36:ARG:NH2	50:1s:72:GLY:O	2.38	0.57
6:2G:41:GLN:O	6:2G:43:LEU:N	2.38	0.57
7:2H:35:VAL:HG13	7:2H:71:LEU:HD22	1.86	0.57
35:2d:18:LYS:HG2	59:2d:303:SF4:S1	2.45	0.57
39:2h:51:VAL:HG11	39:2h:60:ARG:HH11	1.69	0.57
54:2w:11:C:N4	54:2w:24:G:H1	2.00	0.57
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.12	0.57
32:1a:501:C:H2'	32:1a:502:G:C8	2.40	0.57
33:1b:105:PHE:C	33:1b:107:THR:H	2.11	0.57
38:1g:115:ARG:HG2	38:1g:118:VAL:HG12	1.85	0.57
32:2a:1026:G:O6	32:2a:1036:G:N2	2.38	0.57
32:2a:1108:G:O6	61:2a:1911:HOH:O	2.15	0.57
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:1:MET:HE3	24:12:5:GLU:HB3	1.86	0.57
36:1e:41:VAL:HG23	36:1e:67:VAL:HG13	1.87	0.57
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.22	0.57
1:2A:2853:C:H2'	1:2A:2854:G:H8	1.69	0.57
7:2H:86:GLU:OE2	7:2H:130:ARG:NH1	2.37	0.57
32:2a:620:C:C2	35:2d:135:LEU:HG	2.40	0.57
32:2a:973:G:H3'	32:2a:974:A:H5''	1.86	0.57
33:2b:18:GLY:HA2	33:2b:42:ILE:HG13	1.86	0.57
54:2y:51:U:H2'	54:2y:52:G:C8	2.40	0.57
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.39	0.57
6:1G:167:GLU:OE1	6:1G:167:GLU:N	2.38	0.57
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.24	0.57
18:1W:31:GLU:OE1	61:1W:301:HOH:O	2.17	0.57
32:1a:171:A:H2'	32:1a:172:A:C8	2.40	0.57
32:1a:1429:C:H2'	32:1a:1430:C:H6	1.70	0.57
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.87	0.57
33:2b:33:TYR:HB2	33:2b:43:ASP:HB2	1.86	0.57
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.85	0.57
55:2x:40:C:H2'	55:2x:41:C:H6	1.70	0.57
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.86	0.57
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.12	0.57
50:1s:12:ASP:OD1	50:1s:37:ARG:NH2	2.38	0.57
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.86	0.57
1:1A:2234:G:N7	61:1A:4203:HOH:O	2.32	0.56
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.85	0.56
32:1a:1499:A:OP2	61:1a:1903:HOH:O	2.18	0.56
1:2A:1651:G:OP1	13:2R:40:LYS:NZ	2.37	0.56
1:2A:2135:A:C4	1:2A:2136:C:H5	2.23	0.56
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.86	0.56
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.19	0.56
23:21:44:PRO:HB2	23:21:46:LEU:HD12	1.86	0.56
38:2g:151:TYR:OH	42:2k:54:ARG:HD3	2.05	0.56
46:2o:9:GLN:O	46:2o:13:GLN:HG3	2.04	0.56
54:2w:28:G:H2'	54:2w:29:G:O4'	2.05	0.56
1:2A:882:G:H22	1:2A:894:C:N4	2.03	0.56
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.05	0.56
1:2A:2118:U:OP1	1:2A:2148:G:H4'	2.05	0.56
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.70	0.56
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.40	0.56
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.87	0.56
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.38	0.56
48:1q:45:HIS:HB2	48:1q:65:ILE:HD13	1.86	0.56
6:2G:49:ASP:N	6:2G:49:ASP:OD1	2.36	0.56
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.86	0.56
32:2a:266:G:H5''	32:2a:268:C:H41	1.70	0.56
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.87	0.56
1:1A:2296:U:OP2	14:1S:9:ARG:NH2	2.38	0.56
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.70	0.56
11:1P:90:ARG:HG2	11:1P:90:ARG:HH11	1.71	0.56
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.87	0.56
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.41	0.56
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.38	0.56
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.69	0.56
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.88	0.56
26:24:24:THR:OG1	26:24:25:TYR:N	2.37	0.56
35:2d:17:VAL:HG12	35:2d:19:LEU:HD12	1.86	0.56
44:2m:40:ASN:HD22	44:2m:43:THR:HG23	1.70	0.56
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.87	0.56
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.87	0.56
55:1x:23:C:H2'	55:1x:24:U:C6	2.41	0.56
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.06	0.56
25:23:59:VAL:HG12	25:23:60:GLU:H	1.69	0.56
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.40	0.56
9:1N:115:ARG:HA	9:1N:118:LYS:HE3	1.87	0.56
32:1a:167:G:H2'	32:1a:168:G:C8	2.40	0.56
32:1a:450:G:OP1	47:1p:43:LYS:NZ	2.38	0.56
40:1i:53:VAL:O	40:1i:55:ALA:N	2.38	0.56
52:1u:6:ARG:HG2	52:1u:15:ARG:HD2	1.87	0.56
1:2A:208:C:H2'	1:2A:209:C:H6	1.71	0.56
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.40	0.56
20:2Y:43:ASN:HD22	20:2Y:67:LEU:HG	1.71	0.56
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.04	0.56
40:2i:97:LYS:HA	40:2i:102:LEU:HG	1.88	0.56
54:2y:55:PSU:HN1	54:2y:57:G:C5'	2.18	0.56
1:1A:800:A:H8	1:1A:800:A:OP1	1.88	0.56
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.05	0.56
32:1a:1039:C:H2'	32:1a:1040:U:H6	1.69	0.56
34:1c:157:ILE:HD12	34:1c:164:ARG:HB3	1.86	0.56
2:2B:76:G:N7	61:2B:302:HOH:O	2.32	0.56
15:2T:42:ILE:HG13	15:2T:84:GLN:HE21	1.70	0.56
32:2a:996:A:H3'	32:2a:997:U:H5''	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.41	0.56
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.85	0.56
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.88	0.56
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.13	0.56
32:1a:68:G:H1	32:1a:101:A:H61	1.54	0.56
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.88	0.56
6:2G:150:ASP:OD1	6:2G:150:ASP:N	2.38	0.56
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.39	0.56
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.05	0.56
1:1A:1069:A:H5'	1:1A:1070:A:C8	2.41	0.56
15:1T:127:ALA:C	15:1T:129:ARG:H	2.13	0.56
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.40	0.56
32:1a:516:PSU:O2'	32:1a:519:C:N3	2.37	0.56
39:1h:112:LEU:HA	39:1h:134:ILE:HG12	1.87	0.56
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.40	0.56
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.88	0.56
18:2W:84:ARG:HG3	18:2W:98:LYS:HD2	1.88	0.56
41:2j:8:LEU:HB2	41:2j:70:ARG:HB2	1.87	0.56
41:2j:44:VAL:HG13	41:2j:66:ARG:HB3	1.86	0.56
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.70	0.56
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.88	0.56
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.88	0.56
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.88	0.56
32:1a:501:C:H2'	32:1a:502:G:H8	1.71	0.56
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.87	0.56
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.41	0.56
1:2A:1780:A:N6	61:2A:4050:HOH:O	2.39	0.56
1:2A:2134:A:H2	1:2A:2159:G:H1'	1.70	0.56
21:2Z:129:SER:OG	21:2Z:131:ARG:NH1	2.39	0.56
32:2a:377:G:OP1	47:2p:3:LYS:NZ	2.39	0.56
1:1A:536:A:H2'	1:1A:537:C:C6	2.41	0.55
11:1P:95:VAL:HA	11:1P:99:LEU:HD23	1.89	0.55
21:1Z:139:VAL:HG12	21:1Z:140:ASP:H	1.70	0.55
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.41	0.55
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.41	0.55
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.23	0.55
1:2A:2306:C:N4	6:2G:42:GLY:O	2.32	0.55
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.41	0.55
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.38	0.55
1:1A:1055:G:H1	1:1A:1104:C:H42	1.55	0.55
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:376:G:H5''	47:1p:5:ARG:HB2	1.88	0.55
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.17	0.55
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.88	0.55
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.05	0.55
2:2B:72:G:O2'	2:2B:105:A:N6	2.38	0.55
35:2d:187:ARG:NH1	35:2d:190:ASP:OD1	2.38	0.55
54:2y:14:A:H3'	54:2y:15:G:C8	2.40	0.55
1:1A:621:A:OP2	11:1P:108:LYS:NZ	2.39	0.55
1:1A:2712(A):A:OP1	61:1A:4137:HOH:O	2.18	0.55
32:1a:262:A:H2'	32:1a:263:A:C8	2.42	0.55
37:1f:76:ALA:HA	37:1f:79:LEU:HD12	1.88	0.55
34:2c:88:ARG:HA	34:2c:91:LEU:HD13	1.87	0.55
34:2c:157:ILE:HD13	34:2c:166:GLU:HG3	1.89	0.55
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.87	0.55
4:1E:109:LYS:O	4:1E:111:ARG:NH1	2.40	0.55
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.88	0.55
37:1f:11:ASN:HB3	37:1f:14:LEU:HG	1.88	0.55
37:1f:21:LEU:O	37:1f:25:ILE:HG13	2.06	0.55
1:2A:208:C:H2'	1:2A:209:C:C6	2.42	0.55
1:2A:637:A:OP1	11:2P:133:SER:OG	2.17	0.55
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.07	0.55
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.22	0.55
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.88	0.55
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.41	0.55
47:1p:15:PRO:O	47:1p:16:HIS:ND1	2.40	0.55
1:2A:247:G:H4'	1:2A:386:G:C5	2.42	0.55
1:2A:902:C:H2'	1:2A:903:C:C6	2.42	0.55
6:2G:51:ARG:NE	6:2G:51:ARG:H	2.05	0.55
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.73	0.55
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.41	0.55
3:1D:25:THR:HG21	3:1D:113:VAL:HG21	1.88	0.55
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.89	0.55
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.87	0.55
1:2A:888:C:OP1	44:2m:93:ARG:NH1	2.39	0.55
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.07	0.55
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.87	0.55
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.89	0.55
32:2a:1124:G:H4'	41:2j:38:ILE:HD13	1.88	0.55
36:2e:78:HIS:CE1	36:2e:143:ARG:H	2.25	0.55
44:2m:85:GLY:HA2	44:2m:93:ARG:HH21	1.72	0.55
1:1A:1709:U:H2'	1:1A:1710:C:C6	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.89	0.55
32:1a:333:G:H4'	51:1t:16:HIS:CE1	2.42	0.55
32:1a:1027:C:C2	32:1a:1034:G:N2	2.57	0.55
2:2B:114:C:H4'	14:2S:46:VAL:HG12	1.88	0.55
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.89	0.55
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.39	0.55
39:2h:13:ILE:O	39:2h:17:THR:OG1	2.24	0.55
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.06	0.55
32:1a:966:M2G:O2'	40:1i:127:LYS:O	2.25	0.55
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.12	0.55
1:2A:1243:G:O2'	11:2P:7:ARG:NH2	2.39	0.55
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.39	0.55
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.07	0.55
4:1E:29:GLY:HA3	61:1E:404:HOH:O	2.07	0.55
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.71	0.55
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.88	0.55
34:2c:9:GLY:HA2	34:2c:12:LEU:HG	1.89	0.55
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.88	0.55
32:1a:721:G:H4'	32:1a:722:A:O4'	2.07	0.55
32:1a:1500:A:OP2	61:1a:1916:HOH:O	2.18	0.55
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.88	0.55
1:2A:1163:G:OP1	17:2V:24:LYS:NZ	2.33	0.55
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.40	0.55
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.38	0.55
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.89	0.55
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.35	0.54
1:1A:1671:U:O4	61:1A:4106:HOH:O	2.16	0.54
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.23	0.54
33:1b:163:PHE:HD1	33:1b:185:ILE:HG13	1.72	0.54
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.06	0.54
1:2A:652(B):A:N6	1:2A:655:A:O2'	2.36	0.54
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.42	0.54
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.24	0.54
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.42	0.54
32:2a:222:U:H2'	32:2a:223:U:C6	2.42	0.54
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.40	0.54
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.41	0.54
33:2b:53:ARG:HA	33:2b:56:ARG:NH1	2.21	0.54
1:1A:732:C:OP1	61:1A:4135:HOH:O	2.18	0.54
1:1A:2065:C:H4'	1:1A:2251:OMG:HM22	1.89	0.54
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.32	0.54
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.42	0.54
1:2A:921:G:O6	61:2A:3933:HOH:O	2.16	0.54
1:2A:2135:A:OP1	1:2A:2160:G:H1'	2.07	0.54
3:2D:11:PRO:O	3:2D:14:ARG:HG3	2.07	0.54
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.72	0.54
11:2P:29:LYS:HG3	11:2P:30:THR:H	1.71	0.54
41:2j:27:ALA:HB1	41:2j:81:THR:HG23	1.88	0.54
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.06	0.54
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.08	0.54
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.42	0.54
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.90	0.54
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.71	0.54
2:1B:57:A:H1'	6:1G:29:TRP:HB2	1.88	0.54
32:1a:22:G:H4'	32:1a:885:G:C8	2.42	0.54
33:1b:83:MET:N	33:1b:83:MET:SD	2.81	0.54
36:1e:20:GLN:NE2	36:1e:21:ALA:O	2.40	0.54
1:2A:249:C:O2	30:28:12:LYS:NZ	2.36	0.54
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.28	0.54
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.42	0.54
11:2P:37:GLY:O	11:2P:40:SER:OG	2.22	0.54
21:2Z:137:ILE:HA	21:2Z:156:LYS:HE2	1.89	0.54
23:21:32:LYS:O	61:21:201:HOH:O	2.18	0.54
32:2a:396:G:O2'	32:2a:398:C:OP1	2.19	0.54
38:2g:73:MET:HG2	38:2g:90:GLU:HA	1.90	0.54
42:2k:110:ASP:HB3	49:2r:85:LEU:HB3	1.89	0.54
49:2r:52:PRO:HB2	49:2r:54:ARG:HG3	1.88	0.54
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.42	0.54
32:1a:714:G:H2'	32:1a:715:A:C8	2.43	0.54
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.41	0.54
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.89	0.54
13:2R:36:THR:HG22	13:2R:37:THR:H	1.73	0.54
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.40	0.54
32:2a:1191:A:H5''	34:2c:4:LYS:HE3	1.88	0.54
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.37	0.54
39:2h:95:VAL:HB	39:2h:99:GLU:HG3	1.89	0.54
1:1A:586:A:N1	1:1A:809:G:O2'	2.37	0.54
1:1A:1054:A:N6	1:1A:1105:U:H3	2.03	0.54
2:1B:14:U:OP2	2:1B:70:C:O2'	2.24	0.54
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.41	0.54
32:1a:382:A:H2'	32:1a:383:A:C8	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.42	0.54
33:1b:170:GLU:HG3	33:1b:173:ALA:HB3	1.89	0.54
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.72	0.54
35:1d:8:VAL:HG22	35:1d:21:LEU:HD13	1.89	0.54
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	1.89	0.54
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	1.88	0.54
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.05	0.54
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.43	0.54
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.08	0.54
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.42	0.54
1:2A:2318:G:H21	14:2S:3:ARG:HD3	1.72	0.54
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.71	0.54
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.71	0.54
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.43	0.54
1:1A:530:G:N1	1:1A:2023:G:OP1	2.30	0.54
1:1A:2156:G:OP2	1:1A:2156:G:H8	1.91	0.54
32:1a:181:G:H4'	32:1a:182:U:H5'	1.88	0.54
32:1a:250:A:H4'	32:1a:251:G:O5'	2.08	0.54
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.42	0.54
40:1i:23:ASN:OD1	40:1i:23:ASN:N	2.39	0.54
16:2U:105:VAL:HG22	17:2V:45:THR:HG23	1.90	0.54
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.41	0.54
33:2b:185:ILE:HB	33:2b:199:TYR:HB2	1.90	0.54
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.42	0.54
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.07	0.54
51:1t:42:GLN:NE2	51:1t:46:GLU:OE2	2.39	0.54
1:2A:893:C:H2'	1:2A:894:C:C4	2.43	0.54
32:2a:524:G:H2'	32:2a:525:C:C6	2.43	0.54
34:2c:134:ILE:HG23	34:2c:151:VAL:HG13	1.90	0.54
55:2x:50:U:H3	55:2x:64:G:H1	1.56	0.54
54:2y:51:U:H2'	54:2y:52:G:H8	1.73	0.54
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.27	0.54
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.90	0.54
1:2A:579:G:H2'	1:2A:580:C:C6	2.43	0.54
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.26	0.54
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.08	0.54
4:2E:101:ARG:HB2	4:2E:201:THR:HG21	1.90	0.54
6:2G:124:SER:O	6:2G:124:SER:OG	2.26	0.54
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.07	0.54
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.43	0.54
36:2e:41:VAL:O	36:2e:66:MET:HA	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:100:ASN:HD21	49:2r:23:LYS:HE3	1.73	0.54
54:2w:18:G:O2'	54:2w:19:G:OP2	2.25	0.54
1:1A:2371:G:O6	61:1A:4139:HOH:O	2.19	0.54
8:1I:37:VAL:HG13	8:1I:38:LEU:HD23	1.89	0.54
32:1a:1144:G:N2	32:1a:1146:A:H62	2.07	0.54
40:1i:17:VAL:HG23	40:1i:63:ILE:HG12	1.90	0.54
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.90	0.54
9:2N:20:GLY:HA2	9:2N:61:ARG:HE	1.72	0.54
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.90	0.54
32:2a:473:G:H2'	32:2a:474:G:H8	1.73	0.54
36:2e:78:HIS:HE1	36:2e:143:ARG:H	1.56	0.54
1:1A:1364:G:P	23:11:3:LYS:HG3	2.47	0.53
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.54	0.53
24:12:41:ILE:HG13	24:12:43:GLN:HG3	1.90	0.53
32:1a:189(B):C:H2'	32:1a:189(C):C:C6	2.42	0.53
33:1b:118:LEU:HB3	33:1b:142:LEU:HD12	1.90	0.53
1:2A:709:U:H2'	1:2A:710:G:C8	2.44	0.53
1:2A:2379:G:HO2'	14:2S:17:ARG:HH12	1.51	0.53
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.73	0.53
6:2G:167:GLU:HA	6:2G:170:ARG:HB2	1.89	0.53
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.89	0.53
32:2a:1016:A:H2'	32:2a:1017:G:O4'	2.07	0.53
36:2e:43:LEU:HD22	36:2e:136:MET:HG3	1.90	0.53
41:2j:42:THR:HG23	41:2j:68:HIS:HA	1.90	0.53
50:2s:63:THR:HG23	50:2s:66:MET:HE3	1.90	0.53
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.43	0.53
32:1a:692:U:O2'	32:1a:694:A:N7	2.32	0.53
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	1.90	0.53
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.73	0.53
1:2A:2540:C:O2'	1:2A:2740:A:N3	2.40	0.53
21:2Z:106:GLY:HA3	21:2Z:141:VAL:HB	1.89	0.53
28:26:9:LEU:HD13	28:26:51:GLU:HG3	1.90	0.53
32:2a:542:G:OP1	35:2d:10:ARG:NH2	2.33	0.53
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.23	0.53
33:2b:93:VAL:HG11	33:2b:97:TRP:HE3	1.71	0.53
33:2b:97:TRP:NE1	33:2b:176:GLU:OE2	2.36	0.53
33:2b:114:ARG:HD2	33:2b:117:GLU:HB3	1.90	0.53
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.43	0.53
15:1T:84:GLN:HG2	15:1T:85:LYS:HG2	1.89	0.53
21:1Z:138:GLU:H	21:1Z:156:LYS:HE2	1.73	0.53
32:1a:45:U:H2'	32:1a:46:G:C8	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:458:C:H2'	32:1a:460:G:O4'	2.09	0.53
54:1w:26:A:N6	54:1w:44:G:H1	2.05	0.53
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.08	0.53
1:2A:2317:C:N4	1:2A:2318:G:O6	2.40	0.53
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.43	0.53
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.08	0.53
36:2e:100:VAL:HG13	36:2e:118:ILE:HG22	1.90	0.53
1:1A:897:C:N3	1:1A:898:C:N4	2.57	0.53
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.08	0.53
32:1a:812:C:O2	61:1a:1917:HOH:O	2.18	0.53
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.42	0.53
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.11	0.53
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.08	0.53
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.08	0.53
34:2c:8:ILE:HG12	34:2c:184:TYR:HB3	1.90	0.53
44:2m:4:ILE:HG23	44:2m:5:ALA:H	1.73	0.53
55:2x:67:C:H2'	55:2x:68:C:H6	1.74	0.53
1:1A:1082:U:H3	1:1A:1086:A:H61	0.61	0.53
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.41	0.53
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.44	0.53
1:1A:2098:U:H3	1:1A:2191:G:H1	1.54	0.53
1:1A:2102:U:H3	1:1A:2187:G:H1	1.56	0.53
32:1a:731:G:H5'	32:1a:766:A:H4'	1.91	0.53
32:1a:1030(C):G:H8	32:1a:1030(D):A:N7	2.07	0.53
1:2A:2895:U:H2'	1:2A:2896:C:O4'	2.09	0.53
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.42	0.53
3:2D:35:LYS:HD3	3:2D:64:ILE:HD11	1.91	0.53
32:2a:617:G:N7	61:2a:1930:HOH:O	2.34	0.53
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.43	0.53
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.90	0.53
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.05	0.53
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.42	0.53
16:1U:69:CYS:HB3	16:1U:74:LEU:HD12	1.91	0.53
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.74	0.53
33:1b:122:PHE:HE2	33:1b:139:LYS:HB2	1.73	0.53
44:1m:16:ASP:OD1	44:1m:16:ASP:N	2.41	0.53
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.41	0.53
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.91	0.53
28:26:14:THR:O	28:26:17:LYS:NZ	2.42	0.53
32:2a:1236:A:O2'	32:2a:1304:G:H4'	2.09	0.53
38:2g:54:THR:O	38:2g:56:GLN:N	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.90	0.53
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.09	0.53
46:2o:70:LEU:HD11	46:2o:77:ARG:HB3	1.91	0.53
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.88	0.53
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.73	0.53
1:1A:2702:U:OP2	61:1A:4138:HOH:O	2.18	0.53
16:1U:49:HIS:HA	16:1U:52:ARG:HB2	1.89	0.53
32:1a:169:C:H2'	32:1a:170:U:H6	1.74	0.53
32:1a:627:G:H2'	32:1a:628:G:C8	2.44	0.53
33:1b:39:ILE:HG22	33:1b:41:ILE:HD13	1.90	0.53
42:1k:87:THR:O	42:1k:87:THR:OG1	2.27	0.53
51:1t:56:MET:HE3	51:1t:85:MET:HG2	1.89	0.53
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.41	0.53
9:2N:12:ARG:NH2	9:2N:50:ASP:OD2	2.41	0.53
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.23	0.53
33:2b:118:LEU:O	33:2b:122:PHE:HB3	2.09	0.53
35:2d:76:ARG:NE	35:2d:80:GLU:OE2	2.41	0.53
41:2j:13:HIS:HB3	41:2j:68:HIS:CE1	2.44	0.53
54:2y:14:A:H3'	54:2y:15:G:H8	1.74	0.53
7:1H:25:LYS:HE2	7:1H:27:LYS:HE3	1.91	0.53
32:1a:200:G:H2'	32:1a:201:C:C6	2.44	0.53
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.41	0.53
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.42	0.53
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.09	0.53
5:1F:110:LEU:HD11	5:1F:181:LEU:HG	1.89	0.53
28:16:9:LEU:HD13	28:16:51:GLU:HG3	1.90	0.53
32:1a:684:A:N6	61:1a:1953:HOH:O	2.40	0.53
32:1a:1086:U:H3	32:1a:1099:G:H22	1.55	0.53
32:1a:1239:A:H62	32:1a:1299:A:N6	2.07	0.53
33:1b:109:SER:HA	33:1b:112:VAL:HG13	1.89	0.53
36:1e:85:GLY:O	36:1e:87:SER:N	2.42	0.53
54:1w:18:G:H4'	54:1w:60:U:C5	2.44	0.53
1:2A:764:A:H5''	3:2D:210:GLY:CA	2.39	0.53
1:2A:890:A:H2'	1:2A:892:G:C8	2.44	0.53
1:2A:1754:C:H5	15:2T:96:ARG:NH2	2.07	0.53
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.23	0.53
1:2A:2135:A:C5	1:2A:2136:C:H5	2.27	0.53
1:2A:2218:U:N3	23:21:55:GLY:O	2.40	0.53
8:2I:59:ALA:HA	8:2I:62:LYS:HB2	1.89	0.53
32:2a:407:G:H5''	35:2d:115:ARG:HB3	1.90	0.53
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.43	0.53
1:1A:2552:2MU:O5'	1:1A:2552:2MU:H6	2.08	0.53
21:1Z:138:GLU:HB2	21:1Z:156:LYS:HZ3	1.74	0.53
46:1o:43:LEU:HD12	46:1o:56:LEU:HD22	1.91	0.53
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.34	0.53
1:2A:643:A:N1	1:2A:2369:A:O2'	2.39	0.53
1:2A:668:G:H5'	1:2A:669:G:OP2	2.08	0.53
1:2A:1378:A:O2'	1:2A:1380:G:N7	2.42	0.53
9:2N:59:LYS:O	9:2N:61:ARG:NH2	2.43	0.53
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.23	0.52
1:1A:1058:G:N2	1:1A:1081:U:O2	2.42	0.52
7:1H:149:ARG:HH12	7:1H:167:GLU:CD	2.17	0.52
11:1P:89:ALA:O	11:1P:121:LYS:NZ	2.42	0.52
32:1a:673:G:H2'	32:1a:674:G:C8	2.43	0.52
40:1i:23:ASN:HB2	40:1i:25:LYS:HE2	1.91	0.52
1:2A:27:G:N2	1:2A:512:G:H1'	2.23	0.52
1:2A:271(K):U:H4'	1:2A:271(L):U:OP1	2.09	0.52
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.09	0.52
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.44	0.52
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.37	0.52
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	1.90	0.52
22:20:38:VAL:HG12	22:20:40:GLN:HG2	1.92	0.52
32:2a:989:C:H2'	32:2a:990:C:C6	2.44	0.52
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.07	0.52
1:1A:2106:G:H2'	1:1A:2107:C:C6	2.44	0.52
2:2B:20:C:H42	2:2B:63:G:H1	1.58	0.52
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.92	0.52
14:2S:84:GLN:H	14:2S:111:GLU:HB2	1.75	0.52
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.39	0.52
32:2a:1264:C:H42	32:2a:1271:G:H1	1.57	0.52
32:2a:1312:G:H5'	50:2s:5:LEU:HD11	1.90	0.52
33:2b:58:ILE:HG23	33:2b:61:LEU:HD12	1.90	0.52
1:1A:881:G:C2	1:1A:882:G:H1'	2.44	0.52
1:1A:2355:C:H1'	22:10:39:ARG:HH21	1.73	0.52
9:1N:17:ASP:O	9:1N:21:LYS:HE2	2.08	0.52
1:2A:1261:C:OP2	18:2W:83:LYS:NZ	2.39	0.52
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.74	0.52
6:2G:44:GLY:N	6:2G:88:ILE:O	2.41	0.52
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.45	0.52
15:2T:127:ALA:C	15:2T:129:ARG:H	2.17	0.52
21:2Z:31:ARG:NH1	21:2Z:94:GLU:HG2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:50:VAL:HG11	44:2m:64:TRP:C	2.33	0.52
32:2a:157:G:H1	32:2a:164:U:H3	1.57	0.52
32:2a:165:C:H2'	32:2a:166:G:C8	2.43	0.52
32:2a:881:G:OP2	43:2l:12:ARG:NH2	2.42	0.52
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.24	0.52
1:1A:857:C:N4	1:1A:858:U:O4	2.43	0.52
1:1A:1005:C:O2'	9:1N:28:THR:HG21	2.09	0.52
1:1A:1688:U:H1'	1:1A:1701:A:C6	2.44	0.52
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.90	0.52
32:1a:341:C:H2'	32:1a:342:C:C6	2.43	0.52
40:1i:56:LEU:H	40:1i:56:LEU:HD12	1.74	0.52
1:2A:1248:G:C5	16:2U:3:ARG:HB2	2.44	0.52
6:2G:43:LEU:HD12	6:2G:45:GLU:HG3	1.91	0.52
21:2Z:150:LEU:H	21:2Z:171:ILE:HD11	1.74	0.52
32:2a:757:U:H2'	32:2a:758:G:O4'	2.09	0.52
32:2a:1144:G:N2	32:2a:1146:A:H62	2.08	0.52
32:2a:1192:C:OP2	34:2c:4:LYS:NZ	2.36	0.52
33:2b:212:GLN:CD	33:2b:235:SER:HB3	2.35	0.52
42:2k:21:ILE:HG12	42:2k:30:VAL:HG12	1.92	0.52
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.44	0.52
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.92	0.52
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.45	0.52
42:1k:21:ILE:HB	42:1k:84:VAL:HG12	1.92	0.52
54:1y:56:C:H2'	54:1y:57:G:H8	1.74	0.52
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.25	0.52
7:2H:102:ALA:HB2	7:2H:116:GLU:HG2	1.91	0.52
25:23:12:PRO:HB2	25:23:20:LYS:HG2	1.91	0.52
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.92	0.52
54:2y:52:G:H5'	54:2y:53:G:OP2	2.09	0.52
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.42	0.52
61:1A:5289:HOH:O	11:1P:44:GLY:HA2	2.09	0.52
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.09	0.52
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.42	0.52
33:1b:82:ARG:NH1	33:1b:86:GLU:OE2	2.43	0.52
1:2A:492:A:H2'	1:2A:493:G:O4'	2.10	0.52
1:2A:2853:C:H2'	1:2A:2854:G:C8	2.45	0.52
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	1.91	0.52
21:2Z:150:LEU:N	21:2Z:171:ILE:HD11	2.24	0.52
33:2b:55:PHE:HA	33:2b:58:ILE:HD12	1.92	0.52
42:2k:104:GLN:HG2	42:2k:106:LYS:HG3	1.92	0.52
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1762:A:H2'	61:1A:5831:HOH:O	2.08	0.52
1:2A:2727:G:O3'	10:2O:70:LYS:HE2	2.09	0.52
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.44	0.52
6:2G:51:ARG:H	6:2G:51:ARG:HE	1.58	0.52
28:26:12:GLU:HB2	28:26:19:ARG:HG3	1.92	0.52
36:2e:7:GLU:CD	36:2e:37:ARG:HH21	2.17	0.52
50:2s:27:GLU:HB2	50:2s:28:LYS:HA	1.92	0.52
55:2x:67:C:H2'	55:2x:68:C:C6	2.45	0.52
5:1F:24:LEU:HB3	5:1F:115:ALA:HB2	1.91	0.52
8:1I:62:LYS:HA	8:1I:133:HIS:HE1	1.75	0.52
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.45	0.52
32:1a:973:G:H3'	32:1a:974:A:H5''	1.92	0.52
32:1a:976:G:OP1	45:1n:32:SER:N	2.40	0.52
54:1y:38:A:H2'	54:1y:39:PSU:O4'	2.09	0.52
1:2A:2336:A:H61	22:20:43:THR:HG22	1.74	0.52
5:2F:179:GLU:CD	5:2F:179:GLU:H	2.18	0.52
14:2S:105:ALA:HB1	14:2S:110:LEU:HD23	1.90	0.52
32:2a:984:C:H2'	32:2a:985:C:C6	2.44	0.52
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.26	0.52
1:1A:657:U:H2'	1:1A:658:C:C6	2.45	0.52
2:1B:66:A:N6	2:1B:109:C:H5'	2.24	0.52
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.74	0.52
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.45	0.52
1:2A:212:G:H2'	1:2A:213:A:O4'	2.10	0.52
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.45	0.52
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.43	0.52
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.44	0.52
37:2f:70:ASP:OD1	37:2f:70:ASP:N	2.43	0.52
39:2h:17:THR:HG23	39:2h:63:LEU:HD13	1.92	0.52
55:2x:73:A:H5''	55:2x:74:C:H5'	1.91	0.52
54:2y:5:G:H1	54:2y:68:C:H42	1.57	0.52
1:1A:582:G:H2'	1:1A:583:G:C8	2.44	0.52
1:1A:987:G:O2'	1:1A:1000:A:N3	2.40	0.52
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.10	0.52
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.43	0.52
32:1a:562:C:H1'	43:1l:15:ARG:HB3	1.92	0.52
54:1w:5:G:H2'	54:1w:6:G:C8	2.45	0.52
1:2A:597:U:H2'	1:2A:598:G:C8	2.45	0.52
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.10	0.52
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.56	0.52
35:2d:92:VAL:O	35:2d:96:LEU:HG	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2y:18:G:N2	54:2y:55:PSU:C4	2.75	0.52
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.25	0.51
12:1Q:12:GLN:NE2	12:1Q:73:PRO:HD2	2.25	0.51
21:1Z:101:PRO:HA	21:1Z:123:ASP:HB3	1.92	0.51
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.25	0.51
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.06	0.51
32:1a:1023:G:H3'	32:1a:1024:G:H8	1.75	0.51
1:2A:570:G:H2'	1:2A:2030:A:C5	2.44	0.51
1:2A:652(A):A:H3'	1:2A:652(B):A:H5''	1.91	0.51
1:2A:2750:A:OP2	7:2H:62:LYS:NZ	2.43	0.51
2:2B:4:C:H42	2:2B:117:G:H1	1.57	0.51
32:2a:1251:A:N1	32:2a:1354:C:O2'	2.41	0.51
32:2a:1305:G:O2'	32:2a:1331:G:N2	2.44	0.51
1:1A:185:U:H4'	1:1A:218:A:H4'	1.92	0.51
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.45	0.51
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.25	0.51
33:1b:208:ILE:HD13	33:1b:208:ILE:H	1.75	0.51
40:1i:8:GLY:O	40:1i:15:ALA:N	2.43	0.51
44:1m:91:ARG:HB2	44:1m:98:VAL:HG23	1.91	0.51
1:2A:127:A:H5''	1:2A:128:C:C6	2.45	0.51
1:2A:323:G:O2'	1:2A:1205:U:N3	2.40	0.51
1:2A:458:G:C8	29:27:37:LYS:HG2	2.46	0.51
1:2A:2121:G:H1	1:2A:2177:C:H42	1.56	0.51
1:2A:2127:G:N2	1:2A:2161:C:N3	2.56	0.51
11:2P:37:GLY:N	61:2P:303:HOH:O	2.44	0.51
32:2a:600:C:H2'	32:2a:601:C:C6	2.45	0.51
32:2a:646:U:H2'	32:2a:647:C:C6	2.44	0.51
32:2a:1004:A:N6	32:2a:1037:C:O2	2.28	0.51
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.91	0.51
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.91	0.51
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.93	0.51
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.92	0.51
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.45	0.51
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.91	0.51
41:1j:54:PHE:CD2	41:1j:55:LYS:HG2	2.46	0.51
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.42	0.51
2:2B:88:C:H2'	2:2B:89:G:O4'	2.09	0.51
32:2a:17:U:H2'	32:2a:18:C:C6	2.45	0.51
32:2a:546:G:OP1	35:2d:73:ARG:HG2	2.10	0.51
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.43	0.51
1:1A:411:G:OP1	61:1A:4136:HOH:O	2.18	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:101:ILE:HD13	26:14:25:TYR:HB2	1.93	0.51
32:1a:119:A:H4'	32:1a:120:A:C8	2.45	0.51
32:1a:628:G:H2'	32:1a:629:G:C8	2.46	0.51
33:1b:105:PHE:O	33:1b:107:THR:N	2.43	0.51
34:1c:120:VAL:HG23	34:1c:198:VAL:HG11	1.91	0.51
41:1j:38:ILE:HD11	41:1j:71:LEU:HB3	1.92	0.51
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.92	0.51
1:2A:184:C:H2'	1:2A:185:U:C6	2.46	0.51
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.92	0.51
1:2A:2745:C:H2'	1:2A:2746:U:O4'	2.10	0.51
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.43	0.51
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.93	0.51
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.93	0.51
32:2a:662:G:O2'	32:2a:836:G:OP1	2.28	0.51
42:2k:98:LEU:O	42:2k:101:SER:OG	2.20	0.51
44:2m:49:THR:OG1	44:2m:52:GLU:HG3	2.10	0.51
1:1A:796:C:H2'	1:1A:797:C:C6	2.45	0.51
1:1A:1024:G:OP2	61:1A:4111:HOH:O	2.19	0.51
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.44	0.51
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.44	0.51
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.41	0.51
38:1g:78:ARG:HD3	38:1g:79:ARG:HG3	1.91	0.51
39:1h:77:GLU:HG2	39:1h:78:GLN:H	1.75	0.51
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.92	0.51
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.91	0.51
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.11	0.51
1:2A:2121:G:H2'	1:2A:2122:U:O4'	2.09	0.51
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.76	0.51
16:2U:92:ARG:HA	16:2U:95:LEU:HD12	1.91	0.51
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.93	0.51
38:2g:22:LEU:HD21	38:2g:66:VAL:HG21	1.92	0.51
43:2l:56:ALA:HB2	43:2l:70:ILE:HD11	1.91	0.51
1:1A:278:A:H2'	1:1A:279:C:C6	2.45	0.51
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.46	0.51
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.24	0.51
7:1H:15:VAL:HG11	7:1H:76:VAL:HG13	1.93	0.51
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.92	0.51
17:1V:43:GLU:OE1	17:1V:43:GLU:N	2.43	0.51
28:16:18:ARG:HD2	28:16:42:TRP:CG	2.45	0.51
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.92	0.51
55:1x:23:C:H2'	55:1x:24:U:H6	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.46	0.51
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.45	0.51
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.46	0.51
1:2A:2431:U:OP2	61:2A:3937:HOH:O	2.19	0.51
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.41	0.51
37:2f:97:PHE:CD2	49:2r:31:LEU:HD11	2.46	0.51
38:2g:23:VAL:HG13	38:2g:43:PHE:CE2	2.46	0.51
40:2i:23:ASN:OD1	40:2i:23:ASN:N	2.40	0.51
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.76	0.51
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.93	0.51
32:1a:890:G:O2'	32:1a:906:G:O6	2.26	0.51
34:1c:172:ARG:NH2	34:1c:206:GLU:OE2	2.43	0.51
46:1o:3:ILE:HG21	46:1o:34:LEU:HD21	1.92	0.51
1:2A:2143:C:N4	1:2A:2148:G:H1	2.07	0.51
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.40	0.51
32:2a:573:A:N3	32:2a:883:C:O2'	2.43	0.51
41:2j:5:ARG:O	41:2j:98:ILE:HA	2.11	0.51
1:1A:882:G:H1	1:1A:894:C:H42	1.59	0.51
1:1A:1062:G:H1'	1:1A:1088:A:C8	2.46	0.51
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	1.91	0.51
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.46	0.51
5:2F:137:LYS:HA	5:2F:140:LEU:HD12	1.92	0.51
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.91	0.51
21:2Z:6:LYS:HE3	21:2Z:8:TYR:HE2	1.75	0.51
32:2a:157:G:H2'	32:2a:158:G:C8	2.46	0.51
32:2a:473:G:H2'	32:2a:474:G:C8	2.46	0.51
32:2a:921:U:O2'	36:2e:19:MET:O	2.25	0.51
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.45	0.51
41:2j:5:ARG:N	61:2j:3302:HOH:O	2.43	0.51
1:1A:1039:G:H1	1:1A:1116:C:N4	2.09	0.51
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.10	0.51
5:1F:7:TYR:CD2	5:1F:24:LEU:HB2	2.46	0.51
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.76	0.51
24:12:12:GLU:HA	24:12:15:LYS:HE3	1.91	0.51
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.46	0.51
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.46	0.51
36:1e:85:GLY:C	36:1e:87:SER:H	2.19	0.51
1:2A:900:A:HO2'	1:2A:901:A:P	2.33	0.51
26:24:16:CYS:SG	26:24:17:GLY:N	2.83	0.51
32:2a:881:G:P	43:2l:12:ARG:HH22	2.33	0.51
32:2a:973:G:OP1	41:2j:57:LYS:NZ	2.34	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.76	0.51
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.43	0.51
1:1A:1045:A:OP1	1:1A:1046:A:H3'	2.11	0.51
1:1A:1053:C:H42	1:1A:1106:G:H1	1.57	0.51
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.45	0.51
32:1a:627:G:H2'	32:1a:628:G:H8	1.76	0.51
44:1m:20:THR:HA	44:1m:25:ILE:O	2.09	0.51
8:2I:77:LEU:HB3	8:2I:142:VAL:HG13	1.92	0.51
9:2N:35:ARG:O	9:2N:42:TRP:NE1	2.43	0.51
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.44	0.51
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.94	0.51
32:2a:839:U:H3'	32:2a:840:C:H6	1.76	0.51
33:2b:118:LEU:HD11	33:2b:138:LEU:HB3	1.92	0.51
33:2b:185:ILE:HG22	33:2b:199:TYR:CD2	2.46	0.51
36:2e:20:GLN:HG2	36:2e:25:ARG:HD2	1.91	0.51
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	1.93	0.51
36:2e:69:VAL:HG22	36:2e:71:LEU:HD21	1.92	0.51
54:2y:14:A:H61	54:2y:21:A:H2	1.59	0.51
4:1E:13:ARG:HD3	15:1T:58:ASN:HD21	1.75	0.50
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE3	1.76	0.50
32:1a:1036:G:H3'	32:1a:1037:C:H6	1.76	0.50
54:1w:5:G:H2'	54:1w:6:G:H8	1.76	0.50
1:2A:1301:A:O2'	1:2A:1302:A:H3'	2.11	0.50
2:2B:13:A:O2'	2:2B:14:U:H3'	2.11	0.50
32:2a:662:G:H2'	32:2a:663:A:C8	2.46	0.50
32:2a:1263:C:H1'	32:2a:1273:G:N2	2.26	0.50
36:2e:101:ILE:HG13	36:2e:119:LEU:HD23	1.93	0.50
43:2l:7:ILE:O	43:2l:11:VAL:HG13	2.11	0.50
1:1A:271(H):G:H1	1:1A:271(P):C:H42	1.58	0.50
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.41	0.50
4:1E:119:ARG:HG2	4:1E:120:TRP:CE2	2.47	0.50
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.09	0.50
41:1j:54:PHE:O	41:1j:56:HIS:N	2.44	0.50
54:1w:8:4SU:O5'	54:1w:8:4SU:H6	2.10	0.50
1:2A:340:A:H2'	1:2A:341:G:O4'	2.11	0.50
1:2A:1192:G:OP2	11:2P:17:LYS:NZ	2.35	0.50
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.92	0.50
32:2a:533:A:O2'	32:2a:535:A:OP2	2.20	0.50
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.36	0.50
34:2c:79:ARG:H	34:2c:82:GLU:HB3	1.76	0.50
1:1A:1057:A:N6	1:1A:1087:G:OP1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:126:VAL:HG21	5:1F:129:PHE:CZ	2.47	0.50
6:1G:137:GLU:HG2	6:1G:152:LEU:HD22	1.94	0.50
32:1a:662:G:H2'	32:1a:663:A:C8	2.45	0.50
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.26	0.50
35:1d:107:ARG:NH2	35:1d:194:LEU:HD21	2.26	0.50
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.47	0.50
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.46	0.50
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.51	0.50
32:2a:1049:U:O4	45:2n:3:ARG:NH1	2.45	0.50
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	1.92	0.50
33:2b:80:ILE:HD13	33:2b:211:ILE:HB	1.94	0.50
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.93	0.50
1:1A:576:U:H2'	1:1A:577:G:C8	2.46	0.50
1:1A:1003:G:O2'	1:1A:1010:A:N1	2.39	0.50
32:1a:452:A:H4'	47:1p:72:ARG:CZ	2.42	0.50
32:1a:679:C:H2'	32:1a:680:C:C6	2.46	0.50
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.46	0.50
1:2A:686:G:N2	1:2A:788:A:H61	2.09	0.50
4:2E:119:ARG:HG2	4:2E:120:TRP:NE1	2.27	0.50
9:2N:115:ARG:HA	9:2N:118:LYS:HE2	1.94	0.50
33:2b:71:VAL:HG23	33:2b:164:VAL:HA	1.93	0.50
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.93	0.50
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.46	0.50
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.12	0.50
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.46	0.50
32:1a:838:G:H1	32:1a:848:C:H42	1.59	0.50
42:1k:48:ILE:O	42:1k:48:ILE:HG12	2.10	0.50
1:2A:184:C:H2'	1:2A:185:U:H6	1.76	0.50
1:2A:271(K):U:O2	8:2I:50:ARG:NE	2.31	0.50
32:2a:54:C:N4	32:2a:353:A:OP2	2.43	0.50
32:2a:999:C:C4	32:2a:1000:U:C4	2.99	0.50
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.45	0.50
44:2m:82:MET:HE3	44:2m:93:ARG:HG2	1.94	0.50
48:2q:45:HIS:HB2	48:2q:65:ILE:HD13	1.93	0.50
1:1A:604:G:P	11:1P:90:ARG:HH21	2.33	0.50
1:1A:686:G:OP1	29:17:11:LYS:NZ	2.43	0.50
1:1A:1055:G:H2'	1:1A:1056:G:O4'	2.12	0.50
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.46	0.50
7:1H:96:ALA:HB2	7:1H:105:LEU:HD23	1.93	0.50
32:1a:96:U:H2'	32:1a:97:G:C8	2.47	0.50
32:1a:1367:C:H5'	41:1j:60:ARG:NH1	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:403:U:H4'	1:2A:404:C:H5'	1.92	0.50
1:2A:700:G:O2'	1:2A:1632:A:N3	2.33	0.50
1:2A:1027:A:C6	1:2A:1126:A:C4	3.00	0.50
1:2A:1183:G:H5''	25:23:30:ARG:NH2	2.25	0.50
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.26	0.50
10:2O:71:ARG:NE	10:2O:105:GLU:OE2	2.43	0.50
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.11	0.50
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.76	0.50
36:2e:43:LEU:HB3	36:2e:136:MET:HE2	1.93	0.50
38:2g:69:VAL:HG11	38:2g:134:ALA:HB1	1.93	0.50
54:2y:15:G:H22	54:2y:48:C:N4	2.05	0.50
1:1A:2106:G:H1	1:1A:2183:C:N4	2.09	0.50
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.23	0.50
8:1I:48:GLU:HB3	8:1I:52:ARG:NH1	2.27	0.50
15:1T:35:LYS:HG3	15:1T:40:THR:HG22	1.93	0.50
32:1a:946:A:H2'	32:1a:947:G:C8	2.45	0.50
38:1g:50:ILE:HD12	38:1g:61:VAL:HG11	1.93	0.50
1:2A:2336:A:H61	22:20:43:THR:CG2	2.25	0.50
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.93	0.50
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.29	0.50
32:2a:1263:C:C4	32:2a:1272:G:O6	2.65	0.50
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.45	0.50
33:2b:218:ALA:O	33:2b:222:ILE:HG23	2.12	0.50
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.12	0.50
24:12:10:LEU:HB3	24:12:14:ARG:NH1	2.27	0.50
24:12:63:VAL:HA	24:12:66:GLU:HG3	1.94	0.50
26:14:16:CYS:HB2	26:14:36:CYS:HB3	1.93	0.50
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.59	0.50
32:1a:1456:G:N1	51:1t:51:GLU:OE2	2.45	0.50
38:1g:140:ASP:OD1	54:1y:41:C:O2'	2.28	0.50
39:1h:51:VAL:HG11	39:1h:60:ARG:HH12	1.77	0.50
1:2A:651:G:OP1	30:28:19:SER:OG	2.30	0.50
1:2A:796:C:H2'	1:2A:797:C:C6	2.46	0.50
1:2A:922:U:H2'	1:2A:923:C:C6	2.47	0.50
1:2A:2318:G:H21	14:2S:3:ARG:CD	2.24	0.50
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.45	0.50
6:2G:126:ASP:OD2	6:2G:130:ASN:ND2	2.42	0.50
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.47	0.50
32:2a:1053:G:N7	32:2a:1200:C:H5''	2.27	0.50
21:1Z:151:HIS:CE1	21:1Z:170:THR:HG22	2.46	0.50
32:1a:79:G:C6	32:1a:90:U:O2	2.65	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:600:C:H2'	32:1a:601:C:C6	2.47	0.50
36:1e:137:GLU:HG3	36:1e:141:GLN:HE21	1.75	0.50
39:1h:121:ASP:HB2	39:1h:125:ARG:NH2	2.27	0.50
43:1l:54:LYS:HD3	43:1l:54:LYS:N	2.26	0.50
48:1q:67:LYS:HA	48:1q:70:ARG:HH12	1.76	0.50
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.27	0.50
5:2F:10:PRO:HB3	5:2F:17:ARG:NH1	2.26	0.50
7:2H:101:ARG:HH22	7:2H:122:THR:HA	1.77	0.50
8:2I:72:LEU:HA	8:2I:75:LEU:HG	1.92	0.50
9:2N:38:HIS:NE2	9:2N:50:ASP:OD2	2.39	0.50
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.11	0.50
9:2N:123:TYR:CZ	9:2N:129:PRO:HD2	2.46	0.50
1:1A:839:U:H1'	1:1A:1191:G:H1'	1.94	0.49
1:1A:2428:G:OP1	61:1A:4103:HOH:O	2.20	0.49
11:1P:96:THR:OG1	11:1P:98:GLU:HG3	2.12	0.49
32:1a:1025:U:C2	32:1a:1036:G:O6	2.65	0.49
1:2A:2722:G:H5'	13:2R:4:LEU:HD12	1.92	0.49
2:2B:87:G:N2	2:2B:90:A:OP2	2.38	0.49
4:2E:36:ARG:NH2	4:2E:88:GLY:O	2.42	0.49
20:2Y:15:VAL:HG21	20:2Y:42:VAL:HG11	1.93	0.49
21:2Z:151:HIS:CE1	21:2Z:170:THR:HG23	2.47	0.49
32:2a:352:C:O2'	32:2a:354:G:OP1	2.21	0.49
32:2a:1002:G:H1	32:2a:1038:C:N4	2.10	0.49
32:2a:1193:G:O2'	36:2e:25:ARG:NH2	2.45	0.49
42:2k:70:LYS:HA	42:2k:73:MET:HE2	1.93	0.49
1:1A:184:C:H2'	1:1A:185:U:C6	2.47	0.49
3:1D:70:TRP:CE2	3:1D:150:LYS:HD3	2.47	0.49
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.12	0.49
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.12	0.49
1:2A:2058:A:N7	61:2A:4015:HOH:O	2.33	0.49
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.93	0.49
6:2G:67:LYS:HD3	26:24:5:ILE:HD12	1.95	0.49
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.45	0.49
32:2a:56:U:H2'	32:2a:57:G:H8	1.76	0.49
32:2a:381:C:H2'	32:2a:382:A:O4'	2.13	0.49
32:2a:404:U:H2'	32:2a:405:U:C6	2.47	0.49
32:2a:406:G:O3'	35:2d:3:ARG:NH2	2.44	0.49
33:2b:134:GLU:O	33:2b:138:LEU:HG	2.12	0.49
36:2e:5:ASP:N	36:2e:5:ASP:OD1	2.45	0.49
1:1A:1268:A:C2	1:1A:2013:A:C4	3.01	0.49
1:1A:1971:A:C4	3:1D:241:PRO:HD3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.46	0.49
5:1F:9:ILE:HD13	5:1F:22:ALA:HB3	1.94	0.49
7:1H:105:LEU:HD12	7:1H:151:ILE:HD12	1.94	0.49
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.20	0.49
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.47	0.49
32:1a:1218:C:OP2	45:1n:9:LYS:NZ	2.38	0.49
34:1c:66:VAL:HG23	34:1c:101:LEU:HA	1.95	0.49
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.12	0.49
32:2a:109:A:C6	32:2a:326:G:C6	3.00	0.49
32:2a:444:C:H2'	32:2a:445:G:C8	2.47	0.49
54:2w:9:A:O2'	54:2w:10:G:N7	2.43	0.49
1:1A:247:G:H4'	1:1A:386:G:C5	2.47	0.49
1:1A:321:G:O4'	5:1F:165:ARG:HG2	2.13	0.49
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.13	0.49
32:1a:92:C:H2'	32:1a:93:G:C8	2.48	0.49
32:1a:861:G:HO2'	32:1a:874:G:HO2'	1.58	0.49
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.12	0.49
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.40	0.49
25:23:6:VAL:HA	25:23:56:VAL:HG22	1.94	0.49
28:26:2:ALA:HB1	28:26:6:ARG:O	2.11	0.49
32:2a:236:G:OP1	48:2q:40:LYS:NZ	2.44	0.49
32:2a:1202:G:O3'	45:2n:3:ARG:NH1	2.45	0.49
32:2a:1328:C:OP1	52:2u:21:TYR:OH	2.25	0.49
36:2e:71:LEU:HD22	36:2e:115:VAL:HG12	1.93	0.49
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.11	0.49
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.48	0.49
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.95	0.49
21:1Z:155:LEU:HD12	21:1Z:156:LYS:H	1.76	0.49
33:1b:178:ARG:NH2	39:1h:74:PRO:HB3	2.27	0.49
43:1l:60:LEU:HD11	43:1l:66:VAL:HG22	1.95	0.49
1:2A:646:A:H2'	1:2A:647:G:O4'	2.13	0.49
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.45	0.49
1:2A:2602:A:OP1	61:2A:3940:HOH:O	2.19	0.49
1:2A:2782:G:OP2	61:2A:3939:HOH:O	2.19	0.49
32:2a:280:C:N3	48:2q:39:SER:N	2.57	0.49
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.59	0.49
33:2b:61:LEU:HD11	33:2b:68:ILE:HD11	1.94	0.49
54:2y:8:4SU:H1'	54:2y:48:C:H1'	1.95	0.49
1:1A:2467:C:H4'	12:1Q:123:HIS:CD2	2.47	0.49
21:1Z:103:ARG:O	21:1Z:139:VAL:HG23	2.12	0.49
1:2A:1359:A:H2	1:2A:1372:U:O4	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1754:C:H5	15:2T:96:ARG:HH21	1.58	0.49
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.48	0.49
1:2A:2394:C:N3	54:2y:76:A:O2'	2.38	0.49
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	1.95	0.49
6:2G:5:VAL:HG12	6:2G:8:LYS:HE2	1.92	0.49
18:2W:71:VAL:HA	18:2W:107:LEU:HD23	1.95	0.49
20:2Y:68:HIS:ND1	20:2Y:70:SER:HB3	2.27	0.49
26:24:34:GLU:HB2	44:2m:57:ARG:HE	1.78	0.49
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.28	0.49
32:2a:503:C:OP2	43:2l:116:SER:OG	2.27	0.49
37:2f:100:ASN:ND2	49:2r:23:LYS:HE3	2.27	0.49
54:2w:19:G:N2	54:2w:57:G:H1'	2.28	0.49
54:2y:14:A:O2'	54:2y:15:G:OP1	2.24	0.49
1:1A:2188:C:H2'	1:1A:2189:U:O4'	2.12	0.49
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.47	0.49
61:1A:4639:HOH:O	13:1R:15:SER:HB3	2.13	0.49
21:1Z:1:MET:HE2	21:1Z:135:GLU:HB2	1.95	0.49
26:14:69:LYS:HE3	26:14:69:LYS:HA	1.93	0.49
1:2A:90:U:H1'	1:2A:92:A:C8	2.48	0.49
1:2A:800:A:H8	1:2A:800:A:OP1	1.96	0.49
1:2A:1257:C:H4'	5:2F:83:PHE:CD1	2.47	0.49
4:2E:96:PHE:O	4:2E:175:VAL:HG21	2.12	0.49
32:2a:110:C:O2'	47:2p:25:ARG:O	2.28	0.49
38:2g:22:LEU:HD11	38:2g:101:LEU:HD21	1.94	0.49
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.94	0.49
1:1A:818:G:H5'	1:1A:839:U:OP1	2.12	0.49
1:1A:1670:C:O2	4:1E:129:HIS:NE2	2.44	0.49
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.27	0.49
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.48	0.49
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.95	0.49
28:16:25:LYS:HE3	28:16:27:LYS:HA	1.93	0.49
32:1a:625:G:H2'	32:1a:626:U:C6	2.48	0.49
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.80	0.49
1:2A:271(M):G:H4'	1:2A:271(N):U:OP1	2.13	0.49
1:2A:307:G:H21	1:2A:330:A:H62	1.61	0.49
30:28:26:LYS:HB2	30:28:44:LYS:O	2.13	0.49
32:2a:1327:C:OP2	52:2u:12:LYS:NZ	2.42	0.49
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.48	0.49
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.95	0.49
33:1b:107:THR:O	33:1b:110:GLN:HB3	2.13	0.49
54:1w:18:G:O2'	54:1w:57:G:N2	2.34	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:375:C:H2'	1:2A:376:C:C6	2.47	0.49
1:2A:2343:C:O2'	1:2A:2373:G:O2'	2.28	0.49
2:2B:66:A:N6	2:2B:108:U:H3'	2.28	0.49
6:2G:28:VAL:O	6:2G:31:VAL:HG12	2.13	0.49
32:2a:1316:G:H22	32:2a:1319:A:H5''	1.78	0.49
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.47	0.49
1:1A:226:G:H21	1:1A:228:A:H62	1.61	0.49
1:1A:1025:G:O2'	61:1A:4111:HOH:O	2.07	0.49
1:1A:1509(A):A:H3'	1:1A:1509(B):A:H8	1.78	0.49
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.13	0.49
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.95	0.49
5:1F:117:ARG:NH2	5:1F:189:THR:O	2.45	0.49
8:1I:81:VAL:O	8:1I:146:ALA:HA	2.13	0.49
32:1a:713:G:H2'	32:1a:714:G:C8	2.48	0.49
32:1a:1529:G:H4'	32:1a:1530:G:OP2	2.13	0.49
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.78	0.49
32:2a:1055:A:N7	32:2a:1200:C:N4	2.58	0.49
33:2b:17:PHE:HA	33:2b:44:LEU:HD11	1.94	0.49
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.94	0.49
41:2j:33:GLN:HG2	41:2j:34:VAL:H	1.78	0.49
54:2w:18:G:HO2'	54:2w:19:G:P	2.36	0.49
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.12	0.48
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.13	0.48
1:1A:2418:A:H2'	1:1A:2419:U:C6	2.48	0.48
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.13	0.48
4:1E:9:VAL:HG22	4:1E:25:VAL:HB	1.95	0.48
26:14:15:ILE:HG12	26:14:21:VAL:HG22	1.95	0.48
41:1j:46:ARG:HB2	41:1j:46:ARG:HH11	1.78	0.48
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.13	0.48
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.13	0.48
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.45	0.48
24:22:35:LEU:HD12	24:22:53:LEU:HD12	1.95	0.48
26:24:46:GLN:NE2	26:24:48:ARG:HD3	2.27	0.48
40:2i:99:LEU:HB3	40:2i:101:PHE:CD2	2.48	0.48
1:1A:2136:C:N3	1:1A:2155:G:C2	2.81	0.48
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.47	0.48
32:1a:864:A:H2'	32:1a:865:A:C8	2.48	0.48
32:1a:1441:G:H5''	32:1a:1442:G:O5'	2.12	0.48
42:1k:99:GLN:HE21	42:1k:108:ILE:HD11	1.77	0.48
54:1w:18:G:HO2'	54:1w:57:G:H22	1.58	0.48
1:2A:383:U:H2'	1:2A:385:C:H5	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.12	0.48
1:2A:2319:G:H22	14:2S:3:ARG:HD2	1.76	0.48
1:2A:2841:C:H2'	1:2A:2842:G:H8	1.78	0.48
35:2d:59:ARG:HA	35:2d:59:ARG:NH1	2.28	0.48
36:2e:7:GLU:HB3	36:2e:112:LEU:HD22	1.93	0.48
42:2k:73:MET:HG2	42:2k:103:LEU:HD21	1.94	0.48
1:1A:207:A:H2'	1:1A:208:C:O4'	2.12	0.48
1:1A:221:A:N1	1:1A:265:A:O2'	2.45	0.48
1:1A:603:A:O4'	1:1A:655:A:N6	2.46	0.48
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.76	0.48
61:1A:4988:HOH:O	27:15:3:LYS:HE2	2.12	0.48
23:11:56:GLN:HB3	23:11:87:PRO:HG3	1.94	0.48
32:1a:103:C:O2'	32:1a:172:A:N1	2.39	0.48
32:1a:743:U:H2'	32:1a:744:C:C6	2.47	0.48
32:1a:1007:C:H2'	32:1a:1008:C:C6	2.48	0.48
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.95	0.48
1:2A:468:G:N7	29:27:39:ARG:NH2	2.58	0.48
1:2A:2801(A):A:O2'	1:2A:2895:U:H4'	2.13	0.48
4:2E:1:MET:HE3	4:2E:199:ARG:HD2	1.95	0.48
4:2E:56:PRO:HA	4:2E:59:VAL:HG12	1.95	0.48
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.49	0.48
32:2a:457:C:H2'	32:2a:458:C:H6	1.78	0.48
32:2a:685:G:C2	32:2a:686:U:C4	3.02	0.48
32:2a:1272:G:N2	32:2a:1273:G:C8	2.81	0.48
32:2a:1320:C:H42	50:2s:36:ARG:NE	2.10	0.48
34:2c:34:LEU:HD11	34:2c:38:ARG:HH21	1.77	0.48
37:2f:4:TYR:CZ	37:2f:72:VAL:HG21	2.48	0.48
1:1A:592:G:O2'	30:18:4:MET:HG3	2.13	0.48
1:1A:1062:G:H22	1:1A:1077:A:H61	1.62	0.48
1:1A:2336:A:H61	22:10:43:THR:CG2	2.25	0.48
2:1B:24:G:N7	2:1B:56:G:H2'	2.29	0.48
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.28	0.48
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.13	0.48
25:13:35:ARG:HE	25:13:37:LEU:HD21	1.77	0.48
32:1a:737:A:H2'	32:1a:738:C:C6	2.47	0.48
32:1a:1003:G:C4	32:1a:1004:A:H2	2.31	0.48
33:1b:140:HIS:O	33:1b:144:ARG:HG3	2.14	0.48
34:1c:61:ALA:C	34:1c:63:ASN:H	2.21	0.48
38:1g:12:LEU:HD12	38:1g:12:LEU:H	1.77	0.48
46:1o:84:LYS:O	46:1o:84:LYS:HD3	2.14	0.48
51:1t:72:LEU:HD21	51:1t:80:ARG:HD2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:500:G:N1	1:2A:503:A:OP2	2.47	0.48
1:2A:848:G:H2'	1:2A:849:A:C8	2.49	0.48
1:2A:1325:G:OP1	1:2A:1647:G:O2'	2.26	0.48
1:2A:1639:U:C2'	1:2A:1640:C:H5''	2.42	0.48
2:2B:2:C:H2'	2:2B:3:C:C6	2.48	0.48
2:2B:105:A:H5'	2:2B:106:G:OP2	2.12	0.48
3:2D:5:LYS:HG2	3:2D:17:THR:HG22	1.94	0.48
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.26	0.48
32:2a:1187:G:OP1	40:2i:113:LYS:NZ	2.46	0.48
34:2c:7:PRO:HB2	34:2c:182:ILE:HD13	1.94	0.48
34:2c:152:ILE:HD11	34:2c:199:LYS:HZ2	1.78	0.48
40:2i:99:LEU:HB3	40:2i:101:PHE:HE2	1.78	0.48
51:2t:10:LEU:HD23	51:2t:12:ALA:HB2	1.94	0.48
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.48	0.48
1:1A:862:G:H2'	1:1A:863:A:O4'	2.14	0.48
1:1A:2203:U:H4'	3:1D:151:LYS:HG2	1.94	0.48
1:1A:2379:G:O2'	14:1S:17:ARG:NH1	2.40	0.48
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.32	0.48
21:1Z:167:PRO:C	21:1Z:169:GLU:H	2.22	0.48
26:14:49:PHE:HB3	26:14:50:VAL:H	1.49	0.48
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.46	0.48
54:1y:48:C:C2	54:1y:59:U:H1'	2.49	0.48
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.48	0.48
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.28	0.48
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.48	0.48
1:2A:2663:G:H3'	1:2A:2664:G:H8	1.78	0.48
3:2D:26:LYS:HE2	3:2D:28:GLU:O	2.13	0.48
7:2H:125:VAL:HG22	7:2H:131:VAL:HG22	1.94	0.48
15:2T:92:GLY:O	15:2T:120:ARG:NH2	2.47	0.48
21:2Z:153:SER:HB2	21:2Z:167:PRO:HB3	1.96	0.48
34:2c:36:ASP:HA	34:2c:39:ILE:HD12	1.95	0.48
41:2j:47:PHE:N	41:2j:63:PHE:O	2.42	0.48
44:2m:108:ARG:HD3	44:2m:108:ARG:HA	1.68	0.48
55:2x:9:G:O2'	55:2x:10:G:N7	2.35	0.48
1:1A:428:A:H8	1:1A:428:A:OP2	1.96	0.48
1:1A:1203:G:O6	61:1A:4134:HOH:O	2.17	0.48
15:1T:39:ARG:NH2	32:1a:345:C:H5'	2.29	0.48
32:1a:358:U:H2'	32:1a:359:U:C6	2.48	0.48
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.49	0.48
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.14	0.48
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.36	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:55:PHE:CE1	33:1b:218:ALA:HA	2.48	0.48
1:2A:1184:G:P	25:23:30:ARG:HH21	2.36	0.48
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.49	0.48
1:2A:2801(A):A:H1'	1:2A:2895:U:O2'	2.12	0.48
10:2O:13:ASN:ND2	10:2O:97:ARG:HB2	2.27	0.48
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.29	0.48
32:2a:826:C:O2	39:2h:15:ASN:ND2	2.47	0.48
32:2a:1194:U:H2'	32:2a:1195:C:C6	2.49	0.48
32:2a:1274:G:N2	32:2a:1275:A:N7	2.61	0.48
38:2g:90:GLU:OE1	38:2g:90:GLU:N	2.47	0.48
43:2l:53:ARG:HB3	43:2l:69:TYR:HE1	1.79	0.48
46:2o:37:ASN:O	46:2o:41:GLU:HG2	2.14	0.48
1:1A:1253:A:OP1	61:1A:4141:HOH:O	2.20	0.48
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.13	0.48
32:1a:328:C:H4'	32:1a:329:A:H5'	1.95	0.48
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.13	0.48
44:1m:49:THR:HG23	44:1m:52:GLU:HG3	1.94	0.48
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.96	0.48
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.29	0.48
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.53	0.48
23:21:73:LEU:HB3	23:21:94:LEU:HD22	1.95	0.48
32:2a:179:A:H2'	32:2a:180:U:C6	2.48	0.48
41:2j:45:ARG:HG2	41:2j:47:PHE:CZ	2.49	0.48
1:1A:634:C:H2'	1:1A:635:C:C6	2.49	0.48
1:1A:831:G:N2	11:1P:53:GLY:O	2.45	0.48
1:1A:2722:G:OP2	61:1A:4142:HOH:O	2.20	0.48
10:1O:64:ARG:HD2	10:1O:79:PHE:CD1	2.48	0.48
26:14:53:GLU:HB2	26:14:55:ARG:C	2.38	0.48
32:1a:353:A:H5'	32:1a:353:A:H8	1.79	0.48
32:1a:922:G:C6	32:1a:923:A:C6	3.01	0.48
34:1c:65:ALA:O	34:1c:66:VAL:HG13	2.14	0.48
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.48	0.48
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.29	0.48
4:2E:77:ILE:HD13	4:2E:195:LEU:HD22	1.96	0.48
11:2P:89:ALA:HA	11:2P:121:LYS:HD3	1.94	0.48
32:2a:1225:A:OP1	44:2m:103:THR:OG1	2.29	0.48
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.28	0.48
41:2j:16:LEU:HD13	41:2j:70:ARG:HG2	1.95	0.48
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.14	0.48
1:1A:2393:A:H5''	11:1P:63:PRO:HB3	1.95	0.48
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:186:C:H2'	32:1a:187:C:C6	2.48	0.48
32:1a:381:C:H2'	32:1a:382:A:O4'	2.13	0.48
32:1a:690:G:C6	32:1a:691:G:C6	3.02	0.48
32:1a:1236:A:H4'	32:1a:1304:G:H4'	1.96	0.48
54:1w:2:C:C2	54:1w:71:G:N2	2.82	0.48
1:2A:98:G:OP2	24:22:2:LYS:HG2	2.13	0.48
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.48	0.48
1:2A:832:G:H5'	11:2P:45:LEU:HD11	1.96	0.48
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.14	0.48
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.46	0.48
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.13	0.48
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.49	0.48
11:2P:81:GLN:NE2	11:2P:105:LEU:O	2.46	0.48
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.49	0.48
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.21	0.48
34:2c:79:ARG:N	34:2c:82:GLU:HB3	2.29	0.48
54:2y:62:C:H2'	54:2y:63:G:H8	1.78	0.48
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.49	0.48
1:1A:1466:G:O2'	1:1A:1546:C:O2'	2.17	0.48
32:1a:4:U:O4	39:1h:105:ARG:HD3	2.13	0.48
32:1a:985:C:H2'	32:1a:986:A:H8	1.79	0.48
34:1c:47:LEU:HD13	34:1c:68:VAL:HG11	1.96	0.48
38:1g:50:ILE:HD11	38:1g:125:MET:HG3	1.96	0.48
54:1y:19:G:N2	54:1y:56:C:N3	2.61	0.48
1:2A:392:C:H5''	1:2A:409:C:H5''	1.96	0.48
33:2b:119:GLU:CD	33:2b:153:ARG:HH12	2.22	0.48
38:2g:15:ASP:OD1	38:2g:19:GLY:N	2.46	0.48
1:1A:534:U:H2'	1:1A:535:C:C6	2.49	0.47
1:1A:1077:A:H2'	1:1A:1078:U:H4'	1.96	0.47
3:1D:130:ALA:C	3:1D:131:LEU:HD12	2.39	0.47
6:1G:18:GLU:OE2	6:1G:22:ARG:HD2	2.14	0.47
7:1H:84:SER:HA	7:1H:133:VAL:O	2.14	0.47
21:1Z:44:PHE:CZ	21:1Z:86:VAL:HG11	2.48	0.47
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.40	0.47
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.48	0.47
33:1b:82:ARG:HD2	33:1b:92:TYR:OH	2.13	0.47
35:1d:61:LYS:HA	35:1d:203:VAL:HG22	1.95	0.47
45:1n:41:ARG:NH1	45:1n:42:ILE:HG12	2.29	0.47
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.31	0.47
1:2A:2690:C:OP2	13:2R:14:SER:OG	2.24	0.47
6:2G:25:TYR:CE2	6:2G:31:VAL:HG23	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:31:HIS:CD2	19:2X:33:LYS:HB2	2.49	0.47
32:2a:73:G:H1	32:2a:96:U:H3	1.62	0.47
32:2a:157:G:N2	32:2a:164:U:O2	2.40	0.47
32:2a:953:G:H5'	32:2a:965:A:N6	2.18	0.47
32:2a:1058:G:OP1	34:2c:199:LYS:NZ	2.47	0.47
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.79	0.47
32:2a:1232:U:OP1	40:2i:124:GLN:HG2	2.14	0.47
38:2g:27:ILE:HA	38:2g:30:ILE:HD12	1.96	0.47
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.96	0.47
1:1A:363(A):A:H3'	1:1A:363(B):G:H8	1.78	0.47
1:1A:747:U:O2	1:1A:2014:A:H1'	2.15	0.47
1:1A:2134:A:N3	1:1A:2159:G:O2'	2.39	0.47
1:1A:2140:C:H2'	1:1A:2141:G:C8	2.48	0.47
4:1E:47:VAL:HG22	4:1E:84:PHE:O	2.14	0.47
26:14:63:TYR:N	26:14:63:TYR:CD1	2.80	0.47
28:16:6:ARG:HD3	28:16:24:GLU:OE2	2.14	0.47
32:1a:56:U:H2'	32:1a:57:G:C8	2.49	0.47
32:1a:339:C:H2'	32:1a:340:U:H6	1.79	0.47
32:1a:948:C:OP1	44:1m:109:THR:OG1	2.31	0.47
33:1b:16:HIS:HD2	33:1b:204:ASN:H	1.62	0.47
37:1f:3:ARG:NE	37:1f:38:GLU:OE2	2.48	0.47
38:1g:16:LEU:HD21	40:1i:45:ALA:HB2	1.96	0.47
54:1y:55:PSU:N3	54:1y:57:G:H5'	2.28	0.47
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.29	0.47
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.49	0.47
2:2B:8:U:O3'	14:2S:25:ARG:NH2	2.48	0.47
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.96	0.47
16:2U:27:LEU:HB3	16:2U:31:SER:HB3	1.95	0.47
33:2b:47:THR:HA	33:2b:202:PRO:HG2	1.96	0.47
33:2b:185:ILE:HG22	33:2b:199:TYR:HD2	1.78	0.47
34:2c:129:ALA:HB3	34:2c:132:ARG:HB3	1.96	0.47
39:2h:121:ASP:HB2	39:2h:125:ARG:NH2	2.30	0.47
1:1A:918:A:N3	2:1B:80:U:O2'	2.44	0.47
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.49	0.47
1:1A:2149:G:C6	1:1A:2150:U:C2	3.02	0.47
1:1A:2171:A:O2'	1:1A:2172:U:H5''	2.14	0.47
1:1A:2461:C:H2'	1:1A:2462:U:C6	2.49	0.47
8:1I:9:LEU:HD23	8:1I:9:LEU:HA	1.81	0.47
32:1a:254:G:O2'	48:1q:16:GLN:O	2.31	0.47
32:1a:718:G:H5'	42:1k:117:ASN:HB2	1.96	0.47
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:69:LEU:HD11	33:1b:93:VAL:HG23	1.96	0.47
33:1b:102:LEU:HB3	33:1b:180:LEU:CD1	2.45	0.47
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.40	0.47
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.95	0.47
1:2A:121:G:H4'	1:2A:149:A:H5'	1.95	0.47
1:2A:1371:G:O6	61:2A:3936:HOH:O	2.18	0.47
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.49	0.47
8:2I:90:GLY:O	8:2I:121:LYS:HE3	2.14	0.47
17:2V:14:VAL:HA	17:2V:18:LEU:HD23	1.96	0.47
23:21:56:GLN:OE1	23:21:87:PRO:HG3	2.14	0.47
46:2o:87:ILE:O	46:2o:88:ARG:HB2	2.14	0.47
48:2q:80:GLY:O	48:2q:82:MET:N	2.44	0.47
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.49	0.47
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.79	0.47
1:1A:1424:G:H2'	1:1A:1425:G:O4'	2.14	0.47
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.15	0.47
32:1a:7:G:H21	36:1e:121:LYS:HG2	1.80	0.47
32:1a:7:G:H5'	32:1a:298:A:O4'	2.14	0.47
32:1a:627:G:O2'	32:1a:628:G:H5'	2.14	0.47
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.79	0.47
40:1i:36:TYR:CZ	40:1i:70:LYS:HE2	2.49	0.47
1:2A:236:C:H2'	1:2A:237:C:H6	1.77	0.47
1:2A:860:U:C2	1:2A:2268:A:C8	3.02	0.47
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.14	0.47
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.14	0.47
2:2B:94:C:H2'	2:2B:95:C:C6	2.50	0.47
4:2E:12:THR:HG22	4:2E:13:ARG:H	1.80	0.47
4:2E:13:ARG:HH21	15:2T:77:PRO:HB3	1.79	0.47
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	1.96	0.47
8:2I:130:TYR:HD2	8:2I:138:ILE:HD12	1.78	0.47
9:2N:131:GLN:O	9:2N:134:ARG:HG3	2.14	0.47
10:2O:80:ASP:OD2	15:2T:64:ARG:NH2	2.47	0.47
32:2a:7:G:O2'	36:2e:120:THR:O	2.32	0.47
32:2a:337:C:H2'	32:2a:338:A:C8	2.49	0.47
32:2a:512:U:H2'	32:2a:513:C:C6	2.50	0.47
36:2e:80:ILE:HD11	36:2e:141:GLN:HE21	1.78	0.47
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.49	0.47
47:2p:12:LYS:NZ	61:2p:201:HOH:O	2.47	0.47
1:1A:2126:A:N3	1:1A:2127:G:H1'	2.30	0.47
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.50	0.47
1:1A:2820:A:C5	13:1R:4:LEU:HD11	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.49	0.47
32:1a:748:C:H4'	32:1a:749:C:O5'	2.13	0.47
1:2A:191:A:H2'	1:2A:192:C:C6	2.48	0.47
1:2A:1496:A:N3	1:2A:1577:C:O2'	2.42	0.47
3:2D:75:ILE:HG21	3:2D:99:ASP:HB2	1.97	0.47
33:2b:215:LEU:HD23	33:2b:215:LEU:HA	1.77	0.47
54:2y:53:G:H3'	54:2y:54:5MU:H71	1.96	0.47
1:1A:613:G:N2	1:1A:614(C):A:O2'	2.47	0.47
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.14	0.47
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.13	0.47
1:1A:2857:G:N2	1:1A:2860:A:OP2	2.44	0.47
5:1F:152:GLU:OE1	5:1F:191:ARG:HD2	2.15	0.47
8:1I:48:GLU:HB3	8:1I:52:ARG:HH12	1.79	0.47
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	1.98	0.47
32:1a:841:U:OP2	32:1a:841:U:H6	1.98	0.47
34:1c:56:ASP:HB2	34:1c:67:THR:HB	1.96	0.47
39:1h:81:HIS:N	39:1h:138:TRP:O	2.47	0.47
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.49	0.47
1:2A:2857:G:N1	1:2A:2861:G:C6	2.83	0.47
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.44	0.47
32:2a:41:G:H2'	32:2a:42:G:H8	1.80	0.47
40:2i:89:ASN:HD22	40:2i:91:ASP:H	1.61	0.47
42:2k:41:THR:HG21	42:2k:71:LYS:HB2	1.97	0.47
1:1A:9:U:H3	1:1A:2629:A:H2	1.61	0.47
1:1A:1174:A:H1'	1:1A:1175:U:H5''	1.96	0.47
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.49	0.47
1:1A:1789:A:H5''	3:1D:220:HIS:O	2.15	0.47
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.15	0.47
1:1A:2612:C:OP2	27:15:2:ALA:N	2.48	0.47
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	1.95	0.47
6:1G:179:PRO:HG3	26:14:43:TYR:CZ	2.50	0.47
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.95	0.47
21:1Z:31:ARG:NE	21:1Z:94:GLU:OE2	2.45	0.47
28:16:12:GLU:OE1	28:16:52:VAL:HG11	2.14	0.47
32:1a:1136:U:H5''	32:1a:1137:C:C2	2.49	0.47
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.13	0.47
35:1d:138:TYR:HE2	35:1d:140:VAL:HA	1.80	0.47
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.48	0.47
51:1t:13:LEU:HD12	51:1t:14:LYS:N	2.30	0.47
1:2A:764:A:H5''	3:2D:210:GLY:HA2	1.96	0.47
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.15	0.47
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.49	0.47
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.27	0.47
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.29	0.47
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.97	0.47
1:2A:2119:A:N1	1:2A:2170:A:H2'	2.30	0.47
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.29	0.47
1:2A:2786:U:O2'	4:2E:62:PRO:O	2.26	0.47
8:2I:78:THR:HA	8:2I:143:SER:HB3	1.96	0.47
8:2I:114:LEU:HD12	8:2I:130:TYR:HA	1.96	0.47
8:2I:140:LEU:HG	8:2I:142:VAL:HG22	1.96	0.47
10:2O:63:VAL:HG11	10:2O:85:VAL:HG23	1.96	0.47
17:2V:18:LEU:HD12	17:2V:19:LYS:H	1.79	0.47
32:2a:266:G:H2'	32:2a:266:G:N3	2.30	0.47
32:2a:501:C:OP2	43:2l:124:LYS:NZ	2.47	0.47
32:2a:504:C:H2'	32:2a:511:C:H5	1.80	0.47
32:2a:1190:G:O2'	34:2c:3:ASN:HB2	2.15	0.47
33:2b:219:VAL:O	33:2b:223:ILE:HG12	2.15	0.47
43:2l:84:LEU:HB2	43:2l:105:TYR:CE2	2.49	0.47
44:2m:101:GLN:OE1	44:2m:101:GLN:N	2.48	0.47
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.15	0.47
1:1A:27:G:N2	1:1A:512:G:H1'	2.30	0.47
1:1A:421:U:OP1	61:1A:4143:HOH:O	2.20	0.47
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.43	0.47
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.29	0.47
4:1E:34:VAL:HB	4:1E:48:GLN:HE21	1.80	0.47
27:15:45:VAL:HG11	27:15:58:LEU:HD23	1.96	0.47
32:1a:376:G:H5''	47:1p:5:ARG:HD3	1.97	0.47
32:1a:600:C:H42	32:1a:638:G:H1	1.62	0.47
32:1a:828:A:H2'	32:1a:829:G:O4'	2.15	0.47
1:2A:2839:G:H5'	13:2R:46:GLY:CA	2.40	0.47
12:2Q:1:MET:HE1	54:2w:63:G:H5'	1.97	0.47
32:2a:1146:A:H2'	32:2a:1147:C:O4'	2.14	0.47
32:2a:1268:A:H4'	52:2u:19:GLY:HA2	1.96	0.47
42:2k:20:TYR:O	42:2k:30:VAL:HA	2.15	0.47
48:2q:12:SER:HB3	48:2q:20:THR:HB	1.97	0.47
54:2y:14:A:N3	54:2y:14:A:H2'	2.29	0.47
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.15	0.47
1:1A:1907:G:H2'	1:1A:1908:C:C6	2.50	0.47
28:16:39:TYR:OH	28:16:44:ARG:HG3	2.15	0.47
32:1a:175:C:H2'	32:1a:176:C:H6	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:219:C:H2'	32:1a:220:G:O4'	2.15	0.47
32:1a:269:C:H2'	32:1a:270:A:C8	2.49	0.47
32:1a:664:G:N2	32:1a:741:G:H1	2.08	0.47
33:1b:16:HIS:O	33:1b:18:GLY:N	2.48	0.47
1:2A:1263:U:C4	1:2A:1264:G:C6	3.03	0.47
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.15	0.47
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.15	0.47
1:2A:2888:C:H2'	1:2A:2889:C:H6	1.80	0.47
7:2H:101:ARG:HH12	7:2H:122:THR:HG23	1.79	0.47
14:2S:61:ASN:O	14:2S:64:GLU:HG3	2.15	0.47
25:23:46:ASN:O	25:23:50:VAL:HG22	2.15	0.47
32:2a:457:C:H2'	32:2a:458:C:C6	2.50	0.47
32:2a:925:G:H1'	32:2a:1502:A:C4	2.50	0.47
32:2a:1089:G:H1	32:2a:1096:C:N4	2.12	0.47
32:2a:1355:G:H2'	32:2a:1356:G:C8	2.50	0.47
33:2b:16:HIS:O	33:2b:18:GLY:N	2.48	0.47
35:2d:158:ILE:HG22	35:2d:162:LEU:HD12	1.97	0.47
35:2d:176:LEU:HD12	35:2d:182:LYS:O	2.14	0.47
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.22	0.47
1:1A:321:G:N3	5:1F:165:ARG:HD2	2.30	0.47
1:1A:922:U:H2'	1:1A:923:C:C6	2.50	0.47
1:1A:1051:G:H2'	1:1A:1052:C:O4'	2.14	0.47
27:15:48:GLU:O	27:15:60:VAL:HG11	2.14	0.47
32:1a:17:U:H2'	32:1a:18:C:C6	2.49	0.47
32:1a:57:G:H2'	32:1a:58:C:C6	2.50	0.47
32:1a:130:A:O2'	32:1a:131:C:O5'	2.28	0.47
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.32	0.47
1:2A:1020:A:N1	1:2A:1141:U:O2'	2.46	0.47
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.15	0.47
1:2A:1038:C:H42	1:2A:1117:G:H1	1.62	0.47
1:2A:2065:C:H4'	1:2A:2251:OMG:HM22	1.96	0.47
1:2A:2143:C:N3	1:2A:2148:G:N2	2.58	0.47
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.49	0.47
6:2G:56:ALA:HA	6:2G:59:GLU:HG2	1.96	0.47
32:2a:984:C:H2'	32:2a:985:C:H6	1.78	0.47
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.15	0.47
36:2e:10:MET:HE2	36:2e:55:VAL:HG21	1.97	0.47
48:2q:4:LYS:HE2	48:2q:6:LEU:HD21	1.96	0.47
54:2w:19:G:H1	54:2w:56:C:H42	1.62	0.47
4:1E:21:VAL:HG13	4:1E:185:LYS:HD2	1.96	0.46
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.79	0.46
33:1b:212:GLN:O	33:1b:216:SER:N	2.33	0.46
35:1d:104:VAL:HG21	35:1d:140:VAL:HG11	1.97	0.46
37:1f:55:ASP:OD2	37:1f:86:ARG:NH1	2.35	0.46
40:1i:3:GLN:HE21	40:1i:20:ARG:CZ	2.28	0.46
54:1w:2:C:C4	54:1w:71:G:N1	2.83	0.46
1:2A:639:U:H2'	1:2A:640:C:C6	2.50	0.46
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.80	0.46
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.62	0.46
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.80	0.46
12:2Q:10:ARG:NH1	12:2Q:11:LYS:HE2	2.29	0.46
32:2a:1189:C:OP1	34:2c:5:ILE:HD12	2.14	0.46
32:2a:1275:A:H2'	32:2a:1276:G:O4'	2.14	0.46
32:2a:1288:A:H2'	32:2a:1289:A:O4'	2.15	0.46
1:1A:897:C:H5'	54:1w:56:C:OP1	2.14	0.46
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.50	0.46
1:1A:1426:G:O2'	1:1A:1572:A:N6	2.46	0.46
1:1A:2667:C:H2'	1:1A:2668:G:O4'	2.15	0.46
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.16	0.46
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.45	0.46
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD11	1.97	0.46
32:1a:1033:G:H3'	32:1a:1034:G:H8	1.81	0.46
38:1g:58:PRO:O	38:1g:61:VAL:HG12	2.15	0.46
41:1j:5:ARG:NH2	41:1j:73:ASP:OD2	2.40	0.46
54:1w:10:G:H2'	54:1w:11:C:C6	2.50	0.46
1:2A:602:G:N2	1:2A:655:A:OP2	2.47	0.46
1:2A:918:A:N3	2:2B:80:U:O2'	2.42	0.46
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.15	0.46
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.43	0.46
5:2F:172:TRP:CD1	5:2F:172:TRP:H	2.33	0.46
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.98	0.46
32:2a:107:G:H2'	32:2a:108:G:O4'	2.15	0.46
32:2a:406:G:H21	35:2d:119:GLN:NE2	2.11	0.46
33:2b:178:ARG:NH2	39:2h:68:ARG:HH22	2.11	0.46
38:2g:108:ALA:O	38:2g:119:ARG:HD2	2.14	0.46
41:2j:5:ARG:HA	41:2j:73:ASP:OD1	2.15	0.46
42:2k:81:ASP:OD1	42:2k:107:SER:OG	2.21	0.46
44:2m:89:GLY:O	44:2m:93:ARG:HG3	2.15	0.46
1:1A:2115:G:H21	1:1A:2171:A:H61	1.61	0.46
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.50	0.46
20:1Y:92:ASN:O	20:1Y:92:ASN:ND2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.51	0.46
32:1a:257:G:C6	32:1a:258:G:C5	3.04	0.46
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.31	0.46
32:1a:1518:MA6:H93	32:1a:1519:MA6:C9	2.44	0.46
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.15	0.46
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.15	0.46
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.97	0.46
44:1m:11:ARG:C	44:1m:13:LYS:H	2.23	0.46
51:1t:9:ASN:O	51:1t:10:LEU:HB2	2.14	0.46
54:1w:37:MIA:H121	54:1w:37:MIA:H162	1.62	0.46
54:1w:37:MIA:H8	54:1w:37:MIA:O5'	2.15	0.46
1:2A:271(P):C:O3'	8:2I:42:SER:OG	2.27	0.46
1:2A:839:U:H2'	1:2A:840:C:C6	2.50	0.46
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.30	0.46
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.96	0.46
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.48	0.46
26:24:13:ARG:NH1	26:24:13:ARG:HB2	2.31	0.46
35:2d:70:ILE:HD11	35:2d:74:GLN:HB3	1.96	0.46
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.48	0.46
44:2m:91:ARG:HH11	44:2m:96:LEU:HD13	1.79	0.46
51:2t:56:MET:HE2	51:2t:56:MET:HB3	1.73	0.46
1:1A:1697:G:OP2	1:1A:1698:A:O2'	2.31	0.46
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.13	0.46
15:1T:98:LYS:NZ	61:1T:301:HOH:O	2.34	0.46
32:1a:461:A:O2'	32:1a:470:C:H5'	2.15	0.46
32:1a:1136:U:H5''	32:1a:1137:C:N3	2.30	0.46
43:1l:7:ILE:HD13	43:1l:10:LEU:HD12	1.98	0.46
47:1p:55:ARG:HH21	47:1p:59:TRP:NE1	2.13	0.46
50:1s:27:GLU:OE1	50:1s:27:GLU:N	2.44	0.46
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.31	0.46
1:2A:2111:C:N4	1:2A:2144:U:O2'	2.35	0.46
25:23:15:TYR:O	25:23:20:LYS:NZ	2.49	0.46
32:2a:114:U:H2'	32:2a:115:G:C8	2.51	0.46
32:2a:1279:A:O2'	32:2a:1281:U:OP2	2.30	0.46
33:2b:53:ARG:NH2	33:2b:198:ASP:O	2.47	0.46
39:2h:121:ASP:HB2	39:2h:125:ARG:HH21	1.80	0.46
1:1A:388:G:O2'	1:1A:389:G:N7	2.37	0.46
1:1A:414:C:H2'	1:1A:415:A:C8	2.51	0.46
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.51	0.46
1:1A:2134:A:H2'	1:1A:2159:G:O2'	2.16	0.46
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:18:PRO:O	24:12:22:GLU:HG3	2.15	0.46
32:1a:431:A:H2'	32:1a:432:A:O4'	2.15	0.46
32:1a:715:A:H2'	32:1a:716:A:C8	2.51	0.46
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.50	0.46
1:2A:699:A:H2'	1:2A:700:G:O4'	2.16	0.46
1:2A:1021:A:H3'	1:2A:1021:A:C8	2.51	0.46
1:2A:1209:G:O2'	1:2A:1237:A:N1	2.48	0.46
1:2A:2006:C:O2'	1:2A:2823:A:N3	2.48	0.46
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.48	0.46
2:2B:52:A:N6	14:2S:33:LYS:HG2	2.30	0.46
32:2a:1203:C:P	45:2n:3:ARG:HH11	2.39	0.46
34:2c:122:GLU:HA	34:2c:125:GLU:HG2	1.97	0.46
35:2d:155:LEU:HD23	35:2d:156:GLU:H	1.80	0.46
50:2s:38:SER:HB2	50:2s:71:LEU:HD22	1.98	0.46
54:2w:34:G:H2'	54:2w:35:A:C8	2.50	0.46
1:1A:910:A:N1	1:1A:2277:G:H1'	2.30	0.46
1:1A:1693:U:H1'	3:1D:14:ARG:NH2	2.30	0.46
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.16	0.46
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.17	0.46
32:1a:1025:U:O2	32:1a:1036:G:C6	2.68	0.46
35:1d:18:LYS:HG2	59:1d:302:SF4:S1	2.55	0.46
54:1w:4:C:H2'	54:1w:5:G:H8	1.81	0.46
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.98	0.46
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.50	0.46
32:2a:430:A:OP2	35:2d:22:LYS:NZ	2.48	0.46
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.97	0.46
43:2l:117:ARG:NE	43:2l:123:LYS:O	2.49	0.46
54:2y:61:C:H2'	54:2y:62:C:C6	2.51	0.46
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.30	0.46
26:14:49:PHE:HB3	26:14:50:VAL:HG22	1.98	0.46
36:1e:10:MET:H	36:1e:10:MET:HG2	1.50	0.46
1:2A:817:C:O2'	1:2A:839:U:H5''	2.16	0.46
1:2A:1195:G:N7	11:2P:15:ARG:NH1	2.64	0.46
11:2P:38:GLN:HG2	11:2P:45:LEU:H	1.81	0.46
11:2P:121:LYS:O	11:2P:123:LEU:N	2.48	0.46
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.26	0.46
18:2W:92:ARG:HG2	18:2W:93:ALA:N	2.30	0.46
31:29:27:CYS:SG	31:29:28:GLU:N	2.88	0.46
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.28	0.46
34:2c:22:TRP:CH2	34:2c:32:LEU:HB3	2.51	0.46
38:2g:97:GLN:O	38:2g:101:LEU:HG	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:50:ILE:HB	45:2n:41:ARG:NH1	2.31	0.46
49:2r:25:THR:OG1	49:2r:42:ARG:NH2	2.49	0.46
54:2w:70:G:H2'	54:2w:71:G:H8	1.81	0.46
54:2y:55:PSU:N1	54:2y:57:G:H5''	2.26	0.46
1:1A:601:C:OP1	5:1F:108:LYS:HE3	2.16	0.46
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.44	0.46
1:1A:1991:U:H2'	1:1A:1992:G:H5''	1.98	0.46
4:1E:111:ARG:HG2	4:1E:118:LYS:HD3	1.97	0.46
6:1G:36:LYS:HD3	6:1G:95:ARG:NH1	2.31	0.46
6:1G:126:ASP:HB3	6:1G:128:ARG:N	2.31	0.46
26:14:63:TYR:N	26:14:64:GLY:HA2	2.30	0.46
32:1a:399:G:H2'	32:1a:400:C:C6	2.51	0.46
1:2A:881:G:C2	1:2A:882:G:H1'	2.51	0.46
1:2A:910:A:N1	1:2A:2277:G:H1'	2.31	0.46
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.31	0.46
14:2S:11:LYS:O	14:2S:15:ARG:HB2	2.15	0.46
14:2S:11:LYS:HG2	14:2S:91:PRO:HD3	1.97	0.46
32:2a:109:A:H5'	32:2a:110:C:H5	1.80	0.46
32:2a:273:A:H1'	48:2q:16:GLN:NE2	2.31	0.46
32:2a:966:M2G:HM23	32:2a:967:5MC:H1'	1.97	0.46
34:2c:179:ARG:NH1	34:2c:206:GLU:OE1	2.27	0.46
35:2d:22:LYS:HG2	59:2d:303:SF4:S4	2.56	0.46
36:2e:75:THR:OG1	36:2e:117:ASP:O	2.21	0.46
36:2e:95:ALA:O	36:2e:97:GLY:N	2.44	0.46
54:2w:21:A:O2'	54:2w:22:G:OP1	2.32	0.46
1:1A:218:A:C2	1:1A:235:U:H4'	2.50	0.46
1:1A:721:C:H2'	1:1A:722:A:C8	2.51	0.46
1:1A:1399:C:OP1	19:1X:25:LYS:NZ	2.47	0.46
1:1A:1486:A:H2'	1:1A:1487:G:H8	1.80	0.46
1:1A:2532:G:O2'	1:1A:2657:A:N1	2.44	0.46
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.81	0.46
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.98	0.46
32:1a:23:C:OP2	32:1a:561:U:N3	2.47	0.46
32:1a:560:U:H5'	32:1a:566:G:N2	2.31	0.46
32:1a:1021:G:HO2'	32:1a:1022:G:P	2.38	0.46
32:1a:1030(C):G:C8	32:1a:1030(D):A:N7	2.84	0.46
32:1a:1328:C:OP1	52:1u:21:TYR:OH	2.33	0.46
33:1b:72:GLY:HA3	33:1b:81:VAL:HG11	1.96	0.46
37:1f:35:ALA:HA	37:1f:67:MET:HB3	1.98	0.46
39:1h:82:HIS:NE2	39:1h:136:GLU:OE2	2.46	0.46
1:2A:94(A):G:H2'	1:2A:95:G:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.81	0.46
1:2A:1019:U:H3	1:2A:1142(A):A:N6	2.12	0.46
1:2A:1797:C:H4'	3:2D:257:LEU:O	2.16	0.46
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.51	0.46
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.38	0.46
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.33	0.46
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.51	0.46
2:2B:9:G:H1	2:2B:112:U:H3	1.64	0.46
6:2G:53:LEU:HD22	6:2G:53:LEU:HA	1.75	0.46
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.51	0.46
23:21:46:LEU:HD23	23:21:61:ARG:HB3	1.98	0.46
32:2a:1004:A:C8	32:2a:1005:A:H4'	2.50	0.46
32:2a:1028:C:H2'	32:2a:1029:C:O4'	2.16	0.46
32:2a:1133:G:H1	32:2a:1141:C:N4	2.11	0.46
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.21	0.46
36:2e:76:ILE:O	36:2e:93:PRO:HB3	2.16	0.46
39:2h:85:ARG:NH1	39:2h:87:SER:O	2.49	0.46
49:2r:53:ARG:HA	49:2r:56:THR:OG1	2.16	0.46
50:2s:12:ASP:OD1	50:2s:37:ARG:NH2	2.46	0.46
8:1I:54:GLN:HG3	8:1I:57:ARG:HH22	1.80	0.46
14:1S:5:THR:OG1	14:1S:8:GLU:HG3	2.16	0.46
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.79	0.46
32:1a:116:A:H61	32:1a:313:A:H1'	1.81	0.46
32:1a:875:C:O2'	39:1h:14:ARG:HD2	2.16	0.46
32:1a:1136:U:H5''	32:1a:1137:C:C4	2.51	0.46
33:1b:98:LEU:HD12	33:1b:101:MET:HE3	1.98	0.46
36:1e:78:HIS:HE1	36:1e:142:LEU:HA	1.80	0.46
39:1h:121:ASP:O	39:1h:125:ARG:HG3	2.16	0.46
40:1i:9:ARG:HG2	40:1i:14:VAL:HG12	1.98	0.46
44:1m:92:HIS:HA	44:1m:110:ARG:NH2	2.30	0.46
46:1o:32:LEU:HD11	46:1o:62:GLN:HG2	1.97	0.46
1:2A:34:C:N4	1:2A:454:A:O2'	2.48	0.46
1:2A:271(P):C:OP1	8:2I:45:LYS:NZ	2.37	0.46
1:2A:1482:G:H1	1:2A:1506:C:H42	1.63	0.46
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.64	0.46
8:2I:77:LEU:HD11	8:2I:100:ALA:HB3	1.98	0.46
25:23:40:THR:HG22	25:23:42:ALA:H	1.81	0.46
27:25:35:GLU:HG2	27:25:51:TYR:CD1	2.51	0.46
32:2a:741:G:H2'	32:2a:742:G:O4'	2.16	0.46
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.51	0.46
33:2b:149:LEU:HD23	33:2b:152:PHE:HD2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:5:GLU:OE1	49:2r:34:TYR:OH	2.27	0.46
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.98	0.46
1:1A:264:C:O2'	1:1A:265:A:H2'	2.16	0.45
1:1A:489:G:N7	18:1W:49:LYS:NZ	2.64	0.45
1:1A:566:U:H5''	11:1P:29:LYS:HE3	1.98	0.45
1:1A:602:G:N1	1:1A:655:A:OP2	2.38	0.45
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.79	0.45
1:1A:2149:G:C2	1:1A:2150:U:H1'	2.51	0.45
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.31	0.45
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.98	0.45
26:14:33:VAL:HG12	26:14:35:VAL:H	1.81	0.45
32:1a:277:C:P	48:1q:68:ARG:HH12	2.39	0.45
32:1a:767:A:H2'	32:1a:768:A:O4'	2.16	0.45
33:1b:12:GLU:C	33:1b:14:GLY:H	2.23	0.45
33:1b:40:HIS:HB2	33:1b:190:THR:HG21	1.99	0.45
54:1y:19:G:H1	54:1y:56:C:H42	1.62	0.45
1:2A:568:U:H5'	1:2A:945:A:C6	2.51	0.45
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.51	0.45
1:2A:1665:A:OP2	61:2A:3942:HOH:O	2.20	0.45
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.51	0.45
3:2D:168:ARG:HG2	3:2D:173:VAL:HG13	1.97	0.45
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	1.98	0.45
37:2f:14:LEU:HD22	37:2f:18:GLN:HB3	1.98	0.45
44:2m:3:ARG:HB3	44:2m:8:GLU:HA	1.98	0.45
44:2m:91:ARG:NH1	44:2m:96:LEU:HD13	2.29	0.45
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	1.97	0.45
54:2y:9:A:H4'	54:2y:46:G7M:H5'	1.97	0.45
1:1A:226:G:N2	1:1A:228:A:H62	2.14	0.45
1:1A:1071:G:N2	1:1A:1090:U:O4	2.50	0.45
1:1A:1125:G:H5'	31:19:37:GLY:HA2	1.99	0.45
1:1A:1175:U:OP1	1:1A:1177:A:N6	2.49	0.45
1:1A:2778:A:OP2	61:1A:4146:HOH:O	2.21	0.45
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.16	0.45
19:1X:61:GLY:HA3	19:1X:73:ARG:O	2.16	0.45
32:1a:719:C:N4	49:1r:71:LYS:HE2	2.31	0.45
32:1a:1316:G:N1	32:1a:1319:A:OP2	2.42	0.45
35:1d:94:LEU:HA	35:1d:97:LEU:HD12	1.99	0.45
39:1h:20:TYR:HA	39:1h:65:TYR:CZ	2.52	0.45
40:1i:17:VAL:HG11	40:1i:81:ILE:N	2.31	0.45
54:1w:70:G:N2	54:1w:71:G:H1'	2.31	0.45
1:2A:38:A:H2'	1:2A:39:C:C6	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1446:C:H42	1:2A:1465:G:H1	1.64	0.45
1:2A:2331:G:O2'	22:20:43:THR:HG22	2.16	0.45
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.98	0.45
4:2E:7:VAL:HG12	4:2E:51:PHE:CE2	2.51	0.45
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	1.97	0.45
19:2X:5:TYR:CZ	24:22:30:ARG:HB2	2.51	0.45
21:2Z:126:VAL:HG13	21:2Z:161:VAL:HG23	1.98	0.45
34:2c:35:GLU:O	34:2c:39:ILE:HG13	2.16	0.45
38:2g:152:ALA:O	38:2g:155:ARG:HD3	2.17	0.45
55:2x:18:G:O2'	55:2x:19:G:H5'	2.16	0.45
1:1A:55:G:O2'	1:1A:127:A:N1	2.45	0.45
1:1A:289:A:H2'	1:1A:290:G:O4'	2.16	0.45
1:1A:639:U:H2'	1:1A:640:C:C6	2.51	0.45
20:1Y:86:ARG:HB2	20:1Y:98:VAL:HG23	1.98	0.45
35:1d:196:LEU:O	35:1d:198:VAL:N	2.45	0.45
46:1o:17:ARG:HD3	46:1o:26:GLU:OE1	2.17	0.45
1:2A:534:U:H5'	16:2U:42:ALA:HB1	1.99	0.45
1:2A:644:A:H4'	1:2A:645:C:C4	2.51	0.45
1:2A:1451:C:H42	1:2A:1459:G:H1	1.65	0.45
7:2H:9:ILE:HB	7:2H:50:VAL:HB	1.96	0.45
9:2N:69:GLN:O	9:2N:71:ILE:HG13	2.15	0.45
10:2O:111:PHE:HB3	10:2O:114:ILE:HD12	1.98	0.45
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.98	0.45
16:2U:79:PHE:CZ	16:2U:83:LEU:HD11	2.51	0.45
32:2a:978:A:O2'	32:2a:1322:C:N3	2.39	0.45
32:2a:1124:G:N2	32:2a:1125:U:O4	2.45	0.45
33:2b:120:ALA:O	33:2b:125:PRO:HD2	2.16	0.45
34:2c:119:ARG:HG2	34:2c:140:ARG:NH2	2.26	0.45
44:2m:73:GLU:O	44:2m:77:ASN:HB2	2.16	0.45
47:2p:43:LYS:HG2	47:2p:48:TRP:CG	2.50	0.45
1:1A:848:G:H2'	1:1A:849:A:C8	2.52	0.45
1:1A:1368:G:C2	1:1A:1369:G:C8	3.05	0.45
1:1A:2128:C:N4	1:1A:2160:G:N1	2.54	0.45
1:1A:2319:G:H1	14:1S:3:ARG:HD3	1.81	0.45
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.82	0.45
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.99	0.45
21:1Z:70:LEU:HD23	21:1Z:70:LEU:HA	1.84	0.45
25:13:55:ARG:NH2	25:13:57:GLU:HB2	2.31	0.45
32:1a:636:U:H2'	32:1a:637:G:H8	1.82	0.45
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.47	0.45
32:1a:1289:A:N1	32:1a:1371:G:O2'	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:42:GLN:HB3	35:1d:43:HIS:CD2	2.51	0.45
38:1g:28:ASN:HD21	38:1g:36:LYS:NZ	2.15	0.45
1:2A:30:G:H2'	1:2A:31:C:C6	2.51	0.45
1:2A:896:A:H1'	54:2w:56:C:H5'	1.99	0.45
5:2F:32:LEU:HD21	5:2F:105:VAL:HG13	1.99	0.45
14:2S:58:LEU:HD13	14:2S:65:VAL:HB	1.98	0.45
15:2T:108:ARG:NH2	32:2a:1465:C:OP2	2.47	0.45
21:2Z:55:HIS:HE1	21:2Z:135:GLU:HB2	1.81	0.45
32:2a:401:C:P	35:2d:73:ARG:HH21	2.36	0.45
32:2a:671:G:H2'	32:2a:672:U:O4'	2.16	0.45
