



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:22 PM UTC

PDB ID : 9O3K / pdb_00009o3k
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with macrolide erythromycin, mRNA, aminoacylated A-site Lys-tRNA^{Lys}, P-site fMAC-peptidyl-tRNA^{Met}, and deacylated E-site tRNA^{Lys} at 2.70Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Kruglov, A.A.; Paranjpe, M.N.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on : 2025-04-07
Resolution : 2.70 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

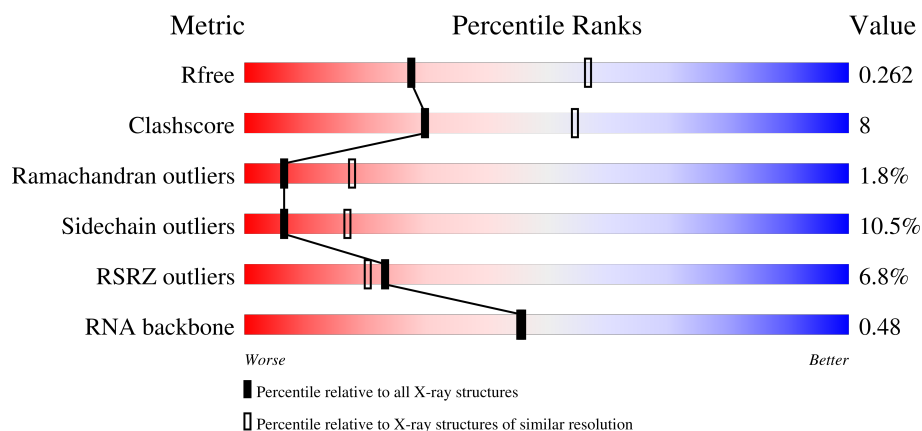
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

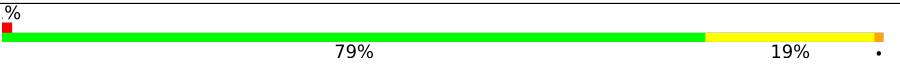
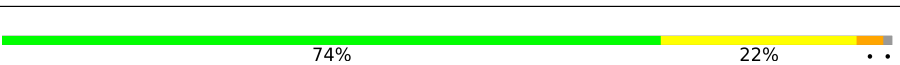
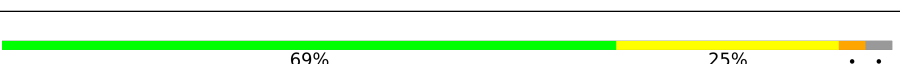
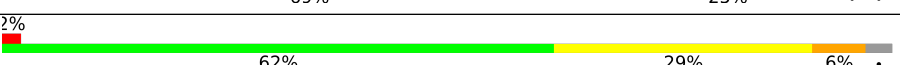
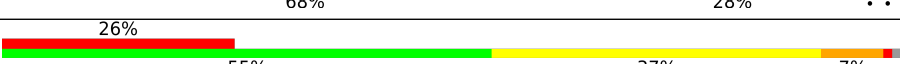
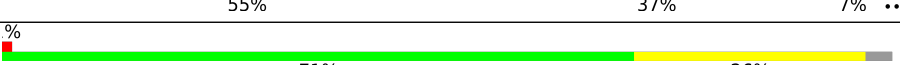
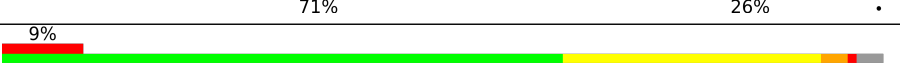
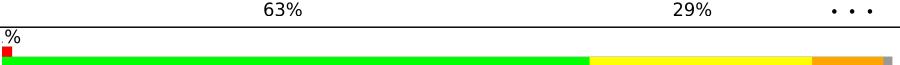
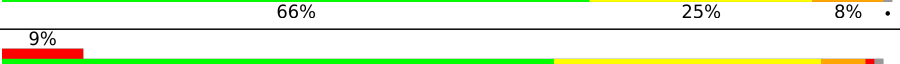
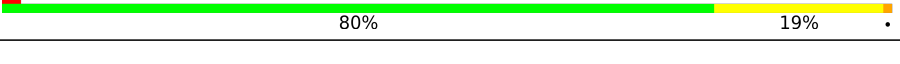
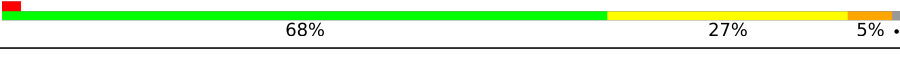
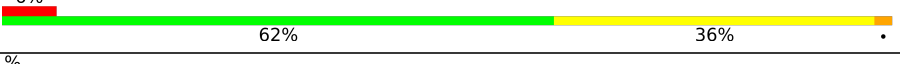
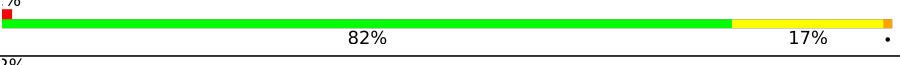
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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% 66% 27% 6% •
1	2A	2915	 4% 57% 32% 6% •