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.51	0.45
32:2a:1438:G:H2'	32:2a:1439:C:C6	2.50	0.45
39:2h:119:LEU:HB3	39:2h:123:GLU:HB3	1.98	0.45
41:2j:36:GLY:O	41:2j:38:ILE:HG12	2.16	0.45
1:1A:1056:G:H5''	1:1A:1057:A:O4'	2.16	0.45
1:1A:1478:G:O2'	1:1A:1558:A:N7	2.50	0.45
1:1A:2134:A:N6	1:1A:2157:G:O4'	2.48	0.45
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.51	0.45
2:1B:88:C:H2'	2:1B:89:G:O4'	2.16	0.45
5:1F:13:SER:HB2	5:1F:127:GLU:HG3	1.98	0.45
6:1G:32:PRO:HB3	6:1G:163:ALA:HB2	1.99	0.45
7:1H:86:GLU:OE2	7:1H:130:ARG:NH1	2.49	0.45
32:1a:332:G:H2'	32:1a:333:G:H8	1.82	0.45
32:1a:435:C:H2'	32:1a:436:C:H6	1.81	0.45
32:1a:881:G:P	43:1l:12:ARG:HH22	2.40	0.45
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.17	0.45
33:1b:139:LYS:O	33:1b:143:GLU:HG2	2.17	0.45
36:1e:147:ASP:O	36:1e:151:LEU:HD12	2.16	0.45
1:2A:272(G):C:H42	1:2A:363(C):G:H1	1.64	0.45
1:2A:751:A:C6	1:2A:789:A:C5	3.04	0.45
1:2A:981:A:N1	1:2A:2027:G:O2'	2.42	0.45
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.16	0.45
1:2A:2818:G:OP1	1:2A:2837:G:O2'	2.22	0.45
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.51	0.45
10:2O:17:ARG:HD3	10:2O:17:ARG:HA	1.81	0.45
32:2a:202:U:H3'	32:2a:203:U:C5	2.52	0.45
32:2a:1264:C:N4	32:2a:1265:G:O6	2.49	0.45
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.82	0.45
50:2s:61:TYR:CE2	50:2s:63:THR:HG22	2.51	0.45
1:1A:271(I):G:H2'	1:1A:271(J):C:C2	2.51	0.45
1:1A:1057:A:N6	1:1A:1081:U:H3	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.52	0.45
5:1F:136:THR:HA	5:1F:166:ALA:O	2.17	0.45
8:1I:130:TYR:O	8:1I:138:ILE:N	2.48	0.45
32:1a:179:A:H2'	32:1a:180:U:C6	2.52	0.45
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.50	0.45
32:1a:857:C:H2'	32:1a:858:G:O4'	2.17	0.45
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.51	0.45
32:1a:1338:G:H2'	32:1a:1339:A:C8	2.52	0.45
32:1a:1346:A:H61	32:1a:1374:A:H3'	1.80	0.45
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.66	0.45
1:2A:673:C:H5''	5:2F:81:PRO:HD2	1.98	0.45
1:2A:921:G:H2'	1:2A:922:U:C6	2.51	0.45
1:2A:2495:G:H5''	12:2Q:82:ARG:HG2	1.98	0.45
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.50	0.45
10:2O:120:GLU:HB2	15:2T:68:TYR:HE2	1.81	0.45
14:2S:49:VAL:HG12	14:2S:73:LEU:HD12	1.98	0.45
25:23:4:LEU:O	25:23:36:VAL:HA	2.17	0.45
32:2a:791:G:H2'	32:2a:792:A:H5'	1.98	0.45
36:2e:102:ALA:HB2	36:2e:120:THR:HG21	1.99	0.45
44:2m:13:LYS:HA	44:2m:44:ARG:NH1	2.31	0.45
45:2n:23:ARG:NH1	45:2n:28:GLY:O	2.49	0.45
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.98	0.45
47:2p:15:PRO:HD2	47:2p:42:ARG:CD	2.47	0.45
1:1A:124:G:OP1	1:1A:1376:C:O2'	2.23	0.45
1:1A:479:A:N3	1:1A:481:G:H5''	2.31	0.45
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.32	0.45
8:1I:77:LEU:HB2	8:1I:142:VAL:HG12	1.98	0.45
14:1S:110:LEU:HA	14:1S:110:LEU:HD12	1.74	0.45
17:1V:38:LEU:HD23	17:1V:50:PRO:O	2.16	0.45
26:14:54:GLY:N	26:14:55:ARG:HA	2.31	0.45
32:1a:527:G7M:HN71	43:1I:92:OTD:H3	1.98	0.45
32:1a:966:M2G:HM13	32:1a:967:5MC:H1'	1.99	0.45
32:1a:1151:A:O2'	32:1a:1152:A:O5'	2.31	0.45
34:1c:52:LEU:HD13	34:1c:68:VAL:HG13	1.98	0.45
42:1k:91:ARG:NH1	42:1k:110:ASP:OD1	2.43	0.45
46:1o:82:ILE:O	46:1o:86:GLY:N	2.49	0.45
1:2A:40:C:H2'	1:2A:41:C:C6	2.51	0.45
1:2A:458:G:O2'	1:2A:469:G:O6	2.34	0.45
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.17	0.45
1:2A:2116:G:H5''	1:2A:2116:G:H8	1.81	0.45
1:2A:2745:C:O2	7:2H:139:GLN:NE2	2.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:77:LEU:HD12	8:2I:97:ILE:HG23	1.99	0.45
17:2V:28:GLU:HG3	17:2V:29:PRO:HD2	1.97	0.45
22:20:48:GLY:HA3	22:20:80:HIS:ND1	2.32	0.45
25:23:22:ALA:HB2	25:23:49:LYS:HD3	1.97	0.45
25:23:30:ARG:HB2	25:23:33:GLN:HB2	1.97	0.45
32:2a:160:A:H1'	32:2a:344:A:N7	2.32	0.45
34:2c:78:GLY:HA3	34:2c:82:GLU:HB3	1.98	0.45
40:2i:17:VAL:HG11	40:2i:81:ILE:HG12	1.97	0.45
42:2k:79:SER:HA	42:2k:104:GLN:HB3	1.99	0.45
1:1A:484:C:H2'	1:1A:485:C:C6	2.52	0.45
1:1A:887:A:H2	1:1A:889:C:H3'	1.81	0.45
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.30	0.45
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.52	0.45
1:1A:2336:A:H61	22:10:43:THR:HG22	1.82	0.45
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.17	0.45
10:1O:113:LYS:HD2	10:1O:113:LYS:HA	1.77	0.45
34:1c:116:VAL:O	34:1c:120:VAL:HG22	2.17	0.45
35:1d:15:GLU:OE2	35:1d:66:ARG:NH1	2.50	0.45
41:1j:55:LYS:HG3	41:1j:56:HIS:H	1.82	0.45
1:2A:479:A:N3	1:2A:481:G:H5''	2.32	0.45
1:2A:2313:C:H4'	6:2G:91:ARG:HG3	1.99	0.45
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.45	0.45
26:24:26:SER:OG	26:24:27:THR:N	2.50	0.45
26:24:46:GLN:O	26:24:48:ARG:N	2.49	0.45
33:2b:25:ASN:HD21	33:2b:27:LYS:HG3	1.80	0.45
33:2b:81:VAL:HG12	33:2b:215:LEU:HD12	1.99	0.45
34:2c:40:ARG:O	34:2c:44:GLU:HB2	2.17	0.45
36:2e:41:VAL:HG22	36:2e:113:ALA:HA	1.98	0.45
40:2i:3:GLN:HE21	40:2i:20:ARG:NE	2.14	0.45
41:2j:74:ILE:HG22	61:2j:3302:HOH:O	2.17	0.45
47:2p:26:ARG:HG3	47:2p:27:LYS:O	2.16	0.45
1:1A:2391:G:O6	1:1A:2425:A:H8	2.00	0.45
21:1Z:70:LEU:HG	21:1Z:91:LEU:HD11	1.99	0.45
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.52	0.45
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.98	0.45
1:2A:31:C:H5''	1:2A:1239:G:OP1	2.17	0.45
1:2A:71:A:H5''	1:2A:73:A:C8	2.52	0.45
1:2A:667:U:O2	30:28:2:PRO:HD2	2.16	0.45
1:2A:987:G:O2'	1:2A:1000:A:N3	2.43	0.45
1:2A:1008:C:H4'	16:2U:59:ARG:HH22	1.82	0.45
26:24:58:ARG:O	26:24:61:ARG:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:142:G:H2'	32:2a:143:A:C8	2.52	0.45
32:2a:410:G:H21	32:2a:432:A:H62	1.65	0.45
32:2a:458:C:H2'	32:2a:460:G:O4'	2.16	0.45
32:2a:1060:C:H2'	32:2a:1061:G:C8	2.50	0.45
33:2b:211:ILE:O	33:2b:215:LEU:HB2	2.17	0.45
34:2c:8:ILE:HG23	34:2c:16:ARG:HG2	1.98	0.45
34:2c:38:ARG:HE	34:2c:38:ARG:HB2	1.53	0.45
40:2i:8:GLY:N	40:2i:15:ALA:O	2.48	0.45
1:1A:1899:G:O2'	1:1A:1900:A:OP2	2.30	0.45
1:1A:2590:A:H2'	1:1A:2591:C:C6	2.51	0.45
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.82	0.45
12:1Q:32:TYR:OH	12:1Q:133:ARG:NH2	2.47	0.45
32:1a:753:A:OP1	46:1o:69:TYR:OH	2.26	0.45
32:1a:963:G:H5'	61:1a:2049:HOH:O	2.17	0.45
32:1a:1157:A:H4'	32:1a:1158:C:O5'	2.17	0.45
33:1b:21:ARG:H	33:1b:21:ARG:HG3	1.52	0.45
34:1c:18:TRP:H	34:1c:18:TRP:HE3	1.65	0.45
35:1d:166:LYS:NZ	35:1d:179:GLU:OE2	2.50	0.45
43:1l:42:THR:HA	43:1l:53:ARG:O	2.17	0.45
43:1l:70:ILE:HG12	43:1l:100:ILE:HD13	1.98	0.45
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.80	0.45
1:2A:143(A):C:O2'	19:2X:2:LYS:NZ	2.47	0.45
1:2A:582:G:H2'	1:2A:583:G:C8	2.52	0.45
1:2A:774:A:H2'	1:2A:774:A:N3	2.31	0.45
1:2A:880:G:C2	1:2A:881:G:C8	3.05	0.45
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.51	0.45
3:2D:44:ASN:HD21	3:2D:46:GLN:CD	2.24	0.45
6:2G:170:ARG:O	6:2G:174:GLU:HB2	2.17	0.45
8:2I:129:THR:HA	8:2I:138:ILE:O	2.17	0.45
15:2T:61:PHE:CE2	15:2T:76:PHE:HB2	2.52	0.45
32:2a:520:A:N1	32:2a:536:C:H1'	2.32	0.45
32:2a:1264:C:C4	32:2a:1272:G:O6	2.69	0.45
36:2e:43:LEU:HD21	36:2e:133:TYR:CD1	2.52	0.45
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.98	0.45
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	1.99	0.45
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.17	0.45
54:2y:36:A:H2'	54:2y:37:MIA:O4'	2.17	0.45
54:2y:68:C:H2'	54:2y:69:G:O4'	2.17	0.45
1:1A:412:A:H8	1:1A:412:A:O5'	2.00	0.44
1:1A:628:G:H2'	1:1A:629:G:C8	2.52	0.44
1:1A:764:A:N3	3:1D:213:ARG:NH1	2.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:24:ILE:HD13	3:1D:84:TYR:HB2	1.99	0.44
3:1D:118:VAL:HG22	3:1D:119:ALA:H	1.82	0.44
8:1I:77:LEU:HD12	8:1I:97:ILE:HG23	1.99	0.44
32:1a:109:A:H2'	32:1a:326:G:N2	2.32	0.44
32:1a:679:C:H2'	32:1a:680:C:H6	1.82	0.44
34:1c:134:ILE:HD11	34:1c:153:VAL:HB	1.99	0.44
46:1o:39:LEU:HB3	46:1o:56:LEU:HD13	1.99	0.44
1:2A:912:C:OP1	12:2Q:9:TYR:OH	2.31	0.44
1:2A:1386:C:H2'	1:2A:1387:C:C6	2.52	0.44
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.30	0.44
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.99	0.44
6:2G:12:TYR:O	6:2G:16:ARG:HB2	2.18	0.44
6:2G:15:VAL:HG13	6:2G:175:LEU:HD12	1.99	0.44
6:2G:106:LEU:HG	6:2G:111:LEU:HD13	1.98	0.44
8:2I:88:ILE:HD11	8:2I:144:VAL:HG11	1.99	0.44
20:2Y:92:ASN:OD1	20:2Y:94:LYS:HG3	2.17	0.44
26:24:62:ARG:HB2	26:24:63:TYR:CE2	2.52	0.44
32:2a:64:G:H4'	32:2a:65:U:H3'	1.99	0.44
32:2a:137:C:H2'	32:2a:138:G:H8	1.82	0.44
32:2a:730:G:C5	32:2a:731:G:H1'	2.52	0.44
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.52	0.44
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	1.99	0.44
1:1A:34:C:H5''	1:1A:35:G:OP2	2.18	0.44
1:1A:444:C:H5''	61:1A:4825:HOH:O	2.17	0.44
1:1A:882:G:H4'	54:1w:19:G:O6	2.17	0.44
1:1A:1062:G:H22	1:1A:1077:A:N6	2.15	0.44
1:1A:1069:A:H4'	1:1A:1070:A:H5''	1.99	0.44
1:1A:2001:A:OP1	13:1R:9:LYS:NZ	2.49	0.44
15:1T:27:THR:HG22	15:1T:89:VAL:HB	1.99	0.44
32:1a:339:C:H2'	32:1a:340:U:C6	2.52	0.44
32:1a:935:A:N6	38:1g:3:ARG:HG3	2.32	0.44
55:1x:8:4SU:O2	55:1x:21:A:H2	2.00	0.44
1:2A:764:A:H5''	3:2D:210:GLY:HA3	1.99	0.44
1:2A:850:C:O3'	25:23:49:LYS:HE2	2.16	0.44
1:2A:894:C:O2'	1:2A:895:U:H5''	2.17	0.44
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.51	0.44
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.32	0.44
1:2A:1372:U:H2'	1:2A:1373:A:O4'	2.17	0.44
1:2A:1857:G:C6	1:2A:1858:G:N1	2.85	0.44
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.32	0.44
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:138:GLU:H	21:2Z:156:LYS:CE	2.30	0.44
22:20:36:ILE:HD12	22:20:58:THR:HG21	1.98	0.44
28:26:8:LYS:HD3	30:28:34:TRP:CD2	2.52	0.44
33:2b:15:VAL:HG12	33:2b:209:ARG:HD2	1.99	0.44
36:2e:123:LEU:HD23	36:2e:123:LEU:HA	1.88	0.44
37:2f:97:PHE:HD2	49:2r:31:LEU:HD11	1.82	0.44
1:1A:37:C:H2'	1:1A:38:A:C8	2.52	0.44
1:1A:272(H):C:H42	1:1A:363(B):G:H1	1.66	0.44
1:1A:764:A:O4'	3:1D:213:ARG:HG3	2.17	0.44
1:1A:863:A:N7	61:1A:4236:HOH:O	2.36	0.44
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.53	0.44
1:1A:2245:U:O2'	1:1A:2436:G:OP2	2.31	0.44
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.47	0.44
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.56	0.44
32:1a:1106:G:H2'	32:1a:1107:C:C6	2.52	0.44
54:1w:4:C:H2'	54:1w:5:G:C8	2.52	0.44
1:2A:311:A:C6	1:2A:328:U:C4	3.06	0.44
1:2A:493:G:H2'	1:2A:494:G:O4'	2.16	0.44
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.52	0.44
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.17	0.44
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.18	0.44
1:2A:2809:A:C6	1:2A:2810:A:C6	3.05	0.44
4:2E:48:GLN:HE21	4:2E:78:LEU:HD22	1.82	0.44
7:2H:149:ARG:HD2	7:2H:164:TYR:CE2	2.52	0.44
14:2S:83:LYS:HE3	14:2S:84:GLN:HG3	1.99	0.44
32:2a:58:C:O2'	32:2a:388:G:N7	2.38	0.44
32:2a:529:G:O6	43:2l:49:ASN:HA	2.17	0.44
32:2a:943:U:H1'	40:2i:124:GLN:HE22	1.82	0.44
36:2e:12:LEU:HB3	36:2e:31:LEU:HB2	1.98	0.44
38:2g:78:ARG:HD3	38:2g:79:ARG:H	1.83	0.44
42:2k:30:VAL:HG21	42:2k:65:ALA:HA	2.00	0.44
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.17	0.44
1:1A:2464:C:H1'	61:1A:4358:HOH:O	2.17	0.44
8:1I:77:LEU:HG	8:1I:101:LEU:HD22	1.98	0.44
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.17	0.44
32:1a:523:A:N1	43:1l:92:OTD:H6	2.32	0.44
32:1a:1503:A:N3	53:1v:13:A:N6	2.65	0.44
33:1b:105:PHE:C	33:1b:107:THR:N	2.74	0.44
37:1f:33:TYR:CE2	37:1f:78:GLU:HG3	2.53	0.44
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	1.99	0.44
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:48:C:C2	54:1w:59:U:H1'	2.53	0.44
54:1y:6:G:C6	54:1y:7:A:C6	3.05	0.44
1:2A:315:G:H2'	1:2A:316:C:C6	2.52	0.44
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.29	0.44
1:2A:2712(A):A:N3	61:2A:4033:HOH:O	2.36	0.44
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.52	0.44
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.18	0.44
30:28:50:LEU:HA	30:28:50:LEU:HD23	1.69	0.44
32:2a:859:A:H2'	32:2a:860:A:O4'	2.17	0.44
32:2a:1080:A:H5'	36:2e:14:ARG:HH21	1.82	0.44
33:2b:16:HIS:CB	33:2b:210:SER:HB2	2.47	0.44
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.81	0.44
34:2c:138:VAL:HG13	34:2c:149:ALA:HB3	1.99	0.44
50:2s:46:GLY:HA2	50:2s:61:TYR:CZ	2.52	0.44
1:1A:899:A:H2'	1:1A:899:A:N3	2.33	0.44
1:1A:1055:G:H3'	1:1A:1056:G:H8	1.83	0.44
1:1A:1062:G:P	1:1A:1070:A:H1'	2.58	0.44
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.83	0.44
1:1A:2168:G:N1	1:1A:2171:A:C8	2.85	0.44
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.53	0.44
32:1a:1498:UR3:O2'	53:1v:17:U:OP1	2.28	0.44
35:1d:141:ARG:HG3	35:1d:144:ASP:OD1	2.18	0.44
54:1w:54:5MU:H2'	54:1w:55:PSU:O4'	2.17	0.44
54:1y:51:U:H2'	54:1y:52:G:C8	2.52	0.44
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.50	0.44
1:2A:903:C:H2'	1:2A:904:C:C6	2.53	0.44
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.30	0.44
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.52	0.44
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.99	0.44
2:2B:41:U:H5	6:2G:70:VAL:H	1.66	0.44
2:2B:80:U:H2'	2:2B:81:G:C8	2.53	0.44
2:2B:83:G:H5''	25:23:52:HIS:CD2	2.52	0.44
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.18	0.44
13:2R:33:ARG:HA	13:2R:114:VAL:O	2.18	0.44
23:21:67:ILE:N	23:21:68:PRO:HD2	2.32	0.44
32:2a:451:A:N6	32:2a:480:U:H2'	2.32	0.44
33:2b:150:SER:O	33:2b:153:ARG:HG2	2.16	0.44
33:2b:150:SER:OG	33:2b:151:GLY:N	2.50	0.44
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	1.99	0.44
35:2d:191:ARG:HD2	35:2d:191:ARG:HA	1.72	0.44
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1071:G:H1	1:1A:1100:C:H42	1.64	0.44
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.53	0.44
1:1A:2406:U:H6	1:1A:2406:U:H2'	1.66	0.44
1:1A:2590:A:H2'	1:1A:2591:C:H6	1.83	0.44
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.76	0.44
32:1a:1002:G:C5	32:1a:1003:G:H1'	2.53	0.44
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.46	0.44
34:1c:180:ALA:HB1	34:1c:203:PHE:CE1	2.53	0.44
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.82	0.44
46:1o:15:PHE:CZ	46:1o:84:LYS:HD2	2.53	0.44
54:1y:65:G:C6	54:1y:66:U:C4	3.06	0.44
1:2A:142(A):C:H2'	1:2A:143:G:O4'	2.18	0.44
1:2A:332:A:O2'	1:2A:334:C:OP2	2.32	0.44
1:2A:478:A:N1	1:2A:500:G:H4'	2.32	0.44
1:2A:645:C:H5''	1:2A:646:A:OP2	2.18	0.44
1:2A:715:G:C2	46:2o:56:LEU:HD21	2.52	0.44
1:2A:720:C:H2'	1:2A:721:C:H6	1.82	0.44
1:2A:992:C:OP1	17:2V:74:LYS:NZ	2.36	0.44
4:2E:7:VAL:HG13	4:2E:27:LEU:HB3	1.99	0.44
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.82	0.44
14:2S:62:LYS:HA	14:2S:65:VAL:HG22	1.99	0.44
21:2Z:31:ARG:HG3	21:2Z:32:HIS:CD2	2.53	0.44
32:2a:309:G:H1'	32:2a:608:A:C2	2.52	0.44
32:2a:719:C:H42	49:2r:71:LYS:HE2	1.83	0.44
32:2a:779:C:O2'	42:2k:120:ARG:HD3	2.18	0.44
32:2a:865:A:H5'	32:2a:1078:U:C5	2.52	0.44
1:1A:548:A:H61	17:1V:18:LEU:HA	1.83	0.44
1:1A:774:A:N3	1:1A:774:A:H2'	2.32	0.44
1:1A:1792:G:O2'	1:1A:1830:C:OP1	2.32	0.44
1:1A:2853:C:H2'	1:1A:2854:G:C8	2.52	0.44
6:1G:44:GLY:O	6:1G:47:LYS:HE3	2.18	0.44
8:1I:123:LEU:HD12	8:1I:123:LEU:HA	1.86	0.44
32:1a:920:U:H2'	32:1a:921:U:C6	2.53	0.44
32:1a:1239:A:H62	32:1a:1299:A:H62	1.66	0.44
34:1c:119:ARG:HE	34:1c:140:ARG:CZ	2.31	0.44
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.83	0.44
37:1f:97:PHE:HD2	49:1r:31:LEU:HD11	1.83	0.44
39:1h:51:VAL:HG11	39:1h:60:ARG:NH1	2.31	0.44
40:1i:79:LEU:HG	40:1i:83:ARG:HD2	2.00	0.44
1:2A:92:A:H2'	1:2A:93:G:O4'	2.17	0.44
1:2A:265:A:C8	1:2A:266:G:H1'	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:84:GLY:O	8:2I:86:THR:N	2.45	0.44
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.25	0.44
12:2Q:75:THR:HG21	12:2Q:87:LYS:HE3	1.99	0.44
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.99	0.44
32:2a:434:U:H2'	32:2a:435:C:C6	2.53	0.44
32:2a:587:G:N2	32:2a:754:C:OP2	2.44	0.44
34:2c:152:ILE:HG22	34:2c:167:TRP:HB2	2.00	0.44
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.58	0.44
1:1A:657:U:H2'	1:1A:658:C:H6	1.83	0.44
1:1A:1557:C:H5''	1:1A:1558:A:OP2	2.17	0.44
1:1A:1924:C:H4'	55:1x:13:C:O2'	2.17	0.44
1:1A:2478:A:H5'	31:19:31:LYS:HD3	1.99	0.44
11:1P:37:GLY:C	11:1P:38:GLN:O	2.61	0.44
32:1a:603:U:H3	32:1a:635:G:H1	1.65	0.44
32:1a:974:A:H8	32:1a:974:A:OP1	2.01	0.44
32:1a:1137:C:H5''	32:1a:1138:G:OP1	2.18	0.44
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.99	0.44
35:1d:107:ARG:HH21	35:1d:194:LEU:HD21	1.82	0.44
39:1h:114:THR:HG22	39:1h:130:GLY:O	2.18	0.44
42:1k:48:ILE:O	42:1k:50:TYR:N	2.47	0.44
1:2A:380:U:H2'	1:2A:381:G:H8	1.83	0.44
1:2A:531:C:OP1	1:2A:561:G:N1	2.43	0.44
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.52	0.44
1:2A:2299:G:N1	1:2A:2318:G:N7	2.65	0.44
2:2B:7:G:H2'	2:2B:8:U:O4'	2.18	0.44
4:2E:48:GLN:NE2	4:2E:78:LEU:HD13	2.32	0.44
7:2H:101:ARG:NH2	7:2H:122:THR:HA	2.32	0.44
32:2a:123:C:OP1	32:2a:312:C:H5'	2.18	0.44
32:2a:1216:G:H5''	45:2n:5:ALA:CB	2.48	0.44
39:2h:77:GLU:HG2	39:2h:78:GLN:H	1.80	0.44
51:2t:56:MET:HG3	51:2t:88:VAL:HG21	2.00	0.44
54:2y:9:A:H5'	54:2y:46:G7M:N3	2.32	0.44
1:1A:302:C:H2'	1:1A:303:U:H6	1.83	0.44
1:1A:593:G:C4'	30:18:4:MET:HE2	2.48	0.44
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.33	0.44
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.51	0.44
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.52	0.44
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.99	0.44
18:1W:23:LEU:HD21	27:15:25:LEU:HB2	1.99	0.44
18:1W:57:ASN:HA	18:1W:61:ASN:HD22	1.83	0.44
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:58:ARG:HG2	50:1s:67:VAL:H	1.82	0.44
32:1a:70:G:H1	32:1a:99:U:H3	1.66	0.44
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.36	0.44
38:1g:37:ASN:O	38:1g:41:ARG:HG3	2.18	0.44
41:1j:7:LYS:HG3	41:1j:71:LEU:HD13	1.99	0.44
1:2A:724:U:H2'	1:2A:725:G:O4'	2.18	0.44
1:2A:2413:G:H2'	1:2A:2414:G:O4'	2.18	0.44
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.18	0.44
4:2E:30:PRO:HB3	4:2E:92:THR:HG22	1.99	0.44
7:2H:35:VAL:O	7:2H:37:VAL:HG23	2.18	0.44
11:2P:63:PRO:HG2	30:28:25:MET:HB2	2.00	0.44
32:2a:994:A:N7	32:2a:1216:G:H4'	2.32	0.44
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.52	0.44
48:2q:51:TYR:HE1	48:2q:76:LEU:HB2	1.83	0.44
50:2s:31:ILE:O	50:2s:50:ALA:N	2.30	0.44
1:1A:278:A:O2'	1:1A:279:C:OP1	2.28	0.43
1:1A:828:U:H4'	1:1A:831:G:N1	2.33	0.43
1:1A:2141:G:C4	1:1A:2142:C:H1'	2.53	0.43
5:1F:72:ARG:HE	5:1F:72:ARG:HB3	1.45	0.43
32:1a:60:A:N1	32:1a:107:G:O2'	2.50	0.43
32:1a:262:A:C6	32:1a:263:A:C6	3.05	0.43
32:1a:403:C:O2'	35:1d:122:ARG:NH2	2.28	0.43
32:1a:762:C:H2'	32:1a:763:G:H8	1.83	0.43
51:1t:77:ALA:O	51:1t:81:LYS:HG3	2.18	0.43
1:2A:380:U:H2'	1:2A:381:G:C8	2.53	0.43
1:2A:458:G:O2'	29:27:39:ARG:HD3	2.18	0.43
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.53	0.43
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.53	0.43
6:2G:43:LEU:HD13	6:2G:43:LEU:HA	1.76	0.43
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	2.00	0.43
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.51	0.43
27:25:41:PRO:O	27:25:44:THR:OG1	2.35	0.43
33:2b:27:LYS:HB2	33:2b:194:PRO:HD2	2.00	0.43
41:2j:9:ARG:O	41:2j:16:LEU:HD21	2.18	0.43
44:2m:54:VAL:HG22	44:2m:57:ARG:NH1	2.25	0.43
1:1A:818:G:O6	61:1A:4140:HOH:O	2.20	0.43
1:1A:1858:G:N2	1:1A:1883:G:H2'	2.32	0.43
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.19	0.43
7:1H:5:GLY:HA2	7:1H:69:ARG:HB2	2.00	0.43
11:1P:59:LEU:HD21	30:18:10:ALA:HB2	2.00	0.43
12:1Q:111:GLU:O	12:1Q:115:MET:HG2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1U:105:VAL:HG11	17:1V:39:LEU:HD21	1.99	0.43
32:1a:382:A:H2'	32:1a:383:A:H8	1.82	0.43
32:1a:540:G:H2'	32:1a:541:G:O4'	2.18	0.43
32:1a:1223:C:OP2	50:1s:78:ARG:NH2	2.42	0.43
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.53	0.43
47:1p:76:GLN:HE21	47:1p:76:GLN:HB3	1.49	0.43
54:1y:23:A:H2'	54:1y:24:G:C8	2.54	0.43
54:1y:36:A:H2'	54:1y:37:MIA:O4'	2.17	0.43
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.18	0.43
1:2A:196:A:N3	1:2A:196:A:H2'	2.33	0.43
1:2A:864:G:H21	1:2A:866:A:H61	1.66	0.43
1:2A:1006:C:C2	1:2A:1138:G:N2	2.87	0.43
1:2A:1021:A:H3'	1:2A:1021:A:H8	1.82	0.43
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.53	0.43
1:2A:1689:A:N6	1:2A:1698:A:H2	2.07	0.43
9:2N:123:TYR:CE2	9:2N:129:PRO:HD2	2.53	0.43
11:2P:81:GLN:NE2	11:2P:106:LEU:HA	2.33	0.43
12:2Q:31:ASP:N	12:2Q:106:VAL:O	2.47	0.43
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.32	0.43
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.33	0.43
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.18	0.43
20:2Y:5:MET:HE1	20:2Y:32:PRO:HA	1.99	0.43
20:2Y:28:LYS:HD2	20:2Y:40:GLU:HG2	1.99	0.43
32:2a:165:C:H2'	32:2a:166:G:H8	1.82	0.43
32:2a:645:C:H2'	32:2a:646:U:C6	2.53	0.43
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.18	0.43
34:2c:108:ASN:HB3	34:2c:111:LEU:HB2	1.99	0.43
39:2h:73:ASP:OD1	39:2h:75:ARG:NE	2.51	0.43
40:2i:85:LEU:HD12	40:2i:96:LEU:HD11	2.00	0.43
1:1A:42:G:H2'	1:1A:43:A:O4'	2.18	0.43
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.83	0.43
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.34	0.43
1:1A:2439:A:H5'	1:1A:2439:A:C8	2.53	0.43
7:1H:104:GLU:HG3	7:1H:114:VAL:HG12	2.00	0.43
12:1Q:16:ARG:HG3	12:1Q:18:LYS:HG3	2.00	0.43
32:1a:925:G:H1'	32:1a:1502:A:C4	2.54	0.43
51:1t:48:LYS:HA	51:1t:48:LYS:HD3	1.74	0.43
54:1y:62:C:H2'	54:1y:63:G:H8	1.83	0.43
1:2A:2807:G:N2	1:2A:2892:A:H62	2.15	0.43
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.18	0.43
6:2G:69:ALA:HB3	6:2G:91:ARG:NH2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:3:ARG:NH2	7:2H:5:GLY:H	2.14	0.43
8:2I:45:LYS:HE2	8:2I:45:LYS:HB3	1.63	0.43
10:2O:71:ARG:NH2	10:2O:77:ILE:HG21	2.32	0.43
16:2U:90:VAL:HG12	16:2U:95:LEU:HG	1.99	0.43
23:21:83:GLU:OE2	23:21:83:GLU:N	2.46	0.43
32:2a:448:A:P	32:2a:485:G:H22	2.40	0.43
32:2a:1265:G:C4	32:2a:1271:G:N2	2.86	0.43
33:2b:50:GLU:HB3	33:2b:200:ILE:O	2.17	0.43
41:2j:74:ILE:HD12	41:2j:74:ILE:HA	1.89	0.43
1:1A:27:G:C2	1:1A:512:G:N3	2.86	0.43
1:1A:1062:G:H5''	1:1A:1070:A:H4'	2.00	0.43
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.53	0.43
3:1D:3:VAL:HG13	3:1D:17:THR:HB	2.00	0.43
32:1a:216:G:H2'	32:1a:217:C:C6	2.53	0.43
32:1a:392:G:OP1	47:1p:8:ARG:NH2	2.51	0.43
32:1a:598:U:H2'	32:1a:599:C:H6	1.84	0.43
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.54	0.43
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	2.00	0.43
37:1f:97:PHE:CD2	49:1r:31:LEU:HD11	2.53	0.43
38:1g:58:PRO:O	38:1g:61:VAL:N	2.51	0.43
38:1g:80:VAL:HB	38:1g:85:TYR:HE2	1.84	0.43
41:1j:4:ILE:N	41:1j:99:LYS:O	2.51	0.43
47:1p:21:VAL:HG13	47:1p:33:ILE:HB	1.99	0.43
49:1r:65:ILE:O	49:1r:69:THR:HG23	2.18	0.43
1:2A:152:G:H2'	1:2A:153:C:C6	2.54	0.43
6:2G:45:GLU:H	6:2G:45:GLU:HG2	1.47	0.43
6:2G:125:PHE:HB3	6:2G:166:ASP:OD2	2.17	0.43
14:2S:19:LYS:C	14:2S:21:THR:H	2.26	0.43
16:2U:81:HIS:O	16:2U:84:LYS:HB3	2.18	0.43
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.53	0.43
32:2a:189(D):C:H2'	32:2a:189(E):U:O4'	2.19	0.43
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.18	0.43
32:2a:1288:A:N3	32:2a:1352:C:O2'	2.41	0.43
32:2a:1508:G:H2'	32:2a:1509:C:C6	2.54	0.43
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	2.00	0.43
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	2.01	0.43
49:2r:58:LEU:HB3	49:2r:62:GLU:HB2	2.00	0.43
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.43	0.43
1:1A:579:G:H2'	1:1A:580:C:C6	2.53	0.43
1:1A:2255:G:N7	61:1A:4234:HOH:O	2.36	0.43
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.34	0.43
32:1a:110:C:H2'	32:1a:111:G:O4'	2.18	0.43
32:1a:271:C:H2'	32:1a:272:C:C6	2.54	0.43
32:1a:1036:G:H5''	32:1a:1037:C:H5	1.83	0.43
33:1b:21:ARG:HA	33:1b:39:ILE:HA	2.01	0.43
40:1i:55:ALA:HB1	40:1i:58:HIS:HB2	1.99	0.43
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.31	0.43
1:2A:2166:G:H3'	1:2A:2167:U:H5''	2.00	0.43
9:2N:67:LEU:O	9:2N:88:GLU:HG3	2.19	0.43
14:2S:36:TYR:CD1	14:2S:52:SER:HB3	2.54	0.43
32:2a:779:C:H2'	32:2a:780:A:O4'	2.19	0.43
32:2a:839:U:H3'	32:2a:840:C:C6	2.54	0.43
32:2a:977:A:H2'	32:2a:978:A:H5''	2.01	0.43
34:2c:53:ALA:HB2	34:2c:115:LEU:HD13	2.00	0.43
38:2g:38:LEU:O	38:2g:42:ILE:HG13	2.18	0.43
48:2q:58:GLU:OE2	48:2q:75:ARG:NH2	2.52	0.43
50:2s:80:TYR:C	50:2s:82:GLY:H	2.27	0.43
1:1A:363(C):G:H2'	1:1A:363(D):G:C8	2.54	0.43
1:1A:1721:G:H2'	1:1A:1722:A:H2'	2.00	0.43
1:1A:2144:U:H3'	1:1A:2146:C:N4	2.33	0.43
6:1G:82:LEU:HD11	6:1G:88:ILE:HG21	2.01	0.43
18:1W:62:HIS:O	18:1W:64:MET:HG3	2.19	0.43
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.49	0.43
32:1a:731:G:OP1	32:1a:766:A:H1'	2.19	0.43
32:1a:750:G:N3	46:1o:23:GLY:HA3	2.33	0.43
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.18	0.43
32:1a:1326:C:H2'	32:1a:1327:C:C6	2.53	0.43
34:1c:22:TRP:CH2	45:1n:54:PRO:HG2	2.54	0.43
34:1c:110:ASN:N	34:1c:110:ASN:OD1	2.50	0.43
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	2.01	0.43
1:2A:252:G:OP1	11:2P:50:ARG:NH1	2.49	0.43
1:2A:611:C:H2'	1:2A:612:C:C6	2.54	0.43
1:2A:1906:G:OP2	1:2A:1929:G:O2'	2.37	0.43
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.53	0.43
10:2O:16:ALA:HB2	10:2O:52:VAL:HG21	2.01	0.43
13:2R:57:ARG:HH22	13:2R:61:HIS:HD2	1.67	0.43
32:2a:664:G:N2	32:2a:741:G:H1	2.13	0.43
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.53	0.43
32:2a:1279:A:H3'	32:2a:1279:A:N3	2.34	0.43
33:2b:52:GLU:O	33:2b:56:ARG:NH1	2.52	0.43
34:2c:16:ARG:HD2	34:2c:16:ARG:HA	1.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:59:LEU:O	38:2g:63:LYS:HG3	2.18	0.43
51:2t:98:PRO:O	51:2t:99:LEU:HB2	2.16	0.43
55:2x:15:G:H2'	55:2x:59:A:N1	2.34	0.43
1:1A:647:G:H2'	1:1A:648:G:O4'	2.18	0.43
1:1A:1054:A:C6	1:1A:1055:G:C6	3.06	0.43
1:1A:1075:C:O2	1:1A:1076:C:H2'	2.19	0.43
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.18	0.43
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.52	0.43
1:1A:2684:U:H1'	10:1O:70:LYS:HD2	2.01	0.43
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.54	0.43
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.59	0.43
7:1H:102:ALA:HB2	7:1H:116:GLU:HG3	2.00	0.43
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.74	0.43
15:1T:39:ARG:HH21	32:1a:345:C:H5'	1.83	0.43
32:1a:1142:G:H2'	32:1a:1143:G:O4'	2.19	0.43
32:1a:1315:U:H2'	32:1a:1316:G:O4'	2.19	0.43
33:1b:174:VAL:O	33:1b:178:ARG:HG2	2.19	0.43
33:1b:196:LEU:HD23	33:1b:196:LEU:HA	1.90	0.43
33:1b:211:ILE:O	33:1b:215:LEU:HB2	2.19	0.43
40:1i:4:TYR:CD1	40:1i:88:TYR:HA	2.54	0.43
1:2A:271(S):G:C6	1:2A:271(T):C:C4	3.06	0.43
1:2A:1657:C:H2'	1:2A:1658:C:H6	1.84	0.43
1:2A:2232:U:P	23:21:40:ARG:HH12	2.41	0.43
1:2A:2483:C:H2'	1:2A:2484:G:O4'	2.19	0.43
10:2O:58:VAL:HG21	10:2O:86:ILE:HG12	1.99	0.43
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	2.01	0.43
14:2S:48:LEU:HG	14:2S:82:ILE:HD11	2.00	0.43
32:2a:630:G:H2'	32:2a:631:G:H8	1.83	0.43
32:2a:673:G:O3'	37:2f:87:ARG:NH2	2.51	0.43
32:2a:769:G:H4'	32:2a:1513:A:H4'	2.01	0.43
43:2l:113:ARG:NE	43:2l:115:LYS:O	2.45	0.43
44:2m:48:LEU:HD23	44:2m:48:LEU:HA	1.91	0.43
1:1A:1027:A:C6	1:1A:1126:A:C4	3.06	0.43
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.17	0.43
21:1Z:45:ASP:O	21:1Z:49:ARG:HB2	2.18	0.43
21:1Z:72:ARG:HD3	21:1Z:72:ARG:HA	1.77	0.43
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.54	0.43
32:1a:31:G:N2	32:1a:47:C:O5'	2.52	0.43
32:1a:236:G:H5''	48:1q:42:TYR:OH	2.19	0.43
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.39	0.43
32:1a:924:C:H2'	32:1a:925:G:C8	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.54	0.43
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.18	0.43
32:1a:1191:A:H5''	34:1c:4:LYS:NZ	2.33	0.43
32:1a:1349:A:H5''	40:1i:121:ARG:HB2	2.00	0.43
35:1d:172:PRO:C	35:1d:174:LEU:H	2.26	0.43
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.25	0.43
50:1s:63:THR:OG1	50:1s:66:MET:HE3	2.18	0.43
1:2A:600:G:O3'	5:2F:108:LYS:HE3	2.18	0.43
1:2A:620:G:H8	1:2A:622:G:O6	2.02	0.43
1:2A:644:A:H4'	1:2A:645:C:N4	2.34	0.43
1:2A:886:C:H2'	1:2A:887:A:O4'	2.19	0.43
6:2G:113:ARG:HH11	26:24:33:VAL:HG23	1.84	0.43
8:2I:66:GLU:HA	8:2I:69:LYS:HB3	2.00	0.43
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.54	0.43
32:2a:34:C:H2'	32:2a:35:G:C8	2.53	0.43
32:2a:974:A:H8	32:2a:974:A:OP1	2.02	0.43
32:2a:1466:C:H2'	32:2a:1467:G:O4'	2.19	0.43
34:2c:138:VAL:O	34:2c:142:MET:HB2	2.19	0.43
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.51	0.43
44:2m:10:PRO:HB2	44:2m:13:LYS:HD2	2.00	0.43
1:1A:279:C:N4	1:1A:361:G:H1	2.16	0.43
1:1A:570:G:H2'	1:1A:2030:A:N7	2.34	0.43
1:1A:603:A:C8	1:1A:655:A:C6	3.06	0.43
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.19	0.43
1:1A:2390:U:P	30:18:35:GLN:HE22	2.42	0.43
3:1D:246:PRO:O	3:1D:254:THR:HG22	2.18	0.43
9:1N:1:MET:HE1	16:1U:94:ASN:ND2	2.33	0.43
23:11:92:LYS:NZ	61:11:202:HOH:O	2.48	0.43
32:1a:841:U:C4	32:1a:848:C:H1'	2.54	0.43
35:1d:144:ASP:OD1	35:1d:144:ASP:N	2.51	0.43
37:1f:70:ASP:O	37:1f:71:ARG:HG3	2.19	0.43
1:2A:1420:U:HO2'	1:2A:1421:G:P	2.38	0.43
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.19	0.43
22:20:53:MET:HG2	22:20:57:PHE:HA	2.00	0.43
32:2a:45:U:H2'	32:2a:46:G:H8	1.81	0.43
32:2a:201:C:H5'	32:2a:202:U:OP2	2.18	0.43
32:2a:714:G:H2'	32:2a:715:A:C8	2.54	0.43
32:2a:1342:C:H4'	40:2i:125:TYR:HB3	2.00	0.43
32:2a:1459:C:OP1	51:2t:31:SER:OG	2.32	0.43
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.47	0.43
33:2b:178:ARG:O	39:2h:72:PRO:HD3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:71:ALA:HA	34:2c:106:VAL:HB	2.01	0.43
36:2e:57:LYS:HD3	36:2e:61:TYR:HE2	1.84	0.43
37:2f:2:ARG:HE	37:2f:69:GLU:HG2	1.84	0.43
41:2j:11:PHE:CE1	41:2j:67:THR:HG22	2.54	0.43
54:2w:8:4SU:O5'	54:2w:8:4SU:H6	2.19	0.43
1:1A:271(L):U:H4'	8:1I:50:ARG:NH2	2.26	0.43
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.53	0.43
1:1A:2808:U:H5''	1:1A:2891:G:O6	2.19	0.43
1:1A:2893:G:H5''	1:1A:2894:G:O4'	2.18	0.43
2:1B:66:A:H61	2:1B:108:U:H2'	1.84	0.43
5:1F:31:HIS:HB2	11:1P:9:ASN:OD1	2.19	0.43
21:1Z:93:ASP:HB3	21:1Z:131:ARG:HH22	1.84	0.43
38:1g:137:LYS:O	38:1g:141:VAL:HG23	2.19	0.43
39:1h:81:HIS:HB2	39:1h:138:TRP:CD1	2.54	0.43
41:1j:5:ARG:HD3	41:1j:71:LEU:HD11	2.01	0.43
1:2A:200:U:O2	1:2A:386:G:N2	2.52	0.43
1:2A:868:U:C4	1:2A:869:G:N7	2.87	0.43
1:2A:947:G:H2'	1:2A:948:G:C8	2.53	0.43
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.54	0.43
1:2A:1999:C:H5''	1:2A:2723:C:O2'	2.19	0.43
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.54	0.43
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.47	0.43
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.19	0.43
21:2Z:171:ILE:CD1	21:2Z:172:ALA:H	2.31	0.43
32:2a:728:A:H2'	32:2a:729:A:C8	2.54	0.43
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	2.00	0.43
54:2y:23:A:C6	54:2y:24:G:C5	3.07	0.43
1:1A:236:C:H2'	1:1A:237:C:C6	2.54	0.42
1:1A:362:U:H6	1:1A:362:U:H2'	1.59	0.42
1:1A:1062:G:H1	1:1A:1077:A:N6	2.12	0.42
1:1A:1639:U:O2'	1:1A:2699:C:H4'	2.19	0.42
7:1H:125:VAL:HG22	7:1H:131:VAL:HG22	2.00	0.42
11:1P:85:LEU:HG	11:1P:115:LEU:O	2.18	0.42
15:1T:65:LYS:HG2	15:1T:66:VAL:N	2.34	0.42
15:1T:108:ARG:NH2	15:1T:112:ARG:HD3	2.34	0.42
34:1c:71:ALA:O	34:1c:73:PRO:HD3	2.19	0.42
37:1f:39:LYS:HE2	37:1f:39:LYS:HB3	1.76	0.42
41:1j:5:ARG:HH21	41:1j:73:ASP:CG	2.25	0.42
41:1j:38:ILE:HG12	41:1j:71:LEU:O	2.19	0.42
43:1l:124:LYS:HA	43:1l:125:PRO:HD3	1.93	0.42
44:1m:2:ALA:HB1	44:1m:6:GLY:HA2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:78:ILE:HG22	44:1m:82:MET:HE2	2.01	0.42
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.34	0.42
54:1y:61:C:H2'	54:1y:62:C:C6	2.54	0.42
1:2A:580:C:H2'	1:2A:581:C:C6	2.54	0.42
1:2A:840:C:H2'	1:2A:841:A:C8	2.54	0.42
1:2A:956:G:H2'	1:2A:957:A:H2'	2.01	0.42
1:2A:1384:A:N3	1:2A:1405:U:H1'	2.33	0.42
1:2A:1702:G:H2'	1:2A:1703:G:O4'	2.20	0.42
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.32	0.42
1:2A:1786:A:C4	1:2A:1938:A:C6	3.07	0.42
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.53	0.42
8:2I:62:LYS:HG3	8:2I:133:HIS:CE1	2.53	0.42
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.34	0.42
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.54	0.42
20:2Y:43:ASN:O	20:2Y:65:ALA:N	2.43	0.42
26:24:46:GLN:C	26:24:48:ARG:N	2.77	0.42
32:2a:116:A:H61	32:2a:313:A:H1'	1.83	0.42
32:2a:983:A:H3'	32:2a:983:A:N3	2.34	0.42
32:2a:1316:G:H22	32:2a:1319:A:C5'	2.31	0.42
32:2a:1380:U:C4	38:2g:3:ARG:HG2	2.54	0.42
1:1A:1673:U:OP1	61:1A:4119:HOH:O	2.21	0.42
5:1F:29:ASN:H	5:1F:112:MET:CE	2.32	0.42
10:1O:1:MET:HE2	10:1O:1:MET:HB3	1.80	0.42
16:1U:79:PHE:CZ	16:1U:83:LEU:HD11	2.54	0.42
32:1a:977:A:H1'	32:1a:982:U:O4	2.18	0.42
32:1a:1121:U:H2'	32:1a:1122:U:C6	2.54	0.42
35:1d:83:SER:HA	35:1d:89:THR:HG21	2.00	0.42
44:1m:20:THR:C	44:1m:22:ILE:H	2.27	0.42
46:1o:10:LYS:HE3	46:1o:10:LYS:HB2	1.87	0.42
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.19	0.42
54:1y:53:G:H3'	54:1y:54:5MU:H73	2.00	0.42
1:2A:223:A:O2'	1:2A:420:C:O2	2.34	0.42
1:2A:747:U:O2	1:2A:2014:A:H1'	2.18	0.42
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.19	0.42
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.83	0.42
1:2A:1919:A:O2'	32:2a:1517:G:N3	2.49	0.42
1:2A:2228:G:C6	1:2A:2229:C:C4	3.07	0.42
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.19	0.42
3:2D:133:LEU:HB3	3:2D:173:VAL:HG21	2.01	0.42
11:2P:138:LEU:HG	11:2P:143:GLY:HA3	2.01	0.42
15:2T:23:ARG:HD3	15:2T:120:ARG:NH1	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:73:GLN:HB3	21:2Z:87:ASP:CG	2.44	0.42
21:2Z:130:PRO:HA	21:2Z:133:ILE:HG13	2.01	0.42
32:2a:523:A:H61	43:2l:92:0TD:CG	2.32	0.42
32:2a:1027:C:O2'	32:2a:1034:G:N2	2.52	0.42
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.54	0.42
32:2a:1292:U:H2'	32:2a:1293:G:C8	2.53	0.42
34:2c:189:ALA:HB3	34:2c:196:LEU:HB2	2.01	0.42
36:2e:84:PHE:CE2	36:2e:133:TYR:HD2	2.37	0.42
39:2h:86:ILE:HG21	39:2h:133:LEU:HD23	2.01	0.42
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	2.01	0.42
42:2k:92:GLU:O	42:2k:96:ARG:HG2	2.19	0.42
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	2.00	0.42
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.53	0.42
1:1A:286:C:H2'	1:1A:287:C:C6	2.54	0.42
1:1A:626:U:O4	11:1P:107:LYS:HE2	2.19	0.42
1:1A:652(S):C:H2'	1:1A:652(T):C:C5	2.54	0.42
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.19	0.42
1:1A:1504:C:H2'	1:1A:1505:C:C6	2.54	0.42
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.54	0.42
1:1A:2399:G:H1'	61:16:202:HOH:O	2.19	0.42
3:1D:34:VAL:HG12	3:1D:63:ARG:HG3	2.00	0.42
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	2.01	0.42
19:1X:25:LYS:HA	19:1X:81:VAL:O	2.19	0.42
26:14:41:PRO:HA	26:14:47:GLN:HE21	1.84	0.42
32:1a:562:C:O2	43:1l:16:GLU:N	2.51	0.42
32:1a:600:C:H2'	32:1a:601:C:H6	1.83	0.42
34:1c:178:LEU:HA	34:1c:178:LEU:HD23	1.79	0.42
54:1y:14:A:C5	54:1y:22:G:C2	3.07	0.42
1:2A:479:A:H4'	1:2A:480:A:OP1	2.18	0.42
1:2A:612:C:H2'	1:2A:613:G:O4'	2.20	0.42
1:2A:851:U:O2'	25:23:42:ALA:O	2.34	0.42
1:2A:2484:G:C2	1:2A:2485:G:C8	3.07	0.42
2:2B:7:G:H21	14:2S:38:GLN:NE2	2.14	0.42
14:2S:80:LEU:HD12	14:2S:80:LEU:HA	1.92	0.42
32:2a:126:G:OP1	32:2a:605:U:O2'	2.36	0.42
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.34	0.42
32:2a:1365:G:H2'	32:2a:1366:C:O4'	2.19	0.42
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.55	0.42
33:2b:7:VAL:HG12	33:2b:9:GLU:OE1	2.19	0.42
35:2d:112:VAL:H	35:2d:116:GLN:NE2	2.18	0.42
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2x:23:C:H2'	55:2x:24:U:C6	2.54	0.42
1:1A:272(A):U:O2'	1:1A:272(B):G:H4'	2.19	0.42
1:1A:1297:C:O2'	1:1A:1302:A:N1	2.50	0.42
1:1A:1507:A:C6	1:1A:1508:A:C5	3.07	0.42
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.53	0.42
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.20	0.42
2:1B:31:C:H4'	6:1G:29:TRP:HH2	1.85	0.42
17:1V:98:GLU:OE2	17:1V:100:ARG:NH1	2.51	0.42
32:1a:447:G:H2'	32:1a:485:G:N2	2.35	0.42
33:1b:48:MET:HA	33:1b:51:LEU:HD12	2.02	0.42
41:1j:75:ILE:O	41:1j:77:PRO:HD3	2.19	0.42
1:2A:471:A:H2'	1:2A:472:A:O4'	2.19	0.42
1:2A:776:G:H4'	1:2A:777:A:O5'	2.20	0.42
1:2A:897:C:H5'	54:2w:56:C:OP1	2.19	0.42
1:2A:1420:U:O5'	1:2A:1420:U:H6	2.02	0.42
1:2A:1592:C:H2'	1:2A:1593:G:C8	2.53	0.42
1:2A:2141:G:C2	1:2A:2142:C:H1'	2.54	0.42
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.19	0.42
12:2Q:27:VAL:O	12:2Q:138:ASP:HB3	2.18	0.42
12:2Q:81:VAL:HB	22:20:7:LEU:HD11	2.01	0.42
12:2Q:130:LYS:HB3	12:2Q:130:LYS:HE2	1.80	0.42
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.20	0.42
18:2W:6:ILE:HG12	18:2W:104:THR:HG23	2.00	0.42
19:2X:46:ALA:HB1	24:22:33:MET:HE1	2.01	0.42
32:2a:72:C:H2'	32:2a:73:G:O4'	2.20	0.42
32:2a:130:A:H1'	32:2a:263:A:O2'	2.20	0.42
32:2a:772:U:H2'	32:2a:773:G:O4'	2.19	0.42
32:2a:983:A:N1	32:2a:1222:G:N2	2.65	0.42
32:2a:1152:A:OP1	41:2j:70:ARG:NH2	2.51	0.42
32:2a:1265:G:C2	32:2a:1271:G:C2	3.07	0.42
36:2e:89:ILE:HD12	36:2e:89:ILE:HA	1.80	0.42
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.19	0.42
1:1A:996:A:H4'	16:1U:91:ASP:OD2	2.20	0.42
1:1A:1021:A:H3'	1:1A:1021:A:N3	2.34	0.42
1:1A:1507:A:O2'	1:1A:1509(A):A:N6	2.53	0.42
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.54	0.42
1:1A:2615:U:H2'	1:1A:2616:C:C6	2.55	0.42
1:1A:2654:A:N1	1:1A:2665:A:H5''	2.34	0.42
2:1B:49:C:H2'	2:1B:50:G:C8	2.55	0.42
5:1F:107:LYS:HE3	5:1F:206:ILE:HA	2.02	0.42
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1V:65:GLY:HA3	17:1V:91:TYR:CZ	2.54	0.42
18:1W:5:ALA:C	18:1W:6:ILE:HG13	2.45	0.42
32:1a:104:G:C2	32:1a:105:G:C8	3.08	0.42
32:1a:123:C:OP1	32:1a:311:C:O2'	2.30	0.42
32:1a:316:G:OP2	32:1a:351:G:O2'	2.36	0.42
32:1a:971:G:N2	32:1a:1363(A):A:OP2	2.45	0.42
32:1a:1343:G:H1'	40:1i:121:ARG:NH1	2.34	0.42
34:1c:58:GLU:O	34:1c:64:VAL:HG23	2.19	0.42
34:1c:112:SER:OG	34:1c:115:LEU:HG	2.19	0.42
35:1d:65:ARG:HG3	35:1d:75:PHE:CD1	2.55	0.42
1:2A:687:C:H5'	29:27:4:THR:O	2.19	0.42
1:2A:877:U:H1'	1:2A:901:A:H61	1.84	0.42
1:2A:1231:G:H2'	1:2A:1232:G:H8	1.84	0.42
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.55	0.42
1:2A:2078:C:C4	1:2A:2079:U:C4	3.08	0.42
2:2B:39:A:O2'	2:2B:46:A:N1	2.49	0.42
9:2N:15:LEU:N	9:2N:136:GLU:O	2.39	0.42
11:2P:28:GLY:O	11:2P:30:THR:N	2.52	0.42
26:24:34:GLU:HB2	44:2m:57:ARG:NE	2.35	0.42
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	2.01	0.42
32:2a:1403:C:H2'	32:2a:1404:5MC:HM53	2.00	0.42
53:2v:12:A:O2'	53:2v:13:A:H5'	2.19	0.42
1:1A:524:U:H2'	1:1A:525:U:C6	2.54	0.42
1:1A:583:G:OP2	16:1U:10:ARG:HD2	2.20	0.42
1:1A:1055:G:OP2	1:1A:1055:G:H8	2.03	0.42
1:1A:1090:U:C2	1:1A:1102:C:H1'	2.54	0.42
1:1A:1190:G:H5''	11:1P:32:THR:O	2.19	0.42
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.18	0.42
25:13:18:ASP:OD1	25:13:18:ASP:N	2.53	0.42
32:1a:146:G:C2	32:1a:147:G:C4	3.08	0.42
32:1a:405:U:H5''	32:1a:495:A:H2	1.84	0.42
32:1a:437:U:OP1	35:1d:155:LEU:HD11	2.19	0.42
32:1a:484:G:H4'	32:1a:485:G:H4'	2.01	0.42
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.55	0.42
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.54	0.42
35:1d:140:VAL:HG21	35:1d:146:ILE:HD11	2.01	0.42
40:1i:4:TYR:CE2	40:1i:88:TYR:HD1	2.38	0.42
49:1r:53:ARG:HA	49:1r:56:THR:OG1	2.20	0.42
1:2A:586:A:N1	1:2A:809:G:O2'	2.38	0.42
1:2A:597:U:H2'	1:2A:598:G:H8	1.84	0.42
1:2A:862:G:H2'	1:2A:863:A:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:974:G:C4	1:2A:989:G:C2	3.08	0.42
1:2A:1556:C:H2'	1:2A:1557:C:C6	2.54	0.42
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.17	0.42
2:2B:94:C:H2'	2:2B:95:C:H6	1.84	0.42
3:2D:38:LYS:HA	3:2D:38:LYS:HD2	1.85	0.42
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	2.00	0.42
8:2I:66:GLU:HG2	8:2I:69:LYS:HD2	2.00	0.42
19:2X:65:ARG:HE	19:2X:70:LEU:CD2	2.32	0.42
24:22:32:LEU:HB2	24:22:53:LEU:HD13	2.01	0.42
32:2a:109:A:H5'	32:2a:110:C:C5	2.55	0.42
32:2a:316:G:OP2	32:2a:351:G:O2'	2.34	0.42
32:2a:583:A:H2'	32:2a:584:G:O4'	2.20	0.42
32:2a:825:G:H2'	32:2a:826:C:H6	1.85	0.42
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.84	0.42
32:2a:1132:C:H2'	32:2a:1133:G:H8	1.82	0.42
44:2m:67:GLU:HG3	44:2m:71:ARG:HH22	1.83	0.42
54:2w:12:U:H2'	54:2w:13:C:H5''	2.01	0.42
1:1A:1179:C:H2'	1:1A:1180:C:H6	1.85	0.42
1:1A:2206:G:H3'	1:1A:2207:G:N7	2.35	0.42
4:1E:79:ARG:HD3	4:1E:79:ARG:HA	1.81	0.42
12:1Q:6:ARG:C	12:1Q:7:MET:HG2	2.44	0.42
24:12:21:LEU:HD23	24:12:21:LEU:HA	1.84	0.42
26:14:50:VAL:HG21	44:1m:65:LYS:HB3	2.02	0.42
32:1a:576:G:O6	32:1a:880:C:O2'	2.31	0.42
32:1a:649:G:H2'	32:1a:650:G:H8	1.85	0.42
32:1a:1066:C:O2'	32:1a:1067:A:H5'	2.19	0.42
32:1a:1118:C:H2'	32:1a:1119:C:C6	2.55	0.42
40:1i:96:LEU:HD22	40:1i:96:LEU:HA	1.84	0.42
42:1k:33:THR:HA	42:1k:39:PRO:HA	2.02	0.42
48:1q:43:LEU:HD12	48:1q:68:ARG:HB3	2.02	0.42
49:1r:58:LEU:HB3	49:1r:62:GLU:HB2	2.00	0.42
1:2A:253:C:H2'	1:2A:254:G:O4'	2.19	0.42
1:2A:468:G:H5''	5:2F:60:SER:HB2	2.01	0.42
1:2A:1186:G:H2'	1:2A:1187:G:O4'	2.20	0.42
1:2A:1213:A:N3	1:2A:1238:G:O2'	2.48	0.42
1:2A:1276:A:N6	1:2A:1295:C:N3	2.68	0.42
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.54	0.42
1:2A:1810:A:H2'	1:2A:1811:G:O4'	2.19	0.42
1:2A:2274:A:O2'	1:2A:2276:G:OP1	2.30	0.42
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.54	0.42
5:2F:28:ILE:HG13	5:2F:119:ARG:HH21	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:29:ASN:HB3	5:2F:112:MET:HE1	2.02	0.42
5:2F:107:LYS:HG3	5:2F:206:ILE:HA	2.01	0.42
7:2H:15:VAL:HG11	7:2H:76:VAL:HG13	2.02	0.42
14:2S:93:LYS:HE2	14:2S:93:LYS:HB2	1.90	0.42
32:2a:102:G:C6	32:2a:103:C:C4	3.08	0.42
32:2a:960:U:H5	50:2s:78:ARG:HD3	1.84	0.42
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.54	0.42
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.35	0.42
38:2g:22:LEU:HG	38:2g:62:PHE:CZ	2.55	0.42
38:2g:69:VAL:HG21	38:2g:104:LEU:HD21	2.02	0.42
46:2o:49:ASP:CG	46:2o:52:SER:HB2	2.44	0.42
49:2r:35:ARG:O	49:2r:37:VAL:N	2.52	0.42
1:1A:251:A:C5	1:1A:252:G:H1'	2.55	0.42
1:1A:529:A:OP2	9:1N:114:ARG:NH2	2.49	0.42
1:1A:1092:C:H2'	1:1A:1093:G:H5'	2.01	0.42
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	2.01	0.42
13:1R:12:ARG:HB3	13:1R:16:HIS:HB3	2.01	0.42
18:1W:4:LYS:HE3	18:1W:6:ILE:HD11	2.01	0.42
32:1a:472:A:OP1	47:1p:75:ARG:NH2	2.44	0.42
32:1a:626:U:H2'	32:1a:627:G:C8	2.55	0.42
32:1a:865:A:H2	32:1a:918:A:H4'	1.84	0.42
32:1a:1152:A:H5'	41:1j:13:HIS:ND1	2.34	0.42
34:1c:156:ARG:HE	34:1c:156:ARG:HB3	1.70	0.42
36:1e:131:ILE:HD13	36:1e:131:ILE:HA	1.95	0.42
36:1e:148:VAL:O	36:1e:152:ARG:HG3	2.20	0.42
40:1i:6:GLY:O	40:1i:17:VAL:HG12	2.19	0.42
54:1w:74:C:H3'	54:1w:75:C:C6	2.55	0.42
1:2A:39:C:H2'	1:2A:40:C:C6	2.55	0.42
1:2A:271(N):U:OP1	1:2A:271(N):U:H2'	2.19	0.42
1:2A:363:G:H2'	1:2A:363(A):A:H8	1.83	0.42
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.20	0.42
1:2A:2184:G:H2'	1:2A:2185:C:C6	2.54	0.42
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.19	0.42
1:2A:2805:G:C6	1:2A:2807:G:C6	3.08	0.42
10:2O:111:PHE:O	10:2O:115:VAL:HG23	2.19	0.42
11:2P:39:LYS:HB2	11:2P:45:LEU:HD22	2.01	0.42
12:2Q:18:LYS:HE2	12:2Q:18:LYS:HB2	1.90	0.42
12:2Q:24:GLY:HA2	12:2Q:67:ARG:NH2	2.35	0.42
19:2X:31:HIS:HD2	19:2X:33:LYS:HB2	1.84	0.42
26:24:50:VAL:HG11	44:2m:64:TRP:O	2.19	0.42
28:26:32:ASN:OD1	28:26:32:ASN:N	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:35:GLU:C	28:26:36:LEU:HD22	2.45	0.42
29:27:24:THR:O	29:27:28:ARG:HG3	2.20	0.42
32:2a:191:G:C6	32:2a:192:U:C4	3.08	0.42
32:2a:715:A:H2'	32:2a:716:A:C8	2.55	0.42
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.55	0.42
32:2a:1052:U:O2'	32:2a:1055:A:OP2	2.20	0.42
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.20	0.42
32:2a:1359:C:H1'	32:2a:1362:C:H41	1.84	0.42
32:2a:1507:A:OP2	53:2v:13:A:N6	2.52	0.42
34:2c:64:VAL:O	34:2c:100:ALA:HB3	2.20	0.42
35:2d:101:LEU:O	35:2d:104:VAL:HG22	2.20	0.42
35:2d:111:ALA:HA	35:2d:116:GLN:HE21	1.84	0.42
43:2l:36:VAL:O	43:2l:58:VAL:HA	2.20	0.42
55:2x:53:G:H2'	55:2x:54:5MU:C6	2.54	0.42
1:1A:271(M):G:O2'	1:1A:271(N):U:H5''	2.20	0.42
1:1A:818:G:H4'	1:1A:838:C:O3'	2.20	0.42
1:1A:1512:U:H2'	1:1A:1513:C:C6	2.54	0.42
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.20	0.42
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.33	0.42
15:1T:99:LEU:O	15:1T:102:ILE:HG12	2.20	0.42
15:1T:127:ALA:C	15:1T:129:ARG:N	2.78	0.42
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.55	0.42
21:1Z:131:ARG:HG3	21:1Z:132:ASN:OD1	2.19	0.42
28:16:40:CYS:O	28:16:44:ARG:N	2.52	0.42
32:1a:376:G:OP2	47:1p:67:THR:HG21	2.20	0.42
32:1a:872:A:C4	32:1a:874:G:N7	2.88	0.42
32:1a:971:G:N1	32:1a:1363(A):A:OP2	2.49	0.42
33:1b:37:ASN:C	33:1b:39:ILE:N	2.76	0.42
37:1f:68:PRO:CG	37:1f:71:ARG:HD2	2.47	0.42
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	2.01	0.42
54:1w:28:G:H2'	54:1w:29:G:C8	2.55	0.42
1:2A:271(X):G:C2	1:2A:271(Y):U:O4	2.73	0.42
1:2A:398:G:OP1	1:2A:2090:G:O2'	2.37	0.42
1:2A:1270:C:H5''	1:2A:1271:G:O5'	2.20	0.42
1:2A:1317:A:H2'	1:2A:1318:C:C6	2.55	0.42
1:2A:1752:C:H2'	1:2A:1753:G:C8	2.55	0.42
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.55	0.42
1:2A:2391:G:O6	1:2A:2425:A:H8	2.03	0.42
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.55	0.42
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.54	0.42
6:2G:36:LYS:HG3	6:2G:160:VAL:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:171:ALA:O	6:2G:175:LEU:HG	2.20	0.42
8:2I:75:LEU:HD13	8:2I:105:HIS:HD2	1.82	0.42
9:2N:67:LEU:C	9:2N:88:GLU:HG3	2.45	0.42
11:2P:62:LEU:HD11	30:28:50:LEU:HD11	2.02	0.42
15:2T:64:ARG:NH1	15:2T:103:ARG:HA	2.35	0.42
19:2X:92:LEU:HD12	19:2X:92:LEU:HA	1.86	0.42
26:24:45:GLY:C	26:24:47:GLN:H	2.27	0.42
32:2a:397:A:H5'	32:2a:398:C:OP1	2.19	0.42
32:2a:499:A:H4'	32:2a:500:G:OP1	2.19	0.42
32:2a:554:C:H2'	32:2a:555:C:C6	2.55	0.42
32:2a:1309:G:O3'	44:2m:77:ASN:ND2	2.53	0.42
32:2a:1465:C:H2'	32:2a:1466:C:O4'	2.19	0.42
33:2b:115:LEU:HD23	33:2b:115:LEU:HA	1.85	0.42
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.53	0.42
40:2i:9:ARG:O	40:2i:104:ARG:HG3	2.19	0.42
47:2p:43:LYS:HG2	47:2p:48:TRP:CD1	2.54	0.42
48:2q:24:GLU:OE2	48:2q:37:LYS:HE3	2.19	0.42
1:1A:493:G:H2'	1:1A:494:G:O4'	2.20	0.42
1:1A:762:U:H5''	61:1A:4741:HOH:O	2.20	0.42
1:1A:1683:C:H2'	1:1A:1684:C:C6	2.55	0.42
1:1A:2600:A:H2'	1:1A:2601:C:C6	2.55	0.42
1:1A:2839:G:H5'	13:1R:46:GLY:CA	2.49	0.42
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.20	0.42
12:1Q:1:MET:HE3	12:1Q:1:MET:HB2	1.88	0.42
22:10:32:ARG:H	22:10:35:ASN:ND2	2.17	0.42
30:18:26:LYS:HG2	30:18:46:ARG:O	2.20	0.42
32:1a:1292:U:H2'	32:1a:1293:G:C8	2.55	0.42
32:1a:1355:G:H2'	32:1a:1356:G:C8	2.55	0.42
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.24	0.42
34:1c:36:ASP:O	34:1c:40:ARG:HG3	2.19	0.42
36:1e:84:PHE:HB2	36:1e:134:ALA:HB2	2.02	0.42
40:1i:6:GLY:N	40:1i:84:ALA:HB2	2.35	0.42
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	2.01	0.42
47:1p:47:ASP:OD1	47:1p:47:ASP:N	2.43	0.42
1:2A:361:G:O2'	1:2A:362:U:H5'	2.20	0.42
1:2A:443:A:H5''	1:2A:444:C:OP1	2.19	0.42
1:2A:783:A:O2'	1:2A:785:G:OP1	2.32	0.42
1:2A:2135:A:H61	1:2A:2156:G:H21	1.67	0.42
3:2D:37:LEU:HD13	3:2D:87:ASN:ND2	2.34	0.42
7:2H:90:LYS:HD2	7:2H:159:GLU:HG2	2.02	0.42
11:2P:135:LEU:HD23	11:2P:135:LEU:HA	1.86	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:81:HIS:HD2	16:2U:84:LYS:HD3	1.84	0.42
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	2.02	0.42
21:2Z:152:ALA:O	21:2Z:155:LEU:HG	2.20	0.42
21:2Z:156:LYS:HG3	21:2Z:157:LEU:H	1.85	0.42
32:2a:302:G:N3	32:2a:556:C:H4'	2.35	0.42
48:2q:81:ARG:HH21	48:2q:83:ASP:CG	2.28	0.42
1:1A:271(K):U:O2	8:1I:50:ARG:HD2	2.20	0.41
1:1A:749:C:H4'	1:1A:1271:G:N3	2.35	0.41
1:1A:978:G:C2	1:1A:986:C:C2	3.08	0.41
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.55	0.41
1:1A:2164:C:OP2	1:1A:2165:G:N2	2.53	0.41
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	2.02	0.41
3:1D:206:LEU:HD23	3:1D:206:LEU:HA	1.82	0.41
15:1T:118:ARG:HA	15:1T:121:ILE:HD12	2.02	0.41
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	2.00	0.41
26:14:62:ARG:HB3	26:14:63:TYR:H	1.49	0.41
29:17:24:THR:HG23	61:17:201:HOH:O	2.20	0.41
32:1a:625:G:H4'	47:1p:16:HIS:CG	2.55	0.41
32:1a:688:G:H5'	42:1k:46:GLY:C	2.45	0.41
32:1a:1118:C:OP1	40:1i:9:ARG:NH1	2.53	0.41
33:1b:126:GLU:HB3	33:1b:127:ILE:H	1.72	0.41
37:1f:50:TYR:OH	37:1f:87:ARG:NH2	2.53	0.41
40:1i:82:ALA:O	40:1i:86:VAL:HG22	2.19	0.41
41:1j:81:THR:C	41:1j:83:GLU:H	2.27	0.41
1:2A:652(A):A:H3'	1:2A:652(B):A:C5'	2.50	0.41
1:2A:1632:A:OP2	61:2A:3944:HOH:O	2.22	0.41
1:2A:1876:A:H2'	1:2A:1877:A:C8	2.55	0.41
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.34	0.41
4:2E:4:ILE:HD11	4:2E:29:GLY:HA2	2.02	0.41
5:2F:158:THR:O	5:2F:164:ARG:HD3	2.19	0.41
9:2N:55:VAL:HG23	9:2N:56:ASN:HD22	1.85	0.41
11:2P:29:LYS:HG3	11:2P:30:THR:N	2.35	0.41
14:2S:78:LEU:HD11	14:2S:109:GLY:HA3	2.02	0.41
19:2X:5:TYR:CE2	24:22:30:ARG:HB2	2.55	0.41
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.47	0.41
32:2a:1131:G:H2'	32:2a:1132:C:C6	2.55	0.41
36:2e:28:PHE:O	36:2e:47:LYS:HA	2.20	0.41
36:2e:78:HIS:NE2	36:2e:142:LEU:HD23	2.35	0.41
54:2w:71:G:N2	54:2w:72:C:H1'	2.35	0.41
54:2y:51:U:H3	54:2y:63:G:H1	1.67	0.41
54:2y:67:C:H2'	54:2y:68:C:H6	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:605:C:H2'	1:1A:606:U:O4'	2.20	0.41
1:1A:2439:A:H5'	1:1A:2439:A:H8	1.84	0.41
8:1I:77:LEU:HD23	8:1I:77:LEU:HA	1.76	0.41
16:1U:74:LEU:HD13	16:1U:79:PHE:HB2	2.01	0.41
19:1X:44:GLU:OE2	61:1X:201:HOH:O	2.21	0.41
23:11:75:GLU:O	23:11:78:LYS:HD3	2.20	0.41
32:1a:1023:G:H3'	32:1a:1024:G:C8	2.53	0.41
32:1a:1060:C:H5''	41:1j:51:ARG:HG2	2.02	0.41
32:1a:1202:G:H1'	45:1n:29:ARG:HD2	2.01	0.41
1:2A:100:G:O2'	24:22:7:ARG:NH2	2.53	0.41
1:2A:263:C:H2'	1:2A:264:C:O4'	2.21	0.41
1:2A:602:G:N1	1:2A:655:A:OP2	2.53	0.41
1:2A:614:U:H2'	1:2A:614(A):U:O4'	2.20	0.41
1:2A:720:C:H2'	1:2A:721:C:C6	2.55	0.41
5:2F:110:LEU:HD21	5:2F:181:LEU:HD23	2.01	0.41
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	2.01	0.41
20:2Y:16:ALA:HB2	20:2Y:73:ARG:HG3	2.01	0.41
22:20:70:GLN:HG2	22:20:72:ARG:HG3	2.01	0.41
26:24:16:CYS:C	26:24:18:CYS:H	2.28	0.41
32:2a:142:G:H2'	32:2a:143:A:H8	1.83	0.41
32:2a:189(A):C:H2'	32:2a:189(B):C:H6	1.84	0.41
32:2a:335:C:H2'	32:2a:336:C:C6	2.55	0.41
32:2a:427:U:OP1	35:2d:13:ARG:NH1	2.53	0.41
32:2a:1121:U:H2'	32:2a:1122:U:C6	2.55	0.41
32:2a:1328:C:O2'	44:2m:29:ARG:NE	2.47	0.41
37:2f:82:ARG:HB2	37:2f:85:VAL:HG23	2.03	0.41
38:2g:28:ASN:HD21	38:2g:36:LYS:NZ	2.18	0.41
44:2m:93:ARG:HG3	44:2m:93:ARG:H	1.66	0.41
55:2x:66:C:H2'	55:2x:67:C:O4'	2.21	0.41
1:1A:422:A:H2'	1:1A:423:A:C8	2.55	0.41
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.56	0.41
1:1A:876:C:H2'	1:1A:877:U:O4'	2.20	0.41
1:1A:881:G:N2	1:1A:897:C:O2	2.53	0.41
1:1A:1773:A:H2'	1:1A:1774:C:O4'	2.20	0.41
1:1A:1826:G:H4'	3:1D:242:ARG:CZ	2.50	0.41
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.21	0.41
1:1A:2056:G:C2	1:1A:2057:A:C8	3.08	0.41
1:1A:2114:A:H2'	1:1A:2115:G:O4'	2.21	0.41
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.41	0.41
2:1B:75:G:H22	21:1Z:73:GLN:HE21	1.66	0.41
3:1D:62:TYR:HA	3:1D:87:ASN:OD1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:96:THR:O	11:1P:100:LEU:HG	2.21	0.41
13:1R:96:ARG:HG2	13:1R:115:GLU:HG2	2.03	0.41
19:1X:1:MET:HE3	19:1X:1:MET:HB2	1.88	0.41
21:1Z:98:MET:O	21:1Z:125:LEU:HD12	2.21	0.41
21:1Z:121:HIS:HB3	21:1Z:123:ASP:O	2.20	0.41
32:1a:433:C:H2'	32:1a:434:U:C6	2.55	0.41
32:1a:437:U:H5''	35:1d:155:LEU:HD21	2.02	0.41
32:1a:667:G:H4'	46:1o:51:HIS:CE1	2.56	0.41
32:1a:833:U:H2'	32:1a:834:C:C6	2.54	0.41
32:1a:860:A:H2'	32:1a:861:G:O4'	2.20	0.41
32:1a:911:U:H2'	32:1a:912:C:C6	2.55	0.41
40:1i:92:TYR:O	40:1i:96:LEU:HB2	2.19	0.41
41:1j:7:LYS:C	41:1j:8:LEU:HD23	2.45	0.41
42:1k:18:ARG:HA	42:1k:81:ASP:H	1.85	0.41
48:1q:15:MET:HE3	48:1q:15:MET:HB2	1.95	0.41
1:2A:1169:G:C2	1:2A:1170:G:N7	2.88	0.41
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.55	0.41
6:2G:61:ALA:HB1	26:24:7:PRO:HG3	2.01	0.41
12:2Q:10:ARG:NH1	12:2Q:90:VAL:H	2.15	0.41
13:2R:78:LYS:HE2	13:2R:83:ILE:HD11	2.01	0.41
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.38	0.41
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.55	0.41
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.20	0.41
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.61	0.41
31:29:13:LYS:HA	31:29:13:LYS:HD3	1.90	0.41
32:2a:37:U:O2'	32:2a:500:G:H4'	2.20	0.41
32:2a:114:U:O2'	32:2a:115:G:H5'	2.20	0.41
32:2a:420:U:O2'	32:2a:423:G:O6	2.37	0.41
32:2a:442:C:H42	32:2a:492:G:H1	1.67	0.41
32:2a:521:G:H4'	43:2l:73:GLU:HG2	2.02	0.41
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.54	0.41
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.55	0.41
32:2a:1057:G:H2'	32:2a:1058:G:O4'	2.21	0.41
33:2b:15:VAL:HG12	33:2b:209:ARG:HB3	2.02	0.41
35:2d:150:GLU:CD	35:2d:150:GLU:H	2.26	0.41
38:2g:49:ILE:H	38:2g:49:ILE:HG12	1.68	0.41
41:2j:85:LEU:C	41:2j:87:THR:H	2.28	0.41
43:2l:102:ARG:HE	43:2l:102:ARG:HB3	1.41	0.41
1:1A:196:A:O2'	1:1A:805:G:O6	2.29	0.41
1:1A:888:C:H2'	1:1A:889:C:C5	2.55	0.41
1:1A:2037:G:H2'	1:1A:2038:G:C8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2322:A:H2'	1:1A:2323:G:O4'	2.19	0.41
4:1E:47:VAL:O	4:1E:80:GLU:HA	2.20	0.41
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	2.01	0.41
13:1R:22:ARG:O	13:1R:26:LYS:HG3	2.20	0.41
16:1U:76:TYR:O	16:1U:80:ILE:HG12	2.20	0.41
26:14:55:ARG:H	26:14:56:VAL:HA	1.82	0.41
32:1a:6:G:H1	36:1e:98:THR:HG21	1.84	0.41
32:1a:375:U:C4	32:1a:376:G:N7	2.89	0.41
32:1a:551:U:H2'	32:1a:552:U:C6	2.56	0.41
32:1a:598:U:H2'	32:1a:599:C:C6	2.54	0.41
32:1a:762:C:H2'	32:1a:763:G:C8	2.54	0.41
35:1d:100:ARG:O	35:1d:104:VAL:HG23	2.20	0.41
36:1e:12:LEU:HD22	36:1e:13:ILE:N	2.35	0.41
36:1e:145:LYS:O	36:1e:149:GLU:HG2	2.19	0.41
38:1g:114:ARG:HB2	38:1g:115:ARG:NH2	2.36	0.41
49:1r:76:LEU:HD23	49:1r:76:LEU:HA	1.93	0.41
1:2A:25:U:H5'	18:2W:79:GLY:HA2	2.02	0.41
1:2A:660:G:H5'	5:2F:99:TYR:CE1	2.55	0.41
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.20	0.41
1:2A:1851:U:H2'	1:2A:1852:C:O4'	2.20	0.41
1:2A:2489:G:C2'	1:2A:2490:G:H5'	2.50	0.41
1:2A:2557:G:H2'	1:2A:2558:C:H6	1.85	0.41
4:2E:111:ARG:HA	13:2R:1:MET:SD	2.59	0.41
6:2G:33:ARG:NH2	6:2G:162:THR:HG21	2.35	0.41
14:2S:19:LYS:C	14:2S:21:THR:N	2.78	0.41
14:2S:25:ARG:HB3	14:2S:40:ILE:HB	2.01	0.41
21:2Z:23:LYS:NZ	21:2Z:40:ASP:HB2	2.35	0.41
23:21:53:VAL:HG22	23:21:74:VAL:HG13	2.02	0.41
25:23:23:LEU:HD13	25:23:50:VAL:HG11	2.02	0.41
32:2a:273:A:H1'	48:2q:16:GLN:HE21	1.85	0.41
32:2a:652:U:O4	32:2a:752:G:O2'	2.31	0.41
32:2a:908:A:H2'	32:2a:909:A:C8	2.55	0.41
32:2a:1029:C:H1'	32:2a:1033:G:H22	1.85	0.41
32:2a:1068:G:H8	32:2a:1068:G:OP2	2.02	0.41
32:2a:1081:G:H5''	36:2e:18:ARG:HG2	2.03	0.41
32:2a:1272:G:H5'	32:2a:1273:G:OP2	2.21	0.41
32:2a:1316:G:H5''	45:2n:17:LYS:HD2	2.03	0.41
32:2a:1517:G:H2'	32:2a:1518:MA6:H8	2.01	0.41
38:2g:65:ALA:O	38:2g:69:VAL:HG23	2.21	0.41
38:2g:73:MET:HE2	38:2g:73:MET:HB3	1.95	0.41
38:2g:79:ARG:O	38:2g:80:VAL:C	2.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:44:SER:OG	42:2k:47:VAL:HG23	2.21	0.41
44:2m:4:ILE:HG23	44:2m:5:ALA:N	2.36	0.41
46:2o:87:ILE:HG22	46:2o:88:ARG:N	2.30	0.41
54:2w:34:G:H2'	54:2w:35:A:H8	1.84	0.41
1:1A:309:G:N3	1:1A:329:G:O2'	2.49	0.41
1:1A:858:U:O2	1:1A:2268:A:H2'	2.20	0.41
1:1A:1041:C:N4	1:1A:1114:G:H1	2.12	0.41
1:1A:1078:U:H5'	1:1A:1079:C:OP1	2.20	0.41
1:1A:1174:A:H1'	1:1A:1175:U:C5'	2.51	0.41
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.36	0.41
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.85	0.41
4:1E:119:ARG:HG2	4:1E:120:TRP:NE1	2.35	0.41
5:1F:107:LYS:NZ	5:1F:207:GLY:O	2.41	0.41
26:14:59:PHE:C	26:14:61:ARG:H	2.29	0.41
32:1a:192:U:O2'	51:1t:60:GLU:OE1	2.32	0.41
32:1a:392:G:H2'	32:1a:393:A:H8	1.86	0.41
47:1p:22:THR:HA	47:1p:33:ILE:HD12	2.01	0.41
54:1w:56:C:H2'	54:1w:57:G:O4'	2.20	0.41
1:2A:35:G:H1'	1:2A:454:A:C4	2.56	0.41
1:2A:1024:G:O2'	1:2A:1144:G:O2'	2.36	0.41
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.56	0.41
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.43	0.41
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.55	0.41
1:2A:2347:C:H2'	1:2A:2348:U:C6	2.55	0.41
1:2A:2685:G:P	15:2T:51:ARG:HH12	2.44	0.41
7:2H:24:VAL:HG22	7:2H:35:VAL:HB	2.03	0.41
8:2I:129:THR:HG22	8:2I:139:GLN:NE2	2.35	0.41
13:2R:44:LEU:HD12	13:2R:44:LEU:HA	1.89	0.41
17:2V:12:TYR:CZ	17:2V:22:VAL:HG12	2.55	0.41
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.85	0.41
32:2a:391:G:C6	32:2a:392:G:C5	3.08	0.41
32:2a:1243:C:H42	32:2a:1294:G:H1	1.68	0.41
35:2d:177:ASP:OD1	35:2d:179:GLU:HB2	2.21	0.41
36:2e:33:VAL:HG21	36:2e:109:ILE:HA	2.02	0.41
44:2m:3:ARG:NH2	44:2m:11:ARG:HG3	2.31	0.41
49:2r:31:LEU:H	49:2r:31:LEU:HG	1.63	0.41
50:2s:47:HIS:O	50:2s:61:TYR:HA	2.20	0.41
1:1A:321:G:C2	5:1F:165:ARG:HD2	2.55	0.41
1:1A:397:G:OP2	23:11:10:LYS:NZ	2.42	0.41
1:1A:632:A:H2'	1:1A:633:A:C8	2.56	0.41
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1398:C:H2'	1:1A:1399:C:C6	2.55	0.41
1:1A:1448:G:H1'	1:1A:1528:A:N1	2.36	0.41
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.20	0.41
1:1A:1815:A:H8	1:1A:1815:A:OP1	2.03	0.41
1:1A:1851:U:C4	1:1A:1852:C:C4	3.09	0.41
1:1A:2183:C:O2'	1:1A:2184:G:OP1	2.34	0.41
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	2.02	0.41
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.50	0.41
5:1F:13:SER:HA	5:1F:127:GLU:HB2	2.03	0.41
5:1F:46:ARG:HB3	5:1F:48:THR:HG23	2.02	0.41
9:1N:67:LEU:HD23	9:1N:87:LEU:HG	2.02	0.41
11:1P:90:ARG:HG2	11:1P:90:ARG:NH1	2.34	0.41
12:1Q:71:ASP:OD1	12:1Q:71:ASP:N	2.51	0.41
21:1Z:138:GLU:HB2	21:1Z:156:LYS:NZ	2.34	0.41
32:1a:92:C:H2'	32:1a:93:G:H8	1.85	0.41
32:1a:555:C:H2'	32:1a:556:C:C6	2.55	0.41
32:1a:684:A:O2'	42:1k:39:PRO:O	2.30	0.41
33:1b:55:PHE:HB3	33:1b:221:LEU:HD22	2.03	0.41
33:1b:84:GLU:OE1	33:1b:87:ARG:NH1	2.53	0.41
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	2.03	0.41
42:1k:33:THR:OG1	42:1k:34:ASP:O	2.36	0.41
54:1y:66:U:C4	54:1y:67:C:C4	3.09	0.41
1:2A:531:C:H4'	1:2A:532:A:H5''	2.02	0.41
1:2A:637:A:C6	1:2A:652:C:H4'	2.56	0.41
1:2A:699:A:H4'	1:2A:1554:A:N6	2.36	0.41
1:2A:1461:G:H2'	1:2A:1462:C:H6	1.86	0.41
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.56	0.41
1:2A:2274:A:C5	1:2A:2276:G:C8	3.09	0.41
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.55	0.41
3:2D:232:PRO:HB3	3:2D:244:ARG:CZ	2.50	0.41
4:2E:203:LYS:HD3	4:2E:203:LYS:HA	1.86	0.41
8:2I:101:LEU:HD12	8:2I:102:SER:N	2.35	0.41
14:2S:83:LYS:NZ	14:2S:84:GLN:HE21	2.19	0.41
32:2a:254:G:H1	32:2a:272:C:H42	1.69	0.41
32:2a:1151:A:O2'	32:2a:1152:A:H8	2.03	0.41
32:2a:1216:G:H5''	45:2n:5:ALA:HB2	2.02	0.41
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.82	0.41
32:2a:1414:U:H2'	32:2a:1415:G:H8	1.86	0.41
41:2j:16:LEU:HD23	41:2j:16:LEU:HA	1.64	0.41
44:2m:33:ALA:HA	44:2m:59:TYR:HE2	1.84	0.41
54:2w:71:G:N3	54:2w:71:G:H2'	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2y:62:C:H2'	54:2y:63:G:C8	2.55	0.41
1:1A:83:G:N7	61:1A:4241:HOH:O	2.37	0.41
1:1A:120:U:OP2	61:1A:4148:HOH:O	2.22	0.41
1:1A:484:C:OP1	20:1Y:51:VAL:HG22	2.20	0.41
1:1A:1359:A:H2'	1:1A:1360:A:H5'	2.03	0.41
3:1D:138:VAL:HA	3:1D:165:ILE:HG22	2.03	0.41
4:1E:13:ARG:HD3	15:1T:58:ASN:ND2	2.35	0.41
8:1I:3:VAL:O	8:1I:18:VAL:HA	2.21	0.41
8:1I:87:LYS:HE2	8:1I:87:LYS:O	2.21	0.41
13:1R:52:ILE:HD11	13:1R:116:LEU:HD22	2.03	0.41
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.21	0.41
26:14:50:VAL:HG11	44:1m:64:TRP:C	2.45	0.41
32:1a:159:G:N2	32:1a:161:A:H3'	2.35	0.41
32:1a:358:U:H2'	32:1a:359:U:H6	1.86	0.41
32:1a:617:G:H4'	47:1p:44:THR:O	2.21	0.41
32:1a:958:A:C6	32:1a:959:A:N1	2.88	0.41
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.55	0.41
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.54	0.41
33:1b:158:LEU:HA	33:1b:159:PRO:HD3	1.93	0.41
35:1d:178:VAL:O	35:1d:180:GLY:N	2.50	0.41
45:1n:6:LEU:HD23	45:1n:23:ARG:NH2	2.36	0.41
49:1r:25:THR:O	49:1r:26:LEU:HD12	2.21	0.41
51:1t:58:LYS:HE3	51:1t:62:LEU:HD11	2.02	0.41
1:2A:30:G:C5	1:2A:31:C:C4	3.08	0.41
1:2A:330:A:H2	1:2A:1210:A:H2'	1.84	0.41
1:2A:729:G:C4	1:2A:1775:U:C2	3.09	0.41
1:2A:847:U:H5'	1:2A:848:G:OP2	2.20	0.41
1:2A:851:U:H5'	25:23:49:LYS:HD2	2.02	0.41
1:2A:869:G:O3'	12:2Q:6:ARG:NH2	2.54	0.41
1:2A:1038:C:N4	1:2A:1117:G:H1	2.18	0.41
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.86	0.41
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.86	0.41
1:2A:2405:G:H5'	11:2P:75:ILE:HD13	2.02	0.41
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.56	0.41
2:2B:49:C:OP1	14:2S:97:ARG:HB2	2.21	0.41
8:2I:44:LEU:HD13	8:2I:44:LEU:HA	1.93	0.41
10:2O:36:GLY:HA2	10:2O:106:LEU:HD23	2.02	0.41
15:2T:108:ARG:HA	15:2T:111:ARG:NH1	2.35	0.41
17:2V:24:LYS:HB3	17:2V:24:LYS:HE2	1.78	0.41
22:20:23:VAL:HG22	22:20:38:VAL:HG22	2.02	0.41
24:22:1:MET:HG2	24:22:5:GLU:OE1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:20:U:H2'	32:2a:21:G:O4'	2.21	0.41
32:2a:23:C:H5	32:2a:561:U:O4	2.04	0.41
32:2a:684:A:C6	32:2a:685:G:C6	3.08	0.41
33:2b:79:ASP:C	33:2b:81:VAL:H	2.29	0.41
33:2b:212:GLN:OE1	33:2b:235:SER:HB3	2.21	0.41
38:2g:89:MET:SD	38:2g:155:ARG:HB2	2.61	0.41
38:2g:92:SER:O	38:2g:96:GLN:HG3	2.20	0.41
39:2h:103:VAL:HG21	39:2h:110:ALA:HB2	2.03	0.41
40:2i:85:LEU:O	40:2i:89:ASN:N	2.51	0.41
51:2t:79:ARG:O	51:2t:83:ARG:HG3	2.20	0.41
1:1A:2066:C:H5''	61:1A:5208:HOH:O	2.21	0.41
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.20	0.41
2:1B:4:C:H2'	2:1B:5:C:O4'	2.21	0.41
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.45	0.41
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	2.02	0.41
32:1a:161:A:H2'	32:1a:162:A:C8	2.56	0.41
32:1a:270:A:H2'	32:1a:271:C:C6	2.55	0.41
32:1a:660:G:H2'	32:1a:661:G:O4'	2.20	0.41
41:1j:95:GLU:HG2	41:1j:96:ILE:N	2.36	0.41
51:1t:71:THR:HG22	51:1t:72:LEU:HD13	2.02	0.41
1:2A:27:G:C2	1:2A:512:G:N3	2.89	0.41
1:2A:218:A:C2	1:2A:235:U:H4'	2.56	0.41
1:2A:539:G:C6	1:2A:540:C:C4	3.09	0.41
1:2A:612:C:C2	1:2A:616:G:N2	2.89	0.41
1:2A:995:C:O2	9:2N:3:THR:OG1	2.34	0.41
1:2A:1031:G:N3	31:29:36:GLN:NE2	2.63	0.41
1:2A:1252:G:O2'	1:2A:1253:A:C8	2.74	0.41
1:2A:1272:A:H3'	1:2A:1273:U:H5''	2.03	0.41
1:2A:1821:A:H2'	1:2A:1822:G:C8	2.55	0.41
2:2B:83:G:N1	2:2B:94:C:N3	2.60	0.41
3:2D:78:LYS:HE3	3:2D:78:LYS:HB2	1.92	0.41
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	2.01	0.41
15:2T:77:PRO:HG2	15:2T:80:SER:HB2	2.03	0.41
23:21:77:ALA:HB2	23:21:94:LEU:HD21	2.03	0.41
24:22:41:ILE:HG13	24:22:43:GLN:HG2	2.03	0.41
28:26:40:CYS:SG	28:26:42:TRP:HB2	2.61	0.41
32:2a:509:A:H5''	35:2d:55:ALA:HB2	2.02	0.41
32:2a:1004:A:H1'	32:2a:1038:C:O2	2.21	0.41
32:2a:1117:G:N2	32:2a:1180:A:O2'	2.54	0.41
32:2a:1178:G:N2	32:2a:1180:A:H3'	2.36	0.41
38:2g:29:LYS:O	38:2g:105:VAL:HG11	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:106:GLY:O	39:2h:122:ARG:NH2	2.53	0.41
40:2i:18:PHE:HD2	40:2i:62:TYR:HD2	1.69	0.41
1:1A:432:A:N6	61:1A:4257:HOH:O	2.40	0.41
1:1A:459:U:H4'	29:17:40:TRP:CZ3	2.56	0.41
1:1A:817:C:H4'	1:1A:932:G:C5	2.56	0.41
1:1A:821:A:H2'	1:1A:946:G:H5''	2.02	0.41
1:1A:1006:C:C2	1:1A:1138:G:N2	2.89	0.41
1:1A:1501:C:O4'	3:1D:100:GLY:HA2	2.21	0.41
1:1A:1622:G:C2	1:1A:1623:G:C8	3.09	0.41
1:1A:2079:U:O3'	23:11:35:THR:OG1	2.36	0.41
1:1A:2141:G:C6	1:1A:2142:C:C2	3.09	0.41
1:1A:2820:A:C8	4:1E:109:LYS:HE2	2.56	0.41
2:1B:11:C:OP2	22:10:72:ARG:NH2	2.37	0.41
6:1G:18:GLU:HG3	6:1G:22:ARG:HD2	2.03	0.41
7:1H:56:SER:OG	7:1H:57:ASP:N	2.52	0.41
8:1I:38:LEU:H	8:1I:38:LEU:CD2	2.34	0.41
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	2.02	0.41
11:1P:63:PRO:HD3	30:18:27:THR:HG22	2.03	0.41
16:1U:54:LYS:H	16:1U:54:LYS:HG3	1.73	0.41
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	2.03	0.41
22:10:11:ARG:HG2	61:10:208:HOH:O	2.20	0.41
26:14:44:THR:OG1	26:14:47:GLN:HB2	2.20	0.41
30:18:23:VAL:HG13	30:18:47:LYS:HB3	2.03	0.41
32:1a:175:C:H2'	32:1a:176:C:C6	2.56	0.41
32:1a:195:A:H1'	32:1a:222:U:O2'	2.21	0.41
32:1a:472:A:H2'	32:1a:473:G:O4'	2.20	0.41
32:1a:620:C:H2'	32:1a:621:A:O4'	2.21	0.41
32:1a:1054:C:C5	54:1w:34:G:H1'	2.56	0.41
32:1a:1151:A:O4'	41:1j:39:PRO:HB2	2.21	0.41
32:1a:1279:A:H4'	32:1a:1281:U:H5	1.86	0.41
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.56	0.41
33:1b:42:ILE:HD12	33:1b:203:GLY:HA2	2.02	0.41
33:1b:80:ILE:HD12	33:1b:211:ILE:HG22	2.03	0.41
33:1b:131:PRO:O	33:1b:135:GLN:N	2.52	0.41
36:1e:57:LYS:HG2	36:1e:61:TYR:CE2	2.56	0.41
38:1g:144:MET:HE2	38:1g:144:MET:HB3	1.88	0.41
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.85	0.41
44:1m:15:VAL:O	44:1m:19:LEU:HD22	2.21	0.41
47:1p:19:ILE:HG22	47:1p:36:ILE:HG13	2.03	0.41
1:2A:655:A:H8	1:2A:656:G:O4'	2.04	0.41
1:2A:815:C:H2'	1:2A:816:C:H6	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:904:C:H4'	21:2Z:169:GLU:OE2	2.21	0.41
1:2A:1508:A:H4'	1:2A:1509(A):A:N7	2.35	0.41
1:2A:1720:U:H2'	1:2A:1721:G:O4'	2.20	0.41
1:2A:1816:G:H3'	3:2D:62:TYR:CE1	2.56	0.41
1:2A:2112:G:C2	1:2A:2113:U:H1'	2.56	0.41
1:2A:2115:G:H5'	1:2A:2116:G:OP1	2.21	0.41
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.35	0.41
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.86	0.41
1:2A:2207:G:H3'	1:2A:2208:A:H5''	2.02	0.41
1:2A:2584:U:H2'	1:2A:2585:U:C6	2.55	0.41
2:2B:34:U:OP1	6:2G:2:PRO:HG3	2.21	0.41
4:2E:11:MET:HE2	4:2E:11:MET:HB3	1.98	0.41
5:2F:176:LEU:HD23	5:2F:176:LEU:HA	1.88	0.41
6:2G:173:LEU:HB3	6:2G:178:PHE:CG	2.56	0.41
11:2P:6:LEU:HA	11:2P:6:LEU:HD23	1.71	0.41
13:2R:13:HIS:CD2	13:2R:13:HIS:H	2.39	0.41
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.46	0.41
21:2Z:97:GLU:HA	21:2Z:126:VAL:O	2.21	0.41
30:28:15:LYS:HB3	30:28:23:VAL:HG12	2.03	0.41
32:2a:336:C:H2'	32:2a:337:C:C6	2.56	0.41
32:2a:382:A:H2'	32:2a:383:A:C8	2.56	0.41
32:2a:407:G:OP1	35:2d:115:ARG:HD3	2.21	0.41
32:2a:598:U:H4'	39:2h:94:TYR:CG	2.56	0.41
32:2a:748:C:H4'	32:2a:749:C:O5'	2.21	0.41
32:2a:975:A:H5'	32:2a:975:A:H8	1.86	0.41
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.55	0.41
32:2a:1130:A:H2'	32:2a:1131:G:H8	1.86	0.41
32:2a:1256:A:H61	32:2a:1278:U:C2'	2.34	0.41
32:2a:1256:A:N1	32:2a:1278:U:H1'	2.36	0.41
32:2a:1258:G:O2'	32:2a:1259:C:H5'	2.20	0.41
32:2a:1281:U:O2'	32:2a:1282:C:H5'	2.21	0.41
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.56	0.41
32:2a:1388:C:H2'	32:2a:1389:C:C6	2.56	0.41
33:2b:16:HIS:C	33:2b:18:GLY:N	2.79	0.41
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.21	0.41
34:2c:120:VAL:HG13	34:2c:133:ALA:HB1	2.03	0.41
34:2c:149:ALA:HA	34:2c:201:TYR:O	2.21	0.41
36:2e:36:ASP:O	36:2e:38:GLN:N	2.48	0.41
38:2g:74:GLU:HG2	38:2g:91:VAL:HG22	2.03	0.41
39:2h:39:LEU:HD13	39:2h:39:LEU:HA	1.86	0.41
44:2m:50:GLU:O	44:2m:54:VAL:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:90:LEU:HA	44:2m:93:ARG:HD2	2.03	0.41
48:2q:45:HIS:O	48:2q:47:PRO:HD3	2.21	0.41
49:2r:22:VAL:HG23	49:2r:55:ARG:O	2.21	0.41
51:2t:10:LEU:HB3	51:2t:12:ALA:H	1.86	0.41
1:1A:1289:C:H2'	1:1A:1290:C:C6	2.56	0.41
1:1A:2389:G:H5''	1:1A:2390:U:O4'	2.21	0.41
1:1A:2691:C:O3'	1:1A:2871:C:H4'	2.20	0.41
16:1U:104:GLN:NE2	16:1U:105:VAL:HG23	2.32	0.41
30:18:62:LEU:HB3	30:18:65:GLU:CG	2.51	0.41
32:1a:234:C:H5''	48:1q:70:ARG:HH21	1.86	0.41
32:1a:901:A:C5	32:1a:902:G:H1'	2.56	0.41
32:1a:1004:A:C5'	32:1a:1024:G:H22	2.34	0.41
32:1a:1007:C:H2'	32:1a:1008:C:H6	1.86	0.41
32:1a:1503:A:N3	53:1v:13:A:C6	2.89	0.41
33:1b:74:LYS:H	33:1b:74:LYS:HG3	1.52	0.41
40:1i:5:TYR:HB2	40:1i:18:PHE:CE1	2.56	0.41
51:1t:99:LEU:HA	51:1t:100:ILE:O	2.21	0.41
1:2A:321:G:H4'	5:2F:165:ARG:O	2.21	0.41
1:2A:443:A:N7	5:2F:45:ARG:HG2	2.36	0.41
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.45	0.41
1:2A:887:A:O2'	1:2A:888:C:H3'	2.21	0.41
1:2A:1260:G:C6	1:2A:1261:C:C4	3.09	0.41
2:2B:58:A:H2'	2:2B:59:A:O4'	2.21	0.41
6:2G:11:TYR:OH	6:2G:16:ARG:HD3	2.20	0.41
10:2O:120:GLU:HG2	10:2O:122:LEU:HG	2.03	0.41
12:2Q:3:MET:HE3	12:2Q:3:MET:HB2	1.97	0.41
18:2W:34:ASN:HA	18:2W:37:ARG:NH1	2.36	0.41
21:2Z:27:VAL:HG12	21:2Z:85:HIS:HE1	1.86	0.41
21:2Z:151:HIS:HB3	21:2Z:152:ALA:H	1.65	0.41
24:22:53:LEU:HD23	24:22:53:LEU:HA	1.81	0.41
32:2a:608:A:H2'	32:2a:609:A:O4'	2.21	0.41
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.20	0.41
32:2a:1307:U:H2'	32:2a:1308:U:C6	2.56	0.41
40:2i:47:LEU:HB3	40:2i:50:LEU:HD21	2.02	0.41
44:2m:117:VAL:HG22	44:2m:118:ALA:H	1.85	0.41
47:2p:5:ARG:NH2	47:2p:28:ARG:HA	2.35	0.41
1:1A:284:U:H2'	1:1A:285:C:C6	2.56	0.40
1:1A:300:A:H2'	1:1A:334:C:H1'	2.03	0.40
1:1A:302:C:H2'	1:1A:303:U:C6	2.56	0.40
1:1A:729:G:OP1	3:1D:10:THR:OG1	2.36	0.40
1:1A:1091:G:H2'	1:1A:1092:C:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2577:A:OP2	27:15:3:LYS:NZ	2.43	0.40
8:1I:114:LEU:HD13	8:1I:130:TYR:HD1	1.86	0.40
24:12:51:ARG:HD3	24:12:55:ARG:NH1	2.36	0.40
26:14:28:LYS:HA	26:14:29:PRO:HD3	1.90	0.40
32:1a:128:G:H4'	48:1q:3:LYS:HG3	2.03	0.40
32:1a:271:C:H2'	32:1a:272:C:H6	1.86	0.40
32:1a:1004:A:H5'	32:1a:1024:G:H22	1.86	0.40
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.56	0.40
32:1a:1228:C:OP1	44:1m:115:LYS:NZ	2.49	0.40
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.56	0.40
32:1a:1505:G:O2'	53:1v:13:A:O2'	2.33	0.40
33:1b:76:GLN:H	33:1b:76:GLN:CD	2.29	0.40
33:1b:84:GLU:O	33:1b:219:VAL:HG21	2.20	0.40
34:1c:6:HIS:HA	34:1c:7:PRO:HD3	1.98	0.40
34:1c:19:GLU:HG2	34:1c:54:ARG:CZ	2.51	0.40
43:1l:7:ILE:O	43:1l:11:VAL:HG12	2.21	0.40
50:1s:48:THR:HG22	50:1s:61:TYR:HD1	1.85	0.40
1:2A:117:G:C6	1:2A:119:A:C6	3.09	0.40
1:2A:702:G:C2	1:2A:731:C:C2	3.08	0.40
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.46	0.40
1:2A:1466:G:O3'	1:2A:1546:C:O2'	2.38	0.40
1:2A:1508:A:H5'	1:2A:1509(A):A:C8	2.56	0.40
1:2A:1889:A:N1	1:2A:2234:G:H1'	2.36	0.40
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.36	0.40
1:2A:2712:U:H2'	1:2A:2714:G:H5''	2.02	0.40
2:2B:24:G:N7	2:2B:56:G:H2'	2.36	0.40
4:2E:52:LEU:HA	4:2E:53:PRO:HD3	1.93	0.40
4:2E:127:ASP:OD2	61:2E:401:HOH:O	2.21	0.40
5:2F:116:ASP:HA	5:2F:119:ARG:NH2	2.36	0.40
5:2F:152:GLU:HA	5:2F:190:GLU:OE1	2.20	0.40
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	2.02	0.40
21:2Z:15:PRO:HA	21:2Z:18:LEU:HB2	2.03	0.40
24:22:1:MET:HE2	24:22:6:VAL:HG23	2.03	0.40
26:24:68:ARG:NE	26:24:68:ARG:HA	2.31	0.40
33:2b:93:VAL:HG11	33:2b:97:TRP:CE3	2.55	0.40
33:2b:215:LEU:O	33:2b:219:VAL:HG12	2.21	0.40
35:2d:112:VAL:HG22	35:2d:116:GLN:HE22	1.85	0.40
55:2x:37:A:H2'	55:2x:38:A:O4'	2.20	0.40
1:1A:1011:G:OP1	16:1U:77:SER:OG	2.31	0.40
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.56	0.40
1:1A:1540:U:H2'	1:1A:1541:G:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2123:G:H1	1:1A:2175:C:H42	1.68	0.40
1:1A:2328:A:H2'	1:1A:2329:G:H8	1.83	0.40
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.36	0.40
1:1A:2741:A:H2'	1:1A:2742:C:O4'	2.20	0.40
11:1P:114:ILE:HG13	11:1P:130:PHE:CE1	2.56	0.40
12:1Q:51:ARG:HG3	12:1Q:66:ILE:HD11	2.02	0.40
15:1T:108:ARG:HG3	15:1T:109:GLU:N	2.36	0.40
16:1U:8:VAL:HG23	16:1U:11:ARG:HH21	1.87	0.40
26:14:61:ARG:NH2	50:1s:41:VAL:HG12	2.36	0.40
32:1a:625:G:H2'	32:1a:626:U:H6	1.85	0.40
32:1a:838:G:H1	32:1a:848:C:N4	2.20	0.40
35:1d:101:LEU:HG	35:1d:121:VAL:HG21	2.02	0.40
35:1d:102:ASP:OD1	35:1d:103:ASN:N	2.54	0.40
36:1e:79:GLU:HA	36:1e:91:LEU:O	2.20	0.40
36:1e:79:GLU:HB3	36:1e:92:LYS:HD3	2.03	0.40
49:1r:54:ARG:H	49:1r:54:ARG:HG3	1.74	0.40
54:1w:67:C:H2'	54:1w:68:C:O4'	2.21	0.40
54:1y:34:G:H2'	54:1y:35:A:H1'	2.03	0.40
1:2A:11:G:C2'	1:2A:12:U:H5'	2.51	0.40
1:2A:614:U:H5'	1:2A:614(C):A:N6	2.36	0.40
1:2A:752:A:H3'	29:27:1:MET:HE1	2.02	0.40
1:2A:1357:U:H2'	1:2A:1358:G:O4'	2.20	0.40
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.56	0.40
1:2A:2393:A:H5''	11:2P:63:PRO:HB3	2.04	0.40
2:2B:40:U:O2'	2:2B:43:C:OP2	2.35	0.40
2:2B:42:C:O2	6:2G:93:THR:N	2.45	0.40
3:2D:77:ALA:HA	3:2D:97:TYR:HA	2.04	0.40
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	2.03	0.40
32:2a:397:A:N3	32:2a:397:A:H3'	2.36	0.40
32:2a:403:C:N4	61:2a:1959:HOH:O	2.54	0.40
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.56	0.40
33:2b:20:GLU:HB2	33:2b:190:THR:OG1	2.21	0.40
33:2b:27:LYS:O	33:2b:194:PRO:HG2	2.21	0.40
33:2b:63:MET:O	33:2b:64:ARG:HD3	2.22	0.40
38:2g:50:ILE:HG22	38:2g:125:MET:HG3	2.03	0.40
51:2t:62:LEU:HD23	51:2t:62:LEU:HA	1.90	0.40
54:2w:59:U:C4	54:2w:60:U:C4	3.10	0.40
55:2x:53:G:H2'	55:2x:54:5MU:H6	1.85	0.40
1:1A:271(G):C:H2'	1:1A:271(H):G:C8	2.57	0.40
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.22	0.40
1:1A:1744:C:H2'	1:1A:1745:C:C6	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1767:C:O2'	1:1A:1768:U:H5'	2.20	0.40
1:1A:2447:G:N2	1:1A:2450:A:OP2	2.54	0.40
32:1a:28:G:O2'	32:1a:296:U:OP1	2.36	0.40
32:1a:983:A:H5'	32:1a:984:C:OP2	2.21	0.40
32:1a:1166:G:N2	32:1a:1170:A:OP2	2.54	0.40
32:1a:1457:G:H5''	51:1t:35:THR:HG21	2.02	0.40
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.56	0.40
32:1a:1530:G:OP1	32:1a:1530:G:H4'	2.21	0.40
33:1b:119:GLU:O	33:1b:123:ALA:HB2	2.21	0.40
33:1b:169:LYS:O	33:1b:169:LYS:HD3	2.21	0.40
34:1c:44:GLU:HA	34:1c:52:LEU:HD23	2.04	0.40
36:1e:91:LEU:HD12	36:1e:91:LEU:HA	1.94	0.40
38:1g:67:GLU:HA	38:1g:70:LYS:HD2	2.04	0.40
39:1h:23:SER:HA	39:1h:61:VAL:O	2.20	0.40
40:1i:82:ALA:HB1	40:1i:96:LEU:HD11	2.02	0.40
42:1k:70:LYS:HE3	42:1k:70:LYS:HB2	1.96	0.40
45:1n:46:GLU:O	45:1n:50:LYS:HG3	2.21	0.40
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.86	0.40
54:1y:55:PSU:C4	54:1y:57:G:H5'	2.56	0.40
1:2A:176:G:O2'	1:2A:177:G:H5'	2.21	0.40
1:2A:407:G:H2'	1:2A:408:G:C8	2.57	0.40
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.36	0.40
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.56	0.40
3:2D:29:PRO:HA	3:2D:83:GLU:OE1	2.21	0.40
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.80	0.40
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.57	0.40
7:2H:70:THR:HA	7:2H:73:ALA:HB3	2.03	0.40
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.21	0.40
13:2R:79:LEU:HA	13:2R:83:ILE:HD12	2.03	0.40
32:2a:345:C:H4'	32:2a:346:G:O5'	2.20	0.40
32:2a:922:G:N3	32:2a:1398:A:H2	2.20	0.40
32:2a:1065:U:H1'	32:2a:1066:C:OP2	2.20	0.40
32:2a:1073:U:H2'	32:2a:1074:G:C8	2.57	0.40
36:2e:102:ALA:HB1	36:2e:106:PRO:HB2	2.03	0.40
49:2r:84:LYS:HE2	49:2r:84:LYS:HB2	1.94	0.40
54:2w:21:A:HO2'	54:2w:22:G:P	2.44	0.40
1:1A:11:G:H2'	1:1A:12:U:H5'	2.03	0.40
1:1A:278:A:OP2	1:1A:278:A:H8	2.05	0.40
1:1A:960:A:C8	1:1A:962:G:C8	3.10	0.40
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.21	0.40
1:1A:2107:C:N4	1:1A:2182:G:H1	2.14	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2175:C:H2'	1:1A:2176:A:O4'	2.22	0.40
1:1A:2206:G:H8	1:1A:2207:G:N7	2.19	0.40
2:1B:40:U:H2'	26:14:2:LYS:HE3	2.03	0.40
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.41	0.40
7:1H:3:ARG:NH2	7:1H:5:GLY:H	2.19	0.40
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.57	0.40
9:1N:91:LEU:HD23	9:1N:91:LEU:HA	1.88	0.40
27:15:8:LYS:O	27:15:9:LYS:HD2	2.22	0.40
31:19:27:CYS:SG	31:19:28:GLU:N	2.94	0.40
32:1a:36:C:OP1	43:1l:123:LYS:NZ	2.32	0.40
32:1a:826:C:H4'	39:1h:12:ARG:HG2	2.04	0.40
33:1b:44:LEU:HA	33:1b:47:THR:OG1	2.22	0.40
33:1b:93:VAL:HG11	33:1b:97:TRP:CD1	2.56	0.40
37:1f:19:LEU:HD11	37:1f:59:TYR:CE1	2.57	0.40
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	2.02	0.40
48:1q:87:LYS:HA	48:1q:87:LYS:HD2	1.86	0.40
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.35	0.40
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.22	0.40
1:2A:1388:G:H2'	1:2A:1389:G:H8	1.86	0.40
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.20	0.40
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.56	0.40
1:2A:2203:U:H2'	1:2A:2205:C:H6	1.86	0.40
1:2A:2489:G:O2'	1:2A:2490:G:H5'	2.22	0.40
4:2E:119:ARG:HG2	4:2E:120:TRP:CD1	2.56	0.40
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	2.03	0.40
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.56	0.40
17:2V:71:LEU:HA	17:2V:71:LEU:HD23	1.78	0.40
32:2a:109:A:H2'	32:2a:326:G:N2	2.36	0.40
32:2a:303:A:O2'	32:2a:555:C:H4'	2.21	0.40
32:2a:328:C:H4'	32:2a:329:A:H5'	2.04	0.40
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.21	0.40
41:2j:6:ILE:HG12	41:2j:98:ILE:HG22	2.04	0.40
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.79	0.40
44:2m:16:ASP:OD1	44:2m:17:VAL:N	2.52	0.40
48:2q:5:VAL:HA	48:2q:59:ILE:O	2.21	0.40
54:2y:8:4SU:O4'	54:2y:48:C:O2'	2.32	0.40
1:1A:570:G:H2'	1:1A:2030:A:C5	2.57	0.40
1:1A:1094:U:H2'	1:1A:1095:A:H8	1.86	0.40
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.85	0.40
1:1A:2467:C:O2	12:1Q:124:LYS:NZ	2.52	0.40
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.56	0.40
1:1A:2727:G:O3'	10:1O:70:LYS:HE2	2.22	0.40
24:12:44:LEU:HD12	24:12:44:LEU:HA	1.90	0.40
32:1a:538:G:H5''	43:1l:114:LYS:HB2	2.04	0.40
32:1a:909:A:H2'	32:1a:910:C:O4'	2.21	0.40
32:1a:1129:C:O2	32:1a:1130:A:N6	2.44	0.40
32:1a:1292:U:H5'	40:1i:38:GLN:OE1	2.22	0.40
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.56	0.40
32:1a:1424:C:H2'	32:1a:1425:U:O4'	2.21	0.40
33:1b:21:ARG:HB3	33:1b:39:ILE:HG13	2.03	0.40
33:1b:105:PHE:HE1	33:1b:155:LEU:HG	1.86	0.40
33:1b:154:LEU:HD12	33:1b:154:LEU:HA	1.94	0.40
36:1e:72:GLN:O	36:1e:75:THR:HG22	2.22	0.40
44:1m:3:ARG:HD3	44:1m:4:ILE:HG22	2.04	0.40
54:1w:9:A:O2'	54:1w:10:G:N7	2.54	0.40
54:1y:40:C:H2'	54:1y:41:C:C6	2.57	0.40
1:2A:582:G:OP2	61:2A:3943:HOH:O	2.22	0.40
1:2A:924:C:H2'	1:2A:925:C:C6	2.56	0.40
1:2A:940:G:N3	1:2A:1191:G:H4'	2.37	0.40
1:2A:1035:U:H5''	7:2H:59:ARG:HD3	2.03	0.40
1:2A:1360:A:OP2	61:2A:3946:HOH:O	2.22	0.40
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.52	0.40
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.57	0.40
1:2A:2406:U:OP2	1:2A:2406:U:H2'	2.21	0.40
8:2I:29:TYR:HD2	8:2I:30:LEU:HD23	1.87	0.40
9:2N:16:ILE:O	9:2N:54:VAL:HA	2.21	0.40
12:2Q:57:HIS:C	12:2Q:59:ARG:H	2.29	0.40
32:2a:630:G:H2'	32:2a:631:G:C8	2.57	0.40
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	2.02	0.40
32:2a:1350:A:C2	32:2a:1351:U:C2	3.10	0.40
51:2t:54:LYS:HB3	51:2t:54:LYS:HE3	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
3	1D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	34
4	2E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	34
5	1F	200/210 (95%)	192 (96%)	7 (4%)	1 (0%)	24	34
5	2F	200/210 (95%)	189 (94%)	9 (4%)	2 (1%)	12	17
6	1G	179/182 (98%)	165 (92%)	12 (7%)	2 (1%)	11	15
6	2G	179/182 (98%)	154 (86%)	21 (12%)	4 (2%)	5	5
7	1H	172/180 (96%)	161 (94%)	11 (6%)	0	100	100
7	2H	172/180 (96%)	156 (91%)	16 (9%)	0	100	100
8	1I	144/148 (97%)	132 (92%)	12 (8%)	0	100	100
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	18	25
9	1N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	25
9	2N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	25
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	22
11	1P	147/150 (98%)	136 (92%)	7 (5%)	4 (3%)	4	3
11	2P	147/150 (98%)	131 (89%)	12 (8%)	4 (3%)	4	3
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	6	7
15	1T	129/146 (88%)	119 (92%)	9 (7%)	1 (1%)	16	22
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	17
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	106 (96%)	3 (3%)	1 (1%)	14	20
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	125 (84%)	20 (14%)	3 (2%)	6	6
21	2Z	156/206 (76%)	122 (78%)	29 (19%)	5 (3%)	3	2
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	75 (93%)	6 (7%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	15
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	15
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	53 (79%)	12 (18%)	2 (3%)	3	2
26	24	67/71 (94%)	51 (76%)	15 (22%)	1 (2%)	8	10
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	193 (84%)	28 (12%)	8 (4%)	3	1
33	2b	229/256 (90%)	185 (81%)	38 (17%)	6 (3%)	4	3
34	1c	204/239 (85%)	186 (91%)	15 (7%)	3 (2%)	8	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	2c	204/239 (85%)	172 (84%)	30 (15%)	2 (1%)	12	17
35	1d	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	24	34
35	2d	206/209 (99%)	190 (92%)	14 (7%)	2 (1%)	12	17
36	1e	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	5	5
36	2e	146/162 (90%)	135 (92%)	9 (6%)	2 (1%)	9	11
37	1f	98/101 (97%)	89 (91%)	9 (9%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	18	25
38	2g	153/156 (98%)	134 (88%)	17 (11%)	2 (1%)	9	12
39	1h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
39	2h	135/138 (98%)	121 (90%)	14 (10%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	16	22
40	2i	125/128 (98%)	108 (86%)	17 (14%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	10 (10%)	4 (4%)	2	1
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	3	2
42	1k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	6	7
42	2k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	14	20
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
44	1m	121/126 (96%)	110 (91%)	10 (8%)	1 (1%)	16	22
44	2m	120/126 (95%)	102 (85%)	17 (14%)	1 (1%)	16	22
45	1n	58/61 (95%)	56 (97%)	1 (2%)	1 (2%)	7	8
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	13
46	2o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
47	1p	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	9	12
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
48	1q	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
48	2q	97/105 (92%)	89 (92%)	5 (5%)	3 (3%)	3	2
49	1r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	10
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	1s	81/93 (87%)	72 (89%)	7 (9%)	2 (2%)	4	4
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	1
51	2t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	5	5
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11368/12128 (94%)	10445 (92%)	822 (7%)	101 (1%)	14	20

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
21	1Z	53	ILE
33	1b	17	PHE
34	1c	66	VAL
40	1i	54	ASP
41	1j	55	LYS
41	1j	56	HIS
44	1m	67	GLU
5	2F	130	ALA
6	2G	51	ARG
8	2I	10	GLU
11	2P	29	LYS
21	2Z	144	LEU
33	2b	17	PHE
42	2k	49	GLY
44	2m	67	GLU
11	1P	44	GLY
15	1T	37	GLY
17	1V	79	VAL
26	14	49	PHE
26	14	62	ARG
33	1b	106	LYS
34	1c	107	GLN
38	1g	52	GLU
50	1s	81	ARG
51	1t	47	GLY
6	2G	42	GLY
6	2G	43	LEU
17	2V	79	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	24	49	PHE
33	2b	21	ARG
38	2g	55	GLY
38	2g	80	VAL
41	2j	79	ARG
48	2q	68	ARG
21	1Z	153	SER
23	1l	3	LYS
33	1b	126	GLU
35	1d	173	TRP
36	1e	86	ALA
41	1j	78	ASN
42	1k	49	GLY
51	1t	100	ILE
4	2E	52	LEU
9	2N	2	LYS
14	2S	84	GLN
21	2Z	52	SER
21	2Z	145	GLU
33	2b	20	GLU
33	2b	226	ARG
36	2e	77	PRO
36	2e	97	GLY
4	1E	52	LEU
6	1G	43	LEU
9	1N	2	LYS
11	1P	38	GLN
33	1b	20	GLU
33	1b	124	SER
34	1c	65	ALA
47	1p	81	ARG
51	1t	10	LEU
6	2G	84	LYS
11	2P	36	LYS
23	2l	3	LYS
41	2j	43	ARG
41	2j	78	ASN
48	2q	67	LYS
48	2q	81	ARG
51	2t	95	ALA
6	1G	124	SER
11	1P	45	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	156	LYS
33	1b	8	LYS
45	1n	60	SER
50	1s	27	GLU
5	2F	21	ALA
10	2O	29	ASN
11	2P	45	LEU
17	2V	53	GLU
18	2W	60	ASN
21	2Z	93	ASP
33	2b	150	SER
34	2c	91	LEU
34	2c	144	SER
35	2d	179	GLU
11	1P	29	LYS
36	1e	85	GLY
42	1k	105	VAL
49	1r	25	THR
14	2S	35	ILE
33	1b	231	GLU
46	1o	87	ILE
41	1j	77	PRO
33	2b	231	GLU
35	2d	5	ILE
36	1e	69	VAL
33	1b	38	GLY
51	1t	102	GLY
21	2Z	146	ILE
51	2t	47	GLY
11	2P	122	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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
3	1D	215/218 (99%)	206 (96%)	9 (4%)	26 40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2D	215/218 (99%)	203 (94%)	12 (6%)	19	29
4	1E	164/166 (99%)	152 (93%)	12 (7%)	13	18
4	2E	164/166 (99%)	152 (93%)	12 (7%)	13	18
5	1F	160/166 (96%)	139 (87%)	21 (13%)	4	4
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	10
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	11
6	2G	143/156 (92%)	124 (87%)	19 (13%)	4	4
7	1H	144/148 (97%)	134 (93%)	10 (7%)	14	20
7	2H	144/148 (97%)	126 (88%)	18 (12%)	4	4
8	1I	113/124 (91%)	91 (80%)	22 (20%)	1	1
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2	2
9	1N	118/119 (99%)	110 (93%)	8 (7%)	14	20
9	2N	118/119 (99%)	112 (95%)	6 (5%)	21	33
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	42
10	2O	100/100 (100%)	95 (95%)	5 (5%)	22	33
11	1P	115/116 (99%)	110 (96%)	5 (4%)	26	39
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	16
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13	18
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	20	30
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	12
13	2R	101/101 (100%)	96 (95%)	5 (5%)	22	33
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	15
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	5
15	1T	115/127 (91%)	106 (92%)	9 (8%)	11	16
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	9
16	1U	93/94 (99%)	91 (98%)	2 (2%)	45	64
16	2U	93/94 (99%)	92 (99%)	1 (1%)	65	79
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42	60
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	4
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	21
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	59
19	2X	77/78 (99%)	73 (95%)	4 (5%)	21	32
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	10	14
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	7
21	1Z	135/179 (75%)	125 (93%)	10 (7%)	13	17
21	2Z	137/179 (76%)	118 (86%)	19 (14%)	3	3
22	10	65/67 (97%)	62 (95%)	3 (5%)	24	36
22	20	65/67 (97%)	63 (97%)	2 (3%)	35	53
23	11	80/83 (96%)	77 (96%)	3 (4%)	29	44
23	21	80/83 (96%)	76 (95%)	4 (5%)	22	33
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	36
24	22	65/67 (97%)	62 (95%)	3 (5%)	24	36
25	13	51/52 (98%)	45 (88%)	6 (12%)	5	5
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	26
26	14	59/63 (94%)	50 (85%)	9 (15%)	3	2
26	24	53/63 (84%)	43 (81%)	10 (19%)	1	1
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	26
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	26
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	9
28	26	50/52 (96%)	46 (92%)	4 (8%)	11	15
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	4
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	9
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	29
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	45
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	55
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	55
33	1b	192/220 (87%)	159 (83%)	33 (17%)	2	1
33	2b	187/220 (85%)	146 (78%)	41 (22%)	1	1
34	1c	142/188 (76%)	126 (89%)	16 (11%)	5	6
34	2c	140/188 (74%)	127 (91%)	13 (9%)	8	10
35	1d	169/181 (93%)	150 (89%)	19 (11%)	6	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	2d	173/181 (96%)	156 (90%)	17 (10%)	7	9
36	1e	113/123 (92%)	97 (86%)	16 (14%)	3	3
36	2e	114/123 (93%)	97 (85%)	17 (15%)	3	2
37	1f	84/90 (93%)	77 (92%)	7 (8%)	10	14
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	7
38	1g	119/127 (94%)	102 (86%)	17 (14%)	3	3
38	2g	120/127 (94%)	108 (90%)	12 (10%)	7	9
39	1h	114/119 (96%)	110 (96%)	4 (4%)	32	48
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9	12
40	1i	90/99 (91%)	83 (92%)	7 (8%)	11	16
40	2i	89/99 (90%)	75 (84%)	14 (16%)	2	2
41	1j	66/92 (72%)	61 (92%)	5 (8%)	12	17
41	2j	69/92 (75%)	65 (94%)	4 (6%)	18	27
42	1k	82/99 (83%)	72 (88%)	10 (12%)	5	4
42	2k	83/99 (84%)	79 (95%)	4 (5%)	23	35
43	1l	96/108 (89%)	88 (92%)	8 (8%)	10	14
43	2l	96/108 (89%)	84 (88%)	12 (12%)	4	4
44	1m	93/101 (92%)	81 (87%)	12 (13%)	4	4
44	2m	92/101 (91%)	78 (85%)	14 (15%)	3	2
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17	25
45	2n	49/50 (98%)	47 (96%)	2 (4%)	27	41
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	23
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	33
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	2
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9	12
48	1q	94/97 (97%)	88 (94%)	6 (6%)	16	23
48	2q	94/97 (97%)	84 (89%)	10 (11%)	6	7
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14	20
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	3
50	1s	69/80 (86%)	66 (96%)	3 (4%)	26	39
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	1t	70/82 (85%)	61 (87%)	9 (13%)	4	4
51	2t	70/82 (85%)	65 (93%)	5 (7%)	13	19
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8463 (91%)	840 (9%)	9	11