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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	2w	76	
55	1x	77	
55	2x	77	
56	1z	3	
56	2z	3	
57	1y	76	
57	2y	76	

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
58	MG	1U	212	-	-	-	X
58	MG	2a	1613	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 298915 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
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	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	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	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 MET-LYS-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			283	128	59	83	13			
53	2v	11	Total	C	N	O	P	0	0	0
			239	108	49	71	11			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Lys-tRNAlys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1599	718	282	524	74	1			
54	2w	74	Total	C	N	O	P	S	0	0	0
			1599	718	282	524	74	1			

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMAC-tRNAcys RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMAC-tRNAcys Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	3	Total	C	N	O	S	0	0	0
			21	12	3	4	2			
56	2z	3	Total	C	N	O	S	0	0	0
			21	12	3	4	2			

- Molecule 57 is a RNA chain called E-site Deacylated tRNAlys.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	74	Total	C	N	O	P	S	0	0	0
			1577	705	277	520	74	1			
57	2y	74	Total	C	N	O	P	S	0	0	0
			1577	705	277	520	74	1			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1096	Total	Mg	0	0
			1096	1096		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	35	Total 35	Mg 35	0	0
58	1D	11	Total 11	Mg 11	0	0
58	1E	13	Total 13	Mg 13	0	0
58	1F	12	Total 12	Mg 12	0	0
58	1G	4	Total 4	Mg 4	0	0
58	1H	1	Total 1	Mg 1	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	5	Total 5	Mg 5	0	0
58	1O	5	Total 5	Mg 5	0	0
58	1P	8	Total 8	Mg 8	0	0
58	1Q	7	Total 7	Mg 7	0	0
58	1R	6	Total 6	Mg 6	0	0
58	1S	2	Total 2	Mg 2	0	0
58	1T	2	Total 2	Mg 2	0	0
58	1U	12	Total 12	Mg 12	0	0
58	1V	7	Total 7	Mg 7	0	0
58	1W	7	Total 7	Mg 7	0	0
58	1X	5	Total 5	Mg 5	0	0
58	1Y	4	Total 4	Mg 4	0	0
58	1Z	2	Total 2	Mg 2	0	0
58	10	9	Total 9	Mg 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	11	4	Total 4 Mg 4	0	0
58	12	2	Total 2 Mg 2	0	0
58	13	3	Total 3 Mg 3	0	0
58	14	1	Total 1 Mg 1	0	0
58	15	4	Total 4 Mg 4	0	0
58	16	1	Total 1 Mg 1	0	0
58	17	5	Total 5 Mg 5	0	0
58	18	7	Total 7 Mg 7	0	0
58	19	1	Total 1 Mg 1	0	0
58	1a	213	Total 213 Mg 213	0	0
58	1b	1	Total 1 Mg 1	0	0
58	1d	2	Total 2 Mg 2	0	0
58	1e	2	Total 2 Mg 2	0	0
58	1f	2	Total 2 Mg 2	0	0
58	1k	1	Total 1 Mg 1	0	0
58	1l	2	Total 2 Mg 2	0	0
58	1m	1	Total 1 Mg 1	0	0
58	1n	2	Total 2 Mg 2	0	0
58	1p	1	Total 1 Mg 1	0	0
58	1t	1	Total 1 Mg 1	0	0
58	1v	1	Total 1 Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1w	7	Total Mg 7 7	0	0
58	1x	11	Total Mg 11 11	0	0
58	2A	687	Total Mg 687 687	0	0
58	2B	15	Total Mg 15 15	0	0
58	2D	6	Total Mg 6 6	0	0
58	2E	7	Total Mg 7 7	0	0
58	2F	4	Total Mg 4 4	0	0
58	2N	1	Total Mg 1 1	0	0
58	2O	1	Total Mg 1 1	0	0
58	2P	1	Total Mg 1 1	0	0
58	2Q	2	Total Mg 2 2	0	0
58	2R	3	Total Mg 3 3	0	0
58	2T	2	Total Mg 2 2	0	0
58	2V	1	Total Mg 1 1	0	0
58	2X	2	Total Mg 2 2	0	0
58	2Z	1	Total Mg 1 1	0	0
58	20	3	Total Mg 3 3	0	0
58	23	3	Total Mg 3 3	0	0
58	25	4	Total Mg 4 4	0	0
58	27	2	Total Mg 2 2	0	0
58	28	1	Total Mg 1 1	0	0

Continued on next page...