All (840) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	106	ILE
3	1D	111	LEU
3	1D	142	VAL
3	1D	204	ILE
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
4	1E	7	VAL
4	1E	9	VAL
4	1E	12	THR
4	1E	13	ARG
4	1E	47	VAL
4	1E	59	VAL
4	1E	73	GLU
4	1E	87	GLU
4	1E	97	LYS
4	1E	116	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	9	ILE
5	1F	24	LEU
5	1F	27	GLU
5	1F	28	ILE
5	1F	43	LYS
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	127	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	132	VAL
5	1F	140	LEU
5	1F	144	LYS
5	1F	145	GLU
5	1F	157	VAL
5	1F	162	LEU
5	1F	168	ARG
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	5	VAL
6	1G	7	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	106	LEU
6	1G	109	VAL
6	1G	126	ASP
6	1G	133	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	149	VAL
6	1G	150	ASP
6	1G	159	VAL
7	1H	2	SER
7	1H	23	ARG
7	1H	45	VAL
7	1H	56	SER
7	1H	84	SER
7	1H	101	ARG
7	1H	116	GLU
7	1H	124	GLU
7	1H	127	GLU
7	1H	155	SER
8	1I	2	LYS
8	1I	10	GLU
8	1I	12	LEU
8	1I	15	VAL
8	1I	20	ASP
8	1I	27	ARG
8	1I	38	LEU
8	1I	41	GLU
8	1I	47	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1I	75	LEU
8	1I	77	LEU
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	102	SER
8	1I	108	THR
8	1I	109	ILE
8	1I	123	LEU
8	1I	129	THR
8	1I	136	VAL
8	1I	140	LEU
9	1N	1	MET
9	1N	5	VAL
9	1N	14	VAL
9	1N	28	THR
9	1N	46	VAL
9	1N	48	MET
9	1N	137	LYS
9	1N	140	VAL
10	1O	28	SER
10	1O	52	VAL
10	1O	106	LEU
10	1O	112	MET
11	1P	40	SER
11	1P	45	LEU
11	1P	95	VAL
11	1P	96	THR
11	1P	148	LEU
12	1Q	1	MET
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	56	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	112	GLU
12	1Q	138	ASP
13	1R	6	SER
13	1R	14	SER
13	1R	15	SER
13	1R	30	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1R	36	THR
13	1R	73	VAL
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	14	VAL
14	1S	36	TYR
14	1S	46	VAL
14	1S	69	VAL
14	1S	73	LEU
14	1S	110	LEU
15	1T	28	VAL
15	1T	49	VAL
15	1T	65	LYS
15	1T	82	LEU
15	1T	84	GLN
15	1T	96	ARG
15	1T	123	GLN
15	1T	125	ARG
15	1T	128	GLU
16	1U	8	VAL
16	1U	77	SER
17	1V	79	VAL
17	1V	100	ARG
18	1W	6	ILE
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	63	ASP
18	1W	96	ILE
19	1X	35	THR
19	1X	72	LYS
20	1Y	7	VAL
20	1Y	43	ASN
20	1Y	50	ARG
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	91	GLU
20	1Y	99	CYS
21	1Z	49	ARG
21	1Z	53	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	56	VAL
21	1Z	102	LEU
21	1Z	132	ASN
21	1Z	138	GLU
21	1Z	140	ASP
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	171	ILE
22	10	7	LEU
22	10	10	THR
22	10	49	LYS
23	11	46	LEU
23	11	59	THR
23	11	78	LYS
24	12	3	LEU
24	12	65	ASN
24	12	66	GLU
25	13	23	LEU
25	13	34	GLU
25	13	37	LEU
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	10	VAL
26	14	21	VAL
26	14	49	PHE
26	14	50	VAL
26	14	53	GLU
26	14	61	ARG
26	14	63	TYR
26	14	67	TYR
26	14	69	LYS
27	15	6	VAL
27	15	40	LYS
27	15	58	LEU
28	16	4	GLU
28	16	9	LEU
28	16	44	ARG
28	16	45	LYS
28	16	47	THR
29	17	1	MET
29	17	14	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	29	LYS
30	18	50	LEU
31	19	4	ARG
33	1b	7	VAL
33	1b	12	GLU
33	1b	17	PHE
33	1b	21	ARG
33	1b	27	LYS
33	1b	35	GLU
33	1b	39	ILE
33	1b	41	ILE
33	1b	54	THR
33	1b	61	LEU
33	1b	67	THR
33	1b	76	GLN
33	1b	80	ILE
33	1b	83	MET
33	1b	101	MET
33	1b	108	ILE
33	1b	111	ARG
33	1b	112	VAL
33	1b	126	GLU
33	1b	128	GLU
33	1b	143	GLU
33	1b	157	ARG
33	1b	160	ASP
33	1b	172	ILE
33	1b	185	ILE
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	217	ARG
33	1b	219	VAL
33	1b	223	ILE
33	1b	231	GLU
33	1b	236	TYR
34	1c	3	ASN
34	1c	28	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	46	GLU
34	1c	49	SER
34	1c	58	GLU
34	1c	64	VAL
34	1c	66	VAL
34	1c	82	GLU
34	1c	89	GLU
34	1c	101	LEU
34	1c	110	ASN
34	1c	112	SER
34	1c	165	THR
34	1c	179	ARG
34	1c	195	VAL
34	1c	198	VAL
35	1d	8	VAL
35	1d	19	LEU
35	1d	70	ILE
35	1d	91	SER
35	1d	115	ARG
35	1d	119	GLN
35	1d	122	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	144	ASP
35	1d	158	ILE
35	1d	170	VAL
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	186	LEU
35	1d	188	LEU
35	1d	194	LEU
36	1e	10	MET
36	1e	12	LEU
36	1e	18	ARG
36	1e	38	GLN
36	1e	41	VAL
36	1e	51	VAL
36	1e	56	GLN
36	1e	63	ARG
36	1e	64	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1e	67	VAL
36	1e	78	HIS
36	1e	79	GLU
36	1e	82	VAL
36	1e	91	LEU
36	1e	149	GLU
36	1e	151	LEU
37	1f	25	ILE
37	1f	46	ARG
37	1f	64	GLN
37	1f	72	VAL
37	1f	81	ILE
37	1f	89	MET
37	1f	92	LYS
38	1g	8	GLU
38	1g	12	LEU
38	1g	16	LEU
38	1g	32	ARG
38	1g	50	ILE
38	1g	59	LEU
38	1g	78	ARG
38	1g	94	ARG
38	1g	98	SER
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	114	ARG
38	1g	115	ARG
38	1g	118	VAL
38	1g	120	ILE
38	1g	135	VAL
39	1h	39	LEU
39	1h	51	VAL
39	1h	52	ASP
39	1h	56	LYS
40	1i	23	ASN
40	1i	25	LYS
40	1i	27	THR
40	1i	64	THR
40	1i	92	TYR
40	1i	96	LEU
40	1i	97	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1j	46	ARG
41	1j	66	ARG
41	1j	72	VAL
41	1j	92	THR
41	1j	96	ILE
42	1k	14	VAL
42	1k	18	ARG
42	1k	31	THR
42	1k	33	THR
42	1k	40	ILE
42	1k	48	ILE
42	1k	87	THR
42	1k	109	VAL
42	1k	114	VAL
42	1k	117	ASN
43	1l	11	VAL
43	1l	18	VAL
43	1l	36	VAL
43	1l	54	LYS
43	1l	58	VAL
43	1l	83	VAL
43	1l	86	ARG
43	1l	100	ILE
44	1m	4	ILE
44	1m	9	ILE
44	1m	17	VAL
44	1m	19	LEU
44	1m	25	ILE
44	1m	32	GLU
44	1m	43	THR
44	1m	49	THR
44	1m	70	LEU
44	1m	94	ARG
44	1m	109	THR
44	1m	117	VAL
45	1n	13	THR
45	1n	18	VAL
45	1n	22	THR
46	1o	6	GLU
46	1o	39	LEU
46	1o	47	LYS
46	1o	62	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	1o	87	ILE
47	1p	5	ARG
47	1p	8	ARG
47	1p	20	VAL
47	1p	27	LYS
47	1p	42	ARG
47	1p	45	THR
47	1p	53	VAL
47	1p	62	VAL
47	1p	72	ARG
47	1p	76	GLN
48	1q	5	VAL
48	1q	9	VAL
48	1q	15	MET
48	1q	25	ARG
48	1q	78	GLU
48	1q	85	VAL
49	1r	31	LEU
49	1r	46	GLU
49	1r	47	THR
49	1r	82	THR
50	1s	5	LEU
50	1s	12	ASP
50	1s	48	THR
51	1t	10	LEU
51	1t	13	LEU
51	1t	18	GLN
51	1t	24	LEU
51	1t	30	LYS
51	1t	31	SER
51	1t	62	LEU
51	1t	71	THR
51	1t	100	ILE
3	2D	3	VAL
3	2D	20	ASP
3	2D	27	THR
3	2D	37	LEU
3	2D	142	VAL
3	2D	173	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	260	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2D	270	ILE
3	2D	275	LYS
3	2D	276	LYS
4	2E	7	VAL
4	2E	9	VAL
4	2E	12	THR
4	2E	38	THR
4	2E	59	VAL
4	2E	73	GLU
4	2E	87	GLU
4	2E	97	LYS
4	2E	116	VAL
4	2E	119	ARG
4	2E	134	ILE
4	2E	181	LEU
5	2F	7	TYR
5	2F	11	VAL
5	2F	17	ARG
5	2F	18	ARG
5	2F	19	GLU
5	2F	20	LEU
5	2F	33	LEU
5	2F	70	THR
5	2F	110	LEU
5	2F	126	VAL
5	2F	157	VAL
5	2F	162	LEU
5	2F	165	ARG
5	2F	183	VAL
5	2F	196	LEU
6	2G	7	LEU
6	2G	28	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	47	LYS
6	2G	49	ASP
6	2G	51	ARG
6	2G	53	LEU
6	2G	70	VAL
6	2G	91	ARG
6	2G	130	ASN
6	2G	140	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	149	VAL
6	2G	150	ASP
6	2G	159	VAL
6	2G	160	VAL
6	2G	162	THR
6	2G	165	THR
6	2G	167	GLU
7	2H	3	ARG
7	2H	23	ARG
7	2H	43	VAL
7	2H	45	VAL
7	2H	46	GLU
7	2H	68	THR
7	2H	70	THR
7	2H	71	LEU
7	2H	76	VAL
7	2H	84	SER
7	2H	95	ARG
7	2H	103	LEU
7	2H	106	THR
7	2H	114	VAL
7	2H	122	THR
7	2H	127	GLU
7	2H	130	ARG
7	2H	133	VAL
8	2I	22	LYS
8	2I	38	LEU
8	2I	44	LEU
8	2I	50	ARG
8	2I	51	ILE
8	2I	58	LEU
8	2I	66	GLU
8	2I	68	LEU
8	2I	77	LEU
8	2I	87	LYS
8	2I	92	VAL
8	2I	102	SER
8	2I	117	GLU
8	2I	121	LYS
8	2I	127	VAL
8	2I	133	HIS
8	2I	142	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	2N	14	VAL
9	2N	28	THR
9	2N	38	HIS
9	2N	61	ARG
9	2N	62	VAL
9	2N	73	THR
10	2O	19	ILE
10	2O	66	LYS
10	2O	69	ILE
10	2O	77	ILE
10	2O	116	SER
11	2P	3	LEU
11	2P	7	ARG
11	2P	57	THR
11	2P	95	VAL
11	2P	96	THR
11	2P	119	GLU
11	2P	121	LYS
11	2P	135	LEU
11	2P	148	LEU
12	2Q	1	MET
12	2Q	56	ARG
12	2Q	85	LYS
12	2Q	106	VAL
12	2Q	110	THR
12	2Q	133	ARG
13	2R	6	SER
13	2R	36	THR
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	28	VAL
14	2S	36	TYR
14	2S	52	SER
14	2S	58	LEU
14	2S	62	LYS
14	2S	63	THR
14	2S	64	GLU
14	2S	75	GLU
14	2S	80	LEU
14	2S	110	LEU
15	2T	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	2T	18	ASP
15	2T	23	ARG
15	2T	34	VAL
15	2T	40	THR
15	2T	63	VAL
15	2T	65	LYS
15	2T	96	ARG
15	2T	99	LEU
15	2T	102	ILE
15	2T	124	ASP
16	2U	31	SER
17	2V	7	THR
17	2V	12	TYR
17	2V	18	LEU
17	2V	38	LEU
17	2V	46	VAL
17	2V	79	VAL
17	2V	85	LYS
17	2V	95	LEU
17	2V	98	GLU
17	2V	100	ARG
18	2W	11	ARG
18	2W	17	VAL
18	2W	60	ASN
18	2W	63	ASP
18	2W	65	LEU
19	2X	23	GLU
19	2X	35	THR
19	2X	81	VAL
19	2X	92	LEU
20	2Y	5	MET
20	2Y	8	LYS
20	2Y	11	ASP
20	2Y	14	LEU
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	88	LYS
20	2Y	90	LEU
20	2Y	99	CYS
21	2Z	5	LEU
21	2Z	24	LEU
21	2Z	31	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	52	SER
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	74	VAL
21	2Z	90	VAL
21	2Z	91	LEU
21	2Z	126	VAL
21	2Z	137	ILE
21	2Z	148	ASP
21	2Z	150	LEU
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	170	THR
21	2Z	171	ILE
22	20	49	LYS
22	20	74	ARG
23	21	35	THR
23	21	46	LEU
23	21	78	LYS
23	21	86	SER
24	22	1	MET
24	22	6	VAL
24	22	53	LEU
25	23	23	LEU
25	23	31	LEU
25	23	59	VAL
26	24	34	GLU
26	24	49	PHE
26	24	50	VAL
26	24	58	ARG
26	24	59	PHE
26	24	61	ARG
26	24	62	ARG
26	24	63	TYR
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	26	THR
27	25	59	GLU
28	26	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	26	19	ARG
28	26	34	LEU
28	26	48	VAL
29	27	24	THR
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	23	VAL
30	28	46	ARG
31	29	26	ILE
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	16	HIS
33	2b	23	ARG
33	2b	25	ASN
33	2b	37	ASN
33	2b	56	ARG
33	2b	58	ILE
33	2b	59	GLU
33	2b	61	LEU
33	2b	67	THR
33	2b	71	VAL
33	2b	76	GLN
33	2b	79	ASP
33	2b	81	VAL
33	2b	87	ARG
33	2b	94	ASN
33	2b	108	ILE
33	2b	111	ARG
33	2b	117	GLU
33	2b	127	ILE
33	2b	137	ARG
33	2b	138	LEU
33	2b	140	HIS
33	2b	142	LEU
33	2b	150	SER
33	2b	164	VAL
33	2b	165	VAL
33	2b	170	GLU
33	2b	184	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	185	ILE
33	2b	189	ASP
33	2b	208	ILE
33	2b	215	LEU
33	2b	217	ARG
33	2b	224	GLN
33	2b	229	VAL
33	2b	235	SER
33	2b	236	TYR
34	2c	15	THR
34	2c	35	GLU
34	2c	43	LEU
34	2c	47	LEU
34	2c	55	VAL
34	2c	58	GLU
34	2c	70	VAL
34	2c	105	GLU
34	2c	115	LEU
34	2c	152	ILE
34	2c	153	VAL
34	2c	182	ILE
34	2c	191	THR
35	2d	8	VAL
35	2d	17	VAL
35	2d	18	LYS
35	2d	34	GLU
35	2d	52	SER
35	2d	53	ASP
35	2d	59	ARG
35	2d	76	ARG
35	2d	119	GLN
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	158	ILE
35	2d	162	LEU
35	2d	188	LEU
35	2d	209	ARG
36	2e	13	ILE
36	2e	20	GLN
36	2e	24	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2e	25	ARG
36	2e	31	LEU
36	2e	32	VAL
36	2e	41	VAL
36	2e	43	LEU
36	2e	51	VAL
36	2e	55	VAL
36	2e	57	LYS
36	2e	67	VAL
36	2e	75	THR
36	2e	91	LEU
36	2e	101	ILE
36	2e	111	GLU
36	2e	115	VAL
37	2f	17	SER
37	2f	19	LEU
37	2f	21	LEU
37	2f	31	GLU
37	2f	37	VAL
37	2f	63	TYR
37	2f	69	GLU
37	2f	92	LYS
37	2f	93	SER
38	2g	9	VAL
38	2g	13	GLN
38	2g	15	ASP
38	2g	24	THR
38	2g	52	GLU
38	2g	53	LYS
38	2g	78	ARG
38	2g	79	ARG
38	2g	98	SER
38	2g	106	GLN
38	2g	139	GLU
38	2g	144	MET
39	2h	13	ILE
39	2h	17	THR
39	2h	26	VAL
39	2h	29	SER
39	2h	39	LEU
39	2h	51	VAL
39	2h	79	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	2h	112	LEU
39	2h	127	LEU
39	2h	137	VAL
40	2i	40	LEU
40	2i	41	VAL
40	2i	47	LEU
40	2i	50	LEU
40	2i	54	ASP
40	2i	56	LEU
40	2i	65	VAL
40	2i	86	VAL
40	2i	89	ASN
40	2i	99	LEU
40	2i	102	LEU
40	2i	103	THR
40	2i	107	ARG
40	2i	113	LYS
41	2j	13	HIS
41	2j	38	ILE
41	2j	44	VAL
41	2j	72	VAL
42	2k	14	VAL
42	2k	84	VAL
42	2k	98	LEU
42	2k	114	VAL
43	2l	11	VAL
43	2l	18	VAL
43	2l	22	SER
43	2l	36	VAL
43	2l	39	VAL
43	2l	42	THR
43	2l	43	VAL
43	2l	60	LEU
43	2l	62	SER
43	2l	83	VAL
43	2l	102	ARG
43	2l	123	LYS
44	2m	3	ARG
44	2m	8	GLU
44	2m	15	VAL
44	2m	19	LEU
44	2m	27	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	2m	47	ASP
44	2m	49	THR
44	2m	50	GLU
44	2m	53	VAL
44	2m	62	ASN
44	2m	65	LYS
44	2m	94	ARG
44	2m	103	THR
44	2m	106	ASN
45	2n	18	VAL
45	2n	33	VAL
46	2o	6	GLU
46	2o	25	THR
46	2o	39	LEU
46	2o	88	ARG
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG
47	2p	20	VAL
47	2p	67	THR
47	2p	74	LEU
48	2q	5	VAL
48	2q	13	ASP
48	2q	25	ARG
48	2q	53	LEU
48	2q	60	ILE
48	2q	63	ARG
48	2q	83	ASP
48	2q	85	VAL
48	2q	90	ILE
48	2q	96	GLU
49	2r	21	LYS
49	2r	31	LEU
49	2r	37	VAL
49	2r	54	ARG
49	2r	61	LYS
49	2r	82	THR
49	2r	84	LYS
49	2r	86	VAL
50	2s	12	ASP
50	2s	27	GLU
50	2s	30	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	2s	41	VAL
50	2s	45	VAL
50	2s	47	HIS
50	2s	58	VAL
50	2s	71	LEU
51	2t	9	ASN
51	2t	33	ILE
51	2t	50	GLU
51	2t	56	MET
51	2t	93	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	126	GLN
3	1D	166	GLN
4	1E	48	GLN
4	1E	180	ASN
5	1F	8	GLN
5	1F	160	ASN
6	1G	26	GLN
8	1I	11	ASN
8	1I	105	HIS
8	1I	133	HIS
9	1N	94	HIS
12	1Q	12	GLN
12	1Q	123	HIS
13	1R	50	HIS
13	1R	71	GLN
15	1T	58	ASN
15	1T	84	GLN
16	1U	81	HIS
16	1U	94	ASN
18	1W	111	HIS
19	1X	31	HIS
19	1X	82	GLN
21	1Z	34	ASN
21	1Z	73	GLN
21	1Z	121	HIS
22	10	17	GLN
25	13	32	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	47	GLN
33	1b	40	HIS
33	1b	78	GLN
33	1b	95	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	162	GLN
34	1c	170	GLN
34	1c	181	ASN
35	1d	45	GLN
35	1d	116	GLN
35	1d	123	HIS
35	1d	160	GLN
36	1e	20	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	57	GLN
37	1f	73	ASN
38	1g	13	GLN
38	1g	28	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	117	HIS
40	1i	124	GLN
41	1j	56	HIS
41	1j	69	ASN
42	1k	116	HIS
43	1l	99	HIS
44	1m	40	ASN
44	1m	77	ASN
46	1o	62	GLN
47	1p	13	HIS
47	1p	76	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
51	1t	16	HIS
3	2D	87	ASN
3	2D	126	GLN
4	2E	48	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	55	ASN
5	2F	75	HIS
6	2G	58	GLN
6	2G	108	ASN
6	2G	121	ASN
7	2H	74	ASN
7	2H	111	HIS
8	2I	133	HIS
8	2I	139	GLN
9	2N	56	ASN
9	2N	94	HIS
11	2P	70	GLN
12	2Q	12	GLN
12	2Q	57	HIS
13	2R	13	HIS
13	2R	50	HIS
13	2R	61	HIS
13	2R	71	GLN
14	2S	38	GLN
14	2S	68	GLN
14	2S	84	GLN
15	2T	84	GLN
16	2U	94	ASN
19	2X	31	HIS
20	2Y	43	ASN
21	2Z	55	HIS
22	20	35	ASN
26	24	20	ASN
26	24	46	GLN
33	2b	40	HIS
33	2b	76	GLN
33	2b	95	GLN
33	2b	135	GLN
34	2c	98	ASN
34	2c	162	GLN
34	2c	170	GLN
34	2c	181	ASN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	160	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2e	20	GLN
36	2e	141	GLN
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	73	GLN
40	2i	89	ASN
40	2i	117	HIS
41	2j	21	GLN
41	2j	69	ASN
42	2k	78	GLN
42	2k	116	HIS
42	2k	117	ASN
43	2l	99	HIS
44	2m	77	ASN
48	2q	16	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	18	GLN
51	2t	45	GLN
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	444 (15%)	30 (1%)
1	2A	2791/2915 (95%)	451 (16%)	26 (0%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	118/121 (97%)	24 (20%)	0
32	1a	1497/1521 (98%)	252 (16%)	0
32	2a	1501/1521 (98%)	278 (18%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	0	0
54	1w	71/76 (93%)	24 (33%)	0
54	1y	72/76 (94%)	30 (41%)	0
54	2w	67/76 (88%)	16 (23%)	0
54	2y	70/76 (92%)	23 (32%)	0
55	1x	74/77 (96%)	11 (14%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	2x	74/77 (96%)	5 (6%)	0
All	All	9342/9620 (97%)	1571 (16%)	56 (0%)