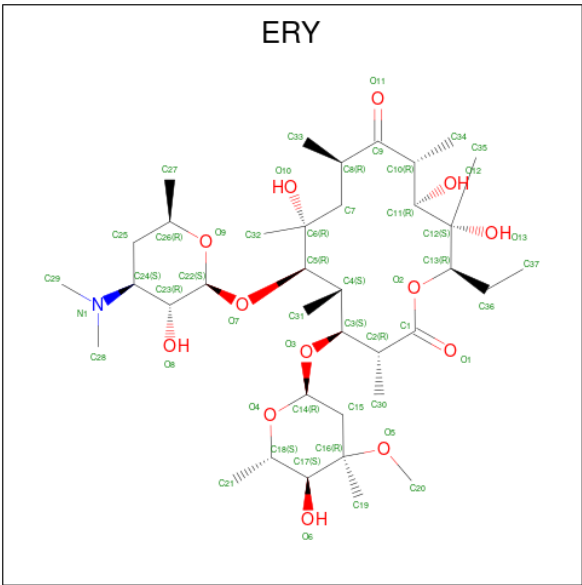
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2a	222	Total 222	Mg 222	0	0
58	2d	2	Total 2	Mg 2	0	0
58	2e	1	Total 1	Mg 1	0	0
58	2f	2	Total 2	Mg 2	0	0
58	2g	1	Total 1	Mg 1	0	0
58	2j	1	Total 1	Mg 1	0	0
58	2l	6	Total 6	Mg 6	0	0
58	2q	2	Total 2	Mg 2	0	0
58	2r	1	Total 1	Mg 1	0	0
58	2t	1	Total 1	Mg 1	0	0
58	2v	2	Total 2	Mg 2	0	0
58	2w	1	Total 1	Mg 1	0	0
58	2x	5	Total 5	Mg 5	0	0

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	1	Total 1	K 1	0	0
59	2x	1	Total 1	K 1	0	0

- Molecule 60 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	1A	1	Total	C	N	O	0	0
			51	37	1	13		
60	2A	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

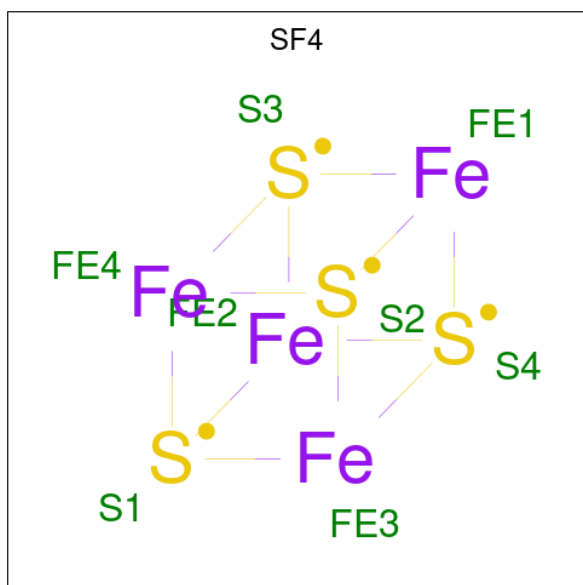
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1Y	1	Total	Zn	0	0
			1	1		
61	14	1	Total	Zn	0	0
			1	1		
61	15	1	Total	Zn	0	0
			1	1		
61	16	1	Total	Zn	0	0
			1	1		
61	19	1	Total	Zn	0	0
			1	1		
61	1n	1	Total	Zn	0	0
			1	1		
61	2Y	1	Total	Zn	0	0
			1	1		
61	24	1	Total	Zn	0	0
			1	1		
61	25	1	Total	Zn	0	0
			1	1		
61	26	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	29	1	Total	Zn	0	0
			1	1		
61	2n	1	Total	Zn	0	0
			1	1		

- Molecule 62 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	1d	1	Total	Fe	S	0	0
			8	4	4		
62	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1A	1715	Total	O	0	0
			1715	1715		
63	1B	53	Total	O	0	0
			53	53		
63	1D	28	Total	O	0	0
			28	28		
63	1E	25	Total	O	0	0
			25	25		
63	1F	13	Total	O	0	0
			13	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1G	3	Total 3	O 3	0	0
63	1H	2	Total 2	O 2	0	0
63	1N	3	Total 3	O 3	0	0
63	1O	4	Total 4	O 4	0	0
63	1P	17	Total 17	O 17	0	0
63	1Q	6	Total 6	O 6	0	0
63	1R	12	Total 12	O 12	0	0
63	1S	5	Total 5	O 5	0	0
63	1T	5	Total 5	O 5	0	0
63	1U	9	Total 9	O 9	0	0
63	1V	9	Total 9	O 9	0	0
63	1W	8	Total 8	O 8	0	0
63	1X	7	Total 7	O 7	0	0
63	1Y	2	Total 2	O 2	0	0
63	1Z	1	Total 1	O 1	0	0
63	10	9	Total 9	O 9	0	0
63	11	8	Total 8	O 8	0	0
63	12	3	Total 3	O 3	0	0
63	13	4	Total 4	O 4	0	0
63	15	6	Total 6	O 6	0	0
63	16	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	17	9	Total 9	O 9	0	0
63	18	9	Total 9	O 9	0	0
63	1a	284	Total 284	O 284	0	0
63	1e	1	Total 1	O 1	0	0
63	1f	1	Total 1	O 1	0	0
63	1i	1	Total 1	O 1	0	0
63	1l	5	Total 5	O 5	0	0
63	1m	2	Total 2	O 2	0	0
63	1o	1	Total 1	O 1	0	0
63	1q	2	Total 2	O 2	0	0
63	1u	1	Total 1	O 1	0	0
63	1v	5	Total 5	O 5	0	0
63	1w	7	Total 7	O 7	0	0
63	1x	6	Total 6	O 6	0	0
63	1z	1	Total 1	O 1	0	0
63	1y	1	Total 1	O 1	0	0
63	2A	624	Total 624	O 624	0	0
63	2B	12	Total 12	O 12	0	0
63	2D	14	Total 14	O 14	0	0
63	2E	5	Total 5	O 5	0	0
63	2F	9	Total 9	O 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2N	1	Total 1	O 1	0	0
63	2O	1	Total 1	O 1	0	0
63	2P	3	Total 3	O 3	0	0
63	2Q	1	Total 1	O 1	0	0
63	2R	1	Total 1	O 1	0	0
63	2T	4	Total 4	O 4	0	0
63	2U	1	Total 1	O 1	0	0
63	2W	3	Total 3	O 3	0	0
63	2Y	1	Total 1	O 1	0	0
63	20	1	Total 1	O 1	0	0
63	21	5	Total 5	O 5	0	0
63	26	1	Total 1	O 1	0	0
63	28	2	Total 2	O 2	0	0
63	2a	161	Total 161	O 161	0	0
63	2d	1	Total 1	O 1	0	0
63	2e	2	Total 2	O 2	0	0
63	2j	1	Total 1	O 1	0	0
63	2l	4	Total 4	O 4	0	0
63	2p	2	Total 2	O 2	0	0
63	2v	1	Total 1	O 1	0	0
63	2w	1	Total 1	O 1	0	0

Continued on next page...

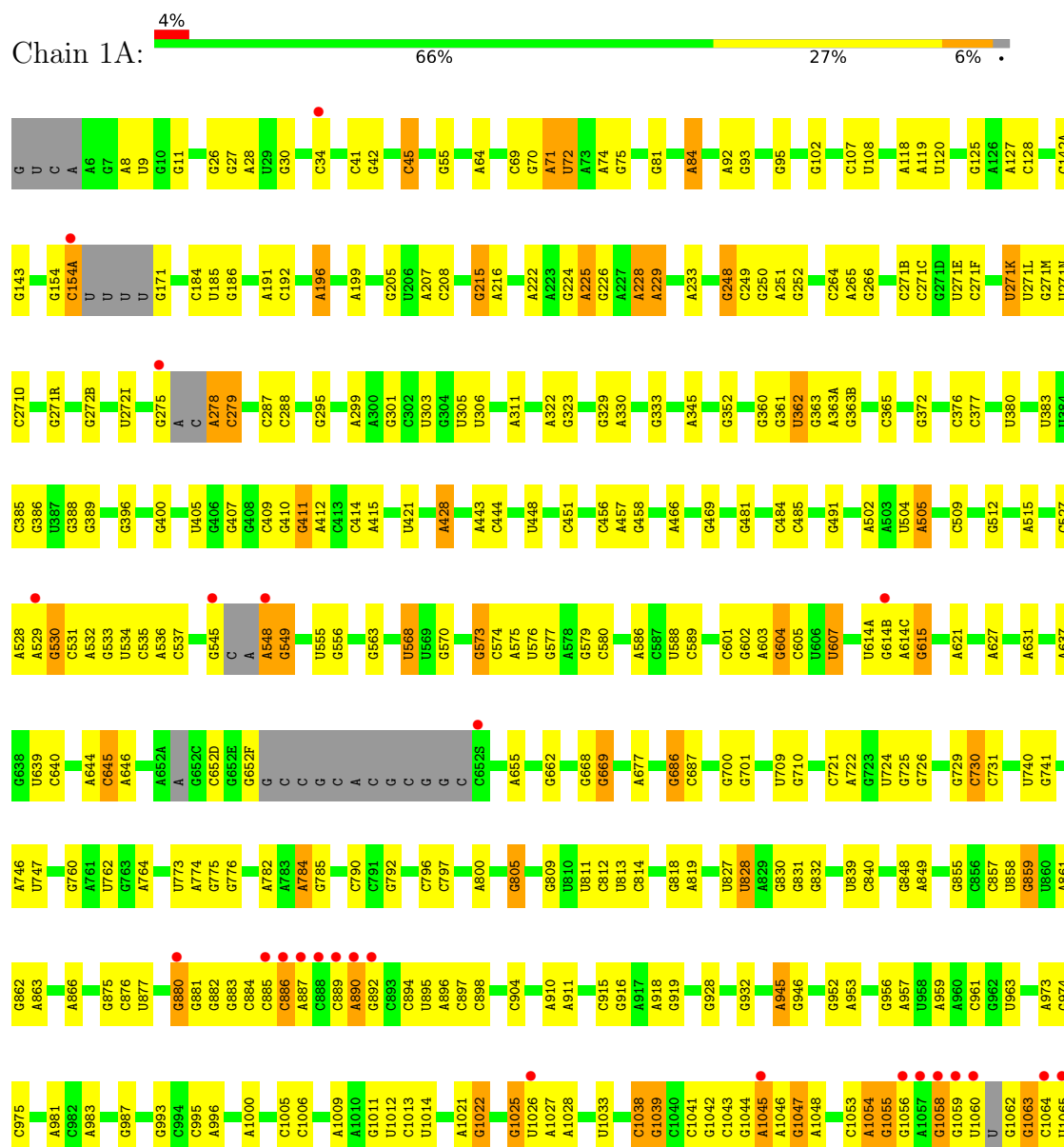
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2x	2	Total	O	0	0
			2	2		