All (1571) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	12	U
1	1A	23	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	92	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	139(A)	G
1	1A	196	A
1	1A	197	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(J)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	327	G
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	440	G
1	1A	443	A
1	1A	444	C
1	1A	448	U
1	1A	454	A
1	1A	456	C
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	740	U
1	1A	746	A
1	1A	747	U
1	1A	764	A
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	892	G
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	899	A
1	1A	910	A
1	1A	919	G
1	1A	931	G
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1041	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1063	G
1	1A	1064	C
1	1A	1065	U
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1082	U
1	1A	1085	A
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1097	U
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1107	G
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1141	U
1	1A	1142	U
1	1A	1149	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1220	A
1	1A	1247	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1276	A
1	1A	1290	C
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1308	A
1	1A	1313	U
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1540	U
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1582	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1584	C
1	1A	1608	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1745	C
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A
1	1A	1847	A
1	1A	1848	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2093	G
1	1A	2099	U
1	1A	2109	U
1	1A	2110	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2120	G
1	1A	2121	G
1	1A	2122	U
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2138	C
1	1A	2141	G
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2149	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2161	C
1	1A	2164	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2218	U
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2449	U
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2498	C
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2601	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2613	U
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2663	G
1	1A	2689	U
1	1A	2691	C
1	1A	2702	U
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2739	U
1	1A	2758	A
1	1A	2762	G
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2825	C
1	1A	2835	A
1	1A	2872	G
1	1A	2873	A
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	12	C
2	1B	13	A
2	1B	15	A
2	1B	25	A
2	1B	35	U
2	1B	45	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	6	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	54	C
32	1a	61	G
32	1a	65	U
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	93	G
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	145	G
32	1a	151	A
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	217	C
32	1a	220	G
32	1a	222	U
32	1a	247	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	345	C
32	1a	347	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	374	A
32	1a	384	G
32	1a	388	G
32	1a	392	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	451	A
32	1a	452	A
32	1a	457	C
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	483	C
32	1a	485	G
32	1a	496	A
32	1a	498	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	607	A
32	1a	616	G
32	1a	627	G
32	1a	628	G
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	686	U
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	717	C
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	876	G
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1001	A
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1044	A
32	1a	1046	A
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A
32	1a	1158	C
32	1a	1159	U
32	1a	1160	G
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1263	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1383	C
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	1v	14	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
54	1w	7	A
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	36	A
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	56	C
54	1w	60	U
54	1w	62	C
54	1w	63	G
54	1w	68	C
54	1w	70	G
54	1w	73	A
54	1w	74	C
54	1w	75	C
55	1x	6	G
55	1x	9	G
55	1x	13	C
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	69	C
55	1x	70	G
54	1y	2	C
54	1y	6	G
54	1y	8	4SU
54	1y	13	C
54	1y	14	A
54	1y	19	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1y	20	U
54	1y	21	A
54	1y	23	A
54	1y	26	A
54	1y	34	G
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	G7M
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	53	G
54	1y	54	5MU
54	1y	56	C
54	1y	57	G
54	1y	58	A
54	1y	59	U
54	1y	61	C
54	1y	64	A
54	1y	65	G
54	1y	66	U
54	1y	70	G
54	1y	71	G
1	2A	8	A
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	265	A
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	311	A
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	391	G
1	2A	396	G
1	2A	405	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	411	G
1	2A	421	U
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	589	C
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	606	U
1	2A	607	U
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(D)	C
1	2A	652(U)	G
1	2A	654	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	957	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1021	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1036	G
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1117	G
1	2A	1118	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1155	A
1	2A	1170	G
1	2A	1171	G
1	2A	1195	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1461	G
1	2A	1466	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1774	C
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1861	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2141	G
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2150	U
1	2A	2151	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2182	G
1	2A	2185	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2268	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2303	G
1	2A	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2400	G
1	2A	2403	C
1	2A	2406	U
1	2A	2414	G
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2459	A
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2534	A
1	2A	2536	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2638	G
1	2A	2646	C
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2760	C
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2780	G
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2820	A
1	2A	2821	A
1	2A	2825	C
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	30	C
2	2B	32	C
2	2B	34	U
2	2B	41	U
2	2B	42	C
2	2B	45	A
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	73	A
2	2B	75	G
2	2B	85	G
2	2B	94	C
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	119	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	40	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	73	G
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	156	G
32	2a	163	C
32	2a	182	U
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	269	C
32	2a	287	U
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	342	C
32	2a	345	C
32	2a	346	G
32	2a	350	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	457	C
32	2a	461	A
32	2a	470	C
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	574	A
32	2a	575	G
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	601	C
32	2a	630	G
32	2a	633	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	756	C
32	2a	759	A
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	870	U
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	931	C
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	962	C
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	984	C
32	2a	990	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1031	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1032	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1045	C
32	2a	1046	A
32	2a	1050	G
32	2a	1053	G
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1108	G
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1126	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1159	U
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1204	A
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1268	A
32	2a	1270	C
32	2a	1273	G
32	2a	1276	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1311	G
32	2a	1320	C
32	2a	1321	C
32	2a	1323	G
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1357	A
32	2a	1358	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1380	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1492	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1519	MA6
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
54	2w	4	C
54	2w	5	G
54	2w	12	U
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	27	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	59	U
54	2w	66	U
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	19	G
55	2x	47	U
55	2x	68	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2y	15	G
54	2y	19	G
54	2y	24	G
54	2y	25	C
54	2y	27	G
54	2y	28	G
54	2y	30	G
54	2y	40	C
54	2y	45	U
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	54	5MU
54	2y	55	PSU
54	2y	56	C
54	2y	58	A
54	2y	60	U
54	2y	62	C
54	2y	64	A
54	2y	65	G
54	2y	68	C
54	2y	69	G
54	2y	70	G

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	573	G
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	827	U
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1067	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1275	A
1	1A	1379	A
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2629	A
1	2A	196	A
1	2A	228	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2406	U
1	2A	2689	U

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

86 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$
1	PSU	2A	2605	1	18,21,22	1.38	3 (16%)	21,30,33	2.06	5 (23%)
32	4OC	2a	1402	32,56	20,23,24	0.76	0	25,32,35	1.05	3 (12%)
32	2MG	1a	1207	32	23,26,27	1.24	2 (8%)	33,38,41	2.20	8 (24%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	1.99	8 (24%)
32	5MC	1a	1407	32	19,22,23	1.50	3 (15%)	26,32,35	1.09	3 (11%)
54	4SU	2w	8	54	18,21,22	1.79	4 (22%)	25,30,33	1.82	5 (20%)
1	PSU	1A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.00	3 (14%)
1	OMC	1A	1920	1	19,22,23	0.82	0	25,31,34	0.99	1 (4%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
55	5MU	1x	54	56,55	19,22,23	1.39	5 (26%)	27,32,35	2.24	8 (29%)
55	31H	1x	76	56,55,60	31,34,35	1.25	3 (9%)	35,47,50	1.83	10 (28%)
54	MIA	2w	37	54	24,27,32	2.13	5 (20%)	32,39,47	2.69	11 (34%)
54	G7M	1y	46	54	23,26,27	1.55	4 (17%)	34,39,42	1.83	4 (11%)
55	31H	2x	76	56,55	31,34,35	1.22	3 (9%)	35,47,50	2.10	11 (31%)
1	5MC	1A	1962	56,1	19,22,23	1.70	3 (15%)	26,32,35	1.22	3 (11%)
54	PSU	2y	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.94	3 (14%)
54	PSU	2w	55	56,54	18,21,22	1.39	2 (11%)	21,30,33	1.96	3 (14%)
32	PSU	1a	516	32	18,21,22	1.42	3 (16%)	21,30,33	2.01	6 (28%)
32	5MC	2a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.26	3 (11%)
54	5MU	2y	54	54	19,22,23	1.49	5 (26%)	27,32,35	1.73	5 (18%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.94	3 (14%)
55	PSU	1x	55	56,55	18,21,22	1.37	2 (11%)	21,30,33	1.99	3 (14%)
54	G7M	2w	46	54	23,26,27	1.52	3 (13%)	34,39,42	1.65	4 (11%)
32	5MC	1a	1404	32	19,22,23	1.83	3 (15%)	26,32,35	1.24	4 (15%)
1	8AH	1A	2503	56,1	22,26,27	1.65	5 (22%)	29,39,42	2.14	6 (20%)
32	G7M	2a	527	32,56	23,26,27	1.49	4 (17%)	34,39,42	1.65	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1939	1	19,22,23	1.39	4 (21%)	27,32,35	2.25	6 (22%)
55	4SU	1x	8	55	18,21,22	2.26	5 (27%)	25,30,33	1.58	6 (24%)
43	0TD	2l	92	43	8,9,10	4.63	1 (12%)	6,11,13	6.84	3 (50%)
54	5MU	1w	54	54	19,22,23	1.41	5 (26%)	27,32,35	2.04	7 (25%)
32	5MC	2a	1407	32,56	19,22,23	1.57	3 (15%)	26,32,35	1.16	3 (11%)
54	4SU	1y	8	54	18,21,22	1.83	4 (22%)	25,30,33	1.75	4 (16%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	21,30,33	2.04	4 (19%)
32	UR3	2a	1498	32	19,22,23	1.07	2 (10%)	26,32,35	1.72	3 (11%)
54	G7M	1w	46	54	23,26,27	1.58	3 (13%)	34,39,42	1.63	4 (11%)
1	OMG	1A	2251	56,55,1	23,26,27	1.29	3 (13%)	32,38,41	1.86	5 (15%)
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.00	3 (14%)
55	5MC	1x	32	55	19,22,23	1.85	3 (15%)	26,32,35	1.32	4 (15%)
1	2MU	1A	2552	56,1	19,22,24	1.32	4 (21%)	25,31,36	1.90	6 (24%)
1	2MU	2A	2552	56,1	19,22,24	1.31	4 (21%)	25,31,36	1.74	5 (20%)
43	0TD	1l	92	43	8,9,10	4.43	1 (12%)	6,11,13	6.07	3 (50%)
1	5MC	1A	1942	56,1	19,22,23	1.56	3 (15%)	26,32,35	1.20	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.39	4 (21%)	27,32,35	2.15	6 (22%)
54	5MU	1y	54	54	19,22,23	1.49	6 (31%)	27,32,35	1.79	5 (18%)
54	PSU	2w	32	54	18,21,22	1.39	2 (11%)	21,30,33	2.00	3 (14%)
54	G7M	2y	46	54	23,26,27	1.59	3 (13%)	34,39,42	1.77	4 (11%)
54	4SU	1w	8	54	18,21,22	1.84	4 (22%)	25,30,33	2.15	5 (20%)
54	PSU	1w	32	56,54	18,21,22	1.32	2 (11%)	21,30,33	1.97	3 (14%)
32	M2G	1a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.91	8 (24%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.88	6 (18%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	21,30,33	2.00	3 (14%)
54	4SU	2y	8	54	18,21,22	1.79	4 (22%)	25,30,33	2.46	5 (20%)
32	MA6	1a	1519	32	23,26,27	0.46	0	33,38,41	2.15	9 (27%)
32	5MC	1a	967	32	19,22,23	1.69	2 (10%)	26,32,35	1.09	2 (7%)
1	5MC	2A	1942	1	19,22,23	1.68	3 (15%)	26,32,35	1.17	3 (11%)
54	MIA	2y	37	54	21,24,32	1.62	4 (19%)	30,35,47	2.00	7 (23%)
54	PSU	1y	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.16	9 (27%)
1	5MU	2A	1939	56,1	19,22,23	1.47	5 (26%)	27,32,35	2.25	5 (18%)
32	5MC	2a	1404	32	19,22,23	1.74	3 (15%)	26,32,35	1.15	2 (7%)
1	OMG	2A	2251	55,1	23,26,27	1.23	3 (13%)	32,38,41	1.96	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	2605	56,1	18,21,22	1.34	2 (11%)	21,30,33	2.04	4 (19%)
54	PSU	2y	55	54	18,21,22	1.35	4 (22%)	21,30,33	2.00	5 (23%)
32	5MC	2a	967	32	19,22,23	1.59	3 (15%)	26,32,35	1.11	3 (11%)
32	2MG	2a	1207	32,56	23,26,27	1.23	2 (8%)	33,38,41	2.16	7 (21%)
55	4SU	2x	8	55	18,21,22	2.01	7 (38%)	25,30,33	1.38	5 (20%)
54	MIA	1y	37	54	21,24,32	1.62	4 (19%)	30,35,47	2.02	7 (23%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	21,30,33	2.03	4 (19%)
55	5MU	2x	54	55	19,22,23	1.40	6 (31%)	27,32,35	2.14	6 (22%)
1	OMC	2A	1920	1	19,22,23	0.81	0	25,31,34	0.95	1 (4%)
54	MIA	1w	37	54	28,31,32	2.28	6 (21%)	38,44,47	2.81	12 (31%)
54	5MU	2w	54	54	19,22,23	1.36	4 (21%)	27,32,35	1.90	7 (25%)
32	UR3	1a	1498	32	19,22,23	0.99	2 (10%)	26,32,35	1.75	5 (19%)
1	5MC	2A	1962	56,1	19,22,23	1.66	3 (15%)	26,32,35	1.08	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	0.99	1 (4%)
54	PSU	1y	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.88	3 (14%)
1	5MU	2A	1915	1	19,22,23	1.44	6 (31%)	27,32,35	2.20	5 (18%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.04	5 (23%)
1	PSU	1A	1911	1	18,21,22	1.46	2 (11%)	21,30,33	1.98	4 (19%)
1	8AH	2A	2503	56,1	22,26,27	1.75	5 (22%)	29,39,42	2.16	5 (17%)
54	PSU	2y	39	54	18,21,22	1.44	2 (11%)	21,30,33	1.66	3 (14%)
54	PSU	1y	32	54	18,21,22	1.32	2 (11%)	21,30,33	1.97	3 (14%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.03	9 (27%)
32	5MC	1a	1400	32	19,22,23	1.63	3 (15%)	26,32,35	1.24	2 (7%)
55	5MC	2x	32	55	19,22,23	1.67	3 (15%)	26,32,35	1.24	3 (11%)
32	G7M	1a	527	32,56	23,26,27	1.53	3 (13%)	34,39,42	1.65	5 (14%)

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
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
55	31H	1x	76	56,55,60	-	4/22/40/41	0/3/3/3
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
54	G7M	1y	46	54	-	1/7/25/26	0/3/3/3
55	31H	2x	76	56,55	-	4/22/40/41	0/3/3/3
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	56,54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
55	PSU	1x	55	56,55	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	8AH	1A	2503	56,1	-	1/7/25/26	0/3/3/3
32	G7M	2a	527	32,56	-	3/7/25/26	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	2/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
1	OMG	1A	2251	56,55,1	-	0/9/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
1	2MU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	5MC	1A	1942	56,1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	G7M	2y	46	54	-	2/7/25/26	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	6/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	0/9/27/28	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
54	MIA	1w	37	54	-	4/15/33/34	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	8AH	2A	2503	56,1	-	1/7/25/26	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	3/7/25/26	0/3/3/3

All (253) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.80	1.69	1.82
43	1l	92	0TD	CB-SB	-12.06	1.70	1.82
54	2w	37	MIA	C2-S10	-7.11	1.69	1.75
54	1w	37	MIA	C13-C14	6.91	1.53	1.32
55	1x	32	5MC	C5-C4	6.83	1.49	1.44
32	1a	1404	5MC	C5-C4	6.70	1.49	1.44
32	2a	1404	5MC	C5-C4	6.37	1.48	1.44
54	1w	37	MIA	C2-S10	-6.37	1.70	1.75
1	1A	1962	5MC	C5-C4	6.36	1.48	1.44
32	1a	967	5MC	C5-C4	6.18	1.48	1.44
1	2A	1962	5MC	C5-C4	6.11	1.48	1.44
55	2x	32	5MC	C5-C4	6.08	1.48	1.44
1	2A	1942	5MC	C5-C4	5.99	1.48	1.44
32	1a	1400	5MC	C5-C4	5.87	1.48	1.44
32	2a	1400	5MC	C5-C4	5.75	1.48	1.44
32	2a	967	5MC	C5-C4	5.68	1.48	1.44
55	1x	8	4SU	C4-N3	-5.57	1.31	1.37
1	1A	1942	5MC	C5-C4	5.56	1.48	1.44
32	2a	1407	5MC	C5-C4	5.38	1.48	1.44
32	1a	1407	5MC	C5-C4	5.37	1.48	1.44
54	1y	37	MIA	C5-C4	5.23	1.48	1.39
54	2y	37	MIA	C5-C4	5.18	1.48	1.39
54	2w	37	MIA	C5-C4	5.13	1.48	1.39
54	2y	8	4SU	C4-S4	-4.97	1.59	1.68
54	1w	8	4SU	C4-S4	-4.91	1.60	1.68
32	1a	527	G7M	C5-N7	-4.89	1.33	1.39
54	1w	46	G7M	C5-N7	-4.88	1.33	1.39
1	2A	2503	8AH	C5-C4	4.79	1.47	1.39
54	2y	46	G7M	C5-N7	-4.76	1.33	1.39
54	1w	37	MIA	C5-C4	4.71	1.47	1.39
54	2w	8	4SU	C4-S4	-4.69	1.60	1.68
54	1y	8	4SU	C4-S4	-4.60	1.60	1.68
55	1x	8	4SU	C4-S4	-4.59	1.60	1.68
54	1y	46	G7M	C5-N7	-4.59	1.33	1.39
55	2x	8	4SU	C4-N3	-4.56	1.32	1.37
54	2w	46	G7M	C5-N7	-4.44	1.34	1.39
1	1A	2503	8AH	C5-C4	4.28	1.46	1.39
32	2a	527	G7M	C5-N7	-4.25	1.34	1.39
55	1x	76	31H	C5-N7	-4.21	1.31	1.39
55	2x	8	4SU	C4-S4	-4.12	1.61	1.68
54	1y	39	PSU	C6-C5	4.01	1.39	1.35
1	1A	1911	PSU	C6-C5	3.99	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	55	PSU	C6-C5	3.98	1.39	1.35
54	2y	39	PSU	C6-C5	3.92	1.39	1.35
54	2w	39	PSU	C6-C5	3.92	1.39	1.35
54	2w	55	PSU	C6-C5	3.91	1.39	1.35
55	1x	8	4SU	C2-N3	-3.86	1.31	1.38
54	1y	55	PSU	C6-C5	3.81	1.39	1.35
54	2y	32	PSU	C6-C5	3.80	1.39	1.35
1	1A	2503	8AH	C4-N9	-3.78	1.33	1.38
54	2w	32	PSU	C6-C5	3.77	1.39	1.35
1	2A	2605	PSU	C6-C5	3.73	1.39	1.35
54	1y	8	4SU	C4-N3	-3.72	1.33	1.37
54	1y	46	G7M	C5-C4	3.65	1.47	1.38
55	2x	76	31H	C5-N7	-3.62	1.32	1.39
55	2x	55	PSU	C6-C5	3.60	1.39	1.35
32	2a	516	PSU	C6-C5	3.59	1.39	1.35
32	1a	516	PSU	C6-C5	3.58	1.39	1.35
1	2A	2503	8AH	C8-N7	3.55	1.36	1.31
54	1y	32	PSU	C6-C5	3.54	1.39	1.35
1	2A	1917	PSU	C6-C5	3.53	1.39	1.35
54	2y	46	G7M	C5-C4	3.49	1.47	1.38
1	1A	1917	PSU	C6-C5	3.42	1.39	1.35
55	1x	8	4SU	C5-C4	-3.42	1.38	1.42
54	2w	46	G7M	C5-C4	3.41	1.46	1.38
1	2A	2503	8AH	C4-N9	-3.41	1.33	1.38
1	2A	1911	PSU	C6-C5	3.41	1.39	1.35
55	2x	76	31H	C5-C4	-3.39	1.33	1.39
54	1w	46	G7M	C5-C4	3.37	1.46	1.38
54	1w	32	PSU	C6-C5	3.35	1.39	1.35
32	2a	527	G7M	C5-C4	3.34	1.46	1.38
55	1x	76	31H	C5-C4	-3.30	1.33	1.39
55	1x	55	PSU	C6-C5	3.26	1.38	1.35
32	1a	527	G7M	C5-C4	3.25	1.46	1.38
32	2a	1207	2MG	C5-C4	3.18	1.47	1.38
55	2x	8	4SU	C2-N3	-3.17	1.32	1.38
1	1A	2251	OMG	C5-C4	3.17	1.47	1.38
1	2A	1939	5MU	C4-N3	-3.16	1.32	1.38
32	2a	966	M2G	C5-C4	3.15	1.47	1.38
54	1w	39	PSU	C6-C5	3.14	1.38	1.35
1	2A	2251	OMG	C5-C4	3.12	1.47	1.38
1	1A	1939	5MU	C6-C5	3.08	1.39	1.34
32	1a	1207	2MG	C5-C4	3.08	1.47	1.38
54	2w	8	4SU	C4-N3	-3.07	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	C5-C4	-3.07	1.38	1.42
1	1A	2552	2MU	C4-N3	-3.06	1.33	1.38
54	2y	54	5MU	C6-C5	3.06	1.39	1.34
55	2x	8	4SU	C5-C4	-3.05	1.38	1.42
32	2a	1404	5MC	C6-C5	3.00	1.39	1.34
54	2w	8	4SU	C5-C4	-2.99	1.38	1.42
1	2A	1942	5MC	C6-C5	2.96	1.39	1.34
1	1A	2251	OMG	C6-N1	-2.95	1.33	1.38
32	1a	1404	5MC	C6-C5	2.94	1.39	1.34
32	1a	966	M2G	C5-C4	2.94	1.46	1.38
54	1w	8	4SU	C4-N3	-2.93	1.34	1.37
55	1x	32	5MC	C6-C5	2.91	1.39	1.34
54	2w	37	MIA	C5-C6	2.91	1.48	1.41
54	1y	54	5MU	C6-C5	2.90	1.39	1.34
32	1a	966	M2G	C2-N2	2.90	1.40	1.35
54	2y	39	PSU	C4-N3	-2.89	1.33	1.38
54	1w	37	MIA	C5-C6	2.89	1.48	1.41
54	1y	54	5MU	C4-N3	-2.89	1.33	1.38
54	2y	54	5MU	C2-N1	2.88	1.43	1.38
1	2A	1915	5MU	C6-C5	2.86	1.39	1.34
54	1y	37	MIA	C5-C6	2.86	1.49	1.41
32	2a	966	M2G	C2-N2	2.86	1.40	1.35
1	2A	2503	8AH	C5-N7	-2.84	1.34	1.39
54	2y	8	4SU	C4-N3	-2.84	1.34	1.37
32	1a	967	5MC	C6-C5	2.84	1.39	1.34
54	2y	37	MIA	C5-C6	2.81	1.48	1.41
1	1A	1915	5MU	C6-C5	2.80	1.39	1.34
32	2a	1407	5MC	C6-C5	2.78	1.39	1.34
54	2y	55	PSU	C4-N3	-2.78	1.33	1.38
32	2a	967	5MC	C6-C5	2.77	1.39	1.34
1	1A	2605	PSU	C6-C5	2.77	1.38	1.35
32	1a	1400	5MC	C6-C5	2.77	1.39	1.34
55	2x	54	5MU	C6-C5	2.75	1.39	1.34
1	1A	2503	8AH	C8-N7	2.72	1.35	1.31
1	1A	2503	8AH	C5-N7	-2.72	1.34	1.39
32	1a	516	PSU	C4-N3	-2.71	1.33	1.38
55	1x	54	5MU	C4-C5	2.70	1.49	1.44
55	2x	32	5MC	C6-C5	2.70	1.39	1.34
1	1A	1942	5MC	C6-C5	2.68	1.39	1.34
32	1a	966	M2G	C6-N1	-2.68	1.33	1.38
54	2w	54	5MU	C6-C5	2.67	1.39	1.34
1	2A	1939	5MU	C6-C5	2.65	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C4-N3	-2.65	1.33	1.38
1	2A	1939	5MU	C6-N1	-2.65	1.33	1.38
55	1x	54	5MU	C6-C5	2.65	1.38	1.34
1	1A	1911	PSU	C4-N3	-2.65	1.33	1.38
55	2x	54	5MU	C4-N3	-2.64	1.33	1.38
1	1A	2605	PSU	C4-N3	-2.64	1.33	1.38
54	1y	8	4SU	C5-C4	-2.59	1.39	1.42
1	2A	1915	5MU	C2-N1	2.58	1.42	1.38
32	1a	1207	2MG	C6-N1	-2.58	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.58	1.34	1.38
54	1w	54	5MU	C2-N1	2.57	1.42	1.38
1	1A	1915	5MU	C4-N3	-2.57	1.34	1.38
54	2y	8	4SU	C5-C4	-2.57	1.39	1.42
55	1x	55	PSU	C4-N3	-2.56	1.34	1.38
54	1w	39	PSU	C4-N3	-2.56	1.34	1.38
54	1y	55	PSU	C4-N3	-2.55	1.34	1.38
54	2y	54	5MU	C4-N3	-2.55	1.34	1.38
54	1w	32	PSU	C4-N3	-2.55	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.54	1.34	1.38
54	2y	8	4SU	C2-N1	2.54	1.42	1.38
32	2a	1400	5MC	C6-C5	2.54	1.38	1.34
54	2y	55	PSU	C6-C5	2.54	1.38	1.35
1	2A	1911	PSU	C4-N3	-2.53	1.34	1.38
54	1w	46	G7M	C6-N1	-2.53	1.34	1.38
55	1x	32	5MC	C6-N1	-2.53	1.33	1.38
1	2A	2552	2MU	C4-N3	-2.53	1.34	1.38
54	1y	54	5MU	C4-C5	2.53	1.48	1.44
55	2x	55	PSU	C4-N3	-2.53	1.34	1.38
54	1y	39	PSU	C4-N3	-2.52	1.34	1.38
54	1w	54	5MU	C6-C5	2.52	1.38	1.34
1	2A	2605	PSU	C4-N3	-2.52	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.51	1.33	1.38
32	2a	1498	UR3	C2-N1	2.51	1.42	1.38
54	1y	32	PSU	C4-N3	-2.50	1.34	1.38
32	2a	527	G7M	C6-N1	-2.49	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.49	1.33	1.38
54	1w	54	5MU	C4-C5	2.48	1.48	1.44
1	2A	2503	8AH	C5-C6	2.48	1.47	1.41
54	1w	8	4SU	C2-N1	2.48	1.42	1.38
55	2x	76	31H	C5-C6	-2.48	1.34	1.41
54	2y	46	G7M	C6-N1	-2.48	1.34	1.38
54	2w	55	PSU	C4-N3	-2.47	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1915	5MU	C4-C5	2.46	1.48	1.44
1	1A	1915	5MU	C2-N1	2.46	1.42	1.38
32	2a	1407	5MC	C6-N1	-2.45	1.33	1.38
54	1y	37	MIA	C8-N7	2.44	1.36	1.31
1	1A	1917	PSU	C4-N3	-2.44	1.34	1.38
32	1a	1407	5MC	C6-C5	2.43	1.38	1.34
55	1x	54	5MU	C4-N3	-2.43	1.34	1.38
1	2A	2552	2MU	C5-C4	2.43	1.49	1.43
1	2A	1917	PSU	C4-N3	-2.42	1.34	1.38
54	2w	54	5MU	C4-N3	-2.42	1.34	1.38
54	2w	54	5MU	C4-C5	2.42	1.48	1.44
55	2x	54	5MU	C4-C5	2.42	1.48	1.44
1	2A	1962	5MC	C6-N1	-2.41	1.33	1.38
32	1a	527	G7M	C6-N1	-2.41	1.34	1.38
1	1A	2251	OMG	C5-N7	-2.41	1.34	1.39
32	2a	1207	2MG	C6-N1	-2.41	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.41	1.33	1.38
54	1w	37	MIA	C5-N7	-2.40	1.34	1.39
54	2w	37	MIA	C5-N7	-2.38	1.34	1.39
54	2w	32	PSU	C4-N3	-2.37	1.34	1.38
1	2A	1962	5MC	C6-C5	2.36	1.38	1.34
1	1A	2503	8AH	C5-C6	2.35	1.47	1.41
54	2y	37	MIA	C8-N7	2.35	1.36	1.31
32	1a	1404	5MC	C6-N1	-2.35	1.34	1.38
54	1y	54	5MU	C2-N1	2.34	1.42	1.38
1	1A	2552	2MU	C2-N3	-2.32	1.33	1.38
32	2a	516	PSU	C4-N3	-2.31	1.34	1.38
55	1x	76	31H	C5-C6	-2.31	1.34	1.41
32	1a	1400	5MC	C6-N1	-2.31	1.34	1.38
55	1x	8	4SU	O2-C2	2.31	1.27	1.23
1	1A	1915	5MU	C4-C5	2.30	1.48	1.44
54	2w	39	PSU	C4-N3	-2.30	1.34	1.38
54	1y	54	5MU	C2-N3	-2.30	1.34	1.38
54	2w	46	G7M	C6-N1	-2.29	1.34	1.38
54	1y	8	4SU	C2-N3	-2.28	1.34	1.38
1	1A	1962	5MC	C6-C5	2.28	1.38	1.34
55	2x	32	5MC	C6-N1	-2.28	1.34	1.38
54	1w	37	MIA	C8-N7	2.27	1.36	1.31
1	2A	1942	5MC	C6-N1	-2.27	1.34	1.38
54	1w	55	PSU	C4-N3	-2.26	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.26	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.25	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	32	PSU	C4-N3	-2.25	1.34	1.38
54	2y	54	5MU	C4-C5	2.24	1.48	1.44
54	1w	54	5MU	C4-N3	-2.24	1.34	1.38
55	2x	54	5MU	C2-N1	2.23	1.42	1.38
1	1A	1939	5MU	C2-N3	-2.21	1.34	1.38
1	2A	2552	2MU	C2-N3	-2.20	1.34	1.38
54	2w	54	5MU	C2-N1	2.20	1.41	1.38
1	2A	2605	PSU	C2-N3	-2.19	1.33	1.37
1	1A	1939	5MU	C6-N1	-2.18	1.34	1.38
54	2w	8	4SU	C2-N3	-2.17	1.34	1.38
55	2x	8	4SU	O2-C2	2.16	1.26	1.23
55	1x	54	5MU	C6-N1	-2.15	1.34	1.38
1	1A	2552	2MU	C2-N1	2.15	1.41	1.38
1	2A	1915	5MU	C6-N1	-2.15	1.34	1.38
32	2a	966	M2G	C6-N1	-2.14	1.34	1.38
54	2y	37	MIA	C5-N7	-2.13	1.35	1.39
1	2A	1939	5MU	C2-N1	2.12	1.41	1.38
54	1w	54	5MU	C6-N1	-2.11	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.10	1.34	1.38
32	2a	967	5MC	C6-N1	-2.10	1.34	1.38
54	1y	54	5MU	C6-N1	-2.10	1.34	1.38
1	1A	2552	2MU	C5-C4	2.09	1.48	1.43
32	1a	1498	UR3	C6-C5	2.08	1.39	1.35
32	1a	1498	UR3	C2-N1	2.08	1.41	1.38
32	2a	966	M2G	C5-N7	-2.08	1.34	1.39
32	2a	1498	UR3	C6-C5	2.08	1.39	1.35
1	2A	2552	2MU	C2-N1	2.07	1.41	1.38
54	2y	55	PSU	C2-N1	-2.07	1.34	1.36
54	1y	46	G7M	C5-C6	2.07	1.49	1.43
55	2x	8	4SU	C2-N1	2.07	1.41	1.38
54	1y	46	G7M	C6-N1	-2.07	1.35	1.38
55	1x	54	5MU	C2-N1	2.07	1.41	1.38
55	2x	54	5MU	C6-N1	-2.07	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.06	1.34	1.38
54	1y	37	MIA	C5-N7	-2.06	1.35	1.39
32	2a	527	G7M	C5-C6	2.06	1.48	1.43
54	2w	37	MIA	C8-N7	2.06	1.35	1.31
55	2x	8	4SU	C6-C5	2.05	1.39	1.35
55	2x	54	5MU	C2-N3	-2.03	1.34	1.38
32	1a	516	PSU	C2-N3	-2.02	1.34	1.37
54	2y	54	5MU	C2-N3	-2.02	1.34	1.38
54	2y	55	PSU	C2-N3	-2.02	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1915	5MU	C2-N3	-2.01	1.34	1.38