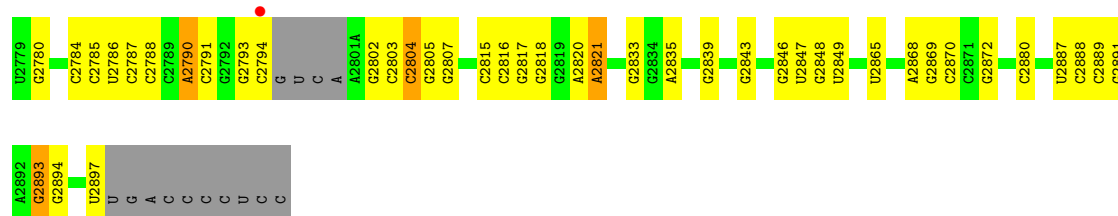
3 Residue-property plots

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.

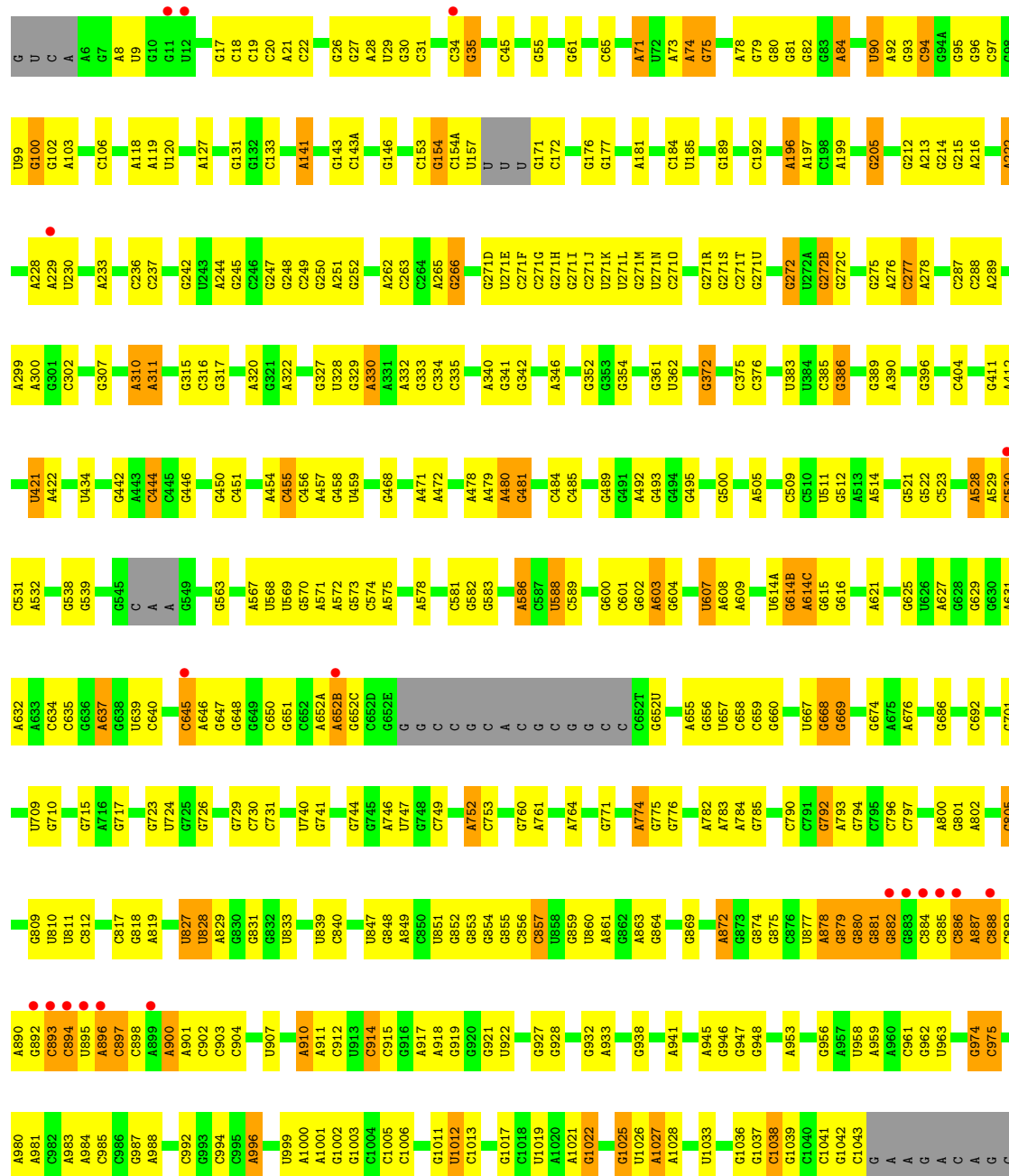
• Molecule 1: 23S Ribosomal RNA



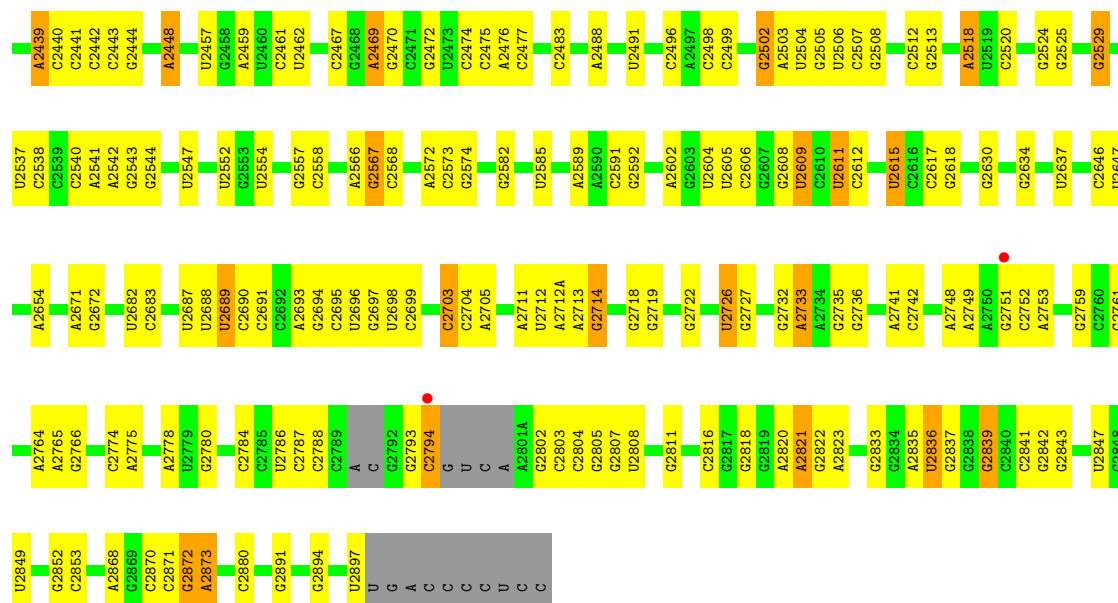
A2654	G2502	G2372	A2266	G2160	G2100	C1967	U1833	G1696	A1558	A1419	U1273	G1138	U1066
C2687	A2503	G2372	A2267	C2161	G2101	G1968	C1943	G1697	A1566	U1420	U1292	G1139	A1067
G2673	U2505	A2376	A2268	C2163	U2102	A1969	G1992	A1698	A1567	G1421	C1293	G1140	G1068
C2680	G2512	A2377	A2269	G2165	G2104	A1971	A1847	A1700	A1568	C1428	U1294	U1141	A1069
	G2513	A2378	A2270	G2166	G2105	A1972	G1858	A1701	A1569	C1429	C1295	A1142	G1070
C2683	A2518	G2379	A2271	U2167	G2106			G1702		C1430	G1296	A1143	C1072
U2684	G2535		A2272	U2168	G2107	U1991		G1703	U1578	U1300		G1144	A1073
G2685	G2536		A2273	A2169	U2108	G1992	U1864		A1579	A1301		G1149	G1074
U2687	G2537		A2274	U2170	U2109	U1993	G1865	U1720	A1580	A1308			G1075
U2688	G2538		A2275	A2171	G2110		G1866	G1721	G1581	A1309		A1156	G1076
U2689	G2550		A2276	U2172	G2111	G1997	A1876	U1722					U1077
C2690	G2551		A2277	A2173	G2112	G2002	A1877	U1723	C1584				U1078
A2693	U2552		A2278	A2174	U2113		G1878	G1740	A1586	G1448		G1164	C1079
G2694	G2553		A2279	C2175	A2114	C2006		A1741	A1587	A1449		C1165	U1081
	G2410		U2291	A2176	G2115		G1882	G1746	C1588	C1315		C1166	U1082
	G2417		C2292	G2177	G2116	G2012	G1883		C1589	G1332		G1167	U1083
			C2295	C2179	U2118	A2013	A1889	G1756	G1593	G1339		G1168	A1084
				U2180	U2119	A2014	A1890		G1594			G1169	A1085
				G2182	G2120	U2022		A1762	U1602	A1342		G1170	A1086
				G2183	G2121	G2023	G1899	G1763	U1603	G1343		G1171	G1087
				G2184	U2122		A1900	G1764	A1608	G1344		G1173	A1088