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-16.22	73.21	102.36
43	1l	92	0TD	CSB-SB-CB	-14.21	76.83	102.36
54	1w	37	MIA	C12-C13-C14	-9.38	110.17	127.01
54	2w	37	MIA	C5-C4-N3	-9.29	117.39	127.18
54	1w	37	MIA	C5-C4-N3	-8.38	118.35	127.18
1	2A	2503	8AH	C5-C4-N3	-8.27	118.47	127.18
54	2w	37	MIA	N3-C4-N9	7.64	136.68	126.99
1	1A	2503	8AH	C5-C4-N3	-7.53	119.25	127.18
54	2y	8	4SU	C4-N3-C2	-7.26	120.36	127.31
32	2a	1498	UR3	C4-N3-C2	-7.01	118.94	124.58
32	1a	1207	2MG	C2-N3-C4	6.98	120.73	112.00
32	2a	1207	2MG	C2-N3-C4	6.88	120.61	112.00
32	1a	1498	UR3	C4-N3-C2	-6.76	119.14	124.58
54	1y	55	PSU	N1-C2-N3	6.49	122.02	115.17
54	1w	37	MIA	N3-C4-N9	6.43	135.15	126.99
1	2A	1911	PSU	N1-C2-N3	6.36	121.88	115.17
55	2x	55	PSU	N1-C2-N3	6.31	121.82	115.17
32	1a	516	PSU	N1-C2-N3	6.27	121.78	115.17
32	2a	516	PSU	N1-C2-N3	6.23	121.74	115.17
1	2A	2605	PSU	N1-C2-N3	6.23	121.74	115.17
55	1x	55	PSU	N1-C2-N3	6.22	121.73	115.17
54	2w	39	PSU	N1-C2-N3	6.16	121.67	115.17
54	1w	39	PSU	N1-C2-N3	6.15	121.66	115.17
54	1w	55	PSU	N1-C2-N3	6.14	121.64	115.17
54	2w	55	PSU	N1-C2-N3	6.09	121.59	115.17
1	2A	2251	OMG	C5-C4-N3	-6.08	118.71	128.39
54	2w	32	PSU	N1-C2-N3	6.07	121.57	115.17
54	1y	46	G7M	N9-C4-N3	6.06	138.08	125.95
54	1y	37	MIA	C5-C4-N3	-6.06	118.38	126.72
1	1A	1917	PSU	N1-C2-N3	6.05	121.55	115.17
32	2a	966	M2G	C5-C4-N3	-6.03	118.80	128.39
1	2A	1917	PSU	N1-C2-N3	6.03	121.53	115.17
54	2y	8	4SU	C5-C4-N3	6.03	120.36	114.75
54	1w	32	PSU	N1-C2-N3	6.01	121.51	115.17
32	1a	966	M2G	C5-C4-N3	-6.00	118.83	128.39
1	1A	2605	PSU	N1-C2-N3	5.96	121.45	115.17
1	1A	2251	OMG	C5-C4-N3	-5.95	118.92	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1911	PSU	N1-C2-N3	5.95	121.44	115.17
54	2y	32	PSU	N1-C2-N3	5.92	121.41	115.17
54	1y	39	PSU	N1-C2-N3	5.90	121.39	115.17
54	2y	46	G7M	N9-C4-N3	5.89	137.73	125.95
55	2x	76	31H	N1-C2-N3	-5.86	119.70	128.58
54	1y	32	PSU	N1-C2-N3	5.86	121.35	115.17
54	2y	55	PSU	N1-C2-N3	5.84	121.33	115.17
32	1a	1207	2MG	C5-C4-N3	-5.83	119.11	128.39
32	2a	1207	2MG	C5-C4-N3	-5.80	119.16	128.39
54	2y	37	MIA	C5-C4-N3	-5.75	118.81	126.72
54	1y	46	G7M	C5-C4-N3	-5.69	117.40	128.15
1	2A	1939	5MU	C4-N3-C2	-5.66	119.91	127.34
54	1w	8	4SU	C4-N3-C2	-5.62	121.93	127.31
55	1x	76	31H	N1-C2-N3	-5.55	120.19	128.58
55	1x	54	5MU	C4-N3-C2	-5.52	120.11	127.34
1	1A	2552	2MU	N3-C2-N1	5.46	121.99	114.89
54	1w	46	G7M	N9-C4-N3	5.45	136.86	125.95
1	1A	1915	5MU	N3-C2-N1	5.42	121.94	114.89
54	1w	8	4SU	C5-C4-N3	5.41	119.78	114.75
54	2w	46	G7M	N9-C4-N3	5.37	136.69	125.95
1	2A	1915	5MU	C4-N3-C2	-5.36	120.31	127.34
54	2y	46	G7M	C5-C4-N3	-5.36	118.03	128.15
1	1A	1939	5MU	C4-N3-C2	-5.34	120.34	127.34
32	2a	527	G7M	N9-C4-N3	5.33	136.61	125.95
55	1x	54	5MU	N3-C2-N1	5.33	121.82	114.89
55	2x	54	5MU	N3-C2-N1	5.28	121.77	114.89
1	2A	1939	5MU	N3-C2-N1	5.28	121.76	114.89
1	1A	1915	5MU	C4-N3-C2	-5.26	120.44	127.34
32	1a	527	G7M	N9-C4-N3	5.22	136.40	125.95
54	2y	39	PSU	N1-C2-N3	5.22	120.67	115.17
55	2x	54	5MU	C4-N3-C2	-5.20	120.52	127.34
1	2A	1939	5MU	C5-C4-N3	5.19	119.83	115.32
55	2x	76	31H	C5-C4-N3	-5.15	119.63	126.72
32	2a	527	G7M	C5-C4-N3	-5.13	118.45	128.15
32	1a	1519	MA6	N1-C2-N3	-5.13	120.82	128.58
1	1A	1939	5MU	O4-C4-C5	-5.09	119.09	124.92
1	2A	1915	5MU	N3-C2-N1	5.07	121.49	114.89
1	1A	1939	5MU	C5-C4-N3	5.05	119.72	115.32
32	2a	1519	MA6	N1-C2-N3	-5.02	120.99	128.58
54	2w	8	4SU	C5-C4-N3	5.01	119.41	114.75
1	2A	1915	5MU	C5-C4-N3	4.94	119.61	115.32
54	1y	8	4SU	C4-N3-C2	-4.93	122.59	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	N1-C2-N3	-4.90	121.17	128.58
32	2a	1518	MA6	N1-C2-N3	-4.89	121.17	128.58
54	1w	54	5MU	C4-N3-C2	-4.89	120.93	127.34
1	1A	2552	2MU	C4-N3-C2	-4.87	120.56	126.61
1	2A	2251	OMG	C2-N3-C4	4.87	120.69	112.30
32	1a	527	G7M	C5-C4-N3	-4.86	118.97	128.15
54	1y	46	G7M	C2-N3-C4	4.85	120.66	112.30
54	2w	46	G7M	C5-C4-N3	-4.85	118.99	128.15
54	2y	37	MIA	N3-C4-N9	4.83	135.39	127.17
54	1y	37	MIA	N3-C4-N9	4.82	135.37	127.17
1	2A	2251	OMG	N9-C4-N3	4.78	135.51	125.95
1	1A	1939	5MU	N3-C2-N1	4.77	121.10	114.89
1	2A	2552	2MU	N3-C2-N1	4.76	121.08	114.89
54	2y	46	G7M	C2-N3-C4	4.75	120.48	112.30
54	1w	46	G7M	C5-C4-N3	-4.71	119.25	128.15
32	2a	966	M2G	N9-C4-N3	4.65	135.26	125.95
54	1w	54	5MU	N3-C2-N1	4.65	120.94	114.89
54	1w	8	4SU	C5-C4-S4	-4.63	119.01	124.31
32	2a	1519	MA6	C5-C4-N3	-4.63	120.34	126.72
1	1A	2251	OMG	C2-N3-C4	4.62	120.26	112.30
32	2a	1518	MA6	C5-C4-N3	-4.61	120.37	126.72
54	2y	8	4SU	C5-C4-S4	-4.61	119.04	124.31
1	1A	2251	OMG	N9-C4-N3	4.58	135.12	125.95
54	1y	8	4SU	C5-C4-N3	4.56	119.00	114.75
32	2a	527	G7M	C2-N3-C4	4.55	120.14	112.30
54	2w	8	4SU	C4-N3-C2	-4.53	122.97	127.31
32	2a	966	M2G	C2-N3-C4	4.52	120.88	112.51
32	1a	966	M2G	C2-N3-C4	4.52	120.87	112.51
1	2A	1915	5MU	O4-C4-C5	-4.51	119.76	124.92
1	1A	1939	5MU	C5-C6-N1	-4.47	118.46	123.31
54	1y	54	5MU	N3-C2-N1	4.47	120.71	114.89
1	1A	1915	5MU	C5-C4-N3	4.43	119.17	115.32
55	2x	55	PSU	C4-N3-C2	-4.42	120.28	126.37
1	2A	2552	2MU	C4-N3-C2	-4.40	121.15	126.61
1	2A	2605	PSU	C4-N3-C2	-4.39	120.32	126.37
54	2y	8	4SU	N3-C2-N1	4.39	120.61	114.89
54	2w	54	5MU	C4-N3-C2	-4.39	121.59	127.34
54	2w	54	5MU	N3-C2-N1	4.39	120.60	114.89
54	2w	46	G7M	C2-N3-C4	4.36	119.81	112.30
55	1x	54	5MU	C5-C4-N3	4.34	119.10	115.32
55	1x	76	31H	C5-C4-N3	-4.34	120.74	126.72
32	1a	1519	MA6	C5-C4-N3	-4.31	120.78	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2605	PSU	C4-N3-C2	-4.30	120.45	126.37
1	2A	2503	8AH	C4-C5-N7	-4.29	106.53	110.91
32	1a	966	M2G	N9-C4-N3	4.27	134.50	125.95
1	2A	1911	PSU	C4-N3-C2	-4.26	120.50	126.37
55	2x	54	5MU	C5-C4-N3	4.25	119.02	115.32
54	1w	54	5MU	C5-C4-N3	4.19	118.97	115.32
1	1A	1917	PSU	C4-N3-C2	-4.19	120.60	126.37
32	2a	1519	MA6	C5-N7-C8	4.17	110.00	103.45
54	2w	39	PSU	C4-N3-C2	-4.16	120.64	126.37
1	2A	1939	5MU	C5-C6-N1	-4.14	118.81	123.31
32	2a	516	PSU	C4-N3-C2	-4.14	120.67	126.37
54	1y	55	PSU	C4-N3-C2	-4.13	120.68	126.37
54	1w	46	G7M	C2-N3-C4	4.12	119.40	112.30
54	1y	54	5MU	C4-N3-C2	-4.12	121.93	127.34
1	1A	1915	5MU	O4-C4-C5	-4.12	120.20	124.92
54	2y	55	PSU	C4-N3-C2	-4.11	120.70	126.37
32	2a	1519	MA6	C4-C5-N7	-4.11	105.88	110.58
32	1a	527	G7M	C2-N3-C4	4.10	119.36	112.30
32	1a	516	PSU	C4-N3-C2	-4.10	120.72	126.37
32	1a	1518	MA6	C2-N1-C6	4.10	121.83	111.83
1	1A	2503	8AH	N6-C6-N1	4.09	122.55	117.03
54	1w	39	PSU	O2-C2-N1	-4.09	118.57	122.79
54	2w	54	5MU	C5-C4-N3	4.09	118.88	115.32
54	1w	54	5MU	O4-C4-C5	-4.08	120.25	124.92
32	1a	1519	MA6	C4-C5-N7	-4.07	105.93	110.58
54	1w	32	PSU	C4-N3-C2	-4.06	120.77	126.37
1	1A	2503	8AH	C6-C5-N7	4.05	135.74	131.72
54	1w	39	PSU	C4-N3-C2	-4.04	120.80	126.37
55	1x	55	PSU	C4-N3-C2	-4.03	120.81	126.37
54	1y	32	PSU	C4-N3-C2	-4.02	120.83	126.37
55	2x	76	31H	O4'-C1'-N9	4.02	115.81	108.09
1	2A	1939	5MU	O4-C4-C5	-4.01	120.33	124.92
32	2a	1519	MA6	C2-N1-C6	4.00	121.61	111.83
1	2A	2503	8AH	C6-C5-N7	4.00	135.68	131.72
1	1A	1911	PSU	C4-N3-C2	-3.99	120.87	126.37
32	1a	1519	MA6	C2-N1-C6	3.99	121.58	111.83
54	1w	37	MIA	C15-C14-C13	-3.98	110.72	122.66
54	2y	54	5MU	N3-C2-N1	3.97	120.06	114.89
54	2w	32	PSU	C4-N3-C2	-3.95	120.93	126.37
32	2a	1518	MA6	C2-N1-C6	3.94	121.45	111.83
32	1a	1519	MA6	C5-N7-C8	3.94	109.64	103.45
55	2x	54	5MU	O4-C4-C5	-3.92	120.43	124.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	C6-C5-N7	3.90	137.39	130.29
1	2A	1917	PSU	C4-N3-C2	-3.90	121.00	126.37
32	1a	1518	MA6	C5-C4-N3	-3.89	121.36	126.72
54	2w	37	MIA	C12-N6-C6	-3.88	119.25	122.85
32	1a	1207	2MG	N9-C4-N3	3.86	133.68	125.95
55	1x	54	5MU	O4-C4-C5	-3.83	120.54	124.92
1	1A	2503	8AH	C4-C5-N7	-3.83	107.00	110.91
54	2w	8	4SU	C5-C4-S4	-3.82	119.94	124.31
32	2a	1207	2MG	N9-C4-N3	3.81	133.57	125.95
1	2A	1942	5MC	C5-C6-N1	-3.80	119.19	123.31
55	1x	32	5MC	C5-C6-N1	-3.79	119.19	123.31
55	1x	54	5MU	O2-C2-N1	-3.79	117.86	122.80
32	1a	1404	5MC	C5-C6-N1	-3.78	119.20	123.31
32	1a	1518	MA6	C5-N7-C8	3.78	109.39	103.45
55	1x	54	5MU	C5-C6-N1	-3.77	119.22	123.31
54	2y	32	PSU	O2-C2-N1	-3.77	118.91	122.79
55	1x	8	4SU	C6-C5-C4	-3.77	116.69	119.95
54	1y	54	5MU	C5-C4-N3	3.75	118.58	115.32
54	1w	55	PSU	C4-N3-C2	-3.75	121.20	126.37
54	2y	55	PSU	O2-C2-N1	-3.75	118.92	122.79
54	2y	54	5MU	C5-C4-N3	3.75	118.58	115.32
54	2y	32	PSU	C4-N3-C2	-3.74	121.21	126.37
54	2w	54	5MU	O4-C4-C5	-3.74	120.64	124.92
54	2y	54	5MU	C4-N3-C2	-3.74	122.44	127.34
54	2w	55	PSU	C4-N3-C2	-3.72	121.25	126.37
32	1a	1400	5MC	C5-C6-N1	-3.71	119.28	123.31
54	1y	32	PSU	O2-C2-N1	-3.71	118.96	122.79
32	2a	1519	MA6	N9-C8-N7	-3.70	108.68	113.94
54	1y	39	PSU	C4-N3-C2	-3.70	121.28	126.37
32	2a	1404	5MC	C5-C6-N1	-3.70	119.30	123.31
1	1A	2605	PSU	O2-C2-N1	-3.69	118.98	122.79
54	1y	37	MIA	C2-N3-C4	3.68	120.83	111.83
55	2x	32	5MC	C5-C6-N1	-3.68	119.31	123.31
1	2A	1911	PSU	O2-C2-N1	-3.67	119.00	122.79
54	2y	54	5MU	O4-C4-C5	-3.67	120.72	124.92
32	2a	1400	5MC	C5-C6-N1	-3.66	119.34	123.31
32	2a	1207	2MG	C6-C5-N7	3.65	136.93	130.29
32	2a	1518	MA6	C5-N7-C8	3.64	109.17	103.45
32	1a	967	5MC	C5-C6-N1	-3.63	119.37	123.31
54	2w	32	PSU	O2-C2-N1	-3.63	119.05	122.79
54	1w	37	MIA	C4-C5-N7	-3.61	106.45	110.58
32	1a	1518	MA6	C4-C5-N7	-3.61	106.45	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	C5-C6-N1	-3.60	119.40	123.31
32	2a	1519	MA6	C2-N3-C4	3.58	120.59	111.83
32	1a	966	M2G	C6-C5-N7	3.55	136.75	130.29
54	1y	8	4SU	N3-C2-N1	3.55	119.51	114.89
54	2y	37	MIA	C2-N3-C4	3.54	120.48	111.83
54	1w	37	MIA	C16-C14-C13	-3.53	112.05	122.66
32	1a	1519	MA6	C2-N3-C4	3.53	120.46	111.83
32	2a	516	PSU	O2-C2-N1	-3.53	119.15	122.79
32	2a	1518	MA6	C2-N3-C4	3.50	120.39	111.83
32	2a	1407	5MC	C5-C6-N1	-3.50	119.52	123.31
54	1w	37	MIA	C2-N3-C4	3.49	121.44	112.29
54	1y	55	PSU	O2-C2-N1	-3.49	119.19	122.79
32	2a	1518	MA6	C4-C5-N7	-3.49	106.59	110.58
55	1x	8	4SU	O2-C2-N1	3.47	127.31	122.80
55	1x	32	5MC	C5-C4-N3	-3.43	118.23	121.75
1	1A	1917	PSU	O2-C2-N1	-3.42	119.26	122.79
54	1y	37	MIA	C4-C5-N7	-3.42	106.67	110.58
1	2A	1915	5MU	C5-C6-N1	-3.42	119.59	123.31
32	1a	1518	MA6	N9-C8-N7	-3.42	109.08	113.94
32	1a	1519	MA6	N9-C8-N7	-3.42	109.09	113.94
55	1x	55	PSU	O2-C2-N1	-3.41	119.28	122.79
1	2A	1917	PSU	O2-C2-N1	-3.40	119.28	122.79
55	2x	76	31H	C2-N3-C4	3.39	120.12	111.83
54	1w	55	PSU	O2-C2-N1	-3.38	119.30	122.79
1	1A	1942	5MC	C5-C4-N3	-3.38	118.29	121.75
55	2x	76	31H	N9-C8-N7	-3.37	109.15	113.94
54	2w	55	PSU	O2-C2-N1	-3.36	119.32	122.79
1	1A	1962	5MC	C5-C6-N1	-3.35	119.68	123.31
43	1l	92	0TD	OD2-CG-CB	3.34	120.37	113.15
55	1x	76	31H	N9-C8-N7	-3.33	109.22	113.94
54	2w	37	MIA	C4-C5-N7	-3.32	106.78	110.58
54	2y	37	MIA	N3-C2-N1	-3.32	123.56	128.58
54	1w	8	4SU	N3-C2-N1	3.31	119.20	114.89
1	1A	1942	5MC	C5-C6-N1	-3.31	119.72	123.31
54	2w	37	MIA	C2-N3-C4	3.29	120.92	112.29
54	1w	32	PSU	O2-C2-N1	-3.28	119.40	122.79
32	2a	1518	MA6	N9-C8-N7	-3.27	109.30	113.94
55	2x	8	4SU	C1'-N1-C2	3.26	123.46	117.59
54	1y	37	MIA	N3-C2-N1	-3.25	123.67	128.58
54	1w	37	MIA	C6-C5-N7	3.24	135.97	132.43
54	1y	54	5MU	C5-C6-N1	-3.24	119.80	123.31
32	1a	1518	MA6	C2-N3-C4	3.23	119.72	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	OD2-CG-CB	3.21	120.09	113.15
1	2A	2503	8AH	N6-C6-N1	3.20	121.35	117.03
54	1w	54	5MU	C5-C6-N1	-3.19	119.85	123.31
1	2A	1962	5MC	C5-C6-N1	-3.19	119.85	123.31
54	1w	8	4SU	C1'-N1-C2	3.16	123.26	117.59
54	2y	37	MIA	C4-C5-N7	-3.15	106.98	110.58
54	2w	39	PSU	O2-C2-N1	-3.15	119.54	122.79
55	1x	8	4SU	C5-C4-N3	3.13	117.66	114.75
32	2a	1498	UR3	C5-C4-N3	3.13	119.16	115.04
55	1x	76	31H	C2-N3-C4	3.11	119.44	111.83
1	1A	1915	5MU	C5-C6-N1	-3.11	119.94	123.31
32	1a	1207	2MG	C4-C5-N7	-3.11	105.74	110.67
32	1a	1400	5MC	C5-C4-N3	-3.11	118.57	121.75
32	1a	1407	5MC	C5-C6-N1	-3.10	119.95	123.31
1	2A	2552	2MU	C5-C4-N3	3.08	119.11	114.80
55	1x	8	4SU	S4-C4-N3	-3.06	117.00	120.20
32	2a	966	M2G	C6-C5-N7	3.06	135.85	130.29
32	2a	1518	MA6	N3-C4-N9	2.99	132.25	127.17
32	2a	1407	5MC	C5-C4-N3	-2.98	118.69	121.75
32	1a	1404	5MC	C5-C4-N3	-2.98	118.70	121.75
1	2A	2251	OMG	C6-C5-N7	2.95	135.66	130.29
1	1A	1939	5MU	O2-C2-N1	-2.93	118.98	122.80
54	2y	39	PSU	C4-N3-C2	-2.93	122.34	126.37
32	2a	967	5MC	C5-C6-N1	-2.92	120.15	123.31
55	1x	76	31H	C5-N7-C8	2.91	108.03	103.45
55	2x	76	31H	C5-C4-N9	2.91	108.98	105.81
1	1A	2251	OMG	C6-C5-N7	2.90	135.56	130.29
32	2a	1207	2MG	C4-C5-N7	-2.88	106.10	110.67
1	1A	2552	2MU	C5-C4-N3	2.87	118.82	114.80
54	1y	54	5MU	O4-C4-C5	-2.87	121.64	124.92
55	2x	54	5MU	O2-C2-N1	-2.86	119.08	122.80
55	2x	8	4SU	O2-C2-N1	2.85	126.51	122.80
32	1a	966	M2G	C4-C5-N7	-2.83	106.19	110.67
54	2w	54	5MU	C5-C6-N1	-2.83	120.25	123.31
1	1A	1911	PSU	C6-C5-C4	-2.82	116.27	118.17
54	2y	54	5MU	C5-C6-N1	-2.82	120.25	123.31
32	2a	1404	5MC	C5-C4-N3	-2.81	118.88	121.75
32	1a	1498	UR3	C5-C4-N3	2.80	118.72	115.04
55	2x	76	31H	C5-N7-C8	2.79	107.83	103.45
1	2A	1942	5MC	C5-C4-N3	-2.78	118.90	121.75
54	2w	8	4SU	N3-C2-N1	2.78	118.51	114.89
32	2a	1519	MA6	N3-C4-N9	2.77	131.88	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	8AH	C2-N1-C6	2.72	122.28	118.10
1	1A	1911	PSU	O2-C2-N1	-2.72	119.99	122.79
54	2y	37	MIA	C4-N9-C8	2.69	108.56	105.74
1	1A	1962	5MC	CM5-C5-C6	-2.69	119.22	122.85
1	1A	1962	5MC	C5-C4-N3	-2.68	119.01	121.75
54	2w	37	MIA	C11-S10-C2	-2.67	100.25	102.25
55	2x	55	PSU	O2-C2-N1	-2.66	120.04	122.79
55	2x	76	31H	C6-C5-C4	2.65	120.80	117.18
55	2x	32	5MC	C5-C4-N3	-2.65	119.03	121.75
32	1a	967	5MC	C5-C4-N3	-2.64	119.05	121.75
1	1A	1915	5MU	O2-C2-N1	-2.63	119.37	122.80
55	2x	76	31H	C4'-O4'-C1'	-2.61	103.70	109.47
1	1A	2552	2MU	O4-C4-C5	-2.61	120.66	125.16
32	2a	1207	2MG	N1-C2-N2	2.61	119.22	116.56
55	2x	8	4SU	C5-C4-N3	2.60	117.17	114.75
32	1a	1402	4OC	C6-C5-C4	2.60	120.13	117.00
54	1w	37	MIA	C5-N7-C8	2.60	107.53	103.45
32	1a	527	G7M	O6-C6-C5	-2.59	122.22	128.01
32	2a	967	5MC	C5-C4-N3	-2.58	119.11	121.75
54	2w	37	MIA	C5-N7-C8	2.55	107.46	103.45
1	2A	1962	5MC	C5-C4-N3	-2.55	119.14	121.75
54	2w	37	MIA	C1'-N9-C8	-2.54	121.47	127.09
32	1a	1207	2MG	N1-C2-N2	2.54	119.15	116.56
32	1a	1407	5MC	C5-C4-N3	-2.53	119.16	121.75
1	1A	2605	PSU	C5-C6-N1	-2.51	118.66	122.14
54	1y	37	MIA	C5-N7-C8	2.49	107.36	103.45
54	1y	39	PSU	O2-C2-N1	-2.48	120.23	122.79
55	2x	76	31H	N3-C4-N9	2.48	131.38	127.17
32	1a	1498	UR3	C6-N1-C2	-2.48	119.78	121.80
32	2a	1400	5MC	O2-C2-N3	-2.46	118.44	122.33
32	2a	1518	MA6	C4-C5-C6	2.46	118.45	115.91
32	1a	516	PSU	O2-C2-N1	-2.45	120.26	122.79
1	2A	2552	2MU	O4-C4-C5	-2.45	120.94	125.16
32	2a	966	M2G	C4-C5-N7	-2.44	106.81	110.67
32	2a	1207	2MG	N2-C2-N3	-2.43	117.41	120.51
1	1A	1920	OMC	O2-C2-N3	-2.43	118.50	122.33
1	2A	2503	8AH	C2-N1-C6	2.43	121.83	118.10
55	2x	8	4SU	C6-C5-C4	-2.42	117.86	119.95
32	1a	516	PSU	O4'-C1'-C2'	2.41	108.49	105.15
54	2w	46	G7M	O6-C6-C5	-2.41	122.63	128.01
54	2w	8	4SU	C1'-N1-C2	2.40	121.90	117.59
54	2y	37	MIA	C5-N7-C8	2.39	107.21	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	N3-C2-N1	-2.39	122.64	127.00
43	2l	92	0TD	OD1-CG-CB	-2.39	117.43	122.44
1	2A	2605	PSU	O2-C2-N1	-2.39	120.33	122.79
1	2A	2605	PSU	C5-C6-N1	-2.38	118.83	122.14
1	2A	2251	OMG	O6-C6-C5	-2.38	120.24	126.53
32	1a	1404	5MC	O2-C2-N3	-2.38	118.57	122.33
55	2x	32	5MC	O2-C2-N3	-2.38	118.58	122.33
32	1a	1519	MA6	N3-C4-N9	2.38	131.21	127.17
32	1a	1518	MA6	N3-C4-N9	2.37	131.20	127.17
43	1l	92	0TD	OD1-CG-CB	-2.37	117.47	122.44
55	1x	76	31H	C4'-O4'-C1'	-2.36	104.26	109.47
54	2w	54	5MU	C5M-C5-C4	2.36	121.30	118.78
55	2x	55	PSU	C5-C6-N1	-2.36	118.87	122.14
32	2a	1519	MA6	C4-C5-C6	2.35	118.34	115.91
54	1w	46	G7M	O6-C6-C5	-2.34	122.78	128.01
32	2a	1402	4OC	O2-C2-N3	-2.34	118.64	122.33
54	1w	37	MIA	C2-N1-C6	2.34	121.98	117.54
55	1x	76	31H	C5-C4-N9	2.33	108.35	105.81
54	2y	8	4SU	C1'-N1-C2	2.33	121.78	117.59
55	1x	32	5MC	O2-C2-N3	-2.33	118.66	122.33
54	1y	46	G7M	O6-C6-C5	-2.33	122.81	128.01
32	2a	966	M2G	O6-C6-C5	-2.33	120.39	126.53
54	2y	46	G7M	O6-C6-C5	-2.33	122.82	128.01
54	1y	8	4SU	C5-C4-S4	-2.32	121.65	124.31
55	2x	8	4SU	O2-C2-N3	-2.31	117.22	121.49
32	2a	1400	5MC	C5-C4-N3	-2.31	119.39	121.75
32	2a	1498	UR3	C3U-N3-C4	2.30	121.06	117.87
1	1A	2503	8AH	C2'-C1'-N9	-2.30	112.13	115.44
54	1w	37	MIA	C4-N9-C8	2.29	108.14	105.74
1	1A	2251	OMG	C4-C5-N7	-2.28	107.05	110.67
32	2a	1402	4OC	CM4-N4-C4	-2.28	117.99	122.45
32	1a	516	PSU	C5-C6-N1	-2.27	118.98	122.14
1	2A	2552	2MU	O2-C2-N1	-2.26	119.85	122.80
54	1y	37	MIA	C4-N9-C8	2.26	108.11	105.74
1	2A	1911	PSU	C5-C6-N1	-2.24	119.03	122.14
55	1x	8	4SU	C1'-N1-C2	2.23	121.60	117.59
54	2w	37	MIA	C4-C5-C6	2.22	118.62	116.78
55	1x	32	5MC	CM5-C5-C6	-2.22	119.85	122.85
54	1w	39	PSU	C5-C6-N1	-2.22	119.06	122.14
55	1x	54	5MU	C5M-C5-C4	2.21	121.14	118.78
1	2A	2605	PSU	O2-C2-N3	-2.21	117.93	121.86
55	1x	76	31H	N3-C4-N9	2.20	130.90	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	76	31H	OCN-CN-N	-2.20	119.64	125.32
1	1A	2552	2MU	O2-C2-N1	-2.19	119.94	122.80
32	1a	516	PSU	O2-C2-N3	-2.19	117.96	121.86
32	2a	1402	4OC	C6-C5-C4	2.19	119.64	117.00
32	1a	1498	UR3	C3U-N3-C4	2.18	120.89	117.87
55	1x	76	31H	CA-N-CN	-2.18	119.47	122.82
32	1a	1207	2MG	N2-C2-N3	-2.18	117.74	120.51
1	2A	2251	OMG	C4-C5-N7	-2.17	107.23	110.67
54	2w	54	5MU	O2-C2-N1	-2.15	120.00	122.80
32	1a	527	G7M	C5-C6-N1	2.15	116.28	111.84
54	2w	37	MIA	C2-N1-C6	2.15	121.62	117.54
32	1a	1404	5MC	CM5-C5-C6	-2.14	119.96	122.85
32	2a	527	G7M	C5-C6-N1	2.14	116.25	111.84
32	1a	966	M2G	O6-C6-C5	-2.13	120.90	126.53
55	1x	54	5MU	C5M-C5-C6	-2.13	119.97	122.85
1	1A	2552	2MU	C2'-C1'-N1	-2.13	110.20	114.24
54	2y	55	PSU	O4'-C1'-C2'	2.12	108.08	105.15
32	1a	1207	2MG	C8-N7-C5	2.11	108.02	104.26
54	2y	55	PSU	C6-C5-C4	-2.10	116.75	118.17
1	2A	2251	OMG	C5-C6-N1	2.10	118.61	113.25
55	2x	55	PSU	O2-C2-N3	-2.10	118.13	121.86
32	2a	1407	5MC	O2-C2-N3	-2.09	119.04	122.33
55	2x	76	31H	C4-C5-N7	-2.09	108.20	110.58
32	2a	967	5MC	O2-C2-N3	-2.08	119.06	122.33
54	2w	37	MIA	C4-N9-C8	2.08	107.92	105.74
54	1w	54	5MU	C5M-C5-C4	2.07	121.00	118.78
32	1a	1407	5MC	O2-C2-N3	-2.07	119.07	122.33
32	2a	516	PSU	O4'-C1'-C2'	2.06	108.01	105.15
1	2A	1942	5MC	O2-C2-N3	-2.06	119.08	122.33
1	2A	1920	OMC	O2-C2-N3	-2.06	119.09	122.33
54	2y	39	PSU	O2-C2-N3	-2.03	118.25	121.86
54	1w	54	5MU	O2-C2-N1	-2.03	120.16	122.80
32	1a	1498	UR3	C1'-N1-C2	2.03	120.36	117.04
55	1x	8	4SU	O2-C2-N3	-2.02	117.75	121.49
32	1a	966	M2G	C5-C6-N1	2.02	118.40	113.25
32	1a	966	M2G	C8-N7-C5	2.01	107.85	104.26
32	1a	1519	MA6	C5-C4-N9	2.01	108.00	105.81

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	N1-C2-S10-C11
54	1w	37	MIA	N3-C2-S10-C11
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
54	1w	46	G7M	C4'-C5'-O5'-P
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12
54	2y	54	5MU	C3'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'
54	2y	55	PSU	C2'-C1'-C5-C4
54	2y	55	PSU	C2'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6
55	1x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
55	1x	76	31H	C4'-C5'-O5'-P
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
54	2y	55	PSU	C3'-C4'-C5'-O5'
55	2x	76	31H	C4'-C5'-O5'-P
54	2y	46	G7M	O4'-C1'-N9-C4
55	2x	76	31H	CB-CG-SD-CE
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
55	1x	76	31H	CB-CA-N-CN
54	2y	55	PSU	O4'-C1'-C5-C4
32	1a	1402	4OC	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	1a	527	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
32	2a	527	G7M	C4'-C5'-O5'-P
54	2w	46	G7M	C4'-C5'-O5'-P
1	1A	2503	8AH	C4'-C5'-O5'-P
54	2y	46	G7M	O4'-C1'-N9-C8
54	2y	55	PSU	O4'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
1	2A	2503	8AH	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2

There are no ring outliers.

41 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1402	4OC	2	0
32	1a	1518	MA6	2	0
54	2w	8	4SU	1	0
32	1a	516	PSU	1	0
54	2y	54	5MU	1	0
1	1A	1939	5MU	2	0
55	1x	8	4SU	2	0
43	2l	92	0TD	1	0
54	1w	54	5MU	1	0
54	1y	8	4SU	1	0
1	1A	2251	OMG	1	0
54	1w	55	PSU	1	0
1	1A	2552	2MU	2	0
1	2A	2552	2MU	2	0
43	1l	92	0TD	2	0
54	1y	54	5MU	1	0
54	2y	46	G7M	2	0
54	1w	8	4SU	1	0
32	1a	966	M2G	2	0
32	2a	966	M2G	1	0
54	2y	8	4SU	2	0
32	1a	1519	MA6	2	0
32	1a	967	5MC	1	0
54	2y	37	MIA	1	0
54	1y	55	PSU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1519	MA6	2	0
1	2A	1939	5MU	1	0
32	2a	1404	5MC	1	0
1	2A	2251	OMG	1	0
54	2y	55	PSU	5	0
32	2a	967	5MC	1	0
54	1y	37	MIA	1	0
55	2x	54	5MU	2	0
54	1w	37	MIA	2	0
32	1a	1498	UR3	1	0
32	1a	1402	4OC	1	0
54	1y	39	PSU	1	0
1	2A	1915	5MU	1	0
54	2y	39	PSU	1	0
32	2a	1518	MA6	3	0
32	1a	527	G7M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2714 ligands modelled in this entry, 2710 are monoatomic - leaving 4 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	$\# Z > 2$
57	6IF	2A	3831	-	30,34,34	1.03	2 (6%)	30,49,49	1.26	3 (10%)
57	6IF	1A	4084	-	30,34,34	1.00	2 (6%)	30,49,49	1.24	3 (10%)
59	SF4	2d	303	35	0,12,12	-	-	-	-	-
59	SF4	1d	302	35	0,12,12	-	-	-	-	-

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
57	6IF	2A	3831	-	-	1/22/65/65	0/3/3/3
57	6IF	1A	4084	-	-	0/22/65/65	0/3/3/3
59	SF4	2d	303	35	-	-	0/6/5/5
59	SF4	1d	302	35	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	4084	6IF	OAF-CAE	3.37	1.49	1.44
57	2A	3831	6IF	OAV-CB	3.07	1.45	1.42
57	2A	3831	6IF	CD2-CAY	-2.29	1.51	1.53
57	1A	4084	6IF	CAG-NAH	2.04	1.49	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3831	6IF	CBB-CBA-CAY	-3.66	109.57	116.68
57	1A	4084	6IF	CD2-CAY-CAX	-2.94	109.39	113.78
57	2A	3831	6IF	CAA-OAF-CAE	-2.87	110.42	114.17
57	1A	4084	6IF	CBB-CBA-CAY	-2.74	111.36	116.68
57	1A	4084	6IF	CAK-CAI-CAG	-2.32	111.11	114.17
57	2A	3831	6IF	CD2-CAY-CAX	-2.19	110.52	113.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	2A	3831	6IF	CAB-CAA-SBE-CBF

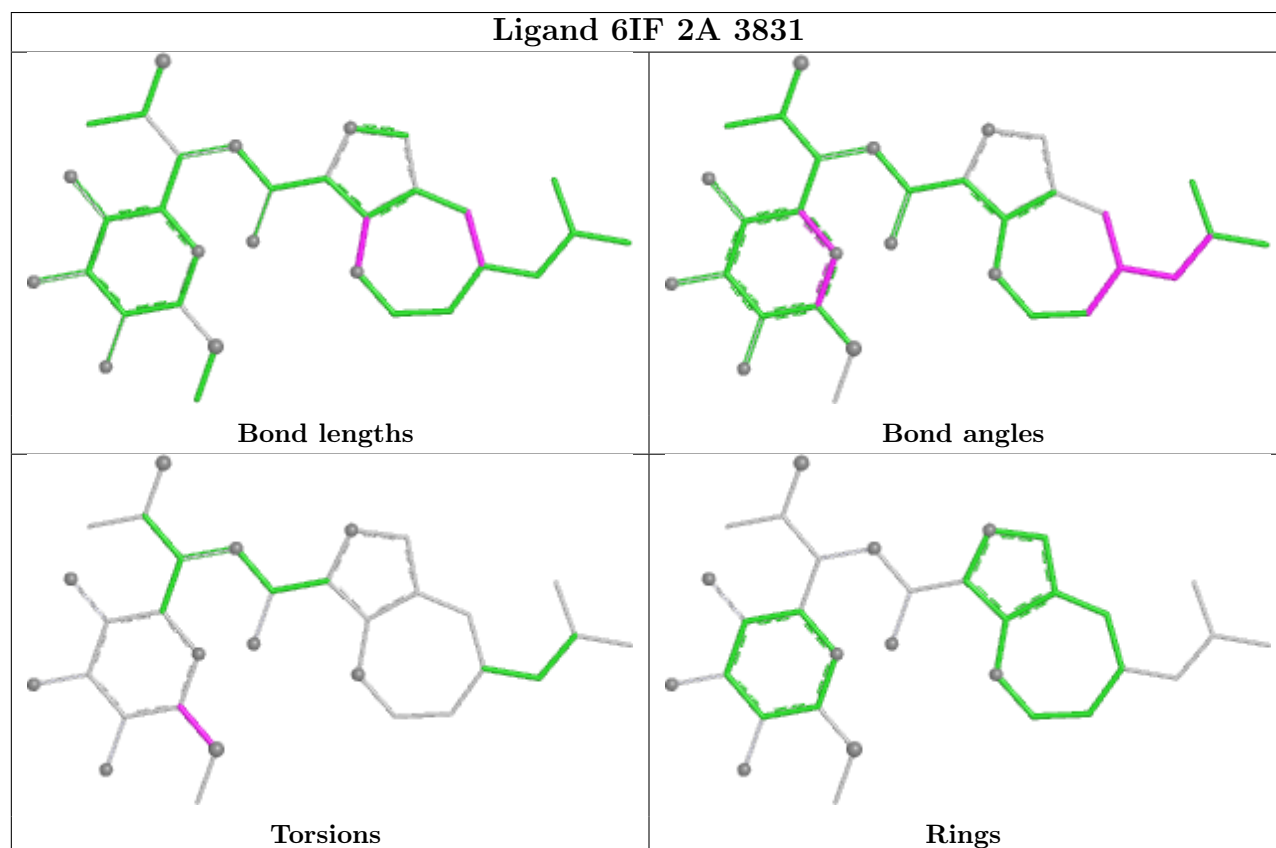
There are no ring outliers.

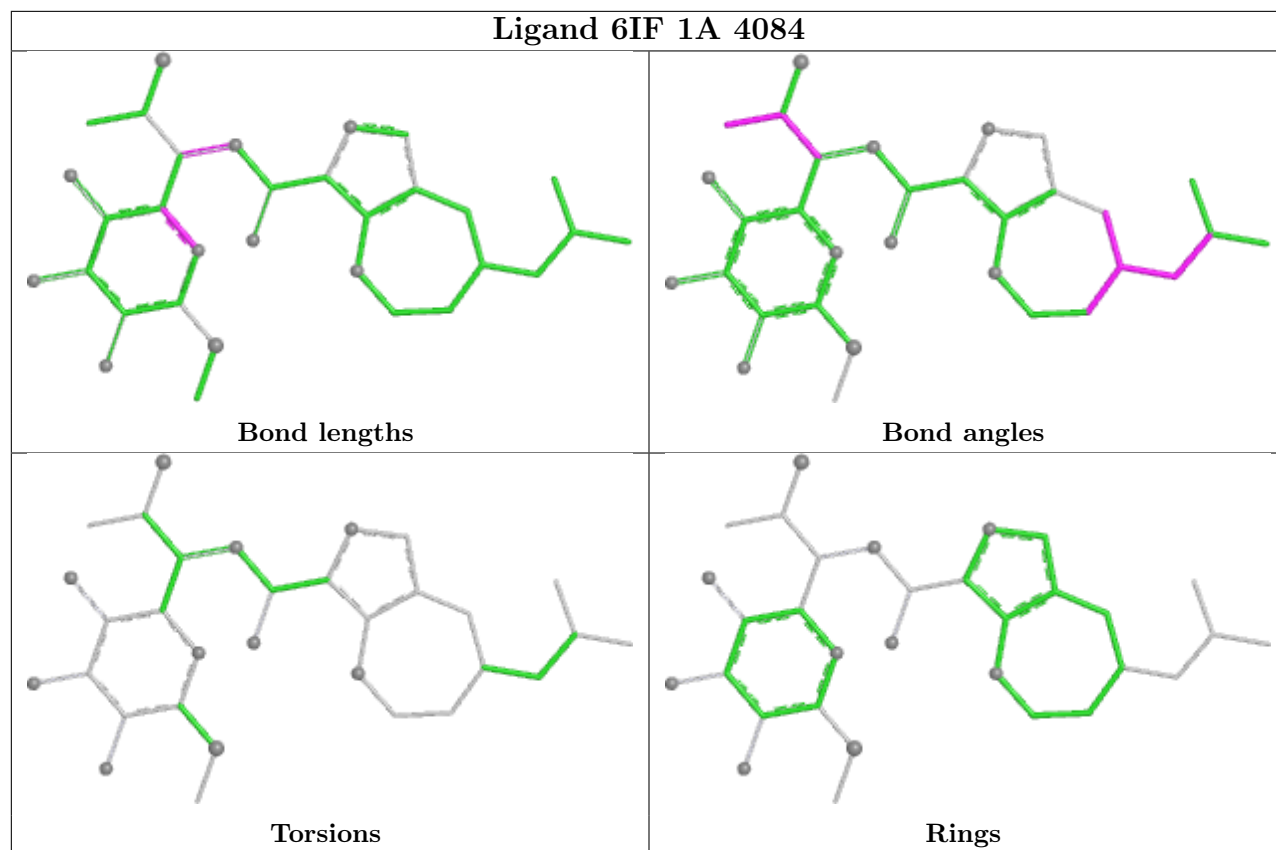
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	2d	303	SF4	2	0
59	1d	302	SF4	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.47	120 (4%)	40	41	23, 40, 97, 111	0
1	2A	2789/2915 (95%)	0.01	102 (3%)	45	46	39, 60, 95, 110	0
2	1B	120/121 (99%)	-0.40	0	100	100	35, 54, 67, 88	0
2	2B	120/121 (99%)	0.54	0	100	100	67, 77, 85, 93	0
3	1D	275/276 (99%)	-0.13	2 (0%)	84	86	25, 39, 53, 76	0
3	2D	275/276 (99%)	0.27	4 (1%)	72	73	32, 52, 65, 80	0
4	1E	204/206 (99%)	-0.10	1 (0%)	87	89	24, 42, 61, 78	0
4	2E	204/206 (99%)	0.59	7 (3%)	48	49	40, 61, 74, 82	0
5	1F	202/210 (96%)	0.00	2 (0%)	79	80	23, 46, 70, 85	0
5	2F	202/210 (96%)	0.66	7 (3%)	47	48	38, 69, 78, 84	0
6	1G	181/182 (99%)	0.56	7 (3%)	43	44	42, 59, 72, 85	0
6	2G	181/182 (99%)	1.04	15 (8%)	17	17	63, 77, 84, 89	0
7	1H	174/180 (96%)	0.33	3 (1%)	69	69	42, 57, 67, 75	0
7	2H	174/180 (96%)	1.62	52 (29%)	1	1	67, 84, 92, 97	0
8	1I	146/148 (98%)	0.79	6 (4%)	41	42	53, 74, 83, 87	0
8	2I	146/148 (98%)	1.00	10 (6%)	23	22	53, 73, 84, 87	0
9	1N	140/140 (100%)	-0.07	1 (0%)	84	86	29, 41, 64, 74	0
9	2N	140/140 (100%)	0.89	6 (4%)	40	40	51, 68, 80, 88	0
10	1O	122/122 (100%)	-0.13	1 (0%)	82	84	31, 44, 61, 66	0
10	2O	122/122 (100%)	0.54	1 (0%)	82	84	49, 61, 73, 76	0
11	1P	149/150 (99%)	0.17	1 (0%)	84	86	24, 51, 72, 79	0
11	2P	149/150 (99%)	0.63	8 (5%)	31	31	41, 68, 84, 92	0
12	1Q	141/141 (100%)	0.04	1 (0%)	84	86	32, 44, 61, 75	0
12	2Q	141/141 (100%)	0.94	11 (7%)	19	18	50, 69, 79, 84	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.20	1 (0%) 82 84	28, 38, 50, 63	0
13	2R	118/118 (100%)	0.29	1 (0%) 82 84	46, 55, 64, 71	0
14	1S	110/112 (98%)	0.23	2 (1%) 67 68	43, 54, 65, 69	0
14	2S	110/112 (98%)	1.06	10 (9%) 15 14	64, 72, 81, 87	0
15	1T	131/146 (89%)	0.25	5 (3%) 44 45	37, 49, 74, 80	0
15	2T	131/146 (89%)	0.72	4 (3%) 51 52	53, 64, 77, 82	0
16	1U	116/118 (98%)	-0.16	0 100 100	24, 32, 47, 63	0
16	2U	116/118 (98%)	0.63	3 (2%) 57 58	48, 66, 75, 80	0
17	1V	101/101 (100%)	-0.17	0 100 100	24, 41, 56, 63	0
17	2V	101/101 (100%)	0.91	6 (5%) 28 27	46, 73, 81, 91	0
18	1W	112/113 (99%)	-0.23	1 (0%) 81 83	26, 34, 52, 85	0
18	2W	112/113 (99%)	0.24	1 (0%) 81 83	43, 52, 70, 82	0
19	1X	95/96 (98%)	-0.02	2 (2%) 63 64	28, 42, 65, 81	0
19	2X	95/96 (98%)	0.64	4 (4%) 40 41	48, 60, 79, 88	0
20	1Y	107/110 (97%)	0.61	5 (4%) 36 36	40, 53, 69, 79	0
20	2Y	107/110 (97%)	1.14	14 (13%) 7 6	62, 72, 83, 90	0
21	1Z	154/206 (74%)	0.96	21 (13%) 7 5	43, 67, 86, 94	0
21	2Z	160/206 (77%)	1.72	51 (31%) 1 0	66, 83, 92, 96	0
22	10	83/85 (97%)	0.24	5 (6%) 27 27	33, 41, 65, 86	0
22	20	83/85 (97%)	1.15	13 (15%) 5 4	48, 65, 77, 89	0
23	11	97/98 (98%)	0.38	1 (1%) 79 80	31, 47, 72, 76	0
23	21	97/98 (98%)	0.50	4 (4%) 41 42	43, 56, 75, 81	0
24	12	70/72 (97%)	0.21	2 (2%) 53 55	39, 52, 63, 73	0
24	22	70/72 (97%)	0.65	1 (1%) 73 74	61, 71, 78, 82	0
25	13	59/60 (98%)	-0.18	1 (1%) 69 69	28, 39, 65, 78	0
25	23	59/60 (98%)	0.71	2 (3%) 48 49	59, 69, 80, 87	0
26	14	69/71 (97%)	0.88	8 (11%) 9 8	56, 77, 88, 91	0
26	24	69/71 (97%)	1.40	14 (20%) 3 2	74, 85, 92, 95	0
27	15	59/60 (98%)	-0.31	0 100 100	23, 33, 57, 63	0
27	25	59/60 (98%)	0.46	1 (1%) 69 69	43, 56, 66, 77	0
28	16	53/54 (98%)	-0.09	0 100 100	37, 45, 60, 66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.59	1 (1%) 66 66	53, 61, 69, 76	0
29	17	48/49 (97%)	-0.21	1 (2%) 63 64	25, 32, 54, 66	0
29	27	48/49 (97%)	0.31	5 (10%) 11 11	37, 44, 68, 73	0
30	18	64/65 (98%)	-0.28	0 100 100	31, 38, 45, 60	0
30	28	64/65 (98%)	0.59	0 100 100	47, 56, 63, 68	0
31	19	37/37 (100%)	-0.00	0 100 100	32, 44, 59, 62	0
31	29	37/37 (100%)	1.08	3 (8%) 18 17	61, 70, 78, 83	0
32	1a	1488/1521 (97%)	0.21	43 (2%) 53 55	35, 68, 94, 109	0
32	2a	1491/1521 (98%)	0.47	59 (3%) 42 43	51, 77, 96, 108	0
33	1b	231/256 (90%)	1.34	44 (19%) 3 2	66, 78, 87, 93	0
33	2b	231/256 (90%)	1.52	57 (24%) 2 1	75, 86, 92, 98	0
34	1c	206/239 (86%)	0.94	18 (8%) 16 15	61, 72, 83, 85	0
34	2c	206/239 (86%)	1.57	57 (27%) 1 1	74, 83, 88, 93	0
35	1d	208/209 (99%)	1.00	23 (11%) 10 9	54, 71, 79, 84	0
35	2d	208/209 (99%)	0.80	5 (2%) 59 61	63, 71, 78, 84	0
36	1e	148/162 (91%)	0.53	3 (2%) 65 65	51, 65, 75, 82	0
36	2e	148/162 (91%)	1.12	14 (9%) 14 13	66, 76, 84, 90	0
37	1f	100/101 (99%)	0.81	2 (2%) 65 65	58, 70, 76, 79	0
37	2f	100/101 (99%)	0.74	4 (4%) 42 43	56, 69, 77, 87	0
38	1g	155/156 (99%)	0.72	13 (8%) 17 16	61, 70, 83, 88	0
38	2g	155/156 (99%)	1.13	16 (10%) 12 11	70, 78, 86, 91	0
39	1h	137/138 (99%)	0.65	3 (2%) 62 63	56, 67, 74, 79	0
39	2h	137/138 (99%)	1.01	7 (5%) 33 33	67, 78, 82, 85	0
40	1i	127/128 (99%)	1.20	17 (13%) 7 5	52, 77, 84, 88	0
40	2i	127/128 (99%)	1.58	34 (26%) 1 1	71, 84, 90, 94	0
41	1j	97/105 (92%)	1.10	9 (9%) 14 13	58, 75, 84, 87	0
41	2j	96/105 (91%)	2.03	48 (50%) 0 0	73, 84, 92, 94	0
42	1k	114/129 (88%)	0.80	8 (7%) 22 21	45, 67, 76, 83	0
42	2k	114/129 (88%)	0.88	11 (9%) 13 13	56, 74, 83, 86	0
43	1l	121/132 (91%)	0.29	1 (0%) 82 84	46, 54, 68, 74	0
43	2l	121/132 (91%)	0.79	9 (7%) 20 19	58, 68, 79, 85	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.01	9 (7%) 21 20	56, 70, 78, 91	0
44	2m	122/126 (96%)	1.61	28 (22%) 2 2	71, 81, 87, 94	0
45	1n	60/61 (98%)	1.07	7 (11%) 9 8	60, 67, 75, 77	0
45	2n	60/61 (98%)	2.46	37 (61%) 0 0	77, 83, 87, 93	0
46	1o	88/89 (98%)	0.87	8 (9%) 15 14	51, 66, 75, 80	0
46	2o	88/89 (98%)	0.83	4 (4%) 38 38	61, 73, 82, 86	0
47	1p	82/88 (93%)	1.34	12 (14%) 6 5	58, 72, 79, 87	0
47	2p	82/88 (93%)	1.13	7 (8%) 16 16	60, 71, 78, 81	0
48	1q	99/105 (94%)	1.00	6 (6%) 27 26	53, 67, 78, 78	0
48	2q	99/105 (94%)	0.98	9 (9%) 15 14	63, 74, 82, 85	0
49	1r	68/88 (77%)	0.71	4 (5%) 28 27	58, 67, 80, 81	0
49	2r	68/88 (77%)	0.64	3 (4%) 39 39	65, 72, 79, 86	0
50	1s	83/93 (89%)	0.84	4 (4%) 35 35	66, 73, 80, 82	0
50	2s	83/93 (89%)	1.67	27 (32%) 1 0	77, 85, 89, 91	0
51	1t	96/106 (90%)	1.19	17 (17%) 4 3	61, 72, 80, 84	0
51	2t	96/106 (90%)	1.12	14 (14%) 6 5	61, 73, 83, 86	0
52	1u	23/27 (85%)	0.95	2 (8%) 16 15	61, 66, 72, 74	0
52	2u	23/27 (85%)	1.84	9 (39%) 1 0	74, 79, 81, 83	0
53	1v	13/24 (54%)	0.26	2 (15%) 5 4	51, 55, 88, 94	0
53	2v	13/24 (54%)	0.84	2 (15%) 5 4	67, 77, 90, 101	0
54	1w	66/76 (86%)	1.00	9 (13%) 7 5	54, 85, 99, 106	0
54	1y	67/76 (88%)	1.05	9 (13%) 7 5	40, 93, 101, 103	0
54	2w	63/76 (82%)	1.06	10 (15%) 5 4	75, 94, 104, 106	0
54	2y	66/76 (86%)	1.12	9 (13%) 7 5	54, 98, 103, 105	0
55	1x	71/77 (92%)	0.26	1 (1%) 73 74	34, 62, 81, 91	0
55	2x	71/77 (92%)	0.54	3 (4%) 40 41	49, 77, 88, 100	0
All	All	20868/21748 (95%)	0.40	1318 (6%) 26 25	23, 65, 90, 111	0

All (1318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	652(U)	G	10.0
44	2m	123	ALA	9.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	652(V)	C	9.8
1	2A	653	A	8.0
1	2A	652(C)	G	7.9
44	2m	124	PRO	7.8
1	1A	653	A	7.5
21	1Z	141	VAL	7.4
1	2A	654	A	7.2
1	1A	652(V)	C	6.9
1	2A	652(T)	C	6.8
21	2Z	172	ALA	6.7
1	1A	652(U)	G	6.6
1	1A	654	A	6.5
45	1n	2	ALA	6.4
22	10	6	GLY	6.3
44	1m	123	ALA	6.2
45	2n	2	ALA	5.8
21	2Z	150	LEU	5.7
41	2j	65	LEU	5.7
23	11	2	SER	5.6
54	1w	71	G	5.5
1	1A	652(C)	G	5.4
22	10	3	HIS	5.3
44	1m	124	PRO	5.2
38	2g	82	GLY	5.2
32	2a	1033	G	5.1
23	21	2	SER	5.1
51	1t	103	GLY	5.1
21	1Z	146	ILE	5.1
1	2A	2802	G	5.0
15	1T	131	ALA	5.0
22	20	2	ALA	5.0
21	1Z	149	SER	4.9
1	1A	1094	U	4.9
34	1c	2	GLY	4.9
1	1A	652(T)	C	4.9
32	1a	1034	G	4.8
45	2n	38	GLY	4.8
21	2Z	171	ILE	4.8
15	1T	130	ALA	4.8
33	2b	237	ALA	4.8
1	2A	2112	G	4.7
44	2m	122	LYS	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	652(S)	C	4.6
40	2i	11	LYS	4.6
41	2j	47	PHE	4.6
40	2i	102	LEU	4.5
1	1A	1087	G	4.5
20	2Y	54	LYS	4.5
21	2Z	173	ALA	4.5
33	2b	165	VAL	4.5
32	2a	1149	C	4.5
1	1A	1078	U	4.4
1	2A	2111	C	4.4
8	2I	146	ALA	4.4
1	1A	896	A	4.4
7	1H	2	SER	4.4
45	2n	34	TYR	4.4
50	2s	2	PRO	4.3
45	2n	7	ILE	4.3
1	2A	2146	C	4.3
41	2j	36	GLY	4.3
1	2A	2803	C	4.3
38	2g	16	LEU	4.3
26	24	56	VAL	4.3
45	2n	55	GLY	4.2
1	2A	883	G	4.2
52	2u	14	TRP	4.2
1	2A	652(B)	A	4.2
54	1w	73	A	4.2
7	2H	36	PRO	4.2
1	1A	1057	A	4.2
1	2A	2804	C	4.2
9	1N	9	VAL	4.2
45	2n	25	VAL	4.2
54	1w	1	G	4.2
12	2Q	15	GLY	4.1
40	1i	2	GLU	4.1
7	2H	136	ILE	4.1
1	2A	652(D)	C	4.1
50	2s	9	VAL	4.1
44	1m	2	ALA	4.1
7	2H	2	SER	4.1
41	2j	63	PHE	4.1
1	2A	2793	G	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	146	ILE	4.1
26	14	56	VAL	4.1
1	1A	1096	A	4.1
38	2g	84	ASN	4.1
54	1w	75	C	4.0
33	1b	237	ALA	4.0
7	1H	174	GLY	4.0
38	1g	80	VAL	4.0
54	2w	73	A	4.0
1	2A	885	C	4.0
32	1a	630	G	4.0
44	2m	102	ARG	4.0
21	2Z	174	VAL	4.0
51	1t	69	GLY	4.0
45	2n	3	ARG	4.0
44	2m	100	GLY	3.9
1	2A	2805	G	3.9
20	2Y	55	TYR	3.9
33	2b	236	TYR	3.9
33	2b	29	ALA	3.9
22	20	3	HIS	3.9
1	2A	2127	G	3.9
34	2c	188	LEU	3.9
25	23	2	PRO	3.9
51	2t	98	PRO	3.9
50	2s	45	VAL	3.9
1	2A	1509	C	3.9
45	2n	21	TYR	3.9
45	2n	20	ALA	3.9
33	2b	121	LEU	3.9
32	1a	1030(A)	G	3.8
21	2Z	147	GLY	3.8
50	2s	13	ASP	3.8
38	1g	2	ALA	3.8
21	2Z	95	PRO	3.8
1	1A	1095	A	3.8
21	2Z	164	ALA	3.8
40	2i	126	SER	3.8
34	2c	189	ALA	3.8
1	2A	2119	A	3.8
1	2A	2126	A	3.8
40	1i	81	ILE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1003	G	3.8
32	1a	1035	A	3.7
33	2b	39	ILE	3.7
38	2g	154	TYR	3.7
26	24	65	ASP	3.7
1	2A	884	C	3.7
1	2A	2145	C	3.7
21	2Z	141	VAL	3.7
32	1a	1001(A)	G	3.7
41	2j	76	ASN	3.7
1	1A	2119	A	3.7
41	2j	32	ALA	3.7
21	2Z	144	LEU	3.7
33	1b	125	PRO	3.7
1	1A	1086	A	3.7
21	2Z	170	THR	3.7
1	1A	897	C	3.7
1	1A	1068	G	3.7
41	2j	55	LYS	3.7
33	2b	17	PHE	3.6
40	2i	9	ARG	3.6
1	1A	1058	G	3.6
38	2g	156	TRP	3.6
50	2s	84	GLY	3.6
32	1a	1033	G	3.6
32	2a	1034	G	3.6
38	2g	80	VAL	3.6
42	2k	89	ALA	3.6
33	1b	11	LEU	3.6
1	2A	2133	G	3.6
45	2n	22	THR	3.6
54	1w	72	C	3.5
32	2a	1002	G	3.5
4	2E	115	GLY	3.5
33	1b	127	ILE	3.5
34	2c	48	TYR	3.5
1	2A	2117	A	3.5
6	1G	51	ARG	3.5
45	2n	12	ARG	3.5
33	2b	33	TYR	3.5
33	1b	10	LEU	3.5
33	2b	187	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	114	GLY	3.5
1	1A	652(E)	G	3.5
1	2A	2893	G	3.5
32	1a	1036	G	3.5
6	1G	146	TYR	3.5
6	1G	50	ALA	3.5
34	2c	2	GLY	3.5
41	2j	37	PRO	3.5
32	1a	1447	A	3.4
32	2a	1003	G	3.4
32	2a	1032	G	3.4
41	2j	49	VAL	3.4
11	1P	44	GLY	3.4
40	2i	49	PRO	3.4
32	2a	1219	U	3.4
54	2w	72	C	3.4
34	2c	8	ILE	3.4
34	2c	190	ARG	3.4
1	1A	1098	A	3.4
32	2a	1001(A)	G	3.4
45	2n	39	LEU	3.4
7	2H	128	PRO	3.4
46	1o	19	PRO	3.4
33	2b	123	ALA	3.4
38	2g	85	TYR	3.4
41	2j	59	SER	3.4
32	1a	1503	A	3.4
40	1i	19	LEU	3.4
44	2m	105	THR	3.4
1	2A	882	G	3.4
1	2A	2113	U	3.4
44	2m	101	GLN	3.4
1	2A	896	A	3.4
33	1b	229	VAL	3.4
33	2b	71	VAL	3.4
26	14	58	ARG	3.4
1	2A	2115	G	3.3
32	1a	1023	G	3.3
50	1s	13	ASP	3.3
40	2i	14	VAL	3.3
41	2j	77	PRO	3.3
45	2n	6	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	188	ALA	3.3
26	24	32	TYR	3.3
1	1A	2113	U	3.3
1	2A	2147	G	3.3
32	1a	1027	C	3.3
7	2H	79	VAL	3.3
51	2t	103	GLY	3.3
29	27	45	ALA	3.3
34	1c	65	ALA	3.3
45	1n	60	SER	3.3
26	24	51	ASP	3.3
32	1a	204	U	3.3
32	2a	1031	G	3.3
1	1A	885	C	3.3
7	2H	33	LEU	3.3
50	1s	71	LEU	3.3
44	2m	104	ARG	3.3
7	2H	19	VAL	3.3
34	2c	55	VAL	3.3
21	2Z	168	GLU	3.3
7	2H	72	ILE	3.3
20	2Y	94	LYS	3.3
32	2a	1035	A	3.3
44	1m	122	LYS	3.3
21	2Z	166	SER	3.3
48	2q	99	SER	3.3
1	1A	1093	G	3.3
32	2a	1030(A)	G	3.3
1	1A	888	C	3.3
32	2a	1038	C	3.3
20	2Y	1	MET	3.3
21	2Z	136	PHE	3.2
21	2Z	167	PRO	3.2
41	2j	90	LEU	3.2
52	2u	2	GLY	3.2
9	2N	83	LYS	3.2
34	2c	182	ILE	3.2
1	1A	652(D)	C	3.2
22	10	2	ALA	3.2
32	2a	1004	A	3.2
49	2r	66	LEU	3.2
33	1b	19	HIS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	52	VAL	3.2
33	1b	7	VAL	3.2
44	2m	6	GLY	3.2
54	2w	74	C	3.2
1	1A	880	G	3.2
55	2x	70	G	3.2
26	24	66	SER	3.2
1	1A	2114	A	3.2
7	2H	64	LEU	3.2
32	1a	1532	U	3.2
34	2c	195	VAL	3.2
54	2y	33	U	3.2
27	25	29	THR	3.2
47	2p	82	GLN	3.2
1	2A	2896	C	3.2
33	1b	17	PHE	3.2
1	2A	2751	G	3.2
1	2A	2894	G	3.2
19	2X	95	LEU	3.2
7	2H	41	MET	3.2
33	1b	172	ILE	3.2
41	2j	38	ILE	3.2
34	2c	53	ALA	3.1
21	2Z	149	SER	3.1
41	2j	35	SER	3.1
45	2n	37	PHE	3.1
21	2Z	159	PRO	3.1
1	2A	2155	G	3.1
26	24	63	TYR	3.1
41	2j	34	VAL	3.1
6	2G	20	ILE	3.1
1	2A	614(A)	U	3.1
47	2p	76	GLN	3.1
1	1A	2136	C	3.1
54	2w	4	C	3.1
1	2A	2131	G	3.1
26	24	50	VAL	3.1
33	2b	7	VAL	3.1
33	2b	66	GLY	3.1
45	2n	33	VAL	3.1
40	2i	10	ARG	3.1
41	1j	4	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	83	ALA	3.1
33	2b	12	GLU	3.1
49	1r	78	LEU	3.1
51	1t	62	LEU	3.1
1	2A	1536	C	3.1
32	2a	1030	C	3.1
40	2i	62	TYR	3.1
1	1A	1067	A	3.1
1	1A	1089	G	3.1
44	2m	121	LYS	3.1
1	2A	1026	U	3.1
9	2N	1	MET	3.1
41	2j	91	PRO	3.1
21	2Z	104	PHE	3.1
33	2b	10	LEU	3.1
33	2b	70	PHE	3.1
21	2Z	106	GLY	3.1
33	2b	136	VAL	3.1
33	2b	185	ILE	3.1
34	2c	137	ALA	3.0
38	1g	7	ALA	3.0
44	2m	33	ALA	3.0
1	2A	2807	G	3.0
25	13	2	PRO	3.0
54	2w	71	G	3.0
7	2H	17	VAL	3.0
44	2m	78	ILE	3.0
42	1k	25	TYR	3.0
21	2Z	151	HIS	3.0
1	1A	1081	U	3.0
21	2Z	125	LEU	3.0
32	1a	1026	G	3.0
21	2Z	143	GLY	3.0
32	1a	1030	C	3.0
33	2b	234	PRO	3.0
1	1A	1060	U	3.0
1	2A	2897	U	3.0
1	1A	883	G	3.0
50	1s	9	VAL	3.0
20	1Y	1	MET	3.0
33	2b	13	ALA	3.0
19	2X	68	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1029	C	3.0
37	2f	21	LEU	3.0
19	1X	94	GLY	3.0
51	1t	102	GLY	3.0
9	2N	5	VAL	2.9
39	2h	9	MET	2.9
40	2i	41	VAL	2.9
32	1a	1002	G	2.9
21	2Z	152	ALA	2.9
33	1b	97	TRP	2.9
45	2n	49	HIS	2.9
51	2t	97	ALA	2.9
41	2j	40	LEU	2.9
1	1A	2803	C	2.9
32	2a	470	C	2.9
1	1A	887	A	2.9
32	1a	344	A	2.9
32	2a	1005	A	2.9
21	2Z	139	VAL	2.9
33	1b	126	GLU	2.9
34	2c	75	VAL	2.9
38	2g	5	ARG	2.9
14	2S	33	LYS	2.9
42	1k	42	TRP	2.9
47	1p	48	TRP	2.9
7	2H	71	LEU	2.9
26	24	49	PHE	2.9
1	2A	2801(A)	A	2.9
21	2Z	96	VAL	2.9
21	2Z	126	VAL	2.9
39	1h	93	VAL	2.9
29	27	47	ARG	2.9
33	2b	21	ARG	2.9
38	1g	4	ARG	2.9
40	2i	128	ARG	2.9
33	1b	22	LYS	2.9
40	2i	82	ALA	2.9
45	2n	4	LYS	2.9
45	2n	30	ALA	2.9
6	1G	139	LEU	2.9
51	1t	13	LEU	2.9
1	2A	652(E)	G	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	1w	70	G	2.9
34	2c	201	TYR	2.9
46	1o	69	TYR	2.9
35	1d	154	ASN	2.9
35	1d	167	GLY	2.9
41	2j	78	ASN	2.9
42	2k	117	ASN	2.9
32	2a	1001	A	2.9
32	2a	1531	A	2.9
33	1b	230	VAL	2.9
40	1i	14	VAL	2.9
21	2Z	158	PRO	2.9
41	2j	100	THR	2.9
33	1b	34	ALA	2.9
33	1b	120	ALA	2.9
40	2i	13	ALA	2.9
45	2n	5	ALA	2.9
34	2c	43	LEU	2.9
34	2c	193	TYR	2.9
39	2h	58	TYR	2.9
11	2P	109	GLY	2.9
35	1d	191	ARG	2.8
33	1b	15	VAL	2.8
1	1A	1064	C	2.8
1	1A	2145	C	2.8
19	1X	95	LEU	2.8
36	2e	20	GLN	2.8
50	2s	12	ASP	2.8
20	1Y	91	GLU	2.8
6	2G	146	TYR	2.8
14	2S	7	TYR	2.8
40	1i	66	ARG	2.8
45	2n	17	LYS	2.8
6	1G	52	ILE	2.8
7	2H	4	ILE	2.8
14	2S	35	ILE	2.8
31	29	20	HIS	2.8
32	1a	1025	U	2.8
43	2l	39	VAL	2.8
54	1w	20	U	2.8
33	1b	131	PRO	2.8
15	2T	130	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	161	ALA	2.8
40	1i	13	ALA	2.8
33	2b	11	LEU	2.8
33	2b	51	LEU	2.8
34	1c	87	LEU	2.8
33	2b	122	PHE	2.8
34	2c	6	HIS	2.8
38	1g	82	GLY	2.8
34	1c	14	ILE	2.8
41	2j	82	ILE	2.8
7	2H	26	VAL	2.8
7	2H	43	VAL	2.8
1	1A	652(F)	G	2.8
1	1A	2793	G	2.8
1	1A	2802	G	2.8
21	1Z	159	PRO	2.8
44	2m	7	VAL	2.8
6	2G	50	ALA	2.8
8	2I	38	LEU	2.8
1	1A	1509	C	2.8
46	1o	47	LYS	2.8
5	1F	207	GLY	2.8
34	2c	158	GLY	2.8
34	2c	157	ILE	2.8
50	2s	80	TYR	2.8
21	1Z	166	SER	2.8
38	2g	77	SER	2.8
7	2H	39	PRO	2.8
1	1A	895	U	2.8
1	1A	2166	G	2.8
1	2A	2125	G	2.8
32	2a	1024	G	2.8
35	1d	192	GLU	2.8
1	1A	2117	A	2.8
1	1A	2790	A	2.8
18	1W	112	GLY	2.7
21	1Z	120	ILE	2.7
51	1t	55	ILE	2.7
26	14	63	TYR	2.7
42	1k	75	TYR	2.7
22	20	7	LEU	2.7
7	2H	175	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	2l	81	LYS	2.7
51	1t	14	LYS	2.7
1	1A	1056	G	2.7
1	1A	1059	G	2.7
1	2A	100	G	2.7
1	1A	548	A	2.7
1	1A	886	C	2.7
1	1A	2138	C	2.7
1	2A	2138	C	2.7
1	2A	2173	A	2.7
32	1a	1028	C	2.7
34	2c	62	ASP	2.7
33	2b	152	PHE	2.7
34	1c	13	GLY	2.7
40	2i	63	ILE	2.7
51	2t	24	LEU	2.7
8	1I	146	ALA	2.7
33	2b	22	LYS	2.7
35	1d	195	ALA	2.7
49	1r	20	ALA	2.7
45	2n	57	ARG	2.7
40	1i	91	ASP	2.7
32	2a	1036	G	2.7
32	2a	1117	G	2.7
1	2A	897	C	2.7
1	2A	2164	C	2.7
34	1c	57	ILE	2.7
4	1E	56	PRO	2.7
20	2Y	53	PRO	2.7
45	2n	14	PRO	2.7
7	2H	133	VAL	2.7
8	1I	91	SER	2.7
13	2R	14	SER	2.7
22	20	84	LEU	2.7
34	1c	72	LYS	2.7
44	2m	64	TRP	2.7
45	2n	44	LEU	2.7
33	1b	186	ALA	2.7
41	2j	5	ARG	2.7
41	2j	61	GLU	2.7
41	2j	73	ASP	2.7
36	2e	22	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	51	GLY	2.7
33	1b	200	ILE	2.7
34	1c	39	ILE	2.7
41	1j	77	PRO	2.7
41	2j	50	ILE	2.7
1	1A	879	G	2.7
1	1A	1063	G	2.7
32	1a	1032	G	2.7
1	1A	898	C	2.7
1	1A	1088	A	2.7
1	1A	2173	A	2.7
3	2D	276	LYS	2.7
32	1a	1030(B)	C	2.7
32	2a	1039	C	2.7
7	2H	24	VAL	2.7
7	2H	38	SER	2.7
9	2N	61	ARG	2.7
22	10	7	LEU	2.7
34	2c	130	VAL	2.7
45	1n	3	ARG	2.7
35	1d	173	TRP	2.7
48	2q	96	GLU	2.7
1	2A	271(K)	U	2.7
1	2A	2118	U	2.7
21	2Z	148	ASP	2.6
47	1p	68	ASP	2.6
21	1Z	147	GLY	2.6
26	14	59	PHE	2.6
15	1T	125	ARG	2.6
10	2O	57	VAL	2.6
32	2a	969	A	2.6
34	2c	116	VAL	2.6
40	1i	17	VAL	2.6
1	1A	2115	G	2.6
1	2A	2792	G	2.6
15	2T	131	ALA	2.6
21	1Z	170	THR	2.6
32	2a	950	U	2.6
40	2i	91	ASP	2.6
54	2w	45	U	2.6
6	1G	182	LYS	2.6
22	20	4	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	88	PHE	2.6
14	2S	3	ARG	2.6
33	2b	48	MET	2.6
21	2Z	2	GLU	2.6
29	27	46	VAL	2.6
38	1g	9	VAL	2.6
1	1A	652(A)	A	2.6
1	1A	2892	A	2.6
32	2a	1225	A	2.6
1	2A	894	C	2.6
1	2A	2137	C	2.6
32	1a	345	C	2.6
32	2a	1037	C	2.6
33	1b	62	ALA	2.6
34	2c	200	ALA	2.6
40	1i	106	ALA	2.6
54	1w	74	C	2.6
1	2A	881	G	2.6
1	2A	2154	G	2.6
1	2A	2166	G	2.6
32	2a	1220	G	2.6
48	2q	14	LYS	2.6
15	1T	129	ARG	2.6
33	1b	232	PRO	2.6
40	2i	96	LEU	2.6
50	2s	20	LEU	2.6
9	2N	45	ASN	2.6
39	2h	26	VAL	2.6
46	2o	60	VAL	2.6
49	1r	86	VAL	2.6
1	2A	1847	A	2.6
1	2A	2169	A	2.6
53	1v	13	A	2.6
1	2A	2136	C	2.6
14	2S	92	TYR	2.6
33	1b	33	TYR	2.6
54	1w	2	C	2.6
1	1A	2792	G	2.6
1	2A	11	G	2.6
1	2A	1533	G	2.6
32	1a	1024	G	2.6
5	2F	134	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	29	PRO	2.6
34	1c	62	ASP	2.6
40	2i	90	PRO	2.6
41	2j	93	GLY	2.6
41	2j	74	ILE	2.6
1	1A	271(K)	U	2.6
1	1A	1082	U	2.6
34	2c	10	PHE	2.6
19	2X	92	LEU	2.6
39	1h	112	LEU	2.6
7	2H	125	VAL	2.6
35	1d	170	VAL	2.6
43	2l	18	VAL	2.6
4	2E	204	ALA	2.6
51	1t	97	ALA	2.6
22	10	4	LYS	2.6
34	1c	184	TYR	2.6
38	1g	85	TYR	2.6
1	1A	884	C	2.5
1	2A	2794	C	2.5
32	1a	1019	C	2.5
37	1f	46	ARG	2.5
41	2j	66	ARG	2.5
7	2H	21	PRO	2.5
32	1a	66	G	2.5
54	1y	19	G	2.5
21	1Z	168	GLU	2.5
34	2c	128	PHE	2.5
40	1i	59	PHE	2.5
17	2V	94	LEU	2.5
20	1Y	106	LEU	2.5
21	1Z	150	LEU	2.5
33	1b	154	LEU	2.5
34	2c	47	LEU	2.5
55	2x	47	U	2.5
7	2H	35	VAL	2.5
21	1Z	139	VAL	2.5
21	2Z	121	HIS	2.5
5	2F	21	ALA	2.5
33	2b	77	ALA	2.5
41	2j	87	THR	2.5
45	1n	57	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2804	C	2.5
26	24	54	GLY	2.5
32	2a	1116	C	2.5
34	2c	145	GLY	2.5
34	2c	18	TRP	2.5
34	2c	124	ILE	2.5
21	2Z	169	GLU	2.5
33	1b	9	GLU	2.5
1	1A	2151	G	2.5
8	2I	75	LEU	2.5
33	1b	28	PHE	2.5
44	1m	56	LEU	2.5
45	1n	6	LEU	2.5
41	2j	13	HIS	2.5
40	1i	15	ALA	2.5
43	2l	68	ALA	2.5
35	1d	181	MET	2.5
34	2c	194	GLY	2.5
21	2Z	53	ILE	2.5
26	24	57	GLU	2.5
34	2c	77	ILE	2.5
47	2p	19	ILE	2.5
1	1A	2174	C	2.5
1	1A	2896	C	2.5
32	2a	1030(B)	C	2.5
54	2w	3	C	2.5
55	2x	69	C	2.5
39	1h	2	LEU	2.5
51	2t	99	LEU	2.5
33	2b	132	LYS	2.5
7	2H	44	VAL	2.5
9	2N	9	VAL	2.5
20	2Y	85	VAL	2.5
22	20	30	VAL	2.5
32	2a	1148	U	2.5
34	1c	207	VAL	2.5
44	2m	53	VAL	2.5
44	2m	60	VAL	2.5
54	1y	20	U	2.5
38	2g	2	ALA	2.5
50	2s	35	SER	2.5
21	1Z	1	MET	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	2U	62	ILE	2.5
1	2A	2158	A	2.5
1	2A	2170	A	2.5
32	2a	1016	A	2.5
3	1D	276	LYS	2.5
29	27	48	LYS	2.5
33	2b	44	LEU	2.5
48	2q	100	LYS	2.5
1	2A	888	C	2.5
1	2A	898	C	2.5
50	2s	14	HIS	2.5
40	2i	17	VAL	2.5
54	1y	45	U	2.5
34	2c	149	ALA	2.5
45	2n	10	ALA	2.5
22	20	43	THR	2.5
1	1A	882	G	2.5
1	2A	2157	G	2.5
1	2A	2168	G	2.5
8	2I	1	MET	2.5
32	1a	1031	G	2.5
32	2a	1021	G	2.5
32	2a	1222	G	2.5
23	21	28	GLY	2.4
33	1b	50	GLU	2.4
50	2s	26	GLY	2.4
52	2u	4	GLY	2.4
35	2d	5	ILE	2.4
41	2j	23	ILE	2.4
42	2k	25	TYR	2.4
43	2l	64	TYR	2.4
52	2u	5	ASP	2.4
1	1A	1103	A	2.4
1	2A	2134	A	2.4
1	2A	2135	A	2.4
38	2g	76	ARG	2.4
45	2n	31	ARG	2.4
50	2s	29	ARG	2.4
50	2s	34	TRP	2.4
1	2A	2163	C	2.4
8	1I	107	VAL	2.4
32	1a	92	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	15	VAL	2.4
33	2b	164	VAL	2.4
40	2i	109	VAL	2.4
6	2G	169	ALA	2.4
40	2i	45	ALA	2.4
45	2n	13	THR	2.4
47	2p	69	THR	2.4
50	2s	4	SER	2.4
33	2b	183	PRO	2.4
1	1A	2124	G	2.4
1	1A	2141	G	2.4
1	1A	2159	G	2.4
1	2A	1171	G	2.4
3	2D	38	LYS	2.4
34	2c	13	GLY	2.4
36	1e	22	GLY	2.4
48	1q	100	LYS	2.4
33	1b	39	ILE	2.4
33	1b	214	ILE	2.4
33	2b	42	ILE	2.4
51	1t	100	ILE	2.4
12	2Q	113	GLN	2.4
33	2b	31	TYR	2.4
35	1d	188	LEU	2.4
40	2i	79	LEU	2.4
42	2k	59	TYR	2.4
22	20	69	PHE	2.4
38	1g	5	ARG	2.4
1	1A	899	A	2.4
1	2A	2892	A	2.4
32	2a	1503	A	2.4
5	2F	6	VAL	2.4
6	2G	159	VAL	2.4
7	2H	114	VAL	2.4
1	1A	889	C	2.4
34	2c	168	ALA	2.4
44	2m	72	ALA	2.4
50	2s	24	ALA	2.4
41	2j	14	LYS	2.4
35	1d	87	GLY	2.4
1	2A	2116	G	2.4
1	2A	2159	G	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	53	LEU	2.4
32	2a	1224	G	2.4
54	2y	57	G	2.4
11	2P	15	ARG	2.4
33	2b	40	HIS	2.4
40	2i	66	ARG	2.4
38	1g	154	TYR	2.4
33	2b	55	PHE	2.4
5	2F	183	VAL	2.4
22	20	66	VAL	2.4
34	2c	153	VAL	2.4
1	1A	1070	A	2.4
1	1A	1073	A	2.4
32	2a	1447	A	2.4
54	2y	36	A	2.4
7	2H	20	ALA	2.4
35	2d	195	ALA	2.4
52	2u	23	PRO	2.4
42	1k	53	SER	2.4
48	2q	39	SER	2.4
33	1b	18	GLY	2.4
52	2u	16	GLY	2.4
11	2P	77	ARG	2.4
21	1Z	148	ASP	2.4
33	1b	40	HIS	2.4
46	1o	31	LEU	2.4
50	2s	15	LEU	2.4
1	1A	2116	G	2.4
1	2A	2148	G	2.4
1	2A	2156	G	2.4
21	2Z	89	PHE	2.4
32	2a	1023	G	2.4
40	2i	36	TYR	2.4
47	1p	80	PHE	2.4
54	2w	70	G	2.4
21	2Z	86	VAL	2.4
21	2Z	105	VAL	2.4
31	29	16	VAL	2.4
36	2e	51	VAL	2.4
45	2n	18	VAL	2.4
41	1j	76	ASN	2.4
22	20	5	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	655	A	2.4
32	1a	1030(D)	A	2.4
32	1a	1531	A	2.4
32	2a	1030(D)	A	2.4
51	2t	95	ALA	2.4
44	2m	58	GLU	2.4
45	2n	8	GLU	2.4
53	2v	12	A	2.4
53	2v	13	A	2.4
21	1Z	95	PRO	2.3
47	2p	45	THR	2.3
32	2a	1532	U	2.3
54	2y	60	U	2.3
1	2A	2128	C	2.3
32	2a	1249	C	2.3
51	2t	101	GLY	2.3
4	2E	77	ILE	2.3
35	1d	132	ARG	2.3
38	2g	32	ARG	2.3
50	2s	31	ILE	2.3
51	2t	25	ARG	2.3
7	2H	7	LEU	2.3
48	1q	13	ASP	2.3
49	2r	76	LEU	2.3
22	20	45	PHE	2.3
50	2s	10	PHE	2.3
14	2S	85	VAL	2.3
21	1Z	165	VAL	2.3
42	2k	14	VAL	2.3
50	2s	18	LYS	2.3
1	1A	1099	G	2.3
1	1A	2110	G	2.3
1	1A	2894	G	2.3
32	2a	1202	G	2.3
54	2y	19	G	2.3
8	1I	65	ALA	2.3
21	2Z	21	ALA	2.3
34	1c	100	ALA	2.3
40	2i	2	GLU	2.3
45	2n	59	ALA	2.3
41	2j	41	PRO	2.3
34	2c	15	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	191	THR	2.3
1	1A	229	A	2.3
1	2A	899	A	2.3
32	1a	143	A	2.3
32	2a	1286	A	2.3
12	2Q	60	ARG	2.3
17	2V	56	SER	2.3
50	2s	36	ARG	2.3
1	1A	1065	U	2.3
1	1A	1097	U	2.3
33	1b	187	LEU	2.3
34	2c	5	ILE	2.3
44	2m	9	ILE	2.3
46	1o	66	LEU	2.3
1	2A	645	C	2.3
32	2a	1006	C	2.3
32	2a	1018	C	2.3
55	1x	69	C	2.3
36	2e	10	MET	2.3
15	2T	22	PHE	2.3
51	2t	27	LYS	2.3
21	1Z	99	TYR	2.3
37	2f	59	TYR	2.3
40	2i	65	VAL	2.3
26	14	57	GLU	2.3
33	2b	34	ALA	2.3
1	2A	171	G	2.3
1	2A	2165	G	2.3
32	1a	79	G	2.3
32	1a	346	G	2.3
32	2a	1182	G	2.3
1	1A	1046	A	2.3
21	1Z	52	SER	2.3
26	14	17	GLY	2.3
32	1a	1286	A	2.3
45	1n	51	GLY	2.3
51	2t	96	GLY	2.3
33	2b	162	ILE	2.3
33	2b	213	LEU	2.3
34	1c	124	ILE	2.3
32	1a	1257	U	2.3
21	2Z	1	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1027	C	2.3
34	2c	135	LYS	2.3
51	1t	68	LYS	2.3
12	2Q	104	PHE	2.3
21	1Z	136	PHE	2.3
26	24	59	PHE	2.3
6	1G	48	GLU	2.3
33	1b	31	TYR	2.3
40	2i	125	TYR	2.3
43	2l	55	VAL	2.3
7	2H	10	PRO	2.3
21	2Z	130	PRO	2.3
44	1m	5	ALA	2.3
49	2r	20	ALA	2.3
21	1Z	103	ARG	2.3
42	2k	54	ARG	2.3
19	2X	94	GLY	2.3
33	2b	19	HIS	2.3
36	2e	23	GLY	2.3
1	1A	2165	G	2.3
1	2A	2149	G	2.3
21	2Z	142	SER	2.3
7	2H	171	LEU	2.3
10	1O	91	LEU	2.3
21	2Z	76	LEU	2.3
32	1a	1021	G	2.3
41	1j	75	ILE	2.3
47	1p	49	LEU	2.3
50	2s	5	LEU	2.3
51	1t	10	LEU	2.3
1	1A	1509(A)	A	2.3
33	2b	83	MET	2.3
40	2i	105	ASP	2.3
1	1A	2109	U	2.3
1	1A	2150	U	2.3
1	1A	34	C	2.3
1	2A	2129	C	2.3
32	2a	1043	C	2.3
32	2a	1115	C	2.3
35	2d	192	GLU	2.3
16	2U	90	VAL	2.3
40	1i	28	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	117	VAL	2.3
12	1Q	32	TYR	2.3
24	12	69	ARG	2.3
33	1b	234	PRO	2.3
38	2g	4	ARG	2.3
38	2g	112	PRO	2.3
34	2c	23	TYR	2.3
45	2n	35	ARG	2.3
34	2c	160	ALA	2.2
44	2m	103	THR	2.2
50	2s	63	THR	2.2
33	2b	14	GLY	2.2
42	2k	49	GLY	2.2
46	1o	89	GLY	2.2
21	2Z	153	SER	2.2
1	1A	1174	A	2.2
1	2A	2114	A	2.2
6	2G	126	ASP	2.2
54	1y	36	A	2.2
1	1A	271(I)	G	2.2
1	1A	2152	G	2.2
1	1A	2190	G	2.2
1	1A	1026	U	2.2
1	1A	2167	U	2.2
1	1A	2897	U	2.2
32	1a	65	U	2.2
32	2a	1025	U	2.2
8	2I	135	GLU	2.2
36	2e	45	PHE	2.2
20	1Y	73	ARG	2.2
26	24	68	ARG	2.2
1	1A	1080	C	2.2
7	2H	15	VAL	2.2
35	2d	112	VAL	2.2
43	2l	41	ARG	2.2
44	1m	53	VAL	2.2
47	1p	21	VAL	2.2
54	2w	2	C	2.2
34	1c	71	ALA	2.2
51	1t	95	ALA	2.2
33	1b	228	GLY	2.2
33	2b	133	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	1i	8	GLY	2.2
42	1k	51	LYS	2.2
6	2G	3	LEU	2.2
6	2G	133	LEU	2.2
34	2c	34	LEU	2.2
34	2c	52	LEU	2.2
41	2j	88	LEU	2.2
44	2m	66	LEU	2.2
12	2Q	66	ILE	2.2
31	29	10	ILE	2.2
33	1b	222	ILE	2.2
7	2H	32	GLU	2.2
1	2A	2144	U	2.2
1	2A	2895	U	2.2
1	1A	2112	G	2.2
1	1A	2125	G	2.2
1	1A	2162	G	2.2
32	1a	1030(C)	G	2.2
32	2a	485	G	2.2
35	1d	122	ARG	2.2
35	1d	153	ARG	2.2
36	2e	27	ARG	2.2
41	1j	79	ARG	2.2
41	2j	79	ARG	2.2
52	2u	6	ARG	2.2
54	2w	19	G	2.2
7	2H	123	PHE	2.2
35	1d	110	PHE	2.2
42	2k	125	PHE	2.2
7	2H	11	VAL	2.2
33	2b	229	VAL	2.2
42	1k	14	VAL	2.2
45	1n	33	VAL	2.2
45	2n	54	PRO	2.2
1	1A	2111	C	2.2
1	2A	271(J)	C	2.2
1	2A	2139	C	2.2
18	2W	60	ASN	2.2
32	1a	1008	C	2.2
34	2c	181	ASN	2.2
38	1g	84	ASN	2.2
7	2H	157	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	2P	39	LYS	2.2
17	2V	12	TYR	2.2
36	1e	20	GLN	2.2
47	1p	39	TYR	2.2
51	1t	74	LYS	2.2
7	2H	120	GLY	2.2
8	1I	38	LEU	2.2
11	2P	6	LEU	2.2
12	2Q	30	GLY	2.2
20	2Y	5	MET	2.2
21	1Z	102	LEU	2.2
39	2h	2	LEU	2.2
6	2G	39	ILE	2.2
35	1d	5	ILE	2.2
20	2Y	91	GLU	2.2
16	2U	12	ARG	2.2
33	2b	24	TRP	2.2
33	2b	36	ARG	2.2
34	1c	190	ARG	2.2
47	1p	59	TRP	2.2
1	1A	1069	A	2.2
1	2A	9	U	2.2
32	2a	983	A	2.2
54	1y	35	A	2.2
8	2I	8	PRO	2.2
14	2S	29	PHE	2.2
21	1Z	104	PHE	2.2
4	2E	196	VAL	2.2
12	2Q	109	VAL	2.2
33	2b	93	VAL	2.2
33	2b	230	VAL	2.2
34	2c	66	VAL	2.2
34	2c	207	VAL	2.2
41	1j	44	VAL	2.2
41	1j	49	VAL	2.2
1	1A	1537	G	2.2
32	2a	1221	G	2.2
7	2H	96	ALA	2.2
8	2I	100	ALA	2.2
33	2b	8	LYS	2.2
34	2c	65	ALA	2.2
36	2e	138	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2k	124	LYS	2.2
1	1A	1079	C	2.2
5	2F	24	LEU	2.2
26	14	32	TYR	2.2
32	2a	1223	C	2.2
33	1b	44	LEU	2.2
33	1b	72	GLY	2.2
34	1c	193	TYR	2.2
42	2k	75	TYR	2.2
47	1p	22	THR	2.2
48	2q	95	TYR	2.2
52	2u	8	THR	2.2
40	2i	99	LEU	2.2
41	1j	40	LEU	2.2
51	1t	53	LEU	2.2
33	2b	214	ILE	2.2
33	2b	223	ILE	2.2
46	2o	3	ILE	2.2
47	1p	33	ILE	2.2
51	2t	63	ILE	2.2
13	1R	15	SER	2.2
21	2Z	52	SER	2.2
4	2E	73	GLU	2.2
20	2Y	107	ASP	2.2
33	2b	86	GLU	2.2
35	1d	150	GLU	2.2
7	2H	59	ARG	2.2
15	2T	112	ARG	2.2
22	20	44	ARG	2.2
35	1d	209	ARG	2.2
41	2j	51	ARG	2.2
6	2G	142	PRO	2.2
1	1A	900	A	2.1
1	2A	895	U	2.2
45	2n	36	PHE	2.2
54	1y	47	U	2.2
54	2y	21	A	2.1
20	2Y	48	ALA	2.1
21	2Z	51	ALA	2.1
41	2j	33	GLN	2.1
1	1A	1091	G	2.1
4	2E	6	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	82	GLY	2.1
20	2Y	58	GLY	2.1
46	2o	89	GLY	2.1
48	1q	98	LEU	2.1
50	2s	33	THR	2.1
7	2H	83	TYR	2.1
7	2H	92	ILE	2.1
33	2b	41	ILE	2.1
35	1d	54	TYR	2.1
35	1d	207	TYR	2.1
6	2G	136	ARG	2.1
11	2P	149	GLU	2.1
22	20	68	GLU	2.1
17	2V	73	SER	2.1
26	24	55	ARG	2.1
44	2m	88	ARG	2.1
52	2u	24	ARG	2.1
21	2Z	140	ASP	2.1
3	2D	275	LYS	2.1
37	2f	96	PRO	2.1
5	2F	142	TRP	2.1
6	2G	29	TRP	2.1
33	1b	163	PHE	2.1
7	2H	45	VAL	2.1
34	2c	68	VAL	2.1
34	2c	76	VAL	2.1
1	1A	1066	U	2.1
32	1a	1020	U	2.1
1	1A	1077	A	2.1
1	2A	2171	A	2.1
8	2I	104	GLN	2.1
5	2F	166	ALA	2.1
29	17	45	ALA	2.1
32	1a	1001	A	2.1
37	1f	27	GLN	2.1
33	1b	13	ALA	2.1
8	2I	16	GLY	2.1
33	1b	61	LEU	2.1
36	2e	119	LEU	2.1
38	1g	81	GLY	2.1
44	2m	90	LEU	2.1
6	2G	52	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	201	ILE	2.1
47	1p	4	ILE	2.1
7	2H	6	ARG	2.1
14	1S	3	ARG	2.1
34	2c	140	ARG	2.1
39	2h	30	ARG	2.1
43	2l	69	TYR	2.1
45	2n	29	ARG	2.1
1	1A	1176	G	2.1
1	1A	2207	G	2.1
1	1A	2893	G	2.1
54	1y	18	G	2.1
1	1A	2137	C	2.1
1	2A	886	C	2.1
6	2G	76	SER	2.1
50	2s	38	SER	2.1
44	2m	31	LYS	2.1
41	2j	39	PRO	2.1
50	2s	76	PRO	2.1
41	2j	11	PHE	2.1
50	2s	47	HIS	2.1
28	26	5	VAL	2.1
36	2e	148	VAL	2.1
32	2a	1257	U	2.1
1	2A	655	A	2.1
12	2Q	19	GLY	2.1
17	2V	54	GLY	2.1
21	2Z	102	LEU	2.1
34	2c	87	LEU	2.1
34	2c	205	GLY	2.1
40	2i	85	LEU	2.1
41	2j	71	LEU	2.1
43	2l	63	GLY	2.1
25	23	29	ARG	2.1
52	1u	24	ARG	2.1
34	2c	14	ILE	2.1
44	2m	4	ILE	2.1
44	1m	87	TYR	2.1
3	2D	99	ASP	2.1
40	2i	70	LYS	2.1
51	1t	38	LYS	2.1
1	1A	2149	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	1114	G	2.1
1	2A	2110	G	2.1
32	2a	1042	G	2.1
32	2a	1127	G	2.1
54	1y	44	G	2.1
54	2y	18	G	2.1
1	2A	2175	C	2.1
11	2P	78	PRO	2.1
44	2m	97	PRO	2.1
54	2y	56	C	2.1
33	1b	48	MET	2.1
15	1T	123	GLN	2.1
20	2Y	57	GLN	2.1
7	2H	50	VAL	2.1
7	2H	107	VAL	2.1
14	2S	28	VAL	2.1
36	2e	90	VAL	2.1
38	1g	91	VAL	2.1
47	2p	20	VAL	2.1
48	1q	27	PHE	2.1
48	1q	71	PHE	2.1
12	2Q	121	ALA	2.1
42	1k	60	ALA	2.1
51	1t	12	ALA	2.1
7	2H	3	ARG	2.1
7	2H	88	LEU	2.1
14	1S	48	LEU	2.1
20	2Y	50	ARG	2.1
20	2Y	90	LEU	2.1
21	2Z	157	LEU	2.1
32	2a	1126	U	2.1
34	1c	47	LEU	2.1
34	1c	178	LEU	2.1
34	2c	167	TRP	2.1
35	2d	154	ASN	2.1
41	1j	78	ASN	2.1
34	2c	79	ARG	2.1
41	2j	46	ARG	2.1
42	1k	126	ARG	2.1
47	1p	5	ARG	2.1
51	2t	86	ARG	2.1
34	2c	19	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	1i	12	GLU	2.1
41	2j	42	THR	2.1
1	1A	1054	A	2.1
7	1H	4	ILE	2.1
34	2c	57	ILE	2.1
41	2j	75	ILE	2.1
45	2n	42	ILE	2.1
53	1v	12	A	2.1
54	1y	58	A	2.1
3	1D	38	LYS	2.1
36	2e	47	LYS	2.1
14	2S	36	TYR	2.1
41	2j	17	ASP	2.1
50	1s	12	ASP	2.1
29	27	1	MET	2.1
1	1A	1092	C	2.1
51	2t	73	HIS	2.1
1	1A	2805	G	2.0
32	1a	70	G	2.0
5	1F	89	VAL	2.0
21	2Z	71	VAL	2.0
38	2g	66	VAL	2.0
40	1i	37	PHE	2.0
41	2j	54	PHE	2.0
43	2l	32	PHE	2.0
47	2p	80	PHE	2.0
8	2I	83	ALA	2.0
12	2Q	59	ARG	2.0
38	1g	3	ARG	2.0
40	1i	20	ARG	2.0
40	2i	20	ARG	2.0
43	1l	19	ARG	2.0
35	1d	77	ASN	2.0
35	1d	120	LEU	2.0
40	1i	50	LEU	2.0
40	2i	19	LEU	2.0
7	2H	58	GLU	2.0
11	2P	82	GLY	2.0
48	2q	80	GLY	2.0
50	2s	68	GLY	2.0
1	1A	2172	U	2.0
7	2H	89	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	122	THR	2.0
12	2Q	22	LYS	2.0
32	2a	1000	U	2.0
32	2a	1150	U	2.0
37	2f	52	ILE	2.0
40	2i	7	THR	2.0
46	1o	12	ILE	2.0
48	1q	20	THR	2.0
1	2A	229	A	2.0
26	14	67	TYR	2.0
33	2b	148	TYR	2.0
42	2k	50	TYR	2.0
46	2o	69	TYR	2.0
36	1e	10	MET	2.0
51	1t	11	SER	2.0
41	2j	62	HIS	2.0
24	12	70	GLN	2.0
35	1d	62	GLN	2.0
1	1A	2128	C	2.0
17	2V	14	VAL	2.0
35	1d	118	ARG	2.0
39	2h	18	ARG	2.0
39	2h	19	VAL	2.0
40	2i	44	VAL	2.0
41	2j	72	VAL	2.0
45	2n	19	ARG	2.0
46	1o	88	ARG	2.0
1	1A	2156	G	2.0
44	2m	30	ALA	2.0
48	2q	98	LEU	2.0
49	1r	73	ALA	2.0
54	2y	44	G	2.0
7	2H	105	LEU	2.0
8	1I	35	LEU	2.0
14	2S	32	LEU	2.0
21	2Z	155	LEU	2.0
23	21	83	GLU	2.0
24	22	60	LEU	2.0
33	2b	61	LEU	2.0
36	2e	112	LEU	2.0
41	2j	16	LEU	2.0
4	2E	106	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	1Y	92	ASN	2.0
44	1m	121	LYS	2.0
51	2t	47	GLY	2.0
21	2Z	57	ILE	2.0
41	2j	48	THR	2.0
1	2A	2130	U	2.0
45	2n	61	TRP	2.0
1	2A	1445	A	2.0
26	24	29	PRO	2.0
34	2c	73	PRO	2.0
47	1p	66	PRO	2.0
48	2q	2	PRO	2.0
40	2i	92	TYR	2.0
52	1u	18	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	PSU	2y	55	20/21	0.55	0.17	92,102,113,117	0
54	G7M	2w	46	24/25	0.61	0.16	85,96,111,121	0
54	G7M	2y	46	24/25	0.63	0.17	96,100,104,123	0
54	G7M	1w	46	24/25	0.64	0.17	78,90,109,132	0
54	G7M	1y	46	24/25	0.65	0.18	84,96,103,119	0
54	4SU	2y	8	20/21	0.67	0.15	93,99,109,120	0
54	5MU	2y	54	21/22	0.70	0.15	88,94,104,118	0
54	PSU	1y	55	20/21	0.73	0.14	92,99,105,112	0
54	5MU	1y	54	21/22	0.73	0.15	88,93,102,111	0
54	MIA	2y	37	22/30	0.74	0.14	85,91,97,107	0
54	4SU	2w	8	20/21	0.76	0.13	86,94,103,115	0
54	4SU	1y	8	20/21	0.79	0.12	91,94,105,106	0
54	PSU	2y	39	20/21	0.80	0.13	86,90,99,105	0
54	PSU	2y	32	20/21	0.80	0.14	84,89,98,101	0
54	MIA	1y	37	22/30	0.83	0.12	80,88,92,96	0
54	PSU	1y	39	20/21	0.84	0.12	83,86,92,99	0
54	PSU	2w	55	20/21	0.85	0.11	79,88,95,101	0
54	PSU	1y	32	20/21	0.85	0.12	80,86,93,94	0
54	MIA	2w	37	25/30	0.88	0.14	67,77,83,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	2w	32	20/21	0.88	0.12	76,83,92,96	0
55	4SU	2x	8	20/21	0.89	0.12	77,81,85,87	0
55	PSU	2x	55	20/21	0.90	0.09	68,74,83,92	0
55	5MU	2x	54	21/22	0.90	0.11	73,78,84,92	0
54	4SU	1w	8	20/21	0.91	0.11	77,84,90,93	0
1	PSU	2A	1917	20/21	0.91	0.10	57,66,72,73	0
54	5MU	2w	54	21/22	0.92	0.11	73,80,83,90	0
43	0TD	2l	92	10/11	0.92	0.11	62,65,71,79	0
54	PSU	1w	55	20/21	0.92	0.09	61,77,81,85	0
55	5MC	2x	32	21/22	0.92	0.15	66,74,78,86	0
32	PSU	2a	516	20/21	0.92	0.10	67,73,77,77	0
32	G7M	2a	527	24/25	0.92	0.11	60,64,70,83	0
1	5MU	2A	1915	21/22	0.92	0.11	60,67,70,77	0
32	2MG	2a	1207	24/25	0.92	0.11	77,86,89,89	0
55	5MC	1x	32	21/22	0.93	0.14	50,57,60,74	0
55	5MU	1x	54	21/22	0.93	0.10	60,66,72,74	0
32	5MC	2a	967	21/22	0.93	0.12	66,71,78,82	0
55	PSU	1x	55	20/21	0.93	0.09	56,62,68,71	0
32	5MC	2a	1400	21/22	0.93	0.15	68,73,78,85	0
32	4OC	2a	1402	22/23	0.93	0.12	56,66,69,71	0
32	5MC	2a	1404	21/22	0.93	0.10	52,60,63,65	0
43	0TD	1l	92	10/11	0.93	0.09	48,54,56,67	0
32	2MG	1a	1207	24/25	0.93	0.11	63,69,74,75	0
32	PSU	1a	516	20/21	0.94	0.09	54,60,66,66	0
54	PSU	1w	32	20/21	0.94	0.10	59,65,72,74	0
1	PSU	2A	1911	20/21	0.94	0.09	57,60,65,66	0
32	M2G	2a	966	25/26	0.94	0.13	65,69,79,83	0
54	MIA	1w	37	29/30	0.94	0.13	44,56,68,91	0
54	PSU	2w	39	20/21	0.95	0.09	70,79,84,85	0
32	MA6	2a	1519	24/25	0.95	0.12	58,66,69,74	0
32	MA6	1a	1519	24/25	0.95	0.09	39,44,49,53	0
55	4SU	1x	8	20/21	0.95	0.10	48,64,70,76	0
1	5MU	1A	1915	21/22	0.95	0.09	52,59,62,64	0
32	G7M	1a	527	24/25	0.95	0.10	43,49,56,60	0
54	5MU	1w	54	21/22	0.95	0.08	53,68,73,74	0
1	OMC	2A	1920	21/22	0.95	0.09	52,61,64,68	0
1	5MC	1A	1942	21/22	0.95	0.11	38,46,51,53	0
1	5MC	2A	1962	21/22	0.95	0.10	40,49,58,64	0
54	PSU	1w	39	20/21	0.96	0.09	58,63,70,77	0
32	5MC	1a	1400	21/22	0.96	0.09	46,52,58,62	0
1	PSU	1A	1911	20/21	0.96	0.08	43,48,57,58	0
32	4OC	1a	1402	22/23	0.96	0.09	43,47,51,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	31H	2x	76	32/33	0.96	0.10	44,50,56,60	0
32	5MC	2a	1407	21/22	0.96	0.09	53,58,61,64	0
1	PSU	1A	1917	20/21	0.96	0.07	46,55,59,59	0
32	UR3	2a	1498	21/22	0.96	0.11	57,64,66,67	0
32	MA6	2a	1518	24/25	0.96	0.10	58,67,71,73	0
1	5MU	2A	1939	21/22	0.96	0.08	35,39,47,49	0
32	5MC	1a	1407	21/22	0.96	0.11	36,42,48,49	0
1	5MC	2A	1942	21/22	0.96	0.09	54,57,63,64	0
32	M2G	1a	966	25/26	0.96	0.10	47,54,57,67	0
1	OMG	2A	2251	24/25	0.96	0.09	43,47,50,54	0
1	2MU	2A	2552	21/23	0.96	0.09	41,48,52,60	0
32	5MC	1a	1404	21/22	0.97	0.08	35,42,47,48	0
55	31H	1x	76	32/33	0.97	0.09	25,34,43,47	10
32	5MC	1a	967	21/22	0.97	0.10	49,54,60,62	0
1	OMC	1A	1920	21/22	0.97	0.07	38,48,55,59	0
32	UR3	1a	1498	21/22	0.97	0.08	39,44,47,49	0
1	8AH	2A	2503	24/25	0.97	0.09	36,43,48,52	0
1	5MU	1A	1939	21/22	0.97	0.07	30,35,39,39	0
1	PSU	2A	2605	20/21	0.97	0.08	39,46,49,51	0
1	8AH	1A	2503	24/25	0.98	0.07	19,29,34,38	0
32	MA6	1a	1518	24/25	0.98	0.07	36,43,46,47	0
1	2MU	1A	2552	21/23	0.98	0.06	27,31,34,38	0
1	OMG	1A	2251	24/25	0.98	0.06	26,29,31,34	0
1	PSU	1A	2605	20/21	0.98	0.07	27,31,35,36	0
1	5MC	1A	1962	21/22	0.98	0.06	30,40,43,46	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3382	1/1	0.60	0.33	86,86,86,86	0
56	MG	1A	3710	1/1	0.60	0.27	78,78,78,78	0
56	MG	20	101	1/1	0.64	0.19	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2q	203	1/1	0.64	0.21	78,78,78,78	0
56	MG	1a	1789	1/1	0.65	0.30	80,80,80,80	0
56	MG	2A	3477	1/1	0.65	0.36	80,80,80,80	0
56	MG	2A	3266	1/1	0.66	0.23	75,75,75,75	0
56	MG	1A	3627	1/1	0.67	0.16	58,58,58,58	0
56	MG	1A	4046	1/1	0.68	0.19	63,63,63,63	0
56	MG	1A	3647	1/1	0.68	0.16	49,49,49,49	0
56	MG	2A	3087	1/1	0.69	0.21	82,82,82,82	0
56	MG	2A	3088	1/1	0.69	0.29	80,80,80,80	0
56	MG	2a	1754	1/1	0.69	0.26	83,83,83,83	0
56	MG	1A	3254	1/1	0.69	0.26	68,68,68,68	0
56	MG	2A	3683	1/1	0.70	0.19	88,88,88,88	0
56	MG	2A	3737	1/1	0.70	0.19	63,63,63,63	0
56	MG	1A	3990	1/1	0.70	0.31	66,66,66,66	0
56	MG	2A	3562	1/1	0.70	0.22	64,64,64,64	0
56	MG	2A	3673	1/1	0.70	0.29	77,77,77,77	0
56	MG	1B	221	1/1	0.71	0.17	75,75,75,75	0
56	MG	2a	1692	1/1	0.71	0.27	69,69,69,69	0
56	MG	1A	3984	1/1	0.71	0.13	78,78,78,78	0
56	MG	2A	3829	1/1	0.71	0.24	69,69,69,69	0
56	MG	2y	105	1/1	0.71	0.18	86,86,86,86	0
56	MG	1A	3590	1/1	0.72	0.24	61,61,61,61	0
56	MG	27	102	1/1	0.72	0.23	77,77,77,77	0
56	MG	2A	3167	1/1	0.72	0.25	82,82,82,82	0
56	MG	2A	3257	1/1	0.72	0.23	79,79,79,79	0
56	MG	1x	116	1/1	0.72	0.14	82,82,82,82	0
56	MG	1A	3816	1/1	0.72	0.27	75,75,75,75	0
56	MG	1a	1729	1/1	0.73	0.19	84,84,84,84	0
56	MG	2A	3191	1/1	0.73	0.22	72,72,72,72	0
56	MG	2A	3755	1/1	0.73	0.17	60,60,60,60	0
56	MG	1a	1745	1/1	0.73	0.18	83,83,83,83	0
56	MG	1A	3772	1/1	0.73	0.24	59,59,59,59	0
56	MG	1A	3529	1/1	0.73	0.32	76,76,76,76	0
56	MG	1A	3821	1/1	0.73	0.16	60,60,60,60	0
56	MG	2A	3604	1/1	0.73	0.17	82,82,82,82	0
56	MG	2j	3200	1/1	0.73	0.18	75,75,75,75	0
56	MG	2A	3620	1/1	0.73	0.19	54,54,54,54	0
56	MG	2v	102	1/1	0.73	0.36	78,78,78,78	0
56	MG	1A	3979	1/1	0.73	0.16	74,74,74,74	0
56	MG	1A	3980	1/1	0.74	0.12	78,78,78,78	0
56	MG	2A	3542	1/1	0.74	0.22	73,73,73,73	0
56	MG	1A	3937	1/1	0.74	0.25	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1680	1/1	0.74	0.52	75,75,75,75	0
56	MG	2A	3219	1/1	0.74	0.17	62,62,62,62	0
56	MG	2a	1797	1/1	0.74	0.18	72,72,72,72	0
56	MG	2A	3085	1/1	0.74	0.30	78,78,78,78	0
56	MG	1A	3733	1/1	0.74	0.12	24,24,24,24	0
56	MG	2v	101	1/1	0.74	0.19	69,69,69,69	0
56	MG	2A	3286	1/1	0.74	0.18	74,74,74,74	0
56	MG	2A	3335	1/1	0.74	0.29	78,78,78,78	0
56	MG	2A	3691	1/1	0.75	0.18	43,43,43,43	0
56	MG	2a	1781	1/1	0.75	0.17	77,77,77,77	0
56	MG	2A	3281	1/1	0.75	0.24	72,72,72,72	0
56	MG	1A	3994	1/1	0.75	0.16	63,63,63,63	0
56	MG	1P	206	1/1	0.75	0.22	55,55,55,55	0
56	MG	1A	4075	1/1	0.75	0.20	65,65,65,65	0
56	MG	2A	3522	1/1	0.75	0.24	70,70,70,70	0
56	MG	2w	104	1/1	0.75	0.32	74,74,74,74	0
56	MG	2A	3534	1/1	0.75	0.19	87,87,87,87	0
56	MG	1A	3383	1/1	0.76	0.12	63,63,63,63	0
56	MG	2a	1685	1/1	0.76	0.35	70,70,70,70	0
56	MG	2A	3659	1/1	0.76	0.21	64,64,64,64	0
56	MG	2B	211	1/1	0.76	0.17	72,72,72,72	0
56	MG	2G	201	1/1	0.76	0.16	72,72,72,72	0
56	MG	1A	4022	1/1	0.76	0.18	61,61,61,61	0
56	MG	2A	3813	1/1	0.77	0.28	70,70,70,70	0
56	MG	2A	3642	1/1	0.77	0.13	78,78,78,78	0
56	MG	1A	3421	1/1	0.77	0.18	68,68,68,68	0
56	MG	2B	215	1/1	0.77	0.24	71,71,71,71	0
56	MG	2A	3670	1/1	0.77	0.19	62,62,62,62	0
56	MG	1a	1694	1/1	0.77	0.20	72,72,72,72	0
56	MG	2a	1677	1/1	0.78	0.27	69,69,69,69	0
56	MG	1A	3499	1/1	0.78	0.17	62,62,62,62	0
56	MG	1A	3331	1/1	0.78	0.20	64,64,64,64	0
56	MG	2a	1739	1/1	0.78	0.13	78,78,78,78	0
56	MG	2A	3597	1/1	0.78	0.18	88,88,88,88	0
56	MG	2A	3289	1/1	0.78	0.23	77,77,77,77	0
56	MG	2A	3814	1/1	0.78	0.24	68,68,68,68	0
56	MG	2a	1798	1/1	0.78	0.16	79,79,79,79	0
56	MG	2A	3312	1/1	0.78	0.16	82,82,82,82	0
56	MG	1w	105	1/1	0.78	0.22	79,79,79,79	0
56	MG	2A	3473	1/1	0.78	0.24	63,63,63,63	0
56	MG	1a	1691	1/1	0.78	0.27	74,74,74,74	0
56	MG	1A	3986	1/1	0.78	0.11	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	230	1/1	0.78	0.21	79,79,79,79	0
56	MG	2A	3065	1/1	0.79	0.15	61,61,61,61	0
56	MG	2A	3299	1/1	0.79	0.15	64,64,64,64	0
56	MG	1A	3796	1/1	0.79	0.20	87,87,87,87	0
56	MG	2A	3590	1/1	0.79	0.22	74,74,74,74	0
56	MG	2a	1750	1/1	0.79	0.20	79,79,79,79	0
56	MG	1A	3687	1/1	0.79	0.13	52,52,52,52	0
56	MG	2A	3343	1/1	0.79	0.12	66,66,66,66	0
56	MG	2A	3357	1/1	0.79	0.17	74,74,74,74	0
56	MG	2A	3006	1/1	0.79	0.31	68,68,68,68	0
56	MG	2A	3643	1/1	0.79	0.18	75,75,75,75	0
56	MG	2A	3164	1/1	0.79	0.14	68,68,68,68	0
56	MG	2P	201	1/1	0.79	0.26	63,63,63,63	0
56	MG	2A	3490	1/1	0.79	0.22	55,55,55,55	0
56	MG	2w	102	1/1	0.79	0.11	86,86,86,86	0
56	MG	2A	3027	1/1	0.79	0.20	76,76,76,76	0
56	MG	2y	104	1/1	0.79	0.22	93,93,93,93	0
56	MG	2a	1635	1/1	0.79	0.14	67,67,67,67	0
56	MG	1A	3903	1/1	0.80	0.18	37,37,37,37	0
56	MG	1A	3915	1/1	0.80	0.15	49,49,49,49	0
56	MG	2A	3427	1/1	0.80	0.29	79,79,79,79	0
56	MG	2A	3436	1/1	0.80	0.18	73,73,73,73	0
56	MG	1a	1771	1/1	0.80	0.13	65,65,65,65	0
56	MG	1B	234	1/1	0.80	0.16	64,64,64,64	0
56	MG	2A	3732	1/1	0.80	0.20	83,83,83,83	0
56	MG	1B	238	1/1	0.80	0.18	65,65,65,65	0
56	MG	2a	1792	1/1	0.80	0.22	61,61,61,61	0
56	MG	2A	3264	1/1	0.80	0.21	63,63,63,63	0
56	MG	1O	203	1/1	0.80	0.12	70,70,70,70	0
56	MG	1A	3337	1/1	0.80	0.14	72,72,72,72	0
56	MG	1T	201	1/1	0.80	0.16	54,54,54,54	0
56	MG	10	107	1/1	0.80	0.16	70,70,70,70	0
56	MG	2A	3292	1/1	0.80	0.30	74,74,74,74	0
56	MG	2w	101	1/1	0.80	0.13	69,69,69,69	0
56	MG	1A	3810	1/1	0.80	0.17	71,71,71,71	0
56	MG	2A	3610	1/1	0.80	0.18	79,79,79,79	0
56	MG	1A	3425	1/1	0.80	0.20	61,61,61,61	0
56	MG	1A	3433	1/1	0.80	0.16	67,67,67,67	0
56	MG	2A	3786	1/1	0.81	0.13	65,65,65,65	0
56	MG	2A	3401	1/1	0.81	0.37	81,81,81,81	0
56	MG	2A	3070	1/1	0.81	0.15	67,67,67,67	0
56	MG	1A	3800	1/1	0.81	0.16	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3367	1/1	0.81	0.21	59,59,59,59	0
56	MG	1a	1670	1/1	0.81	0.29	79,79,79,79	0
56	MG	1a	1671	1/1	0.81	0.29	66,66,66,66	0
56	MG	2A	3517	1/1	0.81	0.17	59,59,59,59	0
56	MG	1A	3377	1/1	0.81	0.43	71,71,71,71	0
56	MG	1A	4044	1/1	0.81	0.28	81,81,81,81	0
56	MG	2A	3209	1/1	0.81	0.20	63,63,63,63	0
56	MG	2A	3210	1/1	0.81	0.27	68,68,68,68	0
56	MG	1A	3603	1/1	0.81	0.14	54,54,54,54	0
56	MG	1A	3380	1/1	0.81	0.20	47,47,47,47	0
56	MG	2a	1702	1/1	0.81	0.27	70,70,70,70	0
56	MG	1A	3241	1/1	0.81	0.10	67,67,67,67	0
56	MG	1B	223	1/1	0.81	0.17	64,64,64,64	0
56	MG	1B	229	1/1	0.81	0.18	69,69,69,69	0
56	MG	2a	1768	1/1	0.81	0.27	78,78,78,78	0
56	MG	2A	3285	1/1	0.81	0.13	71,71,71,71	0
56	MG	1a	1805	1/1	0.81	0.19	61,61,61,61	0
56	MG	1A	3020	1/1	0.81	0.15	59,59,59,59	0
56	MG	1x	112	1/1	0.81	0.22	78,78,78,78	0
56	MG	2a	1802	1/1	0.81	0.21	80,80,80,80	0
56	MG	1A	3326	1/1	0.81	0.18	59,59,59,59	0
56	MG	1A	3087	1/1	0.81	0.16	72,72,72,72	0
56	MG	2A	3021	1/1	0.81	0.34	79,79,79,79	0
56	MG	2A	3696	1/1	0.81	0.14	45,45,45,45	0
56	MG	2A	3724	1/1	0.81	0.12	45,45,45,45	0
56	MG	1A	3336	1/1	0.81	0.22	68,68,68,68	0
56	MG	2A	3350	1/1	0.81	0.49	81,81,81,81	0
56	MG	2A	3747	1/1	0.81	0.12	59,59,59,59	0
56	MG	1A	3216	1/1	0.81	0.18	55,55,55,55	0
56	MG	2F	307	1/1	0.82	0.15	68,68,68,68	0
56	MG	2A	3599	1/1	0.82	0.17	68,68,68,68	0
56	MG	1A	3996	1/1	0.82	0.10	58,58,58,58	0
56	MG	2A	3608	1/1	0.82	0.20	72,72,72,72	0
56	MG	2A	3048	1/1	0.82	0.18	70,70,70,70	0
56	MG	2a	1604	1/1	0.82	0.17	74,74,74,74	0
56	MG	2A	3238	1/1	0.82	0.10	72,72,72,72	0
56	MG	2A	3621	1/1	0.82	0.31	75,75,75,75	0
56	MG	2a	1684	1/1	0.82	0.22	62,62,62,62	0
56	MG	2A	3255	1/1	0.82	0.20	69,69,69,69	0
56	MG	2A	3359	1/1	0.82	0.14	64,64,64,64	0
56	MG	2A	3391	1/1	0.82	0.19	60,60,60,60	0
56	MG	2a	1717	1/1	0.82	0.26	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1718	1/1	0.82	0.12	77,77,77,77	0
56	MG	2A	3064	1/1	0.82	0.38	71,71,71,71	0
56	MG	1A	3308	1/1	0.82	0.20	65,65,65,65	0
56	MG	18	105	1/1	0.82	0.15	68,68,68,68	0
56	MG	1a	1603	1/1	0.82	0.23	66,66,66,66	0
56	MG	2a	1779	1/1	0.82	0.24	72,72,72,72	0
56	MG	2A	3282	1/1	0.82	0.16	65,65,65,65	0
56	MG	2A	3722	1/1	0.82	0.19	75,75,75,75	0
56	MG	2A	3480	1/1	0.82	0.25	60,60,60,60	0
56	MG	1a	1668	1/1	0.82	0.19	56,56,56,56	0
56	MG	2A	3513	1/1	0.82	0.28	64,64,64,64	0
56	MG	1A	3006	1/1	0.82	0.25	69,69,69,69	0
56	MG	1A	3569	1/1	0.82	0.20	72,72,72,72	0
56	MG	1A	4047	1/1	0.82	0.17	80,80,80,80	0
56	MG	2A	3800	1/1	0.82	0.16	74,74,74,74	0
56	MG	2v	103	1/1	0.82	0.20	59,59,59,59	0
56	MG	2A	3294	1/1	0.82	0.19	69,69,69,69	0
56	MG	2A	3546	1/1	0.82	0.22	67,67,67,67	0
56	MG	1A	3403	1/1	0.82	0.18	61,61,61,61	0
56	MG	1A	3479	1/1	0.82	0.18	57,57,57,57	0
56	MG	2A	3320	1/1	0.82	0.16	70,70,70,70	0
56	MG	25	107	1/1	0.83	0.20	69,69,69,69	0
56	MG	1A	4027	1/1	0.83	0.14	52,52,52,52	0
56	MG	2A	3395	1/1	0.83	0.16	61,61,61,61	0
56	MG	1A	3831	1/1	0.83	0.10	42,42,42,42	0
56	MG	2A	3412	1/1	0.83	0.29	72,72,72,72	0
56	MG	2a	1680	1/1	0.83	0.15	72,72,72,72	0
56	MG	2A	3648	1/1	0.83	0.14	67,67,67,67	0
56	MG	2A	3420	1/1	0.83	0.15	68,68,68,68	0
56	MG	2A	3270	1/1	0.83	0.26	70,70,70,70	0
56	MG	2a	1701	1/1	0.83	0.33	66,66,66,66	0
56	MG	2A	3434	1/1	0.83	0.29	73,73,73,73	0
56	MG	1A	3833	1/1	0.83	0.24	57,57,57,57	0
56	MG	1A	3474	1/1	0.83	0.19	73,73,73,73	0
56	MG	1a	1727	1/1	0.83	0.17	70,70,70,70	0
56	MG	2a	1740	1/1	0.83	0.20	77,77,77,77	0
56	MG	1O	204	1/1	0.83	0.19	63,63,63,63	0
56	MG	1A	4071	1/1	0.83	0.19	69,69,69,69	0
56	MG	2a	1763	1/1	0.83	0.31	77,77,77,77	0
56	MG	1A	3198	1/1	0.83	0.23	62,62,62,62	0
56	MG	1a	1780	1/1	0.83	0.10	78,78,78,78	0
56	MG	1A	4076	1/1	0.83	0.20	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	16	101	1/1	0.83	0.28	62,62,62,62	0
56	MG	1v	101	1/1	0.83	0.22	74,74,74,74	0
56	MG	2A	3324	1/1	0.83	0.18	81,81,81,81	0
56	MG	2A	3549	1/1	0.83	0.13	60,60,60,60	0
56	MG	2A	3333	1/1	0.83	0.18	74,74,74,74	0
56	MG	2l	203	1/1	0.83	0.09	68,68,68,68	0
56	MG	1B	207	1/1	0.83	0.23	71,71,71,71	0
56	MG	1A	3390	1/1	0.83	0.29	47,47,47,47	0
56	MG	1a	1637	1/1	0.83	0.19	61,61,61,61	0
56	MG	2A	3602	1/1	0.83	0.18	67,67,67,67	0
56	MG	1A	3960	1/1	0.83	0.17	44,44,44,44	0
56	MG	2A	3358	1/1	0.83	0.14	76,76,76,76	0
56	MG	2W	202	1/1	0.83	0.16	67,67,67,67	0
56	MG	1A	3828	1/1	0.83	0.13	54,54,54,54	0
56	MG	20	103	1/1	0.83	0.23	64,64,64,64	0
56	MG	2a	1607	1/1	0.84	0.22	65,65,65,65	0
56	MG	2a	1629	1/1	0.84	0.26	75,75,75,75	0
56	MG	2A	3514	1/1	0.84	0.25	80,80,80,80	0
56	MG	2a	1638	1/1	0.84	0.12	75,75,75,75	0
56	MG	2A	3689	1/1	0.84	0.18	76,76,76,76	0
56	MG	2A	3251	1/1	0.84	0.26	80,80,80,80	0
56	MG	2a	1681	1/1	0.84	0.14	73,73,73,73	0
56	MG	1A	3481	1/1	0.84	0.17	54,54,54,54	0
56	MG	1A	3446	1/1	0.84	0.13	63,63,63,63	0
56	MG	1A	3904	1/1	0.84	0.11	37,37,37,37	0
56	MG	2A	3731	1/1	0.84	0.17	61,61,61,61	0
56	MG	1A	3235	1/1	0.84	0.19	60,60,60,60	0
56	MG	1A	3082	1/1	0.84	0.24	56,56,56,56	0
56	MG	2A	3274	1/1	0.84	0.16	58,58,58,58	0
56	MG	2a	1732	1/1	0.84	0.12	84,84,84,84	0
56	MG	2A	3360	1/1	0.84	0.17	73,73,73,73	0
56	MG	1R	204	1/1	0.84	0.13	59,59,59,59	0
56	MG	2A	3159	1/1	0.84	0.29	72,72,72,72	0
56	MG	1A	3942	1/1	0.84	0.16	65,65,65,65	0
56	MG	1Y	201	1/1	0.84	0.13	52,52,52,52	0
56	MG	2A	3415	1/1	0.84	0.15	66,66,66,66	0
56	MG	2B	204	1/1	0.84	0.22	68,68,68,68	0
56	MG	2B	210	1/1	0.84	0.24	78,78,78,78	0
56	MG	1A	3824	1/1	0.84	0.18	49,49,49,49	0
56	MG	2A	3613	1/1	0.84	0.15	60,60,60,60	0
56	MG	2B	217	1/1	0.84	0.12	77,77,77,77	0
56	MG	2E	303	1/1	0.84	0.34	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3199	1/1	0.84	0.12	66,66,66,66	0
56	MG	1A	3669	1/1	0.84	0.16	38,38,38,38	0
56	MG	1a	1743	1/1	0.84	0.10	71,71,71,71	0
56	MG	2W	201	1/1	0.84	0.18	68,68,68,68	0
56	MG	2A	3309	1/1	0.84	0.14	74,74,74,74	0
56	MG	2A	3212	1/1	0.84	0.34	77,77,77,77	0
56	MG	1A	3797	1/1	0.84	0.15	45,45,45,45	0
56	MG	20	105	1/1	0.84	0.22	70,70,70,70	0
56	MG	2A	3060	1/1	0.84	0.14	60,60,60,60	0
56	MG	2A	3326	1/1	0.84	0.14	55,55,55,55	0
56	MG	2A	3680	1/1	0.84	0.12	60,60,60,60	0
56	MG	2B	212	1/1	0.85	0.18	74,74,74,74	0
56	MG	1A	4050	1/1	0.85	0.21	70,70,70,70	0
56	MG	1A	3211	1/1	0.85	0.28	49,49,49,49	0
56	MG	2A	3278	1/1	0.85	0.16	68,68,68,68	0
56	MG	1a	1636	1/1	0.85	0.33	58,58,58,58	0
56	MG	2A	3541	1/1	0.85	0.20	71,71,71,71	0
56	MG	2N	201	1/1	0.85	0.18	76,76,76,76	0
56	MG	1A	3753	1/1	0.85	0.20	85,85,85,85	0
56	MG	2A	3026	1/1	0.85	0.33	58,58,58,58	0
56	MG	1a	1659	1/1	0.85	0.10	57,57,57,57	0
56	MG	1a	1663	1/1	0.85	0.19	61,61,61,61	0
56	MG	2A	3583	1/1	0.85	0.15	41,41,41,41	0
56	MG	2A	3049	1/1	0.85	0.12	54,54,54,54	0
56	MG	1A	3966	1/1	0.85	0.22	68,68,68,68	0
56	MG	1A	3763	1/1	0.85	0.11	62,62,62,62	0
56	MG	1A	3654	1/1	0.85	0.11	28,28,28,28	0
56	MG	1a	1678	1/1	0.85	0.21	75,75,75,75	0
56	MG	2a	1613	1/1	0.85	0.16	70,70,70,70	0
56	MG	2a	1617	1/1	0.85	0.33	68,68,68,68	0
56	MG	2A	3316	1/1	0.85	0.13	73,73,73,73	0
56	MG	1A	3458	1/1	0.85	0.18	56,56,56,56	0
56	MG	2A	3323	1/1	0.85	0.13	67,67,67,67	0
56	MG	2a	1641	1/1	0.85	0.30	78,78,78,78	0
56	MG	2a	1663	1/1	0.85	0.17	69,69,69,69	0
56	MG	2A	3619	1/1	0.85	0.22	71,71,71,71	0
56	MG	1a	1686	1/1	0.85	0.27	67,67,67,67	0
56	MG	1A	3832	1/1	0.85	0.22	47,47,47,47	0
56	MG	2A	3629	1/1	0.85	0.23	60,60,60,60	0
56	MG	2A	3110	1/1	0.85	0.34	67,67,67,67	0
56	MG	2a	1688	1/1	0.85	0.15	76,76,76,76	0
56	MG	1A	3461	1/1	0.85	0.36	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1700	1/1	0.85	0.27	79,79,79,79	0
56	MG	1A	3991	1/1	0.85	0.11	50,50,50,50	0
56	MG	2A	3657	1/1	0.85	0.13	58,58,58,58	0
56	MG	2a	1707	1/1	0.85	0.26	67,67,67,67	0
56	MG	2a	1715	1/1	0.85	0.18	67,67,67,67	0
56	MG	1A	3850	1/1	0.85	0.17	42,42,42,42	0
56	MG	2A	3171	1/1	0.85	0.13	58,58,58,58	0
56	MG	2A	3186	1/1	0.85	0.14	61,61,61,61	0
56	MG	2A	3188	1/1	0.85	0.12	62,62,62,62	0
56	MG	2A	3681	1/1	0.85	0.17	60,60,60,60	0
56	MG	1A	3891	1/1	0.85	0.10	57,57,57,57	0
56	MG	1A	4005	1/1	0.85	0.18	44,44,44,44	0
56	MG	2a	1755	1/1	0.85	0.24	74,74,74,74	0
56	MG	2A	3203	1/1	0.85	0.34	66,66,66,66	0
56	MG	2A	3694	1/1	0.85	0.10	48,48,48,48	0
56	MG	2a	1776	1/1	0.85	0.20	65,65,65,65	0
56	MG	2A	3396	1/1	0.85	0.25	59,59,59,59	0
56	MG	1a	1755	1/1	0.85	0.14	71,71,71,71	0
56	MG	2A	3409	1/1	0.85	0.10	74,74,74,74	0
56	MG	2a	1796	1/1	0.85	0.14	71,71,71,71	0
56	MG	1a	1764	1/1	0.85	0.12	83,83,83,83	0
56	MG	2A	3413	1/1	0.85	0.15	68,68,68,68	0
56	MG	1A	4019	1/1	0.85	0.14	44,44,44,44	0
56	MG	2A	3213	1/1	0.85	0.23	68,68,68,68	0
56	MG	1A	3799	1/1	0.85	0.13	55,55,55,55	0
56	MG	2A	3237	1/1	0.85	0.30	59,59,59,59	0
56	MG	1A	3696	1/1	0.85	0.10	67,67,67,67	0
56	MG	1a	1802	1/1	0.85	0.24	78,78,78,78	0
56	MG	1A	3802	1/1	0.85	0.22	63,63,63,63	0
56	MG	2A	3478	1/1	0.85	0.18	55,55,55,55	0
56	MG	2B	202	1/1	0.85	0.19	70,70,70,70	0
56	MG	2w	103	1/1	0.85	0.13	74,74,74,74	0
56	MG	1l	202	1/1	0.85	0.13	69,69,69,69	0
56	MG	1A	3922	1/1	0.85	0.10	29,29,29,29	0
56	MG	1A	3156	1/1	0.85	0.11	52,52,52,52	0
56	MG	1A	3721	1/1	0.86	0.09	25,25,25,25	0
56	MG	2A	3275	1/1	0.86	0.21	67,67,67,67	0
56	MG	2A	3099	1/1	0.86	0.15	60,60,60,60	0
56	MG	1A	3094	1/1	0.86	0.12	67,67,67,67	0
56	MG	2A	3663	1/1	0.86	0.11	73,73,73,73	0
56	MG	2A	3425	1/1	0.86	0.13	64,64,64,64	0
56	MG	2a	1627	1/1	0.86	0.23	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3156	1/1	0.86	0.22	68,68,68,68	0
56	MG	2A	3674	1/1	0.86	0.14	52,52,52,52	0
56	MG	2A	3675	1/1	0.86	0.14	65,65,65,65	0
56	MG	2A	3428	1/1	0.86	0.18	68,68,68,68	0
56	MG	2a	1642	1/1	0.86	0.17	80,80,80,80	0
56	MG	2a	1661	1/1	0.86	0.27	71,71,71,71	0
56	MG	2A	3283	1/1	0.86	0.18	64,64,64,64	0
56	MG	2a	1673	1/1	0.86	0.23	64,64,64,64	0
56	MG	1A	3972	1/1	0.86	0.12	42,42,42,42	0
56	MG	1A	3746	1/1	0.86	0.10	76,76,76,76	0
56	MG	2A	3165	1/1	0.86	0.23	68,68,68,68	0
56	MG	1a	1605	1/1	0.86	0.14	68,68,68,68	0
56	MG	1A	3188	1/1	0.86	0.12	49,49,49,49	0
56	MG	2A	3701	1/1	0.86	0.10	64,64,64,64	0
56	MG	2a	1690	1/1	0.86	0.25	71,71,71,71	0
56	MG	2a	1691	1/1	0.86	0.32	73,73,73,73	0
56	MG	2A	3298	1/1	0.86	0.21	65,65,65,65	0
56	MG	2A	3500	1/1	0.86	0.16	44,44,44,44	0
56	MG	1A	3149	1/1	0.86	0.21	40,40,40,40	0
56	MG	1a	1642	1/1	0.86	0.14	65,65,65,65	0
56	MG	2a	1706	1/1	0.86	0.27	66,66,66,66	0
56	MG	2A	3733	1/1	0.86	0.15	72,72,72,72	0
56	MG	1a	1657	1/1	0.86	0.24	56,56,56,56	0
56	MG	2A	3741	1/1	0.86	0.11	63,63,63,63	0
56	MG	2A	3742	1/1	0.86	0.10	82,82,82,82	0
56	MG	2a	1723	1/1	0.86	0.24	78,78,78,78	0
56	MG	2a	1731	1/1	0.86	0.07	67,67,67,67	0
56	MG	2A	3313	1/1	0.86	0.13	85,85,85,85	0
56	MG	2A	3523	1/1	0.86	0.23	73,73,73,73	0
56	MG	2A	3768	1/1	0.86	0.08	59,59,59,59	0
56	MG	2A	3194	1/1	0.86	0.25	66,66,66,66	0
56	MG	1B	218	1/1	0.86	0.14	54,54,54,54	0
56	MG	2A	3803	1/1	0.86	0.19	60,60,60,60	0
56	MG	1A	3675	1/1	0.86	0.18	51,51,51,51	0
56	MG	1A	3776	1/1	0.86	0.11	63,63,63,63	0
56	MG	1A	3677	1/1	0.86	0.19	61,61,61,61	0
56	MG	2A	3556	1/1	0.86	0.13	37,37,37,37	0
56	MG	1A	3898	1/1	0.86	0.13	58,58,58,58	0
56	MG	2B	206	1/1	0.86	0.21	73,73,73,73	0
56	MG	1A	3681	1/1	0.86	0.12	55,55,55,55	0
56	MG	2A	3584	1/1	0.86	0.14	55,55,55,55	0
56	MG	1A	3319	1/1	0.86	0.14	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1800	1/1	0.86	0.12	46,46,46,46	0
56	MG	1F	303	1/1	0.86	0.27	67,67,67,67	0
56	MG	2a	1806	1/1	0.86	0.35	77,77,77,77	0
56	MG	1A	4013	1/1	0.86	0.14	74,74,74,74	0
56	MG	2A	3250	1/1	0.86	0.18	63,63,63,63	0
56	MG	1A	3613	1/1	0.86	0.12	65,65,65,65	0
56	MG	1a	1714	1/1	0.86	0.25	68,68,68,68	0
56	MG	2A	3379	1/1	0.86	0.29	69,69,69,69	0
56	MG	2O	201	1/1	0.86	0.23	68,68,68,68	0
56	MG	2A	3382	1/1	0.86	0.26	61,61,61,61	0
56	MG	1A	3702	1/1	0.86	0.13	71,71,71,71	0
56	MG	2A	3260	1/1	0.86	0.17	58,58,58,58	0
56	MG	1A	3934	1/1	0.86	0.15	72,72,72,72	0
56	MG	2y	101	1/1	0.86	0.12	62,62,62,62	0
56	MG	1A	3704	1/1	0.86	0.12	30,30,30,30	0
56	MG	1A	3237	1/1	0.86	0.18	71,71,71,71	0
56	MG	2A	3306	1/1	0.87	0.26	70,70,70,70	0
56	MG	1x	105	1/1	0.87	0.15	65,65,65,65	0
56	MG	2a	1636	1/1	0.87	0.18	61,61,61,61	0
56	MG	1A	4043	1/1	0.87	0.14	62,62,62,62	0
56	MG	2A	3503	1/1	0.87	0.19	49,49,49,49	0
56	MG	2A	3208	1/1	0.87	0.22	68,68,68,68	0
56	MG	2a	1644	1/1	0.87	0.26	68,68,68,68	0
56	MG	2a	1660	1/1	0.87	0.23	62,62,62,62	0
56	MG	2A	3714	1/1	0.87	0.19	60,60,60,60	0
56	MG	1A	3550	1/1	0.87	0.25	67,67,67,67	0
56	MG	2a	1670	1/1	0.87	0.18	61,61,61,61	0
56	MG	1A	3300	1/1	0.87	0.17	68,68,68,68	0
56	MG	2A	3321	1/1	0.87	0.12	57,57,57,57	0
56	MG	1A	3719	1/1	0.87	0.18	54,54,54,54	0
56	MG	1A	3576	1/1	0.87	0.11	41,41,41,41	0
56	MG	1A	3441	1/1	0.87	0.14	58,58,58,58	0
56	MG	2A	3223	1/1	0.87	0.24	58,58,58,58	0
56	MG	2a	1686	1/1	0.87	0.16	71,71,71,71	0
56	MG	2a	1687	1/1	0.87	0.22	68,68,68,68	0
56	MG	1A	4074	1/1	0.87	0.20	66,66,66,66	0
56	MG	1A	3163	1/1	0.87	0.24	57,57,57,57	0
56	MG	2A	3248	1/1	0.87	0.21	65,65,65,65	0
56	MG	2A	3352	1/1	0.87	0.18	74,74,74,74	0
56	MG	2a	1696	1/1	0.87	0.15	60,60,60,60	0
56	MG	2A	3779	1/1	0.87	0.10	61,61,61,61	0
56	MG	1l	106	1/1	0.87	0.10	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3797	1/1	0.87	0.16	62,62,62,62	0
56	MG	2A	3061	1/1	0.87	0.24	70,70,70,70	0
56	MG	15	108	1/1	0.87	0.11	55,55,55,55	0
56	MG	2a	1713	1/1	0.87	0.31	66,66,66,66	0
56	MG	1A	3483	1/1	0.87	0.18	57,57,57,57	0
56	MG	2A	3371	1/1	0.87	0.20	57,57,57,57	0
56	MG	2A	3818	1/1	0.87	0.28	75,75,75,75	0
56	MG	1A	3689	1/1	0.87	0.12	63,63,63,63	0
56	MG	2a	1726	1/1	0.87	0.36	68,68,68,68	0
56	MG	2A	3261	1/1	0.87	0.20	66,66,66,66	0
56	MG	1A	3360	1/1	0.87	0.14	59,59,59,59	0
56	MG	1a	1750	1/1	0.87	0.13	54,54,54,54	0
56	MG	1a	1752	1/1	0.87	0.15	68,68,68,68	0
56	MG	2A	3614	1/1	0.87	0.14	58,58,58,58	0
56	MG	2a	1752	1/1	0.87	0.27	76,76,76,76	0
56	MG	2A	3615	1/1	0.87	0.18	65,65,65,65	0
56	MG	2A	3097	1/1	0.87	0.14	68,68,68,68	0
56	MG	2B	216	1/1	0.87	0.15	69,69,69,69	0
56	MG	1A	3938	1/1	0.87	0.13	48,48,48,48	0
56	MG	2a	1773	1/1	0.87	0.12	68,68,68,68	0
56	MG	1a	1759	1/1	0.87	0.11	76,76,76,76	0
56	MG	2E	308	1/1	0.87	0.15	56,56,56,56	0
56	MG	1a	1635	1/1	0.87	0.27	62,62,62,62	0
56	MG	2a	1782	1/1	0.87	0.20	75,75,75,75	0
56	MG	2a	1784	1/1	0.87	0.19	69,69,69,69	0
56	MG	2a	1791	1/1	0.87	0.22	66,66,66,66	0
56	MG	2A	3633	1/1	0.87	0.11	72,72,72,72	0
56	MG	1A	4010	1/1	0.87	0.10	59,59,59,59	0
56	MG	1A	3697	1/1	0.87	0.10	50,50,50,50	0
56	MG	1a	1638	1/1	0.87	0.29	74,74,74,74	0
56	MG	2A	3656	1/1	0.87	0.22	67,67,67,67	0
56	MG	1A	3794	1/1	0.87	0.15	62,62,62,62	0
56	MG	2Z	301	1/1	0.87	0.20	74,74,74,74	0
56	MG	1a	1647	1/1	0.87	0.26	67,67,67,67	0
56	MG	1A	3310	1/1	0.87	0.14	49,49,49,49	0
56	MG	1t	201	1/1	0.87	0.19	57,57,57,57	0
56	MG	2A	3671	1/1	0.87	0.12	60,60,60,60	0
56	MG	26	101	1/1	0.87	0.24	69,69,69,69	0
56	MG	2A	3443	1/1	0.87	0.23	55,55,55,55	0
56	MG	28	102	1/1	0.87	0.15	72,72,72,72	0
56	MG	2A	3451	1/1	0.87	0.17	50,50,50,50	0
56	MG	2A	3460	1/1	0.87	0.12	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1608	1/1	0.87	0.27	68,68,68,68	0
56	MG	2x	102	1/1	0.87	0.22	75,75,75,75	0
56	MG	2x	108	1/1	0.87	0.12	56,56,56,56	0
56	MG	1A	3968	1/1	0.87	0.13	58,58,58,58	0
56	MG	1E	307	1/1	0.87	0.19	59,59,59,59	0
56	MG	2A	3303	1/1	0.87	0.13	63,63,63,63	0
56	MG	1a	1630	1/1	0.88	0.17	65,65,65,65	0
56	MG	1A	4038	1/1	0.88	0.21	62,62,62,62	0
56	MG	2A	3296	1/1	0.88	0.12	65,65,65,65	0
56	MG	1A	3528	1/1	0.88	0.20	46,46,46,46	0
56	MG	1A	3423	1/1	0.88	0.09	49,49,49,49	0
56	MG	2A	3587	1/1	0.88	0.14	63,63,63,63	0
56	MG	1A	4045	1/1	0.88	0.17	70,70,70,70	0
56	MG	1A	3250	1/1	0.88	0.26	68,68,68,68	0
56	MG	1a	1646	1/1	0.88	0.23	71,71,71,71	0
56	MG	1A	3562	1/1	0.88	0.30	58,58,58,58	0
56	MG	29	101	1/1	0.88	0.23	71,71,71,71	0
56	MG	1a	1651	1/1	0.88	0.26	65,65,65,65	0
56	MG	1A	3914	1/1	0.88	0.12	61,61,61,61	0
56	MG	1A	4056	1/1	0.88	0.10	67,67,67,67	0
56	MG	2a	1610	1/1	0.88	0.25	71,71,71,71	0
56	MG	2a	1611	1/1	0.88	0.30	76,76,76,76	0
56	MG	1A	4070	1/1	0.88	0.09	73,73,73,73	0
56	MG	1A	3426	1/1	0.88	0.14	43,43,43,43	0
56	MG	1A	3917	1/1	0.88	0.15	57,57,57,57	0
56	MG	2A	3108	1/1	0.88	0.20	63,63,63,63	0
56	MG	2A	3331	1/1	0.88	0.27	64,64,64,64	0
56	MG	1A	3573	1/1	0.88	0.10	61,61,61,61	0
56	MG	2A	3625	1/1	0.88	0.15	62,62,62,62	0
56	MG	2A	3628	1/1	0.88	0.14	69,69,69,69	0
56	MG	2A	3120	1/1	0.88	0.21	58,58,58,58	0
56	MG	2a	1643	1/1	0.88	0.13	79,79,79,79	0
56	MG	1A	3361	1/1	0.88	0.13	55,55,55,55	0
56	MG	2a	1655	1/1	0.88	0.26	64,64,64,64	0
56	MG	2A	3345	1/1	0.88	0.15	74,74,74,74	0
56	MG	2A	3348	1/1	0.88	0.15	62,62,62,62	0
56	MG	2A	3157	1/1	0.88	0.15	68,68,68,68	0
56	MG	2A	3649	1/1	0.88	0.26	60,60,60,60	0
56	MG	1a	1679	1/1	0.88	0.11	60,60,60,60	0
56	MG	1A	4083	1/1	0.88	0.28	64,64,64,64	0
56	MG	2a	1678	1/1	0.88	0.20	67,67,67,67	0
56	MG	1A	3313	1/1	0.88	0.19	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	213	1/1	0.88	0.19	63,63,63,63	0
56	MG	1a	1692	1/1	0.88	0.18	55,55,55,55	0
56	MG	2A	3361	1/1	0.88	0.15	63,63,63,63	0
56	MG	2A	3362	1/1	0.88	0.10	71,71,71,71	0
56	MG	2A	3368	1/1	0.88	0.22	50,50,50,50	0
56	MG	1A	3771	1/1	0.88	0.16	59,59,59,59	0
56	MG	1a	1700	1/1	0.88	0.12	63,63,63,63	0
56	MG	2A	3380	1/1	0.88	0.14	66,66,66,66	0
56	MG	1a	1704	1/1	0.88	0.32	64,64,64,64	0
56	MG	1A	3253	1/1	0.88	0.08	41,41,41,41	0
56	MG	1a	1717	1/1	0.88	0.14	60,60,60,60	0
56	MG	1A	3945	1/1	0.88	0.13	67,67,67,67	0
56	MG	2A	3398	1/1	0.88	0.33	58,58,58,58	0
56	MG	2A	3399	1/1	0.88	0.34	64,64,64,64	0
56	MG	2A	3704	1/1	0.88	0.27	66,66,66,66	0
56	MG	2A	3708	1/1	0.88	0.15	45,45,45,45	0
56	MG	2a	1714	1/1	0.88	0.09	66,66,66,66	0
56	MG	1A	3454	1/1	0.88	0.18	59,59,59,59	0
56	MG	1a	1734	1/1	0.88	0.14	64,64,64,64	0
56	MG	1A	3162	1/1	0.88	0.21	51,51,51,51	0
56	MG	2A	3729	1/1	0.88	0.12	59,59,59,59	0
56	MG	1a	1744	1/1	0.88	0.23	74,74,74,74	0
56	MG	1B	231	1/1	0.88	0.11	81,81,81,81	0
56	MG	1B	232	1/1	0.88	0.13	64,64,64,64	0
56	MG	2A	3423	1/1	0.88	0.23	74,74,74,74	0
56	MG	1A	3460	1/1	0.88	0.17	53,53,53,53	0
56	MG	2A	3224	1/1	0.88	0.18	61,61,61,61	0
56	MG	1A	3292	1/1	0.88	0.11	53,53,53,53	0
56	MG	2A	3753	1/1	0.88	0.18	47,47,47,47	0
56	MG	2A	3431	1/1	0.88	0.40	75,75,75,75	0
56	MG	2a	1759	1/1	0.88	0.16	73,73,73,73	0
56	MG	2A	3758	1/1	0.88	0.14	60,60,60,60	0
56	MG	2A	3765	1/1	0.88	0.10	75,75,75,75	0
56	MG	2a	1771	1/1	0.88	0.18	71,71,71,71	0
56	MG	2a	1772	1/1	0.88	0.27	56,56,56,56	0
56	MG	1A	3976	1/1	0.88	0.14	50,50,50,50	0
56	MG	2A	3435	1/1	0.88	0.37	65,65,65,65	0
56	MG	2A	3247	1/1	0.88	0.38	67,67,67,67	0
56	MG	1A	3662	1/1	0.88	0.10	28,28,28,28	0
56	MG	1A	3473	1/1	0.88	0.15	65,65,65,65	0
56	MG	2A	3453	1/1	0.88	0.25	73,73,73,73	0
56	MG	2a	1787	1/1	0.88	0.26	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1789	1/1	0.88	0.23	64,64,64,64	0
56	MG	2A	3807	1/1	0.88	0.19	68,68,68,68	0
56	MG	1A	3672	1/1	0.88	0.14	48,48,48,48	0
56	MG	2A	3462	1/1	0.88	0.17	75,75,75,75	0
56	MG	1A	3060	1/1	0.88	0.12	57,57,57,57	0
56	MG	1A	3021	1/1	0.88	0.14	69,69,69,69	0
56	MG	1A	3393	1/1	0.88	0.15	55,55,55,55	0
56	MG	2B	203	1/1	0.88	0.20	74,74,74,74	0
56	MG	1A	3349	1/1	0.88	0.22	65,65,65,65	0
56	MG	1A	3688	1/1	0.88	0.15	61,61,61,61	0
56	MG	2B	208	1/1	0.88	0.16	69,69,69,69	0
56	MG	1A	3484	1/1	0.88	0.12	65,65,65,65	0
56	MG	1w	102	1/1	0.88	0.32	69,69,69,69	0
56	MG	2A	3507	1/1	0.88	0.12	63,63,63,63	0
56	MG	1A	3495	1/1	0.88	0.17	82,82,82,82	0
56	MG	1A	3350	1/1	0.88	0.19	53,53,53,53	0
56	MG	1x	107	1/1	0.88	0.21	62,62,62,62	0
56	MG	1A	3847	1/1	0.88	0.11	26,26,26,26	0
56	MG	1A	3503	1/1	0.88	0.11	62,62,62,62	0
56	MG	1y	101	1/1	0.88	0.28	76,76,76,76	0
56	MG	2x	105	1/1	0.88	0.29	65,65,65,65	0
56	MG	2x	107	1/1	0.88	0.25	61,61,61,61	0
56	MG	2A	3538	1/1	0.88	0.09	71,71,71,71	0
56	MG	2A	3002	1/1	0.88	0.32	68,68,68,68	0
56	MG	1A	3887	1/1	0.88	0.09	32,32,32,32	0
56	MG	1a	1629	1/1	0.88	0.33	70,70,70,70	0
56	MG	2A	3544	1/1	0.89	0.24	70,70,70,70	0
56	MG	2A	3301	1/1	0.89	0.17	63,63,63,63	0
56	MG	1A	3175	1/1	0.89	0.07	54,54,54,54	0
56	MG	2A	3555	1/1	0.89	0.10	39,39,39,39	0
56	MG	2A	3063	1/1	0.89	0.21	65,65,65,65	0
56	MG	2A	3559	1/1	0.89	0.17	52,52,52,52	0
56	MG	1D	312	1/1	0.89	0.12	59,59,59,59	0
56	MG	2A	3564	1/1	0.89	0.15	77,77,77,77	0
56	MG	2A	3577	1/1	0.89	0.13	47,47,47,47	0
56	MG	2A	3579	1/1	0.89	0.10	52,52,52,52	0
56	MG	1A	4014	1/1	0.89	0.06	19,19,19,19	0
56	MG	1E	314	1/1	0.89	0.08	40,40,40,40	0
56	MG	2A	3314	1/1	0.89	0.12	62,62,62,62	0
56	MG	2A	3588	1/1	0.89	0.14	59,59,59,59	0
56	MG	1a	1681	1/1	0.89	0.22	66,66,66,66	0
56	MG	1a	1684	1/1	0.89	0.25	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3467	1/1	0.89	0.21	63,63,63,63	0
56	MG	2A	3093	1/1	0.89	0.17	66,66,66,66	0
56	MG	1a	1689	1/1	0.89	0.31	62,62,62,62	0
56	MG	2A	3325	1/1	0.89	0.18	70,70,70,70	0
56	MG	1F	309	1/1	0.89	0.17	54,54,54,54	0
56	MG	2A	3330	1/1	0.89	0.15	67,67,67,67	0
56	MG	2A	3105	1/1	0.89	0.18	79,79,79,79	0
56	MG	2a	1632	1/1	0.89	0.16	71,71,71,71	0
56	MG	1N	201	1/1	0.89	0.15	63,63,63,63	0
56	MG	1A	3386	1/1	0.89	0.21	69,69,69,69	0
56	MG	2A	3340	1/1	0.89	0.19	72,72,72,72	0
56	MG	2A	3113	1/1	0.89	0.20	57,57,57,57	0
56	MG	2A	3114	1/1	0.89	0.12	61,61,61,61	0
56	MG	1a	1696	1/1	0.89	0.32	64,64,64,64	0
56	MG	2A	3349	1/1	0.89	0.23	65,65,65,65	0
56	MG	2A	3134	1/1	0.89	0.17	68,68,68,68	0
56	MG	2A	3146	1/1	0.89	0.26	59,59,59,59	0
56	MG	1A	3790	1/1	0.89	0.10	53,53,53,53	0
56	MG	2A	3647	1/1	0.89	0.20	67,67,67,67	0
56	MG	1A	3552	1/1	0.89	0.30	70,70,70,70	0
56	MG	1a	1706	1/1	0.89	0.29	74,74,74,74	0
56	MG	1A	4040	1/1	0.89	0.29	65,65,65,65	0
56	MG	1S	202	1/1	0.89	0.10	59,59,59,59	0
56	MG	1A	3555	1/1	0.89	0.10	53,53,53,53	0
56	MG	2A	3169	1/1	0.89	0.13	51,51,51,51	0
56	MG	2a	1682	1/1	0.89	0.14	68,68,68,68	0
56	MG	1T	202	1/1	0.89	0.10	57,57,57,57	0
56	MG	2A	3373	1/1	0.89	0.26	64,64,64,64	0
56	MG	2A	3378	1/1	0.89	0.32	66,66,66,66	0
56	MG	1U	203	1/1	0.89	0.15	59,59,59,59	0
56	MG	1a	1738	1/1	0.89	0.11	65,65,65,65	0
56	MG	1V	206	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3384	1/1	0.89	0.18	59,59,59,59	0
56	MG	2A	3389	1/1	0.89	0.20	63,63,63,63	0
56	MG	2A	3686	1/1	0.89	0.10	73,73,73,73	0
56	MG	2A	3390	1/1	0.89	0.17	78,78,78,78	0
56	MG	1W	209	1/1	0.89	0.18	44,44,44,44	0
56	MG	1A	3307	1/1	0.89	0.12	56,56,56,56	0
56	MG	2a	1705	1/1	0.89	0.12	77,77,77,77	0
56	MG	10	102	1/1	0.89	0.15	54,54,54,54	0
56	MG	1A	3476	1/1	0.89	0.12	52,52,52,52	0
56	MG	2a	1710	1/1	0.89	0.40	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1753	1/1	0.89	0.22	72,72,72,72	0
56	MG	1l	102	1/1	0.89	0.25	57,57,57,57	0
56	MG	2A	3710	1/1	0.89	0.11	69,69,69,69	0
56	MG	2A	3402	1/1	0.89	0.35	53,53,53,53	0
56	MG	2A	3403	1/1	0.89	0.22	64,64,64,64	0
56	MG	1A	3264	1/1	0.89	0.16	55,55,55,55	0
56	MG	1A	3574	1/1	0.89	0.10	35,35,35,35	0
56	MG	2A	3217	1/1	0.89	0.12	67,67,67,67	0
56	MG	1A	3806	1/1	0.89	0.16	64,64,64,64	0
56	MG	2a	1737	1/1	0.89	0.08	77,77,77,77	0
56	MG	1A	3444	1/1	0.89	0.18	66,66,66,66	0
56	MG	1a	1602	1/1	0.89	0.13	58,58,58,58	0
56	MG	2a	1744	1/1	0.89	0.19	49,49,49,49	0
56	MG	2a	1748	1/1	0.89	0.27	63,63,63,63	0
56	MG	2A	3740	1/1	0.89	0.18	75,75,75,75	0
56	MG	1A	3401	1/1	0.89	0.20	71,71,71,71	0
56	MG	1A	3967	1/1	0.89	0.15	67,67,67,67	0
56	MG	1a	1808	1/1	0.89	0.25	62,62,62,62	0
56	MG	2a	1756	1/1	0.89	0.10	73,73,73,73	0
56	MG	1a	1809	1/1	0.89	0.25	66,66,66,66	0
56	MG	1A	4073	1/1	0.89	0.10	57,57,57,57	0
56	MG	2a	1767	1/1	0.89	0.12	71,71,71,71	0
56	MG	1m	3002	1/1	0.89	0.26	63,63,63,63	0
56	MG	2A	3253	1/1	0.89	0.24	69,69,69,69	0
56	MG	1A	3453	1/1	0.89	0.11	44,44,44,44	0
56	MG	2A	3774	1/1	0.89	0.12	65,65,65,65	0
56	MG	2A	3775	1/1	0.89	0.15	58,58,58,58	0
56	MG	2A	3449	1/1	0.89	0.10	60,60,60,60	0
56	MG	2A	3783	1/1	0.89	0.12	76,76,76,76	0
56	MG	1A	3281	1/1	0.89	0.15	50,50,50,50	0
56	MG	2A	3788	1/1	0.89	0.08	55,55,55,55	0
56	MG	1A	3619	1/1	0.89	0.12	51,51,51,51	0
56	MG	1A	3291	1/1	0.89	0.15	55,55,55,55	0
56	MG	1A	3722	1/1	0.89	0.13	52,52,52,52	0
56	MG	1A	3080	1/1	0.89	0.13	53,53,53,53	0
56	MG	2a	1795	1/1	0.89	0.17	71,71,71,71	0
56	MG	2A	3808	1/1	0.89	0.14	78,78,78,78	0
56	MG	1x	111	1/1	0.89	0.25	73,73,73,73	0
56	MG	1A	3842	1/1	0.89	0.14	36,36,36,36	0
56	MG	1A	3738	1/1	0.89	0.11	78,78,78,78	0
56	MG	2a	1801	1/1	0.89	0.17	69,69,69,69	0
56	MG	2A	3489	1/1	0.89	0.10	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1803	1/1	0.89	0.19	81,81,81,81	0
56	MG	2A	3277	1/1	0.89	0.12	63,63,63,63	0
56	MG	2d	301	1/1	0.89	0.10	70,70,70,70	0
56	MG	2A	3497	1/1	0.89	0.13	76,76,76,76	0
56	MG	1A	3515	1/1	0.89	0.33	56,56,56,56	0
56	MG	1a	1652	1/1	0.89	0.10	49,49,49,49	0
56	MG	2t	201	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3004	1/1	0.89	0.23	62,62,62,62	0
56	MG	2A	3510	1/1	0.89	0.09	36,36,36,36	0
56	MG	1A	3861	1/1	0.89	0.14	50,50,50,50	0
56	MG	1a	1658	1/1	0.89	0.12	70,70,70,70	0
56	MG	2B	214	1/1	0.89	0.11	68,68,68,68	0
56	MG	1A	3520	1/1	0.89	0.12	69,69,69,69	0
56	MG	1a	1662	1/1	0.89	0.10	62,62,62,62	0
56	MG	2A	3034	1/1	0.89	0.25	55,55,55,55	0
56	MG	2D	304	1/1	0.89	0.35	49,49,49,49	0
56	MG	2D	305	1/1	0.89	0.30	57,57,57,57	0
56	MG	2A	3043	1/1	0.89	0.12	74,74,74,74	0
56	MG	1A	3759	1/1	0.89	0.12	32,32,32,32	0
56	MG	2y	103	1/1	0.89	0.23	81,81,81,81	0
56	MG	1A	4006	1/1	0.89	0.12	37,37,37,37	0
56	MG	1A	3667	1/1	0.89	0.16	56,56,56,56	0
56	MG	1A	3879	1/1	0.90	0.15	38,38,38,38	0
56	MG	1n	102	1/1	0.90	0.19	69,69,69,69	0
56	MG	1A	3883	1/1	0.90	0.12	49,49,49,49	0
56	MG	1A	3424	1/1	0.90	0.13	68,68,68,68	0
56	MG	1A	3083	1/1	0.90	0.10	48,48,48,48	0
56	MG	2A	3499	1/1	0.90	0.15	45,45,45,45	0
56	MG	1A	3478	1/1	0.90	0.30	62,62,62,62	0
56	MG	2A	3273	1/1	0.90	0.12	67,67,67,67	0
56	MG	2A	3504	1/1	0.90	0.15	61,61,61,61	0
56	MG	1a	1627	1/1	0.90	0.34	68,68,68,68	0
56	MG	1A	4048	1/1	0.90	0.09	63,63,63,63	0
56	MG	1x	110	1/1	0.90	0.15	45,45,45,45	0
56	MG	1A	3339	1/1	0.90	0.11	55,55,55,55	0
56	MG	2E	301	1/1	0.90	0.15	69,69,69,69	0
56	MG	2E	302	1/1	0.90	0.08	62,62,62,62	0
56	MG	1A	3581	1/1	0.90	0.12	12,12,12,12	0
56	MG	1A	4069	1/1	0.90	0.15	54,54,54,54	0
56	MG	2F	303	1/1	0.90	0.09	49,49,49,49	0
56	MG	1A	3340	1/1	0.90	0.13	55,55,55,55	0
56	MG	1A	3343	1/1	0.90	0.17	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1639	1/1	0.90	0.26	67,67,67,67	0
56	MG	2A	3539	1/1	0.90	0.12	53,53,53,53	0
56	MG	2A	3288	1/1	0.90	0.13	56,56,56,56	0
56	MG	1A	3606	1/1	0.90	0.17	59,59,59,59	0
56	MG	2A	3290	1/1	0.90	0.12	61,61,61,61	0
56	MG	1A	3755	1/1	0.90	0.16	57,57,57,57	0
56	MG	1A	3607	1/1	0.90	0.13	61,61,61,61	0
56	MG	2A	3554	1/1	0.90	0.16	68,68,68,68	0
56	MG	2A	3295	1/1	0.90	0.17	56,56,56,56	0
56	MG	25	105	1/1	0.90	0.17	60,60,60,60	0
56	MG	1A	3243	1/1	0.90	0.22	48,48,48,48	0
56	MG	2A	3029	1/1	0.90	0.10	58,58,58,58	0
56	MG	1A	4079	1/1	0.90	0.09	65,65,65,65	0
56	MG	2A	3037	1/1	0.90	0.20	68,68,68,68	0
56	MG	2A	3040	1/1	0.90	0.22	60,60,60,60	0
56	MG	2A	3042	1/1	0.90	0.12	58,58,58,58	0
56	MG	1a	1654	1/1	0.90	0.24	67,67,67,67	0
56	MG	2A	3311	1/1	0.90	0.23	74,74,74,74	0
56	MG	2A	3585	1/1	0.90	0.18	58,58,58,58	0
56	MG	1a	1655	1/1	0.90	0.12	72,72,72,72	0
56	MG	1A	3489	1/1	0.90	0.23	41,41,41,41	0
56	MG	1A	3621	1/1	0.90	0.17	41,41,41,41	0
56	MG	2A	3592	1/1	0.90	0.12	38,38,38,38	0
56	MG	1B	210	1/1	0.90	0.11	57,57,57,57	0
56	MG	1A	3624	1/1	0.90	0.10	26,26,26,26	0
56	MG	1A	3948	1/1	0.90	0.09	36,36,36,36	0
56	MG	2A	3322	1/1	0.90	0.25	57,57,57,57	0
56	MG	1a	1666	1/1	0.90	0.28	69,69,69,69	0
56	MG	2A	3067	1/1	0.90	0.20	58,58,58,58	0
56	MG	1A	3952	1/1	0.90	0.08	35,35,35,35	0
56	MG	2A	3071	1/1	0.90	0.23	76,76,76,76	0
56	MG	1a	1669	1/1	0.90	0.29	64,64,64,64	0
56	MG	2a	1645	1/1	0.90	0.23	47,47,47,47	0
56	MG	2a	1646	1/1	0.90	0.13	67,67,67,67	0
56	MG	1A	3225	1/1	0.90	0.30	45,45,45,45	0
56	MG	2a	1659	1/1	0.90	0.15	63,63,63,63	0
56	MG	1A	3791	1/1	0.90	0.20	55,55,55,55	0
56	MG	1a	1675	1/1	0.90	0.25	71,71,71,71	0
56	MG	2A	3622	1/1	0.90	0.14	70,70,70,70	0
56	MG	2a	1667	1/1	0.90	0.14	72,72,72,72	0
56	MG	2A	3094	1/1	0.90	0.19	71,71,71,71	0
56	MG	1A	3629	1/1	0.90	0.12	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1675	1/1	0.90	0.29	68,68,68,68	0
56	MG	2A	3344	1/1	0.90	0.11	66,66,66,66	0
56	MG	2A	3631	1/1	0.90	0.12	55,55,55,55	0
56	MG	2A	3632	1/1	0.90	0.19	58,58,58,58	0
56	MG	2A	3098	1/1	0.90	0.20	79,79,79,79	0
56	MG	2A	3635	1/1	0.90	0.11	69,69,69,69	0
56	MG	2A	3637	1/1	0.90	0.11	57,57,57,57	0
56	MG	2A	3638	1/1	0.90	0.17	60,60,60,60	0
56	MG	2A	3639	1/1	0.90	0.18	72,72,72,72	0
56	MG	2A	3640	1/1	0.90	0.11	61,61,61,61	0
56	MG	1A	3637	1/1	0.90	0.07	23,23,23,23	0
56	MG	1A	3227	1/1	0.90	0.21	38,38,38,38	0
56	MG	1B	233	1/1	0.90	0.12	64,64,64,64	0
56	MG	2A	3351	1/1	0.90	0.10	73,73,73,73	0
56	MG	2a	1695	1/1	0.90	0.13	67,67,67,67	0
56	MG	1A	3653	1/1	0.90	0.14	32,32,32,32	0
56	MG	1A	3395	1/1	0.90	0.12	58,58,58,58	0
56	MG	1a	1688	1/1	0.90	0.27	51,51,51,51	0
56	MG	2A	3658	1/1	0.90	0.19	66,66,66,66	0
56	MG	2A	3117	1/1	0.90	0.17	67,67,67,67	0
56	MG	2A	3661	1/1	0.90	0.09	54,54,54,54	0
56	MG	1A	3505	1/1	0.90	0.17	47,47,47,47	0
56	MG	2A	3665	1/1	0.90	0.18	72,72,72,72	0
56	MG	2A	3125	1/1	0.90	0.10	49,49,49,49	0
56	MG	1A	3509	1/1	0.90	0.26	63,63,63,63	0
56	MG	2A	3363	1/1	0.90	0.18	72,72,72,72	0
56	MG	2A	3145	1/1	0.90	0.17	50,50,50,50	0
56	MG	1E	308	1/1	0.90	0.23	66,66,66,66	0
56	MG	2A	3679	1/1	0.90	0.12	67,67,67,67	0
56	MG	2A	3147	1/1	0.90	0.20	65,65,65,65	0
56	MG	2A	3376	1/1	0.90	0.14	62,62,62,62	0
56	MG	1E	309	1/1	0.90	0.07	24,24,24,24	0
56	MG	1A	3455	1/1	0.90	0.14	56,56,56,56	0
56	MG	2A	3688	1/1	0.90	0.12	73,73,73,73	0
56	MG	1A	3811	1/1	0.90	0.11	54,54,54,54	0
56	MG	2a	1741	1/1	0.90	0.15	63,63,63,63	0
56	MG	2a	1743	1/1	0.90	0.11	67,67,67,67	0
56	MG	2A	3690	1/1	0.90	0.20	61,61,61,61	0
56	MG	2A	3160	1/1	0.90	0.21	58,58,58,58	0
56	MG	1A	3086	1/1	0.90	0.18	58,58,58,58	0
56	MG	2A	3695	1/1	0.90	0.09	49,49,49,49	0
56	MG	2A	3388	1/1	0.90	0.20	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1F	313	1/1	0.90	0.19	59,59,59,59	0
56	MG	1A	3521	1/1	0.90	0.15	58,58,58,58	0
56	MG	2A	3705	1/1	0.90	0.16	61,61,61,61	0
56	MG	2a	1762	1/1	0.90	0.21	68,68,68,68	0
56	MG	1A	3366	1/1	0.90	0.14	27,27,27,27	0
56	MG	1A	4000	1/1	0.90	0.07	26,26,26,26	0
56	MG	2A	3178	1/1	0.90	0.19	60,60,60,60	0
56	MG	1A	4003	1/1	0.90	0.11	58,58,58,58	0
56	MG	2A	3723	1/1	0.90	0.15	60,60,60,60	0
56	MG	1Q	206	1/1	0.90	0.15	44,44,44,44	0
56	MG	2a	1774	1/1	0.90	0.19	63,63,63,63	0
56	MG	1A	3418	1/1	0.90	0.13	35,35,35,35	0
56	MG	2a	1777	1/1	0.90	0.11	70,70,70,70	0
56	MG	1A	3544	1/1	0.90	0.13	60,60,60,60	0
56	MG	2A	3198	1/1	0.90	0.15	53,53,53,53	0
56	MG	2A	3405	1/1	0.90	0.15	49,49,49,49	0
56	MG	2a	1783	1/1	0.90	0.43	71,71,71,71	0
56	MG	1A	3546	1/1	0.90	0.23	51,51,51,51	0
56	MG	2A	3739	1/1	0.90	0.14	70,70,70,70	0
56	MG	1A	4012	1/1	0.90	0.11	56,56,56,56	0
56	MG	1A	3466	1/1	0.90	0.10	57,57,57,57	0
56	MG	1A	3002	1/1	0.90	0.13	60,60,60,60	0
56	MG	2A	3743	1/1	0.90	0.14	74,74,74,74	0
56	MG	2A	3746	1/1	0.90	0.15	70,70,70,70	0
56	MG	1A	4016	1/1	0.90	0.12	53,53,53,53	0
56	MG	2A	3752	1/1	0.90	0.13	82,82,82,82	0
56	MG	1A	3470	1/1	0.90	0.13	52,52,52,52	0
56	MG	2A	3424	1/1	0.90	0.15	58,58,58,58	0
56	MG	1Z	301	1/1	0.90	0.13	68,68,68,68	0
56	MG	2A	3216	1/1	0.90	0.12	57,57,57,57	0
56	MG	1Z	302	1/1	0.90	0.16	76,76,76,76	0
56	MG	2a	1809	1/1	0.90	0.20	82,82,82,82	0
56	MG	2A	3772	1/1	0.90	0.11	58,58,58,58	0
56	MG	1a	1765	1/1	0.90	0.14	60,60,60,60	0
56	MG	2A	3221	1/1	0.90	0.24	52,52,52,52	0
56	MG	2p	101	1/1	0.90	0.14	64,64,64,64	0
56	MG	2A	3777	1/1	0.90	0.20	75,75,75,75	0
56	MG	1A	3560	1/1	0.90	0.09	43,43,43,43	0
56	MG	1A	3859	1/1	0.90	0.14	73,73,73,73	0
56	MG	1a	1783	1/1	0.90	0.08	65,65,65,65	0
56	MG	1A	4033	1/1	0.90	0.10	55,55,55,55	0
56	MG	2A	3793	1/1	0.90	0.09	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3372	1/1	0.90	0.17	45,45,45,45	0
56	MG	1a	1804	1/1	0.90	0.27	64,64,64,64	0
56	MG	12	101	1/1	0.90	0.11	59,59,59,59	0
56	MG	2A	3461	1/1	0.90	0.15	60,60,60,60	0
56	MG	2x	103	1/1	0.90	0.26	71,71,71,71	0
56	MG	2x	104	1/1	0.90	0.13	71,71,71,71	0
56	MG	13	103	1/1	0.90	0.11	51,51,51,51	0
56	MG	2A	3812	1/1	0.90	0.17	79,79,79,79	0
56	MG	2A	3465	1/1	0.90	0.10	54,54,54,54	0
56	MG	2A	3467	1/1	0.90	0.11	43,43,43,43	0
56	MG	2A	3472	1/1	0.90	0.18	70,70,70,70	0
56	MG	14	101	1/1	0.90	0.23	71,71,71,71	0
56	MG	1A	3865	1/1	0.90	0.10	47,47,47,47	0
56	MG	2A	3327	1/1	0.91	0.17	65,65,65,65	0
56	MG	2F	304	1/1	0.91	0.16	67,67,67,67	0
56	MG	2A	3328	1/1	0.91	0.22	65,65,65,65	0
56	MG	2A	3329	1/1	0.91	0.28	69,69,69,69	0
56	MG	1A	3556	1/1	0.91	0.21	62,62,62,62	0
56	MG	2A	3127	1/1	0.91	0.09	73,73,73,73	0
56	MG	2A	3332	1/1	0.91	0.19	73,73,73,73	0
56	MG	2U	201	1/1	0.91	0.17	53,53,53,53	0
56	MG	2A	3131	1/1	0.91	0.21	58,58,58,58	0
56	MG	1A	3112	1/1	0.91	0.08	42,42,42,42	0
56	MG	2A	3593	1/1	0.91	0.26	63,63,63,63	0
56	MG	2A	3336	1/1	0.91	0.20	67,67,67,67	0
56	MG	2A	3136	1/1	0.91	0.20	61,61,61,61	0
56	MG	1A	3664	1/1	0.91	0.11	34,34,34,34	0
56	MG	21	102	1/1	0.91	0.22	60,60,60,60	0
56	MG	25	102	1/1	0.91	0.10	43,43,43,43	0
56	MG	25	103	1/1	0.91	0.10	70,70,70,70	0
56	MG	1A	3494	1/1	0.91	0.09	61,61,61,61	0
56	MG	1A	3564	1/1	0.91	0.18	53,53,53,53	0
56	MG	2A	3609	1/1	0.91	0.13	61,61,61,61	0
56	MG	1a	1604	1/1	0.91	0.18	64,64,64,64	0
56	MG	27	103	1/1	0.91	0.42	58,58,58,58	0
56	MG	1A	3671	1/1	0.91	0.11	40,40,40,40	0
56	MG	1a	1613	1/1	0.91	0.11	67,67,67,67	0
56	MG	1a	1773	1/1	0.91	0.09	60,60,60,60	0
56	MG	2A	3617	1/1	0.91	0.11	56,56,56,56	0
56	MG	2A	3618	1/1	0.91	0.12	64,64,64,64	0
56	MG	2a	1609	1/1	0.91	0.23	69,69,69,69	0
56	MG	1a	1620	1/1	0.91	0.24	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3356	1/1	0.91	0.12	67,67,67,67	0
56	MG	1a	1624	1/1	0.91	0.20	56,56,56,56	0
56	MG	2a	1616	1/1	0.91	0.28	78,78,78,78	0
56	MG	2A	3166	1/1	0.91	0.15	70,70,70,70	0
56	MG	1A	3957	1/1	0.91	0.10	47,47,47,47	0
56	MG	2a	1628	1/1	0.91	0.27	67,67,67,67	0
56	MG	1a	1791	1/1	0.91	0.10	75,75,75,75	0
56	MG	2a	1630	1/1	0.91	0.34	69,69,69,69	0
56	MG	1B	204	1/1	0.91	0.23	66,66,66,66	0
56	MG	2A	3173	1/1	0.91	0.17	63,63,63,63	0
56	MG	2A	3175	1/1	0.91	0.23	58,58,58,58	0
56	MG	2A	3364	1/1	0.91	0.14	60,60,60,60	0
56	MG	2a	1640	1/1	0.91	0.08	71,71,71,71	0
56	MG	1A	3568	1/1	0.91	0.10	37,37,37,37	0
56	MG	2A	3369	1/1	0.91	0.19	51,51,51,51	0
56	MG	1a	1632	1/1	0.91	0.16	64,64,64,64	0
56	MG	2A	3372	1/1	0.91	0.23	48,48,48,48	0
56	MG	2A	3187	1/1	0.91	0.17	64,64,64,64	0
56	MG	2A	3641	1/1	0.91	0.17	74,74,74,74	0
56	MG	2A	3375	1/1	0.91	0.17	57,57,57,57	0
56	MG	1A	3402	1/1	0.91	0.34	69,69,69,69	0
56	MG	1B	211	1/1	0.91	0.15	55,55,55,55	0
56	MG	2A	3192	1/1	0.91	0.21	58,58,58,58	0
56	MG	1l	201	1/1	0.91	0.12	69,69,69,69	0
56	MG	2a	1665	1/1	0.91	0.20	53,53,53,53	0
56	MG	2A	3195	1/1	0.91	0.12	61,61,61,61	0
56	MG	1A	3317	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3387	1/1	0.91	0.29	60,60,60,60	0
56	MG	2a	1674	1/1	0.91	0.18	72,72,72,72	0
56	MG	1B	215	1/1	0.91	0.10	60,60,60,60	0
56	MG	2A	3202	1/1	0.91	0.16	73,73,73,73	0
56	MG	1A	3280	1/1	0.91	0.07	45,45,45,45	0
56	MG	1A	3970	1/1	0.91	0.09	25,25,25,25	0
56	MG	1a	1644	1/1	0.91	0.12	53,53,53,53	0
56	MG	1A	3213	1/1	0.91	0.11	44,44,44,44	0
56	MG	2A	3211	1/1	0.91	0.15	63,63,63,63	0
56	MG	1w	103	1/1	0.91	0.14	60,60,60,60	0
56	MG	1A	3122	1/1	0.91	0.11	73,73,73,73	0
56	MG	2A	3676	1/1	0.91	0.09	60,60,60,60	0
56	MG	2A	3678	1/1	0.91	0.14	52,52,52,52	0
56	MG	2A	3215	1/1	0.91	0.12	53,53,53,53	0
56	MG	1x	102	1/1	0.91	0.16	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3817	1/1	0.91	0.10	70,70,70,70	0
56	MG	2A	3408	1/1	0.91	0.23	64,64,64,64	0
56	MG	1A	3513	1/1	0.91	0.24	57,57,57,57	0
56	MG	1A	3982	1/1	0.91	0.14	55,55,55,55	0
56	MG	1A	3823	1/1	0.91	0.13	58,58,58,58	0
56	MG	1A	3598	1/1	0.91	0.12	52,52,52,52	0
56	MG	2A	3232	1/1	0.91	0.14	60,60,60,60	0
56	MG	2A	3422	1/1	0.91	0.18	60,60,60,60	0
56	MG	1A	3249	1/1	0.91	0.13	66,66,66,66	0
56	MG	1D	310	1/1	0.91	0.12	45,45,45,45	0
56	MG	2A	3697	1/1	0.91	0.18	57,57,57,57	0
56	MG	2A	3241	1/1	0.91	0.14	65,65,65,65	0
56	MG	2A	3001	1/1	0.91	0.29	65,65,65,65	0
56	MG	1A	3604	1/1	0.91	0.09	25,25,25,25	0
56	MG	1A	3294	1/1	0.91	0.17	50,50,50,50	0
56	MG	2a	1721	1/1	0.91	0.17	73,73,73,73	0
56	MG	2A	3709	1/1	0.91	0.15	67,67,67,67	0
56	MG	1A	3189	1/1	0.91	0.10	45,45,45,45	0
56	MG	2a	1727	1/1	0.91	0.13	81,81,81,81	0
56	MG	2A	3008	1/1	0.91	0.19	65,65,65,65	0
56	MG	2A	3014	1/1	0.91	0.16	69,69,69,69	0
56	MG	2a	1736	1/1	0.91	0.17	68,68,68,68	0
56	MG	1A	3715	1/1	0.91	0.11	47,47,47,47	0
56	MG	2a	1738	1/1	0.91	0.12	70,70,70,70	0
56	MG	1A	3717	1/1	0.91	0.08	49,49,49,49	0
56	MG	2A	3727	1/1	0.91	0.09	64,64,64,64	0
56	MG	1A	3610	1/1	0.91	0.08	31,31,31,31	0
56	MG	1A	3432	1/1	0.91	0.12	58,58,58,58	0
56	MG	1A	3860	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3267	1/1	0.91	0.08	68,68,68,68	0
56	MG	2A	3734	1/1	0.91	0.10	59,59,59,59	0
56	MG	1A	3302	1/1	0.91	0.23	35,35,35,35	0
56	MG	2A	3464	1/1	0.91	0.15	64,64,64,64	0
56	MG	1A	3729	1/1	0.91	0.13	34,34,34,34	0
56	MG	2A	3466	1/1	0.91	0.11	62,62,62,62	0
56	MG	1A	3868	1/1	0.91	0.18	57,57,57,57	0
56	MG	1A	3869	1/1	0.91	0.07	41,41,41,41	0
56	MG	1A	3877	1/1	0.91	0.11	30,30,30,30	0
56	MG	2a	1764	1/1	0.91	0.24	69,69,69,69	0
56	MG	1a	1685	1/1	0.91	0.26	54,54,54,54	0
56	MG	2A	3750	1/1	0.91	0.11	66,66,66,66	0
56	MG	2a	1770	1/1	0.91	0.17	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3280	1/1	0.91	0.09	58,58,58,58	0
56	MG	2A	3056	1/1	0.91	0.22	68,68,68,68	0
56	MG	1A	3531	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3623	1/1	0.91	0.07	29,29,29,29	0
56	MG	1A	3885	1/1	0.91	0.09	66,66,66,66	0
56	MG	2A	3498	1/1	0.91	0.10	50,50,50,50	0
56	MG	1a	1690	1/1	0.91	0.21	52,52,52,52	0
56	MG	2a	1780	1/1	0.91	0.08	70,70,70,70	0
56	MG	1A	4034	1/1	0.91	0.14	48,48,48,48	0
56	MG	1U	202	1/1	0.91	0.14	53,53,53,53	0
56	MG	1A	3092	1/1	0.91	0.16	66,66,66,66	0
56	MG	2A	3506	1/1	0.91	0.11	41,41,41,41	0
56	MG	1A	3442	1/1	0.91	0.15	67,67,67,67	0
56	MG	2A	3785	1/1	0.91	0.15	43,43,43,43	0
56	MG	2a	1790	1/1	0.91	0.16	60,60,60,60	0
56	MG	2A	3079	1/1	0.91	0.15	68,68,68,68	0
56	MG	2A	3511	1/1	0.91	0.11	52,52,52,52	0
56	MG	1A	3548	1/1	0.91	0.08	42,42,42,42	0
56	MG	2A	3086	1/1	0.91	0.08	52,52,52,52	0
56	MG	1A	3630	1/1	0.91	0.08	31,31,31,31	0
56	MG	2A	3802	1/1	0.91	0.27	75,75,75,75	0
56	MG	1A	3760	1/1	0.91	0.11	22,22,22,22	0
56	MG	1a	1713	1/1	0.91	0.23	72,72,72,72	0
56	MG	2A	3525	1/1	0.91	0.09	57,57,57,57	0
56	MG	2A	3533	1/1	0.91	0.10	66,66,66,66	0
56	MG	1A	3205	1/1	0.91	0.13	52,52,52,52	0
56	MG	1A	3642	1/1	0.91	0.14	53,53,53,53	0
56	MG	1a	1720	1/1	0.91	0.11	69,69,69,69	0
56	MG	1A	3257	1/1	0.91	0.22	65,65,65,65	0
56	MG	2A	3830	1/1	0.91	0.11	65,65,65,65	0
56	MG	2B	201	1/1	0.91	0.20	73,73,73,73	0
56	MG	2q	201	1/1	0.91	0.25	69,69,69,69	0
56	MG	2A	3101	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3543	1/1	0.91	0.10	47,47,47,47	0
56	MG	2A	3102	1/1	0.91	0.15	82,82,82,82	0
56	MG	2A	3545	1/1	0.91	0.20	56,56,56,56	0
56	MG	1A	3920	1/1	0.91	0.07	37,37,37,37	0
56	MG	2A	3548	1/1	0.91	0.20	71,71,71,71	0
56	MG	2A	3106	1/1	0.91	0.31	68,68,68,68	0
56	MG	1A	3353	1/1	0.91	0.28	47,47,47,47	0
56	MG	2B	213	1/1	0.91	0.15	54,54,54,54	0
56	MG	1A	4061	1/1	0.91	0.12	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	12	102	1/1	0.91	0.15	50,50,50,50	0
56	MG	2A	3558	1/1	0.91	0.10	52,52,52,52	0
56	MG	1A	3925	1/1	0.91	0.14	49,49,49,49	0
56	MG	2x	106	1/1	0.91	0.08	71,71,71,71	0
56	MG	2A	3561	1/1	0.91	0.17	47,47,47,47	0
56	MG	1A	3779	1/1	0.91	0.10	54,54,54,54	0
56	MG	2A	3119	1/1	0.91	0.20	76,76,76,76	0
56	MG	2A	3571	1/1	0.91	0.12	46,46,46,46	0
56	MG	2A	3573	1/1	0.91	0.10	46,46,46,46	0
56	MG	1a	1748	1/1	0.91	0.30	67,67,67,67	0
56	MG	2A	3268	1/1	0.92	0.15	72,72,72,72	0
56	MG	1x	109	1/1	0.92	0.15	68,68,68,68	0
56	MG	2A	3524	1/1	0.92	0.11	34,34,34,34	0
56	MG	1A	3140	1/1	0.92	0.27	42,42,42,42	0
56	MG	2A	3529	1/1	0.92	0.15	67,67,67,67	0
56	MG	2A	3531	1/1	0.92	0.21	70,70,70,70	0
56	MG	17	105	1/1	0.92	0.14	62,62,62,62	0
56	MG	2D	301	1/1	0.92	0.17	56,56,56,56	0
56	MG	18	103	1/1	0.92	0.11	58,58,58,58	0
56	MG	1A	4021	1/1	0.92	0.08	45,45,45,45	0
56	MG	2D	307	1/1	0.92	0.11	62,62,62,62	0
56	MG	1A	3670	1/1	0.92	0.14	61,61,61,61	0
56	MG	2A	3279	1/1	0.92	0.25	61,61,61,61	0
56	MG	1A	3539	1/1	0.92	0.15	54,54,54,54	0
56	MG	1A	3434	1/1	0.92	0.15	56,56,56,56	0
56	MG	1A	3840	1/1	0.92	0.10	48,48,48,48	0
56	MG	1A	3352	1/1	0.92	0.16	48,48,48,48	0
56	MG	1A	3242	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	4042	1/1	0.92	0.10	56,56,56,56	0
56	MG	2A	3287	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	3849	1/1	0.92	0.08	35,35,35,35	0
56	MG	1A	3549	1/1	0.92	0.10	50,50,50,50	0
56	MG	2P	202	1/1	0.92	0.08	59,59,59,59	0
56	MG	2Q	202	1/1	0.92	0.18	47,47,47,47	0
56	MG	1A	3855	1/1	0.92	0.07	28,28,28,28	0
56	MG	2V	202	1/1	0.92	0.11	57,57,57,57	0
56	MG	2A	3557	1/1	0.92	0.13	62,62,62,62	0
56	MG	2A	3291	1/1	0.92	0.19	70,70,70,70	0
56	MG	2Y	201	1/1	0.92	0.24	63,63,63,63	0
56	MG	1A	3858	1/1	0.92	0.09	27,27,27,27	0
56	MG	2A	3293	1/1	0.92	0.20	69,69,69,69	0
56	MG	1A	3355	1/1	0.92	0.14	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3201	1/1	0.92	0.16	61,61,61,61	0
56	MG	2I	101	1/1	0.92	0.38	53,53,53,53	0
56	MG	1A	4049	1/1	0.92	0.16	37,37,37,37	0
56	MG	25	101	1/1	0.92	0.20	67,67,67,67	0
56	MG	2A	3572	1/1	0.92	0.13	66,66,66,66	0
56	MG	2A	3297	1/1	0.92	0.09	54,54,54,54	0
56	MG	1A	3448	1/1	0.92	0.21	51,51,51,51	0
56	MG	1A	4055	1/1	0.92	0.17	49,49,49,49	0
56	MG	1A	3864	1/1	0.92	0.09	52,52,52,52	0
56	MG	1A	3306	1/1	0.92	0.09	55,55,55,55	0
56	MG	1A	3867	1/1	0.92	0.13	38,38,38,38	0
56	MG	2A	3057	1/1	0.92	0.21	60,60,60,60	0
56	MG	2A	3310	1/1	0.92	0.18	61,61,61,61	0
56	MG	1A	3558	1/1	0.92	0.19	64,64,64,64	0
56	MG	2A	3591	1/1	0.92	0.14	49,49,49,49	0
56	MG	1A	3700	1/1	0.92	0.09	55,55,55,55	0
56	MG	1A	3701	1/1	0.92	0.10	57,57,57,57	0
56	MG	1A	3053	1/1	0.92	0.14	61,61,61,61	0
56	MG	1A	3172	1/1	0.92	0.15	44,44,44,44	0
56	MG	1A	3884	1/1	0.92	0.09	42,42,42,42	0
56	MG	2a	1615	1/1	0.92	0.15	73,73,73,73	0
56	MG	2A	3603	1/1	0.92	0.10	70,70,70,70	0
56	MG	1A	3707	1/1	0.92	0.06	19,19,19,19	0
56	MG	2a	1624	1/1	0.92	0.22	51,51,51,51	0
56	MG	2a	1626	1/1	0.92	0.33	58,58,58,58	0
56	MG	1A	4081	1/1	0.92	0.07	46,46,46,46	0
56	MG	1A	3251	1/1	0.92	0.14	57,57,57,57	0
56	MG	1A	3713	1/1	0.92	0.08	68,68,68,68	0
56	MG	1a	1664	1/1	0.92	0.23	66,66,66,66	0
56	MG	1B	206	1/1	0.92	0.22	50,50,50,50	0