				G2185	G2123	U2028	G1903	A1773	A1609			U1175	G1089
				G2186	G2124	G2029			A1610	U1352		G1176	U1090
				G2187	A2126	A2030	G1906	U1778		A1353		A1177	G1091
				G2188	G2127	A2031		U1779	A1614	A1354		C1178	G1092
				U2189	C2128	G2032	U1911	A1780	A1614	A1355		C1179	G1093
				G2190	C2129	A2033		G1781	G1627	G1356		C1180	U1094
				G2191	U2130	G2037	C1914	G1782		A1359		C1181	A1095
				G2192	G2131		U1915	A1783	G1633	A1360		G1187	A1096
				G2193	U2132	C2043	A1916	A1784	A1636	U1507		U1188	U1097
				A2198	G2133	G2049	U1917	A1785	A1637	A1508		C1201	A1098
					A2135		A1918	G1786		A1365			U1099
					G2136	G2053	A1919		A1641	A1509A		A1220	U1101
					G2137		C1920	U1791	G1642				G1102
					C2138	A2054		U1794		U1512		G1227	A1103
					G2139	C2055	G1929	C1795	C1648	C1513		U1105	C1104
					C2140	G2056	G1930	U1796				G1239	U1106
					G2141		U1931	C1797	A1655	U1518			G1107
					C2142	A2059	A1932	U1798	A1656	G1519		G1244	U1108
					G2143	A2060	G1933	G1799	C1657	A1528A			C1109
					U2144	G2061	A1938	C1800	C1658			A1283	G1110
					G2145		U1939	A1801		C1532			A1111
					C2146	C2065		G1802	A1669	G		G1256	G1112
					G2147	C2066	C1942	A1803	C1670	U1396		C1257	U1113
					G2148				U1671			C1258	G1114
					G2149	G2069	A1952	G1807	C1672	U1405		G1259	G1115
					U2150		A1953		U1673	C1407			C1116
					G2151	U2074	G1954	G1813	G1674			G1284	G1117
					G2152	U2075	U1955	G1814	C1675	C1411		A1285	
					G2153		U1956	A1815	U1540	A1412		G1286	G1125
					G2154	G2080	C1957	G1816	A1541	G1413		U1267	
					G2155		U1958		A1677	G1414		U1268	A1128
					G2156	U2086	C1962	G1823	U1688	G1415		A1289	
					G2157	C2097	U1963			G1416		C1270	C1186
					G2158	U2098	U1962	A1829	U1693	G1417		G1137	G1136
					G2159	U2099				G1418			



• Molecule 1: 23S Ribosomal RNA

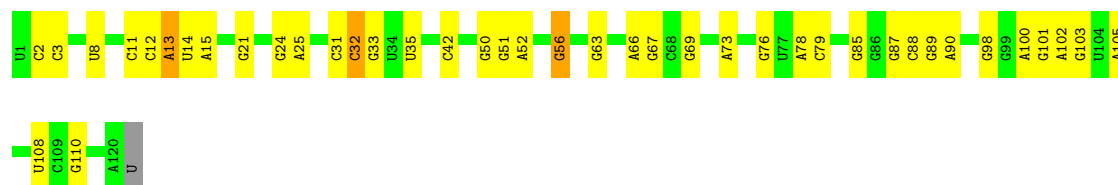


C350	A268	A2158	C2006	G1910	C1782	C1640	U1518	U1431	A1317	U1211	G1115	C
G351	A269	G2159	G2010	U1911	A1783	G1647	G1519	C1432	G1324	G1212	G1116	A
G354	G2160	G2101	U2011	A1912	A1784	G1648	G1519	U1433	G1324	A1220	G1117	G
C359	G2162	G2102	G2012	A1913	A1785	G1649	G1529	U1434	A1336	C1221	G1125	A
A360	G2163	G2103	A2013	C1914	C1786	G1650	G1530	C1437	G1337	A1226	A1126	G
A361	G2164	G2104	A2014	U1915	C1790	G1651	C1531	G1442	U1341	A1226	A1127	U
C364	G2165	C2105	A2015	A1916	A1791	A1652	G1532	G1443	U1352	G1229	U1130	U
C365	G2166	G2106	U2016	A1917	U1794	A1653	G1533	G1444	U1353	C1230	U1131	G
C366	G2167	C2107	A2017	A1918	U1795	A1654	U	A1445	A1354	G1231	U1132	G
A366	G2168	C2108	U2018	A1919	U1796	C1662	G1536	C1445A	G1355	G1232	C1135	C
C370	A2169	G2109	A2019	G1920	U1797	C1663	G1537	A1449	G1356	A1237	G1136	U
G371	A2170	G2110	C2021	U1923	U1798	A1664	G1538	G1450	U1357	G1238	G1139	A
G372	A2171	C2111	U2022	C1924	U1799	A1665	G1539	G1451	U1358	G1239	G1140	G
A286	U2172	G2112	G2023	U1925	C1800	A1666	U1540	G1455	U1359	U1240	U1141	A
C2372	A2173	U2113	G2023	C1926	G1801	G1667	U1541	G1455	A1360	A1241	U1142	A
A2288	C2174	A2114	G2027	A1927	A1802	G1674	A1542	A1460	G1364	U1249	A1142A	G
G2289	G2175	G2115	A2030	U1928	C1803	U1688	C1543	G1461	A1365	U1249	G1149	C
G2290	A2176	G2116	A2031	G1929	A1804	U1689	A1544	G1462	A1366	A1253	C1150	A
U291	C2177	A2117	A2032	G1930	C1805	A1689	A1545	G1466	A1367	G1256	G1153	C
A2376	C2178	U2118	A2033	U1931	A1812	G1696	C1547	G1467	G1368	G1257	G1158	A
G2375	G2179	G2119	A2034	G1932	A1815	G1697	C1557	G1469	C1370	G1260	U1159	U
A2377	G2180	G2120	G2035	U1933	G1816	A1698	A1558	G1470	G1371	C1261	G1160	C
G2378	G2181	G2121	C2036	A1936	G1824	G1699	A1566	A1471	A1373	G1264	C1161	U
G2382	G2182	U2122	G2037	G1937	G1828	A1701	A1569	A1477	A1379	U1265	U1165	U
G2383	G2183	G2123	G2038	A1938	C1829	A1702	U1578	G1478	G1380	G1266	C1166	A
G2384	G2184	G2124	C2039	U1939	C1830	G1711	U1579	G1482	A1384	U1267	G1171	A
G2385	G2185	G2125	G2040	A1942	G1831	G1712	A1580	G1487	G1385	A1268	G1172	G