56	MG	2a	1633	1/1	0.92	0.17	56,56,56,56	0
56	MG	1A	3565	1/1	0.92	0.13	58,58,58,58	0
56	MG	2A	3090	1/1	0.92	0.20	61,61,61,61	0
56	MG	2A	3091	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3900	1/1	0.92	0.10	49,49,49,49	0
56	MG	1A	3459	1/1	0.92	0.18	54,54,54,54	0
56	MG	2A	3095	1/1	0.92	0.13	58,58,58,58	0
56	MG	1B	212	1/1	0.92	0.14	63,63,63,63	0
56	MG	1A	3718	1/1	0.92	0.14	58,58,58,58	0
56	MG	2A	3627	1/1	0.92	0.17	63,63,63,63	0
56	MG	1A	3252	1/1	0.92	0.12	62,62,62,62	0
56	MG	2a	1648	1/1	0.92	0.28	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1650	1/1	0.92	0.19	59,59,59,59	0
56	MG	1A	3314	1/1	0.92	0.28	64,64,64,64	0
56	MG	2a	1656	1/1	0.92	0.26	60,60,60,60	0
56	MG	2a	1657	1/1	0.92	0.16	63,63,63,63	0
56	MG	1A	3465	1/1	0.92	0.13	54,54,54,54	0
56	MG	1A	3728	1/1	0.92	0.09	30,30,30,30	0
56	MG	1B	226	1/1	0.92	0.15	64,64,64,64	0
56	MG	1A	3174	1/1	0.92	0.15	50,50,50,50	0
56	MG	1A	3730	1/1	0.92	0.11	51,51,51,51	0
56	MG	2A	3111	1/1	0.92	0.35	67,67,67,67	0
56	MG	1A	3930	1/1	0.92	0.14	51,51,51,51	0
56	MG	1A	3318	1/1	0.92	0.23	58,58,58,58	0
56	MG	1A	3385	1/1	0.92	0.12	35,35,35,35	0
56	MG	1A	3739	1/1	0.92	0.08	48,48,48,48	0
56	MG	1A	3127	1/1	0.92	0.14	49,49,49,49	0
56	MG	2A	3122	1/1	0.92	0.07	68,68,68,68	0
56	MG	2A	3123	1/1	0.92	0.15	73,73,73,73	0
56	MG	1D	301	1/1	0.92	0.12	46,46,46,46	0
56	MG	2A	3655	1/1	0.92	0.12	64,64,64,64	0
56	MG	1A	3943	1/1	0.92	0.08	60,60,60,60	0
56	MG	1A	3748	1/1	0.92	0.08	34,34,34,34	0
56	MG	1a	1703	1/1	0.92	0.07	64,64,64,64	0
56	MG	2A	3367	1/1	0.92	0.17	60,60,60,60	0
56	MG	1D	313	1/1	0.92	0.18	39,39,39,39	0
56	MG	2A	3662	1/1	0.92	0.13	63,63,63,63	0
56	MG	1A	3947	1/1	0.92	0.10	24,24,24,24	0
56	MG	1a	1707	1/1	0.92	0.21	58,58,58,58	0
56	MG	2a	1694	1/1	0.92	0.24	56,56,56,56	0
56	MG	1A	3751	1/1	0.92	0.08	42,42,42,42	0
56	MG	1A	3601	1/1	0.92	0.12	42,42,42,42	0
56	MG	2A	3672	1/1	0.92	0.12	60,60,60,60	0
56	MG	1E	310	1/1	0.92	0.12	31,31,31,31	0
56	MG	1A	3320	1/1	0.92	0.16	51,51,51,51	0
56	MG	2a	1704	1/1	0.92	0.15	75,75,75,75	0
56	MG	1a	1725	1/1	0.92	0.19	60,60,60,60	0
56	MG	1a	1726	1/1	0.92	0.09	61,61,61,61	0
56	MG	1A	3391	1/1	0.92	0.14	59,59,59,59	0
56	MG	2a	1708	1/1	0.92	0.27	73,73,73,73	0
56	MG	1a	1728	1/1	0.92	0.13	64,64,64,64	0
56	MG	1A	3321	1/1	0.92	0.10	60,60,60,60	0
56	MG	2A	3385	1/1	0.92	0.23	58,58,58,58	0
56	MG	1A	3394	1/1	0.92	0.09	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1736	1/1	0.92	0.09	62,62,62,62	0
56	MG	1G	3603	1/1	0.92	0.12	64,64,64,64	0
56	MG	2A	3174	1/1	0.92	0.21	63,63,63,63	0
56	MG	1A	3324	1/1	0.92	0.17	39,39,39,39	0
56	MG	2A	3392	1/1	0.92	0.17	45,45,45,45	0
56	MG	1A	3398	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3180	1/1	0.92	0.12	64,64,64,64	0
56	MG	2A	3182	1/1	0.92	0.23	59,59,59,59	0
56	MG	2A	3183	1/1	0.92	0.14	68,68,68,68	0
56	MG	2A	3698	1/1	0.92	0.21	60,60,60,60	0
56	MG	2A	3700	1/1	0.92	0.18	66,66,66,66	0
56	MG	1A	3180	1/1	0.92	0.10	59,59,59,59	0
56	MG	2A	3702	1/1	0.92	0.13	58,58,58,58	0
56	MG	1P	205	1/1	0.92	0.07	36,36,36,36	0
56	MG	1A	3262	1/1	0.92	0.12	63,63,63,63	0
56	MG	2A	3190	1/1	0.92	0.14	55,55,55,55	0
56	MG	2a	1746	1/1	0.92	0.19	59,59,59,59	0
56	MG	2a	1747	1/1	0.92	0.21	62,62,62,62	0
56	MG	1Q	203	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3332	1/1	0.92	0.07	55,55,55,55	0
56	MG	2A	3193	1/1	0.92	0.26	63,63,63,63	0
56	MG	2a	1753	1/1	0.92	0.12	71,71,71,71	0
56	MG	2A	3720	1/1	0.92	0.11	54,54,54,54	0
56	MG	1A	3226	1/1	0.92	0.10	58,58,58,58	0
56	MG	1A	3981	1/1	0.92	0.09	59,59,59,59	0
56	MG	2A	3196	1/1	0.92	0.20	69,69,69,69	0
56	MG	2A	3725	1/1	0.92	0.14	72,72,72,72	0
56	MG	2A	3421	1/1	0.92	0.12	55,55,55,55	0
56	MG	2A	3197	1/1	0.92	0.08	67,67,67,67	0
56	MG	2a	1765	1/1	0.92	0.16	64,64,64,64	0
56	MG	1a	1762	1/1	0.92	0.08	66,66,66,66	0
56	MG	1A	3157	1/1	0.92	0.12	37,37,37,37	0
56	MG	2a	1769	1/1	0.92	0.15	76,76,76,76	0
56	MG	1A	3422	1/1	0.92	0.09	50,50,50,50	0
56	MG	1a	1770	1/1	0.92	0.13	52,52,52,52	0
56	MG	2A	3206	1/1	0.92	0.19	58,58,58,58	0
56	MG	2A	3207	1/1	0.92	0.22	66,66,66,66	0
56	MG	1A	3159	1/1	0.92	0.33	46,46,46,46	0
56	MG	1A	3633	1/1	0.92	0.10	50,50,50,50	0
56	MG	1U	207	1/1	0.92	0.38	42,42,42,42	0
56	MG	2A	3437	1/1	0.92	0.18	61,61,61,61	0
56	MG	2A	3745	1/1	0.92	0.10	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3438	1/1	0.92	0.09	39,39,39,39	0
56	MG	2A	3441	1/1	0.92	0.27	63,63,63,63	0
56	MG	1U	210	1/1	0.92	0.09	52,52,52,52	0
56	MG	2A	3446	1/1	0.92	0.15	63,63,63,63	0
56	MG	2a	1786	1/1	0.92	0.09	52,52,52,52	0
56	MG	2A	3447	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3236	1/1	0.92	0.25	62,62,62,62	0
56	MG	2A	3450	1/1	0.92	0.08	51,51,51,51	0
56	MG	2A	3759	1/1	0.92	0.12	62,62,62,62	0
56	MG	1V	207	1/1	0.92	0.08	51,51,51,51	0
56	MG	1a	1797	1/1	0.92	0.09	62,62,62,62	0
56	MG	1a	1801	1/1	0.92	0.21	67,67,67,67	0
56	MG	2A	3773	1/1	0.92	0.09	50,50,50,50	0
56	MG	1W	208	1/1	0.92	0.14	31,31,31,31	0
56	MG	1A	3640	1/1	0.92	0.07	31,31,31,31	0
56	MG	1A	3805	1/1	0.92	0.08	39,39,39,39	0
56	MG	1A	3998	1/1	0.92	0.11	60,60,60,60	0
56	MG	1A	3195	1/1	0.92	0.08	46,46,46,46	0
56	MG	2A	3225	1/1	0.92	0.25	63,63,63,63	0
56	MG	2A	3470	1/1	0.92	0.08	49,49,49,49	0
56	MG	2a	1810	1/1	0.92	0.20	78,78,78,78	0
56	MG	2A	3230	1/1	0.92	0.18	62,62,62,62	0
56	MG	2g	201	1/1	0.92	0.19	69,69,69,69	0
56	MG	1a	1810	1/1	0.92	0.09	64,64,64,64	0
56	MG	1a	1811	1/1	0.92	0.11	61,61,61,61	0
56	MG	2A	3799	1/1	0.92	0.12	71,71,71,71	0
56	MG	1f	201	1/1	0.92	0.12	50,50,50,50	0
56	MG	2q	202	1/1	0.92	0.09	73,73,73,73	0
56	MG	1A	4002	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3246	1/1	0.92	0.12	63,63,63,63	0
56	MG	1A	3345	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3518	1/1	0.92	0.11	62,62,62,62	0
56	MG	2A	3809	1/1	0.92	0.17	54,54,54,54	0
56	MG	2A	3249	1/1	0.92	0.16	72,72,72,72	0
56	MG	1A	3815	1/1	0.92	0.17	43,43,43,43	0
56	MG	1A	3427	1/1	0.92	0.16	57,57,57,57	0
56	MG	1A	3660	1/1	0.92	0.09	37,37,37,37	0
56	MG	2A	3824	1/1	0.92	0.20	65,65,65,65	0
56	MG	2A	3827	1/1	0.92	0.10	60,60,60,60	0
56	MG	1A	3430	1/1	0.92	0.19	57,57,57,57	0
56	MG	2A	3256	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3431	1/1	0.92	0.34	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	15	103	1/1	0.92	0.18	42,42,42,42	0
56	MG	15	104	1/1	0.92	0.18	40,40,40,40	0
56	MG	15	105	1/1	0.92	0.48	32,32,32,32	0
56	MG	1x	106	1/1	0.92	0.19	61,61,61,61	0
56	MG	2A	3516	1/1	0.92	0.12	72,72,72,72	0
56	MG	1A	3293	1/1	0.92	0.13	60,60,60,60	0
56	MG	2A	3580	1/1	0.93	0.08	41,41,41,41	0
56	MG	2A	3582	1/1	0.93	0.19	59,59,59,59	0
56	MG	1V	203	1/1	0.93	0.13	34,34,34,34	0
56	MG	2A	3116	1/1	0.93	0.10	47,47,47,47	0
56	MG	1A	3645	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3118	1/1	0.93	0.16	58,58,58,58	0
56	MG	1A	3074	1/1	0.93	0.14	39,39,39,39	0
56	MG	1a	1733	1/1	0.93	0.38	71,71,71,71	0
56	MG	2T	202	1/1	0.93	0.19	66,66,66,66	0
56	MG	1W	201	1/1	0.93	0.17	45,45,45,45	0
56	MG	2V	201	1/1	0.93	0.17	49,49,49,49	0
56	MG	1W	202	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3554	1/1	0.93	0.32	63,63,63,63	0
56	MG	2A	3334	1/1	0.93	0.13	62,62,62,62	0
56	MG	2A	3126	1/1	0.93	0.10	63,63,63,63	0
56	MG	1A	3754	1/1	0.93	0.14	60,60,60,60	0
56	MG	1A	3373	1/1	0.93	0.23	46,46,46,46	0
56	MG	1Y	204	1/1	0.93	0.11	56,56,56,56	0
56	MG	1a	1747	1/1	0.93	0.09	50,50,50,50	0
56	MG	2A	3144	1/1	0.93	0.21	62,62,62,62	0
56	MG	2A	3347	1/1	0.93	0.13	66,66,66,66	0
56	MG	2A	3611	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3612	1/1	0.93	0.11	64,64,64,64	0
56	MG	1A	3882	1/1	0.93	0.09	64,64,64,64	0
56	MG	1A	3078	1/1	0.93	0.18	36,36,36,36	0
56	MG	1Z	303	1/1	0.93	0.20	51,51,51,51	0
56	MG	2A	3151	1/1	0.93	0.16	46,46,46,46	0
56	MG	2A	3155	1/1	0.93	0.17	62,62,62,62	0
56	MG	2A	3355	1/1	0.93	0.06	61,61,61,61	0
56	MG	10	101	1/1	0.93	0.14	44,44,44,44	0
56	MG	1A	3557	1/1	0.93	0.29	55,55,55,55	0
56	MG	2a	1602	1/1	0.93	0.20	75,75,75,75	0
56	MG	2A	3158	1/1	0.93	0.14	48,48,48,48	0
56	MG	2a	1605	1/1	0.93	0.09	78,78,78,78	0
56	MG	2a	1606	1/1	0.93	0.27	60,60,60,60	0
56	MG	1A	3246	1/1	0.93	0.08	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3626	1/1	0.93	0.28	61,61,61,61	0
56	MG	1a	1760	1/1	0.93	0.08	73,73,73,73	0
56	MG	1A	3764	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3766	1/1	0.93	0.07	27,27,27,27	0
56	MG	2A	3630	1/1	0.93	0.11	52,52,52,52	0
56	MG	1A	3893	1/1	0.93	0.07	38,38,38,38	0
56	MG	1A	3428	1/1	0.93	0.08	51,51,51,51	0
56	MG	2A	3365	1/1	0.93	0.26	65,65,65,65	0
56	MG	2a	1620	1/1	0.93	0.19	67,67,67,67	0
56	MG	2a	1621	1/1	0.93	0.29	65,65,65,65	0
56	MG	2a	1623	1/1	0.93	0.25	64,64,64,64	0
56	MG	2A	3168	1/1	0.93	0.31	67,67,67,67	0
56	MG	2a	1625	1/1	0.93	0.23	54,54,54,54	0
56	MG	13	102	1/1	0.93	0.08	47,47,47,47	0
56	MG	1A	3312	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3901	1/1	0.93	0.08	55,55,55,55	0
56	MG	1a	1782	1/1	0.93	0.11	74,74,74,74	0
56	MG	1A	4051	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3774	1/1	0.93	0.14	45,45,45,45	0
56	MG	1A	3775	1/1	0.93	0.10	57,57,57,57	0
56	MG	2A	3645	1/1	0.93	0.11	73,73,73,73	0
56	MG	2A	3646	1/1	0.93	0.08	31,31,31,31	0
56	MG	2a	1637	1/1	0.93	0.14	79,79,79,79	0
56	MG	1A	4057	1/1	0.93	0.15	48,48,48,48	0
56	MG	1A	3905	1/1	0.93	0.12	66,66,66,66	0
56	MG	1A	3907	1/1	0.93	0.06	52,52,52,52	0
56	MG	2A	3654	1/1	0.93	0.09	44,44,44,44	0
56	MG	1a	1803	1/1	0.93	0.22	65,65,65,65	0
56	MG	18	101	1/1	0.93	0.20	51,51,51,51	0
56	MG	1A	3051	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3386	1/1	0.93	0.23	58,58,58,58	0
56	MG	1A	3777	1/1	0.93	0.17	66,66,66,66	0
56	MG	2a	1649	1/1	0.93	0.18	65,65,65,65	0
56	MG	1A	3341	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3783	1/1	0.93	0.06	30,30,30,30	0
56	MG	1A	3785	1/1	0.93	0.09	36,36,36,36	0
56	MG	1A	3924	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3667	1/1	0.93	0.09	55,55,55,55	0
56	MG	1a	1608	1/1	0.93	0.22	58,58,58,58	0
56	MG	2A	3393	1/1	0.93	0.23	52,52,52,52	0
56	MG	2a	1662	1/1	0.93	0.20	59,59,59,59	0
56	MG	1a	1612	1/1	0.93	0.19	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3290	1/1	0.93	0.18	58,58,58,58	0
56	MG	1n	101	1/1	0.93	0.19	56,56,56,56	0
56	MG	2A	3200	1/1	0.93	0.12	52,52,52,52	0
56	MG	1a	1616	1/1	0.93	0.07	48,48,48,48	0
56	MG	1A	3674	1/1	0.93	0.12	50,50,50,50	0
56	MG	1a	1621	1/1	0.93	0.07	56,56,56,56	0
56	MG	2a	1676	1/1	0.93	0.20	67,67,67,67	0
56	MG	2A	3404	1/1	0.93	0.17	63,63,63,63	0
56	MG	1A	4082	1/1	0.93	0.18	65,65,65,65	0
56	MG	2A	3682	1/1	0.93	0.07	78,78,78,78	0
56	MG	1a	1626	1/1	0.93	0.15	52,52,52,52	0
56	MG	2A	3684	1/1	0.93	0.14	57,57,57,57	0
56	MG	1w	104	1/1	0.93	0.20	69,69,69,69	0
56	MG	2A	3410	1/1	0.93	0.16	57,57,57,57	0
56	MG	1A	3933	1/1	0.93	0.14	58,58,58,58	0
56	MG	1A	3387	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3572	1/1	0.93	0.07	29,29,29,29	0
56	MG	2A	3693	1/1	0.93	0.08	56,56,56,56	0
56	MG	1A	3436	1/1	0.93	0.15	69,69,69,69	0
56	MG	2A	3214	1/1	0.93	0.37	47,47,47,47	0
56	MG	1A	3437	1/1	0.93	0.21	41,41,41,41	0
56	MG	1A	3315	1/1	0.93	0.16	48,48,48,48	0
56	MG	1A	3100	1/1	0.93	0.26	40,40,40,40	0
56	MG	2a	1698	1/1	0.93	0.13	51,51,51,51	0
56	MG	1A	3045	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3508	1/1	0.93	0.17	57,57,57,57	0
56	MG	1x	113	1/1	0.93	0.29	73,73,73,73	0
56	MG	2a	1703	1/1	0.93	0.28	61,61,61,61	0
56	MG	1A	3808	1/1	0.93	0.07	48,48,48,48	0
56	MG	1A	3809	1/1	0.93	0.11	59,59,59,59	0
56	MG	2A	3226	1/1	0.93	0.08	58,58,58,58	0
56	MG	2A	3229	1/1	0.93	0.10	57,57,57,57	0
56	MG	1A	3445	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3711	1/1	0.93	0.08	64,64,64,64	0
56	MG	2a	1711	1/1	0.93	0.23	53,53,53,53	0
56	MG	1B	224	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3715	1/1	0.93	0.15	79,79,79,79	0
56	MG	2A	3233	1/1	0.93	0.14	68,68,68,68	0
56	MG	2A	3234	1/1	0.93	0.22	65,65,65,65	0
56	MG	2A	3445	1/1	0.93	0.15	58,58,58,58	0
56	MG	2A	3236	1/1	0.93	0.38	72,72,72,72	0
56	MG	2A	3003	1/1	0.93	0.17	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3961	1/1	0.93	0.08	20,20,20,20	0
56	MG	2A	3728	1/1	0.93	0.07	43,43,43,43	0
56	MG	1A	3511	1/1	0.93	0.07	22,22,22,22	0
56	MG	2A	3244	1/1	0.93	0.08	55,55,55,55	0
56	MG	2A	3452	1/1	0.93	0.19	61,61,61,61	0
56	MG	1A	3814	1/1	0.93	0.08	23,23,23,23	0
56	MG	2A	3456	1/1	0.93	0.08	27,27,27,27	0
56	MG	2A	3457	1/1	0.93	0.16	52,52,52,52	0
56	MG	1A	3351	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3114	1/1	0.93	0.29	45,45,45,45	0
56	MG	1A	3047	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3609	1/1	0.93	0.08	37,37,37,37	0
56	MG	1a	1660	1/1	0.93	0.26	65,65,65,65	0
56	MG	2A	3030	1/1	0.93	0.12	45,45,45,45	0
56	MG	2A	3031	1/1	0.93	0.10	42,42,42,42	0
56	MG	1B	235	1/1	0.93	0.10	74,74,74,74	0
56	MG	1A	3978	1/1	0.93	0.09	51,51,51,51	0
56	MG	2A	3751	1/1	0.93	0.12	59,59,59,59	0
56	MG	1A	3296	1/1	0.93	0.24	59,59,59,59	0
56	MG	1A	3358	1/1	0.93	0.13	63,63,63,63	0
56	MG	2A	3754	1/1	0.93	0.09	48,48,48,48	0
56	MG	2A	3263	1/1	0.93	0.17	63,63,63,63	0
56	MG	2a	1760	1/1	0.93	0.18	66,66,66,66	0
56	MG	1A	3826	1/1	0.93	0.08	48,48,48,48	0
56	MG	2A	3485	1/1	0.93	0.07	37,37,37,37	0
56	MG	2A	3045	1/1	0.93	0.22	57,57,57,57	0
56	MG	1A	3827	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3771	1/1	0.93	0.12	47,47,47,47	0
56	MG	2A	3492	1/1	0.93	0.10	40,40,40,40	0
56	MG	1A	3457	1/1	0.93	0.08	40,40,40,40	0
56	MG	2A	3269	1/1	0.93	0.21	67,67,67,67	0
56	MG	2A	3051	1/1	0.93	0.14	67,67,67,67	0
56	MG	2A	3271	1/1	0.93	0.28	76,76,76,76	0
56	MG	2A	3272	1/1	0.93	0.26	59,59,59,59	0
56	MG	2A	3052	1/1	0.93	0.14	61,61,61,61	0
56	MG	2a	1775	1/1	0.93	0.20	63,63,63,63	0
56	MG	2A	3784	1/1	0.93	0.07	63,63,63,63	0
56	MG	2A	3053	1/1	0.93	0.11	55,55,55,55	0
56	MG	2a	1778	1/1	0.93	0.08	74,74,74,74	0
56	MG	1A	3065	1/1	0.93	0.21	55,55,55,55	0
56	MG	2A	3787	1/1	0.93	0.08	47,47,47,47	0
56	MG	1A	3409	1/1	0.93	0.10	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3058	1/1	0.93	0.23	58,58,58,58	0
56	MG	2A	3796	1/1	0.93	0.10	62,62,62,62	0
56	MG	1A	3537	1/1	0.93	0.19	44,44,44,44	0
56	MG	2A	3798	1/1	0.93	0.11	70,70,70,70	0
56	MG	1E	311	1/1	0.93	0.09	62,62,62,62	0
56	MG	2a	1788	1/1	0.93	0.19	56,56,56,56	0
56	MG	2A	3062	1/1	0.93	0.34	66,66,66,66	0
56	MG	1A	3834	1/1	0.93	0.23	36,36,36,36	0
56	MG	2A	3518	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3836	1/1	0.93	0.15	44,44,44,44	0
56	MG	1a	1682	1/1	0.93	0.08	63,63,63,63	0
56	MG	1A	3997	1/1	0.93	0.06	44,44,44,44	0
56	MG	2A	3811	1/1	0.93	0.11	64,64,64,64	0
56	MG	1A	3411	1/1	0.93	0.10	44,44,44,44	0
56	MG	2A	3526	1/1	0.93	0.15	56,56,56,56	0
56	MG	1A	3725	1/1	0.93	0.08	42,42,42,42	0
56	MG	2A	3816	1/1	0.93	0.08	55,55,55,55	0
56	MG	2A	3076	1/1	0.93	0.15	51,51,51,51	0
56	MG	2a	1805	1/1	0.93	0.13	65,65,65,65	0
56	MG	2A	3077	1/1	0.93	0.16	54,54,54,54	0
56	MG	2a	1807	1/1	0.93	0.17	68,68,68,68	0
56	MG	2a	1808	1/1	0.93	0.12	86,86,86,86	0
56	MG	2A	3826	1/1	0.93	0.14	62,62,62,62	0
56	MG	1A	4001	1/1	0.93	0.13	49,49,49,49	0
56	MG	2A	3082	1/1	0.93	0.21	60,60,60,60	0
56	MG	2d	302	1/1	0.93	0.19	56,56,56,56	0
56	MG	1O	202	1/1	0.93	0.10	56,56,56,56	0
56	MG	1A	3541	1/1	0.93	0.12	73,73,73,73	0
56	MG	2l	202	1/1	0.93	0.07	68,68,68,68	0
56	MG	1A	3325	1/1	0.93	0.13	66,66,66,66	0
56	MG	1A	3463	1/1	0.93	0.13	47,47,47,47	0
56	MG	1a	1693	1/1	0.93	0.45	62,62,62,62	0
56	MG	1A	3854	1/1	0.93	0.08	26,26,26,26	0
56	MG	1A	3635	1/1	0.93	0.08	27,27,27,27	0
56	MG	2B	209	1/1	0.93	0.20	69,69,69,69	0
56	MG	1a	1697	1/1	0.93	0.25	53,53,53,53	0
56	MG	1A	3735	1/1	0.93	0.10	19,19,19,19	0
56	MG	2A	3096	1/1	0.93	0.09	53,53,53,53	0
56	MG	1a	1702	1/1	0.93	0.19	59,59,59,59	0
56	MG	1R	201	1/1	0.93	0.15	59,59,59,59	0
56	MG	1A	3365	1/1	0.93	0.19	27,27,27,27	0
56	MG	1A	3136	1/1	0.93	0.09	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4015	1/1	0.93	0.12	59,59,59,59	0
56	MG	2B	219	1/1	0.93	0.33	75,75,75,75	0
56	MG	2A	3103	1/1	0.93	0.18	59,59,59,59	0
56	MG	1A	3742	1/1	0.93	0.11	47,47,47,47	0
56	MG	2A	3317	1/1	0.93	0.21	67,67,67,67	0
56	MG	2A	3565	1/1	0.93	0.07	44,44,44,44	0
56	MG	1A	4017	1/1	0.93	0.07	54,54,54,54	0
56	MG	1A	4018	1/1	0.93	0.08	58,58,58,58	0
56	MG	2y	102	1/1	0.93	0.09	80,80,80,80	0
56	MG	1A	3743	1/1	0.93	0.09	51,51,51,51	0
56	MG	1A	3258	1/1	0.93	0.10	41,41,41,41	0
56	MG	1V	202	1/1	0.93	0.20	39,39,39,39	0
56	MG	1A	3381	1/1	0.94	0.12	57,57,57,57	0
56	MG	2A	3502	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3120	1/1	0.94	0.21	56,56,56,56	0
56	MG	1A	3247	1/1	0.94	0.21	38,38,38,38	0
56	MG	2B	205	1/1	0.94	0.16	61,61,61,61	0
56	MG	1A	3062	1/1	0.94	0.11	36,36,36,36	0
56	MG	1A	3712	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3239	1/1	0.94	0.12	71,71,71,71	0
56	MG	2A	3240	1/1	0.94	0.18	61,61,61,61	0
56	MG	2A	3512	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	3124	1/1	0.94	0.21	47,47,47,47	0
56	MG	2A	3242	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3566	1/1	0.94	0.19	52,52,52,52	0
56	MG	1A	3186	1/1	0.94	0.46	35,35,35,35	0
56	MG	1x	108	1/1	0.94	0.23	64,64,64,64	0
56	MG	1A	3388	1/1	0.94	0.10	57,57,57,57	0
56	MG	1a	1601	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3389	1/1	0.94	0.07	56,56,56,56	0
56	MG	1A	3720	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	3001	1/1	0.94	0.11	46,46,46,46	0
56	MG	2D	306	1/1	0.94	0.09	68,68,68,68	0
56	MG	2A	3254	1/1	0.94	0.11	82,82,82,82	0
56	MG	1A	3468	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3871	1/1	0.94	0.06	45,45,45,45	0
56	MG	1A	3724	1/1	0.94	0.08	25,25,25,25	0
56	MG	2E	305	1/1	0.94	0.12	57,57,57,57	0
56	MG	2E	306	1/1	0.94	0.10	41,41,41,41	0
56	MG	2A	3535	1/1	0.94	0.26	69,69,69,69	0
56	MG	2F	301	1/1	0.94	0.11	47,47,47,47	0
56	MG	2F	302	1/1	0.94	0.20	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3878	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	4053	1/1	0.94	0.10	42,42,42,42	0
56	MG	2A	3540	1/1	0.94	0.12	60,60,60,60	0
56	MG	1a	1618	1/1	0.94	0.09	59,59,59,59	0
56	MG	1A	4054	1/1	0.94	0.07	37,37,37,37	0
56	MG	1A	3131	1/1	0.94	0.11	41,41,41,41	0
56	MG	2A	3009	1/1	0.94	0.21	58,58,58,58	0
56	MG	2A	3012	1/1	0.94	0.10	56,56,56,56	0
56	MG	1a	1623	1/1	0.94	0.14	63,63,63,63	0
56	MG	2Q	203	1/1	0.94	0.09	61,61,61,61	0
56	MG	2R	201	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3016	1/1	0.94	0.13	62,62,62,62	0
56	MG	2T	203	1/1	0.94	0.11	67,67,67,67	0
56	MG	2A	3017	1/1	0.94	0.09	47,47,47,47	0
56	MG	2A	3550	1/1	0.94	0.06	62,62,62,62	0
56	MG	2A	3553	1/1	0.94	0.17	68,68,68,68	0
56	MG	2A	3018	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	3880	1/1	0.94	0.11	52,52,52,52	0
56	MG	2A	3022	1/1	0.94	0.07	59,59,59,59	0
56	MG	1a	1625	1/1	0.94	0.23	58,58,58,58	0
56	MG	1A	3190	1/1	0.94	0.16	47,47,47,47	0
56	MG	1A	3587	1/1	0.94	0.07	39,39,39,39	0
56	MG	1a	1628	1/1	0.94	0.21	57,57,57,57	0
56	MG	1A	4064	1/1	0.94	0.12	53,53,53,53	0
56	MG	2A	3563	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	4065	1/1	0.94	0.08	78,78,78,78	0
56	MG	1A	3255	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3038	1/1	0.94	0.11	58,58,58,58	0
56	MG	2A	3039	1/1	0.94	0.25	64,64,64,64	0
56	MG	25	106	1/1	0.94	0.10	53,53,53,53	0
56	MG	1a	1633	1/1	0.94	0.18	65,65,65,65	0
56	MG	2A	3575	1/1	0.94	0.13	68,68,68,68	0
56	MG	2A	3041	1/1	0.94	0.17	67,67,67,67	0
56	MG	2A	3578	1/1	0.94	0.24	56,56,56,56	0
56	MG	1a	1634	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3256	1/1	0.94	0.09	47,47,47,47	0
56	MG	2a	1601	1/1	0.94	0.08	63,63,63,63	0
56	MG	1A	3886	1/1	0.94	0.09	59,59,59,59	0
56	MG	2A	3047	1/1	0.94	0.16	37,37,37,37	0
56	MG	1A	3193	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3888	1/1	0.94	0.07	50,50,50,50	0
56	MG	2A	3586	1/1	0.94	0.10	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3327	1/1	0.94	0.17	38,38,38,38	0
56	MG	1a	1640	1/1	0.94	0.11	67,67,67,67	0
56	MG	1A	3328	1/1	0.94	0.29	42,42,42,42	0
56	MG	2A	3055	1/1	0.94	0.33	65,65,65,65	0
56	MG	1A	4078	1/1	0.94	0.12	44,44,44,44	0
56	MG	2a	1614	1/1	0.94	0.24	68,68,68,68	0
56	MG	1A	3740	1/1	0.94	0.07	33,33,33,33	0
56	MG	1A	3899	1/1	0.94	0.07	41,41,41,41	0
56	MG	2A	3302	1/1	0.94	0.10	59,59,59,59	0
56	MG	2a	1618	1/1	0.94	0.25	67,67,67,67	0
56	MG	2A	3600	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3605	1/1	0.94	0.06	17,17,17,17	0
56	MG	2a	1622	1/1	0.94	0.07	78,78,78,78	0
56	MG	2A	3304	1/1	0.94	0.07	52,52,52,52	0
56	MG	2A	3305	1/1	0.94	0.22	62,62,62,62	0
56	MG	2A	3605	1/1	0.94	0.12	65,65,65,65	0
56	MG	2A	3606	1/1	0.94	0.13	71,71,71,71	0
56	MG	1A	3134	1/1	0.94	0.10	45,45,45,45	0
56	MG	1B	202	1/1	0.94	0.19	57,57,57,57	0
56	MG	1A	3745	1/1	0.94	0.08	25,25,25,25	0
56	MG	1A	3407	1/1	0.94	0.15	55,55,55,55	0
56	MG	2a	1631	1/1	0.94	0.13	62,62,62,62	0
56	MG	1A	3487	1/1	0.94	0.25	39,39,39,39	0
56	MG	1B	209	1/1	0.94	0.08	45,45,45,45	0
56	MG	2a	1634	1/1	0.94	0.09	79,79,79,79	0
56	MG	2A	3068	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3315	1/1	0.94	0.09	61,61,61,61	0
56	MG	2A	3069	1/1	0.94	0.08	57,57,57,57	0
56	MG	1A	3070	1/1	0.94	0.05	35,35,35,35	0
56	MG	1A	3913	1/1	0.94	0.09	66,66,66,66	0
56	MG	2A	3073	1/1	0.94	0.21	45,45,45,45	0
56	MG	1A	3491	1/1	0.94	0.27	65,65,65,65	0
56	MG	1A	3618	1/1	0.94	0.09	41,41,41,41	0
56	MG	2A	3623	1/1	0.94	0.09	48,48,48,48	0
56	MG	2A	3624	1/1	0.94	0.19	58,58,58,58	0
56	MG	1a	1665	1/1	0.94	0.24	60,60,60,60	0
56	MG	2A	3080	1/1	0.94	0.15	52,52,52,52	0
56	MG	1B	214	1/1	0.94	0.21	54,54,54,54	0
56	MG	2A	3084	1/1	0.94	0.10	56,56,56,56	0
56	MG	2a	1653	1/1	0.94	0.19	68,68,68,68	0
56	MG	1A	3916	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3492	1/1	0.94	0.10	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3918	1/1	0.94	0.14	59,59,59,59	0
56	MG	2a	1658	1/1	0.94	0.10	62,62,62,62	0
56	MG	1B	222	1/1	0.94	0.09	54,54,54,54	0
56	MG	1a	1672	1/1	0.94	0.17	62,62,62,62	0
56	MG	2A	3634	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3493	1/1	0.94	0.12	62,62,62,62	0
56	MG	1a	1676	1/1	0.94	0.21	69,69,69,69	0
56	MG	1a	1677	1/1	0.94	0.22	68,68,68,68	0
56	MG	1A	3335	1/1	0.94	0.09	53,53,53,53	0
56	MG	2a	1668	1/1	0.94	0.16	59,59,59,59	0
56	MG	2a	1669	1/1	0.94	0.27	57,57,57,57	0
56	MG	2A	3337	1/1	0.94	0.19	68,68,68,68	0
56	MG	2A	3339	1/1	0.94	0.25	67,67,67,67	0
56	MG	1B	225	1/1	0.94	0.09	60,60,60,60	0
56	MG	2A	3341	1/1	0.94	0.22	49,49,49,49	0
56	MG	2A	3644	1/1	0.94	0.09	62,62,62,62	0
56	MG	2A	3342	1/1	0.94	0.09	69,69,69,69	0
56	MG	1A	3139	1/1	0.94	0.07	34,34,34,34	0
56	MG	2a	1679	1/1	0.94	0.22	56,56,56,56	0
56	MG	1A	3625	1/1	0.94	0.07	27,27,27,27	0
56	MG	1A	3927	1/1	0.94	0.12	45,45,45,45	0
56	MG	2A	3346	1/1	0.94	0.24	66,66,66,66	0
56	MG	2a	1683	1/1	0.94	0.10	70,70,70,70	0
56	MG	2A	3650	1/1	0.94	0.08	61,61,61,61	0
56	MG	1A	3928	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3626	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	3269	1/1	0.94	0.18	34,34,34,34	0
56	MG	1A	3274	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3935	1/1	0.94	0.07	66,66,66,66	0
56	MG	2A	3107	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3354	1/1	0.94	0.23	69,69,69,69	0
56	MG	1A	3050	1/1	0.94	0.08	45,45,45,45	0
56	MG	1A	3147	1/1	0.94	0.15	43,43,43,43	0
56	MG	1D	306	1/1	0.94	0.08	41,41,41,41	0
56	MG	2a	1697	1/1	0.94	0.14	62,62,62,62	0
56	MG	1A	3939	1/1	0.94	0.07	60,60,60,60	0
56	MG	2a	1699	1/1	0.94	0.19	57,57,57,57	0
56	MG	1A	3282	1/1	0.94	0.09	55,55,55,55	0
56	MG	1a	1695	1/1	0.94	0.26	65,65,65,65	0
56	MG	1A	3075	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3944	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3638	1/1	0.94	0.10	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3512	1/1	0.94	0.21	48,48,48,48	0
56	MG	1A	3641	1/1	0.94	0.06	36,36,36,36	0
56	MG	2A	3366	1/1	0.94	0.21	45,45,45,45	0
56	MG	1A	3949	1/1	0.94	0.10	44,44,44,44	0
56	MG	2a	1709	1/1	0.94	0.24	58,58,58,58	0
56	MG	2A	3124	1/1	0.94	0.08	55,55,55,55	0
56	MG	1A	3950	1/1	0.94	0.08	25,25,25,25	0
56	MG	2A	3370	1/1	0.94	0.20	40,40,40,40	0
56	MG	1A	3789	1/1	0.94	0.07	46,46,46,46	0
56	MG	1A	3953	1/1	0.94	0.11	58,58,58,58	0
56	MG	1A	3956	1/1	0.94	0.07	57,57,57,57	0
56	MG	2A	3374	1/1	0.94	0.17	46,46,46,46	0
56	MG	2a	1720	1/1	0.94	0.10	77,77,77,77	0
56	MG	1a	1716	1/1	0.94	0.39	66,66,66,66	0
56	MG	1A	3347	1/1	0.94	0.12	49,49,49,49	0
56	MG	2a	1724	1/1	0.94	0.10	71,71,71,71	0
56	MG	2a	1725	1/1	0.94	0.07	81,81,81,81	0
56	MG	2A	3377	1/1	0.94	0.24	63,63,63,63	0
56	MG	2A	3140	1/1	0.94	0.11	60,60,60,60	0
56	MG	2A	3142	1/1	0.94	0.19	47,47,47,47	0
56	MG	1I	201	1/1	0.94	0.08	59,59,59,59	0
56	MG	2A	3381	1/1	0.94	0.21	58,58,58,58	0
56	MG	1A	3514	1/1	0.94	0.16	56,56,56,56	0
56	MG	1N	202	1/1	0.94	0.09	52,52,52,52	0
56	MG	1N	203	1/1	0.94	0.07	48,48,48,48	0
56	MG	2A	3148	1/1	0.94	0.15	64,64,64,64	0
56	MG	2A	3150	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	3793	1/1	0.94	0.21	63,63,63,63	0
56	MG	2A	3153	1/1	0.94	0.11	69,69,69,69	0
56	MG	2A	3707	1/1	0.94	0.13	45,45,45,45	0
56	MG	2A	3154	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	3042	1/1	0.94	0.06	24,24,24,24	0
56	MG	1a	1730	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	3649	1/1	0.94	0.10	61,61,61,61	0
56	MG	2A	3394	1/1	0.94	0.18	52,52,52,52	0
56	MG	1A	3516	1/1	0.94	0.19	58,58,58,58	0
56	MG	2A	3716	1/1	0.94	0.06	62,62,62,62	0
56	MG	2A	3717	1/1	0.94	0.10	82,82,82,82	0
56	MG	1A	3224	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3397	1/1	0.94	0.26	68,68,68,68	0
56	MG	2a	1761	1/1	0.94	0.08	64,64,64,64	0
56	MG	1A	3519	1/1	0.94	0.12	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3163	1/1	0.94	0.09	63,63,63,63	0
56	MG	2A	3400	1/1	0.94	0.24	56,56,56,56	0
56	MG	1Q	205	1/1	0.94	0.11	47,47,47,47	0
56	MG	2a	1766	1/1	0.94	0.22	61,61,61,61	0
56	MG	1A	3104	1/1	0.94	0.14	42,42,42,42	0
56	MG	1A	3663	1/1	0.94	0.17	58,58,58,58	0
56	MG	2A	3730	1/1	0.94	0.11	68,68,68,68	0
56	MG	1A	3107	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3665	1/1	0.94	0.07	29,29,29,29	0
56	MG	1S	203	1/1	0.94	0.06	59,59,59,59	0
56	MG	1A	3160	1/1	0.94	0.20	67,67,67,67	0
56	MG	1A	3668	1/1	0.94	0.08	31,31,31,31	0
56	MG	1A	3297	1/1	0.94	0.13	51,51,51,51	0
56	MG	1a	1756	1/1	0.94	0.09	54,54,54,54	0
56	MG	2A	3176	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3419	1/1	0.94	0.09	77,77,77,77	0
56	MG	1a	1757	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3744	1/1	0.94	0.13	60,60,60,60	0
56	MG	1a	1758	1/1	0.94	0.15	67,67,67,67	0
56	MG	1A	3357	1/1	0.94	0.14	57,57,57,57	0
56	MG	1A	3987	1/1	0.94	0.11	43,43,43,43	0
56	MG	1A	3989	1/1	0.94	0.06	45,45,45,45	0
56	MG	1A	3161	1/1	0.94	0.10	58,58,58,58	0
56	MG	2A	3426	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3440	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3301	1/1	0.94	0.17	44,44,44,44	0
56	MG	2A	3430	1/1	0.94	0.08	62,62,62,62	0
56	MG	1A	3043	1/1	0.94	0.14	34,34,34,34	0
56	MG	1A	3303	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3761	1/1	0.94	0.22	51,51,51,51	0
56	MG	1a	1774	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3305	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3769	1/1	0.94	0.11	62,62,62,62	0
56	MG	2a	1799	1/1	0.94	0.15	59,59,59,59	0
56	MG	1A	3999	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	3686	1/1	0.94	0.10	51,51,51,51	0
56	MG	1X	104	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3113	1/1	0.94	0.27	53,53,53,53	0
56	MG	1a	1795	1/1	0.94	0.08	65,65,65,65	0
56	MG	1A	3239	1/1	0.94	0.26	58,58,58,58	0
56	MG	2A	3201	1/1	0.94	0.10	60,60,60,60	0
56	MG	2A	3782	1/1	0.94	0.07	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1799	1/1	0.94	0.17	67,67,67,67	0
56	MG	1a	1800	1/1	0.94	0.25	58,58,58,58	0
56	MG	2a	1811	1/1	0.94	0.11	88,88,88,88	0
56	MG	2A	3204	1/1	0.94	0.12	63,63,63,63	0
56	MG	2A	3205	1/1	0.94	0.14	46,46,46,46	0
56	MG	2f	201	1/1	0.94	0.08	50,50,50,50	0
56	MG	1A	3829	1/1	0.94	0.07	36,36,36,36	0
56	MG	1A	3449	1/1	0.94	0.21	53,53,53,53	0
56	MG	1A	3690	1/1	0.94	0.07	59,59,59,59	0
56	MG	2A	3795	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3692	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3164	1/1	0.94	0.09	51,51,51,51	0
56	MG	1a	1806	1/1	0.94	0.12	59,59,59,59	0
56	MG	10	105	1/1	0.94	0.10	53,53,53,53	0
56	MG	2r	101	1/1	0.94	0.20	69,69,69,69	0
56	MG	1A	3004	1/1	0.94	0.08	28,28,28,28	0
56	MG	11	101	1/1	0.94	0.34	47,47,47,47	0
56	MG	1A	3837	1/1	0.94	0.13	37,37,37,37	0
56	MG	2A	3804	1/1	0.94	0.17	45,45,45,45	0
56	MG	1b	301	1/1	0.94	0.17	71,71,71,71	0
56	MG	11	103	1/1	0.94	0.06	50,50,50,50	0
56	MG	2A	3218	1/1	0.94	0.11	49,49,49,49	0
56	MG	1k	201	1/1	0.94	0.15	53,53,53,53	0
56	MG	11	104	1/1	0.94	0.19	63,63,63,63	0
56	MG	2A	3222	1/1	0.94	0.36	46,46,46,46	0
56	MG	2A	3483	1/1	0.94	0.15	56,56,56,56	0
56	MG	2A	3815	1/1	0.94	0.12	65,65,65,65	0
56	MG	1A	3838	1/1	0.94	0.18	37,37,37,37	0
56	MG	1A	3699	1/1	0.94	0.14	49,49,49,49	0
56	MG	2A	3820	1/1	0.94	0.12	68,68,68,68	0
56	MG	1A	3841	1/1	0.94	0.13	36,36,36,36	0
56	MG	1A	3173	1/1	0.94	0.11	52,52,52,52	0
56	MG	1r	101	1/1	0.94	0.20	56,56,56,56	0
56	MG	1A	3846	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3456	1/1	0.94	0.08	54,54,54,54	0
56	MG	1A	3622	1/1	0.95	0.05	29,29,29,29	0
56	MG	2Q	204	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3207	1/1	0.95	0.13	52,52,52,52	0
56	MG	2T	201	1/1	0.95	0.08	57,57,57,57	0
56	MG	1B	220	1/1	0.95	0.05	44,44,44,44	0
56	MG	2A	3319	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	3209	1/1	0.95	0.19	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3079	1/1	0.95	0.17	38,38,38,38	0
56	MG	1A	3761	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3594	1/1	0.95	0.20	57,57,57,57	0
56	MG	2A	3595	1/1	0.95	0.17	49,49,49,49	0
56	MG	1A	3919	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3506	1/1	0.95	0.14	39,39,39,39	0
56	MG	1a	1673	1/1	0.95	0.17	52,52,52,52	0
56	MG	2A	3601	1/1	0.95	0.15	65,65,65,65	0
56	MG	20	104	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3212	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3142	1/1	0.95	0.20	36,36,36,36	0
56	MG	1A	3510	1/1	0.95	0.20	51,51,51,51	0
56	MG	1A	3631	1/1	0.95	0.04	24,24,24,24	0
56	MG	1A	3773	1/1	0.95	0.07	36,36,36,36	0
56	MG	1A	3144	1/1	0.95	0.18	49,49,49,49	0
56	MG	25	104	1/1	0.95	0.11	46,46,46,46	0
56	MG	1A	3368	1/1	0.95	0.29	47,47,47,47	0
56	MG	1A	3370	1/1	0.95	0.30	42,42,42,42	0
56	MG	1a	1683	1/1	0.95	0.18	45,45,45,45	0
56	MG	1B	236	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3316	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3936	1/1	0.95	0.07	63,63,63,63	0
56	MG	1A	3778	1/1	0.95	0.07	29,29,29,29	0
56	MG	2A	3104	1/1	0.95	0.08	47,47,47,47	0
56	MG	1D	309	1/1	0.95	0.12	55,55,55,55	0
56	MG	1A	3217	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	3438	1/1	0.95	0.15	48,48,48,48	0
56	MG	1A	3940	1/1	0.95	0.07	62,62,62,62	0
56	MG	1A	3439	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3786	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3112	1/1	0.95	0.15	57,57,57,57	0
56	MG	1A	3788	1/1	0.95	0.07	34,34,34,34	0
56	MG	1A	3644	1/1	0.95	0.06	30,30,30,30	0
56	MG	1A	3375	1/1	0.95	0.09	46,46,46,46	0
56	MG	2a	1612	1/1	0.95	0.12	62,62,62,62	0
56	MG	1E	312	1/1	0.95	0.11	43,43,43,43	0
56	MG	1E	313	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3353	1/1	0.95	0.22	53,53,53,53	0
56	MG	1A	3376	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3792	1/1	0.95	0.14	43,43,43,43	0
56	MG	2A	3121	1/1	0.95	0.06	52,52,52,52	0
56	MG	2a	1619	1/1	0.95	0.12	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3115	1/1	0.95	0.14	46,46,46,46	0
56	MG	1F	311	1/1	0.95	0.10	52,52,52,52	0
56	MG	1a	1709	1/1	0.95	0.21	40,40,40,40	0
56	MG	1A	3951	1/1	0.95	0.06	30,30,30,30	0
56	MG	1A	3652	1/1	0.95	0.11	38,38,38,38	0
56	MG	1a	1715	1/1	0.95	0.17	64,64,64,64	0
56	MG	1A	3795	1/1	0.95	0.07	53,53,53,53	0
56	MG	1A	3954	1/1	0.95	0.13	40,40,40,40	0
56	MG	1a	1718	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3527	1/1	0.95	0.15	44,44,44,44	0
56	MG	2A	3141	1/1	0.95	0.13	60,60,60,60	0
56	MG	1a	1722	1/1	0.95	0.05	40,40,40,40	0
56	MG	1A	3443	1/1	0.95	0.10	55,55,55,55	0
56	MG	1N	205	1/1	0.95	0.13	49,49,49,49	0
56	MG	1N	206	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3659	1/1	0.95	0.09	41,41,41,41	0
56	MG	2A	3653	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3176	1/1	0.95	0.11	75,75,75,75	0
56	MG	1A	3273	1/1	0.95	0.11	50,50,50,50	0
56	MG	2a	1639	1/1	0.95	0.39	67,67,67,67	0
56	MG	1a	1732	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3803	1/1	0.95	0.05	42,42,42,42	0
56	MG	1A	3535	1/1	0.95	0.20	39,39,39,39	0
56	MG	1a	1735	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3177	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3447	1/1	0.95	0.10	49,49,49,49	0
56	MG	1a	1741	1/1	0.95	0.08	56,56,56,56	0
56	MG	2a	1647	1/1	0.95	0.09	69,69,69,69	0
56	MG	1A	3277	1/1	0.95	0.11	57,57,57,57	0
56	MG	1A	3542	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3161	1/1	0.95	0.13	43,43,43,43	0
56	MG	1R	202	1/1	0.95	0.22	46,46,46,46	0
56	MG	1A	3278	1/1	0.95	0.20	49,49,49,49	0
56	MG	1R	205	1/1	0.95	0.22	40,40,40,40	0
56	MG	1S	201	1/1	0.95	0.21	55,55,55,55	0
56	MG	1a	1751	1/1	0.95	0.10	63,63,63,63	0
56	MG	1A	3812	1/1	0.95	0.10	50,50,50,50	0
56	MG	2A	3677	1/1	0.95	0.07	64,64,64,64	0
56	MG	1A	3450	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3547	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3451	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3985	1/1	0.95	0.09	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3673	1/1	0.95	0.10	55,55,55,55	0
56	MG	1U	205	1/1	0.95	0.16	46,46,46,46	0
56	MG	2A	3177	1/1	0.95	0.11	41,41,41,41	0
56	MG	1U	206	1/1	0.95	0.25	40,40,40,40	0
56	MG	1A	3820	1/1	0.95	0.09	37,37,37,37	0
56	MG	2A	3181	1/1	0.95	0.08	57,57,57,57	0
56	MG	1U	208	1/1	0.95	0.21	36,36,36,36	0
56	MG	1A	3044	1/1	0.95	0.16	35,35,35,35	0
56	MG	1a	1766	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3231	1/1	0.95	0.07	37,37,37,37	0
56	MG	1A	3233	1/1	0.95	0.35	51,51,51,51	0
56	MG	1A	3678	1/1	0.95	0.05	20,20,20,20	0
56	MG	1A	3679	1/1	0.95	0.15	65,65,65,65	0
56	MG	1A	3284	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3683	1/1	0.95	0.06	42,42,42,42	0
56	MG	1W	203	1/1	0.95	0.18	46,46,46,46	0
56	MG	1a	1787	1/1	0.95	0.06	85,85,85,85	0
56	MG	1A	3684	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3285	1/1	0.95	0.10	33,33,33,33	0
56	MG	1X	101	1/1	0.95	0.31	44,44,44,44	0
56	MG	1a	1796	1/1	0.95	0.07	60,60,60,60	0
56	MG	1X	103	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3333	1/1	0.95	0.21	72,72,72,72	0
56	MG	1X	105	1/1	0.95	0.06	52,52,52,52	0
56	MG	1A	3182	1/1	0.95	0.14	34,34,34,34	0
56	MG	1A	3184	1/1	0.95	0.08	50,50,50,50	0
56	MG	1A	4004	1/1	0.95	0.09	26,26,26,26	0
56	MG	1A	3150	1/1	0.95	0.06	48,48,48,48	0
56	MG	2A	3433	1/1	0.95	0.07	53,53,53,53	0
56	MG	1A	3096	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	4009	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3839	1/1	0.95	0.24	38,38,38,38	0
56	MG	10	104	1/1	0.95	0.22	66,66,66,66	0
56	MG	2A	3726	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3694	1/1	0.95	0.05	26,26,26,26	0
56	MG	1A	3563	1/1	0.95	0.13	40,40,40,40	0
56	MG	10	108	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3400	1/1	0.95	0.22	52,52,52,52	0
56	MG	1A	3843	1/1	0.95	0.12	71,71,71,71	0
56	MG	1A	3844	1/1	0.95	0.10	35,35,35,35	0
56	MG	1A	3097	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3295	1/1	0.95	0.10	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3736	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	3848	1/1	0.95	0.05	31,31,31,31	0
56	MG	2A	3738	1/1	0.95	0.07	66,66,66,66	0
56	MG	1A	3081	1/1	0.95	0.12	44,44,44,44	0
56	MG	2a	1719	1/1	0.95	0.18	71,71,71,71	0
56	MG	1A	3404	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3853	1/1	0.95	0.09	45,45,45,45	0
56	MG	13	104	1/1	0.95	0.05	48,48,48,48	0
56	MG	1A	4032	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3570	1/1	0.95	0.11	29,29,29,29	0
56	MG	1A	3706	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	4037	1/1	0.95	0.14	42,42,42,42	0
56	MG	2A	3231	1/1	0.95	0.08	63,63,63,63	0
56	MG	1A	3856	1/1	0.95	0.09	26,26,26,26	0
56	MG	2a	1733	1/1	0.95	0.14	57,57,57,57	0
56	MG	1x	104	1/1	0.95	0.11	52,52,52,52	0
56	MG	2A	3469	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3405	1/1	0.95	0.09	52,52,52,52	0
56	MG	2A	3471	1/1	0.95	0.07	45,45,45,45	0
56	MG	17	103	1/1	0.95	0.06	45,45,45,45	0
56	MG	2A	3757	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3708	1/1	0.95	0.21	59,59,59,59	0
56	MG	17	106	1/1	0.95	0.07	47,47,47,47	0
56	MG	2a	1745	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3129	1/1	0.95	0.32	38,38,38,38	0
56	MG	18	102	1/1	0.95	0.08	44,44,44,44	0
56	MG	1A	3475	1/1	0.95	0.09	64,64,64,64	0
56	MG	2a	1749	1/1	0.95	0.13	68,68,68,68	0
56	MG	18	104	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3488	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3408	1/1	0.95	0.24	52,52,52,52	0
56	MG	1x	114	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3578	1/1	0.95	0.08	51,51,51,51	0
56	MG	2A	3493	1/1	0.95	0.06	53,53,53,53	0
56	MG	2A	3496	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3866	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3477	1/1	0.95	0.21	44,44,44,44	0
56	MG	1A	3585	1/1	0.95	0.11	30,30,30,30	0
56	MG	1A	3586	1/1	0.95	0.09	34,34,34,34	0
56	MG	2A	3252	1/1	0.95	0.19	53,53,53,53	0
56	MG	1a	1606	1/1	0.95	0.21	53,53,53,53	0
56	MG	2A	3005	1/1	0.95	0.13	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3505	1/1	0.95	0.07	60,60,60,60	0
56	MG	2A	3789	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3298	1/1	0.95	0.10	46,46,46,46	0
56	MG	1a	1609	1/1	0.95	0.08	28,28,28,28	0
56	MG	2A	3509	1/1	0.95	0.07	43,43,43,43	0
56	MG	1a	1611	1/1	0.95	0.13	67,67,67,67	0
56	MG	2A	3258	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	4052	1/1	0.95	0.15	55,55,55,55	0
56	MG	1A	3873	1/1	0.95	0.12	43,43,43,43	0
56	MG	2A	3801	1/1	0.95	0.14	62,62,62,62	0
56	MG	2A	3015	1/1	0.95	0.12	51,51,51,51	0
56	MG	1a	1615	1/1	0.95	0.13	56,56,56,56	0
56	MG	2A	3265	1/1	0.95	0.20	58,58,58,58	0
56	MG	2A	3805	1/1	0.95	0.13	72,72,72,72	0
56	MG	2A	3806	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	3588	1/1	0.95	0.13	47,47,47,47	0
56	MG	2A	3521	1/1	0.95	0.16	59,59,59,59	0
56	MG	1A	3410	1/1	0.95	0.07	58,58,58,58	0
56	MG	2a	1785	1/1	0.95	0.13	64,64,64,64	0
56	MG	1a	1619	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3480	1/1	0.95	0.23	32,32,32,32	0
56	MG	2A	3024	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3245	1/1	0.95	0.08	59,59,59,59	0
56	MG	1a	1622	1/1	0.95	0.18	52,52,52,52	0
56	MG	1A	4059	1/1	0.95	0.18	52,52,52,52	0
56	MG	1A	3602	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3413	1/1	0.95	0.13	57,57,57,57	0
56	MG	2A	3821	1/1	0.95	0.11	65,65,65,65	0
56	MG	1A	3414	1/1	0.95	0.11	47,47,47,47	0
56	MG	2A	3036	1/1	0.95	0.10	27,27,27,27	0
56	MG	1A	4068	1/1	0.95	0.13	58,58,58,58	0
56	MG	1A	3034	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3420	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3490	1/1	0.95	0.14	32,32,32,32	0
56	MG	1A	4072	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3284	1/1	0.95	0.13	71,71,71,71	0
56	MG	1A	3056	1/1	0.95	0.12	45,45,45,45	0
56	MG	1A	3889	1/1	0.95	0.10	52,52,52,52	0
56	MG	2A	3547	1/1	0.95	0.17	57,57,57,57	0
56	MG	1A	3200	1/1	0.95	0.14	38,38,38,38	0
56	MG	2A	3046	1/1	0.95	0.12	50,50,50,50	0
56	MG	1A	3611	1/1	0.95	0.06	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3551	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3552	1/1	0.95	0.08	55,55,55,55	0
56	MG	2e	201	1/1	0.95	0.05	75,75,75,75	0
56	MG	1A	3894	1/1	0.95	0.05	71,71,71,71	0
56	MG	2f	202	1/1	0.95	0.23	74,74,74,74	0
56	MG	1A	3897	1/1	0.95	0.05	35,35,35,35	0
56	MG	1A	4080	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3007	1/1	0.95	0.06	41,41,41,41	0
56	MG	1A	3744	1/1	0.95	0.11	60,60,60,60	0
56	MG	2B	218	1/1	0.95	0.19	71,71,71,71	0
56	MG	1A	3615	1/1	0.95	0.09	42,42,42,42	0
56	MG	1a	1645	1/1	0.95	0.15	55,55,55,55	0
56	MG	2A	3560	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	3028	1/1	0.95	0.30	34,34,34,34	0
56	MG	1B	203	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3747	1/1	0.95	0.08	46,46,46,46	0
56	MG	2A	3300	1/1	0.95	0.12	67,67,67,67	0
56	MG	1A	3206	1/1	0.95	0.10	51,51,51,51	0
56	MG	2A	3567	1/1	0.95	0.12	60,60,60,60	0
56	MG	2A	3568	1/1	0.95	0.15	54,54,54,54	0
56	MG	2A	3570	1/1	0.95	0.10	63,63,63,63	0
56	MG	1a	1653	1/1	0.95	0.20	57,57,57,57	0
56	MG	2E	309	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3620	1/1	0.95	0.06	48,48,48,48	0
56	MG	1B	208	1/1	0.95	0.11	60,60,60,60	0
56	MG	1a	1656	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3906	1/1	0.95	0.12	64,64,64,64	0
56	MG	2A	3308	1/1	0.95	0.15	56,56,56,56	0
56	MG	1A	3752	1/1	0.95	0.08	23,23,23,23	0
56	MG	1A	3910	1/1	0.95	0.07	71,71,71,71	0
56	MG	1A	3911	1/1	0.95	0.09	71,71,71,71	0
56	MG	1A	3912	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3496	1/1	0.95	0.10	62,62,62,62	0
56	MG	2A	3074	1/1	0.95	0.09	50,50,50,50	0
56	MG	2E	307	1/1	0.96	0.17	65,65,65,65	0
56	MG	1A	3656	1/1	0.96	0.11	66,66,66,66	0
56	MG	2A	3054	1/1	0.96	0.15	67,67,67,67	0
56	MG	1A	3533	1/1	0.96	0.14	40,40,40,40	0
56	MG	1A	3534	1/1	0.96	0.26	37,37,37,37	0
56	MG	1A	3801	1/1	0.96	0.10	58,58,58,58	0
56	MG	1E	301	1/1	0.96	0.18	32,32,32,32	0
56	MG	2F	306	1/1	0.96	0.17	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1E	302	1/1	0.96	0.24	51,51,51,51	0
56	MG	1E	303	1/1	0.96	0.15	33,33,33,33	0
56	MG	1A	3661	1/1	0.96	0.10	34,34,34,34	0
56	MG	1A	3155	1/1	0.96	0.18	50,50,50,50	0
56	MG	1A	3214	1/1	0.96	0.09	65,65,65,65	0
56	MG	1A	3955	1/1	0.96	0.06	57,57,57,57	0
56	MG	2A	3574	1/1	0.96	0.07	60,60,60,60	0
56	MG	1a	1674	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3287	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3540	1/1	0.96	0.26	35,35,35,35	0
56	MG	2R	202	1/1	0.96	0.20	55,55,55,55	0
56	MG	2R	203	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3959	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3666	1/1	0.96	0.05	18,18,18,18	0
56	MG	2A	3072	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3288	1/1	0.96	0.09	50,50,50,50	0
56	MG	1F	305	1/1	0.96	0.05	35,35,35,35	0
56	MG	2A	3075	1/1	0.96	0.14	34,34,34,34	0
56	MG	1F	307	1/1	0.96	0.15	30,30,30,30	0
56	MG	1F	308	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3962	1/1	0.96	0.14	34,34,34,34	0
56	MG	2A	3318	1/1	0.96	0.12	66,66,66,66	0
56	MG	1F	310	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3067	1/1	0.96	0.06	28,28,28,28	0
56	MG	2A	3083	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3102	1/1	0.96	0.05	36,36,36,36	0
56	MG	1a	1687	1/1	0.96	0.27	47,47,47,47	0
56	MG	2A	3596	1/1	0.96	0.09	76,76,76,76	0
56	MG	1G	3602	1/1	0.96	0.10	57,57,57,57	0
56	MG	2A	3598	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3545	1/1	0.96	0.07	37,37,37,37	0
56	MG	1G	3604	1/1	0.96	0.11	63,63,63,63	0
56	MG	1A	3969	1/1	0.96	0.05	33,33,33,33	0
56	MG	1A	3219	1/1	0.96	0.09	52,52,52,52	0
56	MG	2A	3092	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3971	1/1	0.96	0.04	32,32,32,32	0
56	MG	1A	3220	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3974	1/1	0.96	0.05	41,41,41,41	0
56	MG	28	101	1/1	0.96	0.27	57,57,57,57	0
56	MG	2A	3607	1/1	0.96	0.06	33,33,33,33	0
56	MG	1A	3975	1/1	0.96	0.06	43,43,43,43	0
56	MG	1A	3222	1/1	0.96	0.13	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1699	1/1	0.96	0.06	60,60,60,60	0
56	MG	1A	3819	1/1	0.96	0.11	28,28,28,28	0
56	MG	1a	1701	1/1	0.96	0.17	50,50,50,50	0
56	MG	1A	3069	1/1	0.96	0.15	48,48,48,48	0
56	MG	1A	3105	1/1	0.96	0.18	37,37,37,37	0
56	MG	1A	3676	1/1	0.96	0.07	62,62,62,62	0
56	MG	2A	3616	1/1	0.96	0.34	47,47,47,47	0
56	MG	1A	3551	1/1	0.96	0.19	34,34,34,34	0
56	MG	1Q	204	1/1	0.96	0.09	57,57,57,57	0
56	MG	1a	1708	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3825	1/1	0.96	0.08	52,52,52,52	0
56	MG	2A	3109	1/1	0.96	0.42	68,68,68,68	0
56	MG	1A	3033	1/1	0.96	0.16	32,32,32,32	0
56	MG	1A	3108	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3111	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3046	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3234	1/1	0.96	0.09	50,50,50,50	0
56	MG	1A	3165	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3170	1/1	0.96	0.07	24,24,24,24	0
56	MG	1a	1721	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3384	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3017	1/1	0.96	0.07	53,53,53,53	0
56	MG	1A	3077	1/1	0.96	0.18	31,31,31,31	0
56	MG	1A	3691	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	3035	1/1	0.96	0.20	34,34,34,34	0
56	MG	1A	3119	1/1	0.96	0.22	36,36,36,36	0
56	MG	1A	3311	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3036	1/1	0.96	0.22	36,36,36,36	0
56	MG	1A	3698	1/1	0.96	0.05	50,50,50,50	0
56	MG	2A	3128	1/1	0.96	0.13	52,52,52,52	0
56	MG	1A	3244	1/1	0.96	0.11	38,38,38,38	0
56	MG	2A	3132	1/1	0.96	0.18	51,51,51,51	0
56	MG	1U	211	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3571	1/1	0.96	0.07	46,46,46,46	0
56	MG	2A	3138	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	3469	1/1	0.96	0.16	34,34,34,34	0
56	MG	1a	1739	1/1	0.96	0.10	59,59,59,59	0
56	MG	1a	1740	1/1	0.96	0.15	43,43,43,43	0
56	MG	1V	205	1/1	0.96	0.14	35,35,35,35	0
56	MG	1a	1742	1/1	0.96	0.13	57,57,57,57	0
56	MG	1A	3392	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3703	1/1	0.96	0.06	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3471	1/1	0.96	0.18	41,41,41,41	0
56	MG	1A	3851	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3472	1/1	0.96	0.15	56,56,56,56	0
56	MG	1W	204	1/1	0.96	0.07	50,50,50,50	0
56	MG	1W	206	1/1	0.96	0.07	41,41,41,41	0
56	MG	1W	207	1/1	0.96	0.13	40,40,40,40	0
56	MG	2a	1652	1/1	0.96	0.16	41,41,41,41	0
56	MG	2A	3383	1/1	0.96	0.22	54,54,54,54	0
56	MG	1A	3577	1/1	0.96	0.06	34,34,34,34	0
56	MG	2A	3664	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3052	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3579	1/1	0.96	0.06	26,26,26,26	0
56	MG	1X	102	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	3857	1/1	0.96	0.06	25,25,25,25	0
56	MG	1A	3711	1/1	0.96	0.07	43,43,43,43	0
56	MG	2A	3162	1/1	0.96	0.09	56,56,56,56	0
56	MG	1A	3580	1/1	0.96	0.05	36,36,36,36	0
56	MG	2a	1664	1/1	0.96	0.12	62,62,62,62	0
56	MG	1a	1761	1/1	0.96	0.07	65,65,65,65	0
56	MG	2a	1666	1/1	0.96	0.27	58,58,58,58	0
56	MG	1A	4025	1/1	0.96	0.10	18,18,18,18	0
56	MG	1Y	203	1/1	0.96	0.05	60,60,60,60	0
56	MG	1A	3123	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	3181	1/1	0.96	0.15	47,47,47,47	0
56	MG	2a	1671	1/1	0.96	0.26	43,43,43,43	0
56	MG	1a	1768	1/1	0.96	0.06	64,64,64,64	0
56	MG	1a	1769	1/1	0.96	0.08	64,64,64,64	0
56	MG	2A	3172	1/1	0.96	0.20	59,59,59,59	0
56	MG	1A	3862	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3863	1/1	0.96	0.08	30,30,30,30	0
56	MG	1a	1772	1/1	0.96	0.06	76,76,76,76	0
56	MG	1A	4035	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3397	1/1	0.96	0.17	38,38,38,38	0
56	MG	10	103	1/1	0.96	0.19	45,45,45,45	0
56	MG	2A	3406	1/1	0.96	0.08	68,68,68,68	0
56	MG	2A	3407	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3179	1/1	0.96	0.09	50,50,50,50	0
56	MG	1A	3040	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3399	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3589	1/1	0.96	0.07	53,53,53,53	0
56	MG	1A	3054	1/1	0.96	0.13	50,50,50,50	0
56	MG	2A	3699	1/1	0.96	0.09	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3414	1/1	0.96	0.20	61,61,61,61	0
56	MG	2A	3184	1/1	0.96	0.38	67,67,67,67	0
56	MG	2A	3416	1/1	0.96	0.26	65,65,65,65	0
56	MG	2A	3703	1/1	0.96	0.17	50,50,50,50	0
56	MG	2A	3418	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3593	1/1	0.96	0.05	36,36,36,36	0
56	MG	2A	3706	1/1	0.96	0.06	43,43,43,43	0
56	MG	1a	1794	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3595	1/1	0.96	0.05	22,22,22,22	0
56	MG	2A	3189	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	3872	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3597	1/1	0.96	0.08	27,27,27,27	0
56	MG	1A	3875	1/1	0.96	0.05	27,27,27,27	0
56	MG	1A	3726	1/1	0.96	0.05	31,31,31,31	0
56	MG	1A	3727	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3185	1/1	0.96	0.28	40,40,40,40	0
56	MG	2A	3719	1/1	0.96	0.05	55,55,55,55	0
56	MG	2A	3429	1/1	0.96	0.05	37,37,37,37	0
56	MG	2A	3721	1/1	0.96	0.09	62,62,62,62	0
56	MG	1A	3600	1/1	0.96	0.07	27,27,27,27	0
56	MG	1A	3881	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3432	1/1	0.96	0.05	63,63,63,63	0
56	MG	1A	3128	1/1	0.96	0.21	30,30,30,30	0
56	MG	2a	1716	1/1	0.96	0.06	70,70,70,70	0
56	MG	15	101	1/1	0.96	0.18	37,37,37,37	0
56	MG	1a	1807	1/1	0.96	0.17	61,61,61,61	0
56	MG	1A	3055	1/1	0.96	0.08	44,44,44,44	0
56	MG	1A	3322	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3323	1/1	0.96	0.16	39,39,39,39	0
56	MG	2a	1722	1/1	0.96	0.12	75,75,75,75	0
56	MG	15	106	1/1	0.96	0.15	42,42,42,42	0
56	MG	1A	4058	1/1	0.96	0.07	34,34,34,34	0
56	MG	1e	201	1/1	0.96	0.08	69,69,69,69	0
56	MG	1e	202	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3488	1/1	0.96	0.13	40,40,40,40	0
56	MG	2a	1728	1/1	0.96	0.06	45,45,45,45	0
56	MG	2a	1729	1/1	0.96	0.14	58,58,58,58	0
56	MG	2A	3448	1/1	0.96	0.08	70,70,70,70	0
56	MG	1A	4060	1/1	0.96	0.16	56,56,56,56	0
56	MG	1A	3085	1/1	0.96	0.11	27,27,27,27	0
56	MG	1A	3041	1/1	0.96	0.17	34,34,34,34	0
56	MG	1m	3001	1/1	0.96	0.11	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3608	1/1	0.96	0.14	28,28,28,28	0
56	MG	1A	4066	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	4067	1/1	0.96	0.09	34,34,34,34	0
56	MG	2A	3459	1/1	0.96	0.11	53,53,53,53	0
56	MG	2a	1742	1/1	0.96	0.10	65,65,65,65	0
56	MG	1A	3890	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3191	1/1	0.96	0.22	50,50,50,50	0
56	MG	2A	3749	1/1	0.96	0.05	50,50,50,50	0
56	MG	19	101	1/1	0.96	0.12	49,49,49,49	0
56	MG	2A	3463	1/1	0.96	0.09	47,47,47,47	0
56	MG	1w	101	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3220	1/1	0.96	0.15	51,51,51,51	0
56	MG	1A	3135	1/1	0.96	0.08	57,57,57,57	0
56	MG	2a	1751	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3059	1/1	0.96	0.04	34,34,34,34	0
56	MG	2A	3756	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3896	1/1	0.96	0.04	40,40,40,40	0
56	MG	1A	3412	1/1	0.96	0.18	43,43,43,43	0
56	MG	1w	106	1/1	0.96	0.06	77,77,77,77	0
56	MG	2a	1757	1/1	0.96	0.23	68,68,68,68	0
56	MG	2a	1758	1/1	0.96	0.17	69,69,69,69	0
56	MG	1w	107	1/1	0.96	0.16	64,64,64,64	0
56	MG	2A	3762	1/1	0.96	0.09	59,59,59,59	0
56	MG	2A	3228	1/1	0.96	0.14	49,49,49,49	0
56	MG	2A	3474	1/1	0.96	0.07	35,35,35,35	0
56	MG	2A	3475	1/1	0.96	0.09	49,49,49,49	0
56	MG	1A	3614	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3329	1/1	0.96	0.14	46,46,46,46	0
56	MG	2A	3479	1/1	0.96	0.08	53,53,53,53	0
56	MG	1a	1607	1/1	0.96	0.06	52,52,52,52	0
56	MG	2A	3481	1/1	0.96	0.13	49,49,49,49	0
56	MG	1A	3616	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3617	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3486	1/1	0.96	0.08	48,48,48,48	0
56	MG	2A	3487	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3330	1/1	0.96	0.16	31,31,31,31	0
56	MG	1A	3498	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3757	1/1	0.96	0.04	20,20,20,20	0
56	MG	1a	1614	1/1	0.96	0.16	65,65,65,65	0
56	MG	1A	3259	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3502	1/1	0.96	0.14	43,43,43,43	0
56	MG	2A	3790	1/1	0.96	0.14	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1617	1/1	0.96	0.08	55,55,55,55	0
56	MG	1x	115	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3243	1/1	0.96	0.07	61,61,61,61	0
56	MG	1A	3260	1/1	0.96	0.29	44,44,44,44	0
56	MG	2A	3501	1/1	0.96	0.07	55,55,55,55	0
56	MG	2A	3245	1/1	0.96	0.08	63,63,63,63	0
56	MG	1A	3504	1/1	0.96	0.18	46,46,46,46	0
56	MG	1A	3196	1/1	0.96	0.07	20,20,20,20	0
56	MG	1A	3765	1/1	0.96	0.05	53,53,53,53	0
56	MG	1A	3088	1/1	0.96	0.13	42,42,42,42	0
56	MG	1A	3768	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3265	1/1	0.96	0.16	41,41,41,41	0
56	MG	1A	3267	1/1	0.96	0.16	32,32,32,32	0
56	MG	2a	1794	1/1	0.96	0.10	70,70,70,70	0
56	MG	1A	3089	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3271	1/1	0.96	0.57	43,43,43,43	0
56	MG	1A	3141	1/1	0.96	0.20	32,32,32,32	0
56	MG	1A	3342	1/1	0.96	0.06	46,46,46,46	0
56	MG	2A	3515	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3923	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3429	1/1	0.96	0.24	53,53,53,53	0
56	MG	2A	3259	1/1	0.96	0.10	55,55,55,55	0
56	MG	2A	3519	1/1	0.96	0.07	41,41,41,41	0
56	MG	2A	3817	1/1	0.96	0.10	60,60,60,60	0
56	MG	2A	3520	1/1	0.96	0.09	43,43,43,43	0
56	MG	1B	219	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3023	1/1	0.96	0.10	30,30,30,30	0
56	MG	2A	3822	1/1	0.96	0.06	71,71,71,71	0
56	MG	2A	3262	1/1	0.96	0.18	50,50,50,50	0
56	MG	2A	3825	1/1	0.96	0.09	70,70,70,70	0
56	MG	2A	3020	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3275	1/1	0.96	0.13	46,46,46,46	0
56	MG	1A	3780	1/1	0.96	0.20	26,26,26,26	0
56	MG	2A	3527	1/1	0.96	0.09	55,55,55,55	0
56	MG	2A	3528	1/1	0.96	0.09	58,58,58,58	0
56	MG	2A	3023	1/1	0.96	0.15	60,60,60,60	0
56	MG	1A	3781	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	3931	1/1	0.96	0.10	60,60,60,60	0
56	MG	1A	3143	1/1	0.96	0.09	40,40,40,40	0
56	MG	1A	3003	1/1	0.96	0.06	30,30,30,30	0
56	MG	2B	207	1/1	0.96	0.08	67,67,67,67	0
56	MG	1a	1641	1/1	0.96	0.17	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	228	1/1	0.96	0.08	40,40,40,40	0
56	MG	2A	3033	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	3279	1/1	0.96	0.11	28,28,28,28	0
56	MG	2A	3035	1/1	0.96	0.13	53,53,53,53	0
56	MG	2A	3276	1/1	0.96	0.28	65,65,65,65	0
56	MG	1A	3787	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3643	1/1	0.96	0.14	60,60,60,60	0
56	MG	1A	3435	1/1	0.96	0.07	43,43,43,43	0
56	MG	1a	1649	1/1	0.96	0.12	48,48,48,48	0
56	MG	1A	3522	1/1	0.96	0.24	41,41,41,41	0
56	MG	1A	3526	1/1	0.96	0.20	39,39,39,39	0
56	MG	1A	3095	1/1	0.96	0.06	33,33,33,33	0
56	MG	2D	302	1/1	0.96	0.21	52,52,52,52	0
56	MG	1A	3063	1/1	0.96	0.15	34,34,34,34	0
56	MG	2A	3044	1/1	0.96	0.17	65,65,65,65	0
56	MG	1B	237	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3029	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3283	1/1	0.96	0.16	65,65,65,65	0
56	MG	1D	303	1/1	0.96	0.15	43,43,43,43	0
56	MG	1D	304	1/1	0.96	0.12	36,36,36,36	0
56	MG	1A	3655	1/1	0.96	0.07	21,21,21,21	0
56	MG	1a	1661	1/1	0.96	0.10	55,55,55,55	0
58	ZN	24	501	1/1	0.96	0.10	119,119,119,119	0
58	ZN	2n	501	1/1	0.96	0.06	85,85,85,85	0
60	K	1x	101	1/1	0.96	0.13	66,66,66,66	0
60	K	2x	101	1/1	0.96	0.12	73,73,73,73	0
56	MG	1B	217	1/1	0.97	0.15	44,44,44,44	0
56	MG	1A	3187	1/1	0.97	0.30	41,41,41,41	0
56	MG	1A	3101	1/1	0.97	0.28	32,32,32,32	0
56	MG	1A	3818	1/1	0.97	0.11	22,22,22,22	0
56	MG	1A	3030	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3103	1/1	0.97	0.09	34,34,34,34	0
56	MG	1A	3695	1/1	0.97	0.10	55,55,55,55	0
56	MG	1A	3822	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3396	1/1	0.97	0.21	43,43,43,43	0
56	MG	1A	3009	1/1	0.97	0.05	28,28,28,28	0
56	MG	1a	1775	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3508	1/1	0.97	0.06	44,44,44,44	0
56	MG	1a	1777	1/1	0.97	0.05	58,58,58,58	0
56	MG	2A	3307	1/1	0.97	0.11	63,63,63,63	0
56	MG	1A	3583	1/1	0.97	0.10	39,39,39,39	0
56	MG	1a	1781	1/1	0.97	0.06	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3057	1/1	0.97	0.11	58,58,58,58	0
56	MG	1A	3482	1/1	0.97	0.16	50,50,50,50	0
56	MG	1A	3194	1/1	0.97	0.06	33,33,33,33	0
56	MG	1a	1788	1/1	0.97	0.09	69,69,69,69	0
56	MG	1A	3010	1/1	0.97	0.07	38,38,38,38	0
56	MG	1a	1790	1/1	0.97	0.07	67,67,67,67	0
56	MG	1A	3145	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3963	1/1	0.97	0.10	25,25,25,25	0
56	MG	2A	3129	1/1	0.97	0.26	48,48,48,48	0
56	MG	2A	3130	1/1	0.97	0.05	50,50,50,50	0
56	MG	1A	3146	1/1	0.97	0.14	36,36,36,36	0
56	MG	2a	1651	1/1	0.97	0.19	63,63,63,63	0
56	MG	1A	3022	1/1	0.97	0.16	32,32,32,32	0
56	MG	1A	3594	1/1	0.97	0.04	40,40,40,40	0
56	MG	2A	3135	1/1	0.97	0.15	45,45,45,45	0
56	MG	1a	1798	1/1	0.97	0.16	56,56,56,56	0
56	MG	2A	3137	1/1	0.97	0.24	53,53,53,53	0
56	MG	1A	3835	1/1	0.97	0.03	28,28,28,28	0
56	MG	2A	3530	1/1	0.97	0.04	43,43,43,43	0
56	MG	2A	3139	1/1	0.97	0.14	49,49,49,49	0
56	MG	2A	3532	1/1	0.97	0.06	68,68,68,68	0
56	MG	1A	3109	1/1	0.97	0.19	30,30,30,30	0
56	MG	1D	302	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3596	1/1	0.97	0.05	30,30,30,30	0
56	MG	2A	3143	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3261	1/1	0.97	0.17	32,32,32,32	0
56	MG	1A	3202	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3599	1/1	0.97	0.11	34,34,34,34	0
56	MG	1A	3263	1/1	0.97	0.22	41,41,41,41	0
56	MG	1A	3204	1/1	0.97	0.13	34,34,34,34	0
56	MG	1A	3013	1/1	0.97	0.29	35,35,35,35	0
56	MG	2a	1672	1/1	0.97	0.21	59,59,59,59	0
56	MG	1A	3266	1/1	0.97	0.17	29,29,29,29	0
56	MG	2A	3152	1/1	0.97	0.10	53,53,53,53	0
56	MG	2A	3760	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3845	1/1	0.97	0.05	37,37,37,37	0
56	MG	1A	3497	1/1	0.97	0.24	57,57,57,57	0
56	MG	1A	3983	1/1	0.97	0.08	60,60,60,60	0
56	MG	2A	3766	1/1	0.97	0.09	47,47,47,47	0
56	MG	1d	301	1/1	0.97	0.17	55,55,55,55	0
56	MG	1A	3151	1/1	0.97	0.10	35,35,35,35	0
56	MG	2A	3770	1/1	0.97	0.11	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1631	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3268	1/1	0.97	0.18	41,41,41,41	0
56	MG	1A	3334	1/1	0.97	0.18	39,39,39,39	0
56	MG	1A	3415	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3988	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3416	1/1	0.97	0.13	40,40,40,40	0
56	MG	2a	1689	1/1	0.97	0.13	58,58,58,58	0
56	MG	2A	3778	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3152	1/1	0.97	0.09	30,30,30,30	0
56	MG	2A	3781	1/1	0.97	0.11	60,60,60,60	0
56	MG	2a	1693	1/1	0.97	0.08	54,54,54,54	0
56	MG	1A	3419	1/1	0.97	0.10	59,59,59,59	0
56	MG	1F	304	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	3612	1/1	0.97	0.05	28,28,28,28	0
56	MG	1A	3507	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3731	1/1	0.97	0.12	35,35,35,35	0
56	MG	1a	1643	1/1	0.97	0.15	57,57,57,57	0
56	MG	1A	3732	1/1	0.97	0.04	36,36,36,36	0
56	MG	2A	3566	1/1	0.97	0.08	35,35,35,35	0
56	MG	1A	3154	1/1	0.97	0.34	35,35,35,35	0
56	MG	2A	3791	1/1	0.97	0.16	49,49,49,49	0
56	MG	1A	3048	1/1	0.97	0.14	37,37,37,37	0
56	MG	2A	3569	1/1	0.97	0.05	42,42,42,42	0
56	MG	1F	312	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	3338	1/1	0.97	0.14	38,38,38,38	0
56	MG	1G	3601	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3084	1/1	0.97	0.07	55,55,55,55	0
56	MG	1x	103	1/1	0.97	0.27	71,71,71,71	0
56	MG	1A	3049	1/1	0.97	0.06	37,37,37,37	0
56	MG	2a	1712	1/1	0.97	0.43	69,69,69,69	0
56	MG	2A	3576	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3741	1/1	0.97	0.05	26,26,26,26	0
56	MG	1G	3605	1/1	0.97	0.07	48,48,48,48	0
56	MG	1H	201	1/1	0.97	0.22	48,48,48,48	0
56	MG	1A	3276	1/1	0.97	0.10	51,51,51,51	0
56	MG	1A	3066	1/1	0.97	0.08	33,33,33,33	0
56	MG	1A	4007	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	4008	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3215	1/1	0.97	0.19	39,39,39,39	0
56	MG	1A	3117	1/1	0.97	0.16	34,34,34,34	0
56	MG	1A	4011	1/1	0.97	0.08	24,24,24,24	0
56	MG	1A	3517	1/1	0.97	0.12	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3589	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3037	1/1	0.97	0.10	40,40,40,40	0
56	MG	1P	201	1/1	0.97	0.26	34,34,34,34	0
56	MG	1a	1667	1/1	0.97	0.07	50,50,50,50	0
56	MG	2A	3819	1/1	0.97	0.05	51,51,51,51	0
56	MG	1P	203	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3348	1/1	0.97	0.09	40,40,40,40	0
56	MG	1A	3749	1/1	0.97	0.04	48,48,48,48	0
56	MG	2A	3823	1/1	0.97	0.06	72,72,72,72	0
56	MG	1Q	202	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3874	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3218	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3876	1/1	0.97	0.04	32,32,32,32	0
56	MG	2A	3010	1/1	0.97	0.06	39,39,39,39	0
56	MG	2A	3011	1/1	0.97	0.07	55,55,55,55	0
56	MG	1A	3068	1/1	0.97	0.19	46,46,46,46	0
56	MG	1A	3121	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3524	1/1	0.97	0.08	53,53,53,53	0
56	MG	1A	3221	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3756	1/1	0.97	0.07	55,55,55,55	0
56	MG	1A	4028	1/1	0.97	0.05	21,21,21,21	0
56	MG	1A	4029	1/1	0.97	0.14	53,53,53,53	0
56	MG	1A	3039	1/1	0.97	0.04	30,30,30,30	0
56	MG	1A	3634	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3354	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3090	1/1	0.97	0.10	26,26,26,26	0
56	MG	1A	4036	1/1	0.97	0.10	35,35,35,35	0
56	MG	1U	204	1/1	0.97	0.18	37,37,37,37	0
56	MG	2A	3028	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3762	1/1	0.97	0.05	47,47,47,47	0
56	MG	1A	3356	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3166	1/1	0.97	0.34	39,39,39,39	0
56	MG	2A	3032	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3289	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3169	1/1	0.97	0.08	35,35,35,35	0
56	MG	1A	3536	1/1	0.97	0.11	42,42,42,42	0
56	MG	1V	201	1/1	0.97	0.25	30,30,30,30	0
56	MG	2A	3227	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3770	1/1	0.97	0.30	32,32,32,32	0
56	MG	1A	3024	1/1	0.97	0.19	28,28,28,28	0
56	MG	2A	3417	1/1	0.97	0.19	42,42,42,42	0
56	MG	1A	3538	1/1	0.97	0.17	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1698	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3362	1/1	0.97	0.17	55,55,55,55	0
56	MG	1A	3363	1/1	0.97	0.19	45,45,45,45	0
56	MG	1A	3364	1/1	0.97	0.32	30,30,30,30	0
56	MG	2A	3235	1/1	0.97	0.21	61,61,61,61	0
56	MG	1A	3228	1/1	0.97	0.21	33,33,33,33	0
56	MG	1A	3229	1/1	0.97	0.15	52,52,52,52	0
56	MG	2A	3636	1/1	0.97	0.05	63,63,63,63	0
56	MG	1A	3230	1/1	0.97	0.18	38,38,38,38	0
56	MG	1a	1705	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3171	1/1	0.97	0.07	28,28,28,28	0
56	MG	1A	3369	1/1	0.97	0.07	56,56,56,56	0
56	MG	2A	3050	1/1	0.97	0.18	60,60,60,60	0
56	MG	1A	3125	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3782	1/1	0.97	0.04	40,40,40,40	0
56	MG	1a	1710	1/1	0.97	0.04	70,70,70,70	0
56	MG	1a	1711	1/1	0.97	0.14	45,45,45,45	0
56	MG	2Q	201	1/1	0.97	0.06	67,67,67,67	0
56	MG	1a	1712	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3909	1/1	0.97	0.07	61,61,61,61	0
56	MG	1A	3126	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3784	1/1	0.97	0.09	30,30,30,30	0
56	MG	1A	3071	1/1	0.97	0.10	46,46,46,46	0
56	MG	2a	1793	1/1	0.97	0.18	50,50,50,50	0
56	MG	2A	3651	1/1	0.97	0.17	54,54,54,54	0
56	MG	1A	4063	1/1	0.97	0.08	28,28,28,28	0
56	MG	1A	3374	1/1	0.97	0.09	46,46,46,46	0
56	MG	1Y	202	1/1	0.97	0.19	47,47,47,47	0
56	MG	1A	3299	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3553	1/1	0.97	0.14	43,43,43,43	0
56	MG	1A	3072	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3073	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3378	1/1	0.97	0.06	39,39,39,39	0
56	MG	2W	203	1/1	0.97	0.06	54,54,54,54	0
56	MG	2a	1804	1/1	0.97	0.05	75,75,75,75	0
56	MG	1A	3379	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3130	1/1	0.97	0.10	42,42,42,42	0
56	MG	2A	3454	1/1	0.97	0.10	38,38,38,38	0
56	MG	20	102	1/1	0.97	0.07	56,56,56,56	0
56	MG	2A	3455	1/1	0.97	0.12	58,58,58,58	0
56	MG	1A	3921	1/1	0.97	0.12	57,57,57,57	0
56	MG	2A	3668	1/1	0.97	0.06	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3669	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3559	1/1	0.97	0.25	43,43,43,43	0
56	MG	1A	3462	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3561	1/1	0.97	0.11	32,32,32,32	0
56	MG	1A	3240	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	3464	1/1	0.97	0.05	47,47,47,47	0
56	MG	2A	3078	1/1	0.97	0.15	58,58,58,58	0
56	MG	2I	201	1/1	0.97	0.08	68,68,68,68	0
56	MG	1a	1737	1/1	0.97	0.09	48,48,48,48	0
56	MG	1A	3304	1/1	0.97	0.17	34,34,34,34	0
56	MG	2A	3081	1/1	0.97	0.06	51,51,51,51	0
56	MG	27	101	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3929	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3179	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3005	1/1	0.97	0.10	48,48,48,48	0
56	MG	1A	3132	1/1	0.97	0.14	34,34,34,34	0
56	MG	1B	201	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3804	1/1	0.97	0.13	54,54,54,54	0
56	MG	2A	3685	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	3680	1/1	0.97	0.06	29,29,29,29	0
56	MG	2A	3687	1/1	0.97	0.12	43,43,43,43	0
56	MG	2A	3089	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3098	1/1	0.97	0.05	25,25,25,25	0
56	MG	1A	3682	1/1	0.97	0.18	47,47,47,47	0
56	MG	1A	3309	1/1	0.97	0.13	49,49,49,49	0
56	MG	15	102	1/1	0.97	0.24	29,29,29,29	0
56	MG	1A	3099	1/1	0.97	0.21	41,41,41,41	0
56	MG	1A	3019	1/1	0.97	0.09	36,36,36,36	0
56	MG	2A	3484	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3941	1/1	0.97	0.04	53,53,53,53	0
56	MG	1A	3138	1/1	0.97	0.12	34,34,34,34	0
56	MG	15	107	1/1	0.97	0.26	38,38,38,38	0
56	MG	1A	3813	1/1	0.97	0.11	34,34,34,34	0
56	MG	1A	3248	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	3575	1/1	0.97	0.07	45,45,45,45	0
57	6IF	1A	4084	32/32	0.97	0.08	25,32,37,38	0
57	6IF	2A	3831	32/32	0.97	0.09	38,44,50,53	0
56	MG	2A	3491	1/1	0.97	0.09	44,44,44,44	0
58	ZN	29	102	1/1	0.97	0.04	74,74,74,74	0
56	MG	1A	3946	1/1	0.97	0.07	47,47,47,47	0
56	MG	1B	216	1/1	0.97	0.09	70,70,70,70	0
56	MG	1a	1763	1/1	0.97	0.06	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3718	1/1	0.98	0.05	59,59,59,59	0
56	MG	1A	3658	1/1	0.98	0.06	45,45,45,45	0
56	MG	2A	3581	1/1	0.98	0.07	42,42,42,42	0
56	MG	2F	305	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3995	1/1	0.98	0.07	48,48,48,48	0
56	MG	1A	3008	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3014	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3852	1/1	0.98	0.10	52,52,52,52	0
56	MG	1A	3015	1/1	0.98	0.09	45,45,45,45	0
56	MG	1A	3076	1/1	0.98	0.10	36,36,36,36	0
56	MG	1A	3064	1/1	0.98	0.05	19,19,19,19	0
56	MG	17	101	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3926	1/1	0.98	0.07	31,31,31,31	0
56	MG	17	104	1/1	0.98	0.06	36,36,36,36	0
56	MG	1N	204	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3406	1/1	0.98	0.22	37,37,37,37	0
56	MG	1A	3106	1/1	0.98	0.04	34,34,34,34	0
56	MG	1O	201	1/1	0.98	0.07	54,54,54,54	0
56	MG	2A	3735	1/1	0.98	0.11	42,42,42,42	0
56	MG	1A	3167	1/1	0.98	0.16	34,34,34,34	0
56	MG	1A	3168	1/1	0.98	0.07	29,29,29,29	0
56	MG	1A	3223	1/1	0.98	0.15	42,42,42,42	0
56	MG	1A	3932	1/1	0.98	0.11	67,67,67,67	0
56	MG	1P	202	1/1	0.98	0.18	37,37,37,37	0
56	MG	2A	3338	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3091	1/1	0.98	0.08	35,35,35,35	0
56	MG	1P	204	1/1	0.98	0.33	32,32,32,32	0
56	MG	2X	101	1/1	0.98	0.04	62,62,62,62	0
56	MG	1A	3346	1/1	0.98	0.10	42,42,42,42	0
56	MG	1A	3032	1/1	0.98	0.17	33,33,33,33	0
56	MG	1v	102	1/1	0.98	0.04	50,50,50,50	0
56	MG	1Q	201	1/1	0.98	0.05	27,27,27,27	0
56	MG	1A	3798	1/1	0.98	0.04	34,34,34,34	0
56	MG	2a	1734	1/1	0.98	0.11	46,46,46,46	0
56	MG	2a	1735	1/1	0.98	0.09	79,79,79,79	0
56	MG	2A	3476	1/1	0.98	0.08	67,67,67,67	0
56	MG	2A	3100	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3093	1/1	0.98	0.10	40,40,40,40	0
56	MG	1A	3736	1/1	0.98	0.06	29,29,29,29	0
56	MG	23	101	1/1	0.98	0.05	58,58,58,58	0
56	MG	1a	1610	1/1	0.98	0.04	65,65,65,65	0
56	MG	1A	3567	1/1	0.98	0.07	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3482	1/1	0.98	0.05	49,49,49,49	0
56	MG	1A	3523	1/1	0.98	0.07	28,28,28,28	0
56	MG	1A	3199	1/1	0.98	0.09	38,38,38,38	0
56	MG	1A	3525	1/1	0.98	0.14	38,38,38,38	0
56	MG	1R	203	1/1	0.98	0.10	32,32,32,32	0
56	MG	1a	1719	1/1	0.98	0.06	55,55,55,55	0
56	MG	1A	3485	1/1	0.98	0.17	30,30,30,30	0
56	MG	2A	3763	1/1	0.98	0.05	41,41,41,41	0
56	MG	2A	3764	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	4020	1/1	0.98	0.03	27,27,27,27	0
56	MG	1A	3486	1/1	0.98	0.13	30,30,30,30	0
56	MG	2A	3767	1/1	0.98	0.04	61,61,61,61	0
56	MG	1a	1723	1/1	0.98	0.11	32,32,32,32	0
56	MG	1A	3807	1/1	0.98	0.05	58,58,58,58	0
56	MG	2a	1603	1/1	0.98	0.06	70,70,70,70	0
56	MG	2A	3115	1/1	0.98	0.12	44,44,44,44	0
56	MG	2A	3494	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3495	1/1	0.98	0.09	32,32,32,32	0
56	MG	1A	4023	1/1	0.98	0.05	46,46,46,46	0
56	MG	1A	4024	1/1	0.98	0.03	49,49,49,49	0
56	MG	1A	3148	1/1	0.98	0.26	35,35,35,35	0
56	MG	1U	201	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3417	1/1	0.98	0.18	36,36,36,36	0
56	MG	1A	3530	1/1	0.98	0.11	48,48,48,48	0
56	MG	2A	3780	1/1	0.98	0.07	60,60,60,60	0
56	MG	1A	3452	1/1	0.98	0.08	56,56,56,56	0
56	MG	1B	227	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	4031	1/1	0.98	0.11	56,56,56,56	0
56	MG	1A	3532	1/1	0.98	0.09	26,26,26,26	0
56	MG	1A	3016	1/1	0.98	0.08	27,27,27,27	0
56	MG	1U	209	1/1	0.98	0.24	34,34,34,34	0
56	MG	1A	3750	1/1	0.98	0.04	41,41,41,41	0
56	MG	1A	3628	1/1	0.98	0.08	46,46,46,46	0
56	MG	1A	3011	1/1	0.98	0.05	40,40,40,40	0
56	MG	1A	3203	1/1	0.98	0.12	48,48,48,48	0
56	MG	1A	3018	1/1	0.98	0.07	19,19,19,19	0
56	MG	2A	3792	1/1	0.98	0.04	45,45,45,45	0
56	MG	2A	3133	1/1	0.98	0.14	42,42,42,42	0
56	MG	2A	3794	1/1	0.98	0.05	59,59,59,59	0
56	MG	1A	4039	1/1	0.98	0.18	57,57,57,57	0
56	MG	2A	3013	1/1	0.98	0.06	51,51,51,51	0
56	MG	1A	3026	1/1	0.98	0.16	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4041	1/1	0.98	0.06	43,43,43,43	0
56	MG	1A	3958	1/1	0.98	0.04	54,54,54,54	0
56	MG	1a	1749	1/1	0.98	0.05	60,60,60,60	0
56	MG	1A	3133	1/1	0.98	0.05	19,19,19,19	0
56	MG	1A	3027	1/1	0.98	0.31	28,28,28,28	0
56	MG	1A	3758	1/1	0.98	0.06	24,24,24,24	0
56	MG	1W	205	1/1	0.98	0.17	39,39,39,39	0
56	MG	1a	1754	1/1	0.98	0.06	52,52,52,52	0
56	MG	1D	305	1/1	0.98	0.08	20,20,20,20	0
56	MG	2A	3025	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3208	1/1	0.98	0.16	44,44,44,44	0
56	MG	1D	307	1/1	0.98	0.11	39,39,39,39	0
56	MG	2A	3810	1/1	0.98	0.10	51,51,51,51	0
56	MG	2A	3149	1/1	0.98	0.05	48,48,48,48	0
56	MG	1D	308	1/1	0.98	0.09	42,42,42,42	0
56	MG	1a	1650	1/1	0.98	0.09	51,51,51,51	0
56	MG	1A	3359	1/1	0.98	0.16	29,29,29,29	0
56	MG	1A	3639	1/1	0.98	0.05	24,24,24,24	0
56	MG	1D	311	1/1	0.98	0.24	31,31,31,31	0
56	MG	1A	3238	1/1	0.98	0.13	34,34,34,34	0
56	MG	2A	3537	1/1	0.98	0.04	46,46,46,46	0
56	MG	1A	3543	1/1	0.98	0.07	39,39,39,39	0
56	MG	1X	106	1/1	0.98	0.04	40,40,40,40	0
56	MG	2a	1654	1/1	0.98	0.10	55,55,55,55	0
56	MG	1A	3591	1/1	0.98	0.05	27,27,27,27	0
56	MG	1a	1767	1/1	0.98	0.04	55,55,55,55	0
56	MG	1A	3592	1/1	0.98	0.04	51,51,51,51	0
56	MG	1A	3500	1/1	0.98	0.06	42,42,42,42	0
56	MG	1E	304	1/1	0.98	0.18	32,32,32,32	0
56	MG	1E	305	1/1	0.98	0.08	32,32,32,32	0
56	MG	1A	3767	1/1	0.98	0.06	28,28,28,28	0
56	MG	2A	3411	1/1	0.98	0.12	24,24,24,24	0
56	MG	1A	3501	1/1	0.98	0.17	33,33,33,33	0
56	MG	1A	3769	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3646	1/1	0.98	0.08	29,29,29,29	0
56	MG	1a	1776	1/1	0.98	0.05	68,68,68,68	0
56	MG	1A	3058	1/1	0.98	0.13	33,33,33,33	0
56	MG	1a	1778	1/1	0.98	0.06	56,56,56,56	0
56	MG	1a	1779	1/1	0.98	0.07	64,64,64,64	0
56	MG	1A	3648	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3118	1/1	0.98	0.13	38,38,38,38	0
56	MG	2A	3692	1/1	0.98	0.06	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	10	106	1/1	0.98	0.05	56,56,56,56	0
56	MG	1A	3908	1/1	0.98	0.04	46,46,46,46	0
56	MG	1a	1785	1/1	0.98	0.06	66,66,66,66	0
56	MG	1a	1786	1/1	0.98	0.06	62,62,62,62	0
56	MG	1F	302	1/1	0.98	0.12	35,35,35,35	0
56	MG	1A	4062	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3650	1/1	0.98	0.04	26,26,26,26	0
56	MG	1A	3709	1/1	0.98	0.06	53,53,53,53	0
56	MG	1F	306	1/1	0.98	0.07	42,42,42,42	0
56	MG	1a	1792	1/1	0.98	0.05	57,57,57,57	0
56	MG	2A	3185	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3651	1/1	0.98	0.06	36,36,36,36	0
56	MG	2D	303	1/1	0.98	0.05	28,28,28,28	0
56	MG	1A	3158	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3270	1/1	0.98	0.19	31,31,31,31	0
56	MG	2A	3066	1/1	0.98	0.07	38,38,38,38	0
56	MG	13	101	1/1	0.98	0.08	39,39,39,39	0
56	MG	1A	3137	1/1	0.98	0.22	31,31,31,31	0
56	MG	1A	3714	1/1	0.98	0.04	45,45,45,45	0
56	MG	2A	3439	1/1	0.98	0.14	41,41,41,41	0
56	MG	2E	304	1/1	0.98	0.11	41,41,41,41	0
56	MG	2A	3712	1/1	0.98	0.07	70,70,70,70	0
58	ZN	14	102	1/1	0.98	0.07	95,95,95,95	0
56	MG	2A	3713	1/1	0.98	0.06	58,58,58,58	0
56	MG	2A	3440	1/1	0.98	0.05	53,53,53,53	0
56	MG	1A	3272	1/1	0.98	0.09	46,46,46,46	0
56	MG	1A	3038	1/1	0.98	0.04	36,36,36,36	0
56	MG	1A	3657	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3964	1/1	0.99	0.04	36,36,36,36	0
56	MG	1A	3965	1/1	0.99	0.08	52,52,52,52	0
56	MG	11	105	1/1	0.99	0.05	48,48,48,48	0
56	MG	1A	3902	1/1	0.99	0.03	40,40,40,40	0
56	MG	1A	3183	1/1	0.99	0.20	39,39,39,39	0
56	MG	2A	3468	1/1	0.99	0.06	51,51,51,51	0
56	MG	2A	3019	1/1	0.99	0.14	28,28,28,28	0
56	MG	2A	3652	1/1	0.99	0.03	33,33,33,33	0
56	MG	1A	3031	1/1	0.99	0.07	22,22,22,22	0
56	MG	2a	1730	1/1	0.99	0.04	63,63,63,63	0
56	MG	1A	3025	1/1	0.99	0.12	24,24,24,24	0
56	MG	1A	3012	1/1	0.99	0.03	27,27,27,27	0
56	MG	1A	3716	1/1	0.99	0.03	25,25,25,25	0
56	MG	1V	204	1/1	0.99	0.15	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	205	1/1	0.99	0.07	53,53,53,53	0
56	MG	2A	3536	1/1	0.99	0.05	41,41,41,41	0
56	MG	2A	3660	1/1	0.99	0.03	45,45,45,45	0
56	MG	1A	3693	1/1	0.99	0.03	32,32,32,32	0
56	MG	1A	3973	1/1	0.99	0.03	25,25,25,25	0
56	MG	1A	3632	1/1	0.99	0.08	25,25,25,25	0
56	MG	1A	3232	1/1	0.99	0.13	33,33,33,33	0
56	MG	1a	1724	1/1	0.99	0.05	38,38,38,38	0
56	MG	2A	3666	1/1	0.99	0.07	39,39,39,39	0
56	MG	1A	3371	1/1	0.99	0.03	29,29,29,29	0
56	MG	1A	3977	1/1	0.99	0.04	44,44,44,44	0
56	MG	1A	3197	1/1	0.99	0.04	36,36,36,36	0
56	MG	1A	3636	1/1	0.99	0.07	29,29,29,29	0
56	MG	1A	3286	1/1	0.99	0.12	27,27,27,27	0
56	MG	1A	3582	1/1	0.99	0.08	37,37,37,37	0
56	MG	1a	1731	1/1	0.99	0.04	38,38,38,38	0
56	MG	17	102	1/1	0.99	0.08	31,31,31,31	0
56	MG	1E	306	1/1	0.99	0.05	36,36,36,36	0
56	MG	1a	1784	1/1	0.99	0.04	53,53,53,53	0
56	MG	1A	3830	1/1	0.99	0.04	44,44,44,44	0
56	MG	1A	3178	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3584	1/1	0.99	0.06	57,57,57,57	0
56	MG	1A	3344	1/1	0.99	0.10	49,49,49,49	0
56	MG	1A	3210	1/1	0.99	0.11	44,44,44,44	0
56	MG	1A	3705	1/1	0.99	0.10	29,29,29,29	0
56	MG	1A	3061	1/1	0.99	0.09	19,19,19,19	0
56	MG	2A	3748	1/1	0.99	0.06	53,53,53,53	0
56	MG	1A	4026	1/1	0.99	0.10	38,38,38,38	0
56	MG	1a	1793	1/1	0.99	0.04	71,71,71,71	0
56	MG	1F	301	1/1	0.99	0.11	39,39,39,39	0
56	MG	1A	3892	1/1	0.99	0.03	14,14,14,14	0
56	MG	2A	3442	1/1	0.99	0.04	67,67,67,67	0
56	MG	1a	1648	1/1	0.99	0.04	46,46,46,46	0
56	MG	2A	3444	1/1	0.99	0.03	65,65,65,65	0
56	MG	1A	3110	1/1	0.99	0.11	41,41,41,41	0
56	MG	1a	1746	1/1	0.99	0.08	55,55,55,55	0
56	MG	1A	3685	1/1	0.99	0.06	21,21,21,21	0
56	MG	1A	4030	1/1	0.99	0.07	40,40,40,40	0
56	MG	1A	3992	1/1	0.99	0.04	27,27,27,27	0
56	MG	1A	3993	1/1	0.99	0.05	45,45,45,45	0
56	MG	2A	3828	1/1	0.99	0.06	66,66,66,66	0
56	MG	2A	3059	1/1	0.99	0.05	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3170	1/1	0.99	0.07	38,38,38,38	0
56	MG	1A	3895	1/1	0.99	0.05	35,35,35,35	0
56	MG	1A	3734	1/1	0.99	0.05	59,59,59,59	0
56	MG	2A	3007	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	3116	1/1	0.99	0.19	31,31,31,31	0
58	ZN	1Y	205	1/1	0.99	0.03	72,72,72,72	0
56	MG	1A	3153	1/1	0.99	0.17	34,34,34,34	0
58	ZN	15	109	1/1	0.99	0.04	44,44,44,44	0
58	ZN	1n	103	1/1	0.99	0.04	63,63,63,63	0
58	ZN	2Y	202	1/1	0.99	0.04	101,101,101,101	0
56	MG	2A	3458	1/1	0.99	0.05	47,47,47,47	0
58	ZN	25	108	1/1	0.99	0.06	60,60,60,60	0
58	ZN	26	102	1/1	0.99	0.04	63,63,63,63	0
56	MG	1A	3737	1/1	0.99	0.03	39,39,39,39	0
56	MG	1A	4077	1/1	0.99	0.03	51,51,51,51	0
59	SF4	1d	302	8/8	0.99	0.04	59,63,68,73	0
59	SF4	2d	303	8/8	0.99	0.04	62,73,81,82	0
56	MG	1A	3870	1/1	0.99	0.04	47,47,47,47	0
56	MG	1A	3192	1/1	0.99	0.12	23,23,23,23	0
58	ZN	19	102	1/1	1.00	0.04	48,48,48,48	0
56	MG	2A	3776	1/1	1.00	0.07	39,39,39,39	0
56	MG	1A	3723	1/1	1.00	0.06	42,42,42,42	0
58	ZN	16	102	1/1	1.00	0.04	47,47,47,47	0

6.5 Other polymers

There are no such residues in this entry.