G2386	G2186	A2126	C2043	U1955	U1833	G1717	C1581	G1488	A1386	A1269	G1173	A
U2387	G2187	G2127	A2042	C1962	U1834	G1718	C1582	U1489	U1394	G1271	G1174	U
C2306	G2188	C2128	C2043	U1965	G1839	G1721	C1583	A1490	A1395	A1272	G1175	U
G2307	U2189	C2129	C2055	C1967	A1847	U1739	C1584	C1493	U1405	A1275	G1178	C
G2308	G2192	U2130	G2056	G1968	A1948	G1740	G1589	C1494	U1406	A1278	C1179	G
A2311	G2196	G2131	U2056	A1969	U1851	A1741	U1590	A1495	A1407	G1278	C1180	U
G2315	U2197	U2132	A2059	G1968	C1852	G1746	G1591	A1496	C1408	U1288	A1181	A
C2316	A2198	A2134	A2060	A1970	A1853	G1747	G1592	U1497	U1394	G1292	G1183	U
G2395	G2317	A2135	G2061	G1964	G1861	G1747A	G1593	U1503	A1412	U1292	G1188	A
G2396	G2206	C2136	A2062	C1967	A1876	G1748	G1594	C1504	G1413	C1293	G1187	C
G2397	G2207	C2137	C2063	U1967	A1877	G1756	C1604	C1505	G1416	G1295	U1189	U
C2404	G2208	C2138	U2068	G1968	G1878	A1762	U1608	A1507	U1420	U1300	G1190	C
U2405	U2218	C2139	G2069	A1969	A1889	G1763	A1609	C1508	G1421	A1301	G1191	A
G2406	G2219	C2140	G2070	A1971	A1890	G1764	A1610	A1509A	G1422	G1302	G1192	U
G2407	G2224	G2141	A2071	A1972	A1773	A1773	G1626	A1509B	G1423	G1303	G1195	G
U2408	A2225	C2142	A2072	A1972	G1899	U1777	C1636	G1510	G1424	C1306	A1204	U
G2409	G2226	C2143	G2072	G1975	A1901	U1778	A1637	C1511	G1428	C1314	U1205	C
U2419	G2238	C2144	U2074	G1975	C1902	U1779	C1638	C1512	G1429	G1315	G1210	G
C2420	U2245	C2145	U2075	G1983	G1907	U1780	U1639	U1513	C1430	U1316	A1210	A
G2421	G2246	G2146	U2076	G1984	A2001	U1781		U1514				
A2422	A2247	U2149	G2080	U1991	G2002							
A2425	C2248	G2151	A2086	G1992								
C2443	G2249	G2152	G2087	U1993								
U2449	G2250	G2153	G2087	G1997								
A2450	G2251	G2154	G2087	A2001								
A2456	G2252	G2155	G2087	G2002								
G2436	G2253	G2156	G2087	G2002								
G2437	G2254	G2157	G2087	G2002								



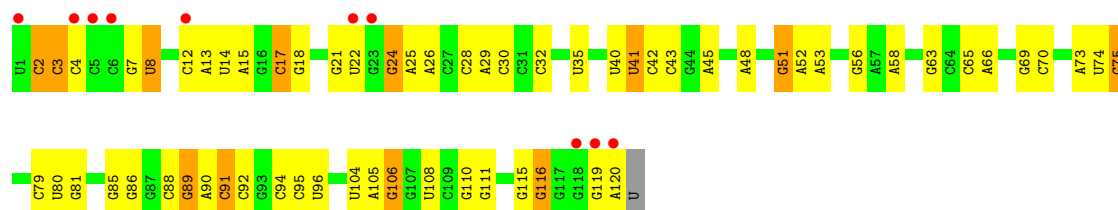
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 65% 31% ..



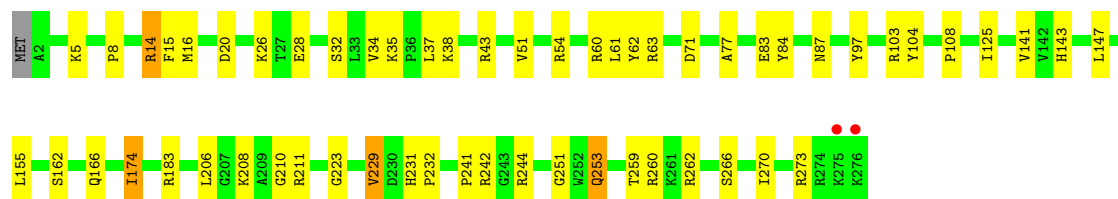
- Molecule 2: 5S Ribosomal RNA

Chain 2B: 8% 47% 42% 10% .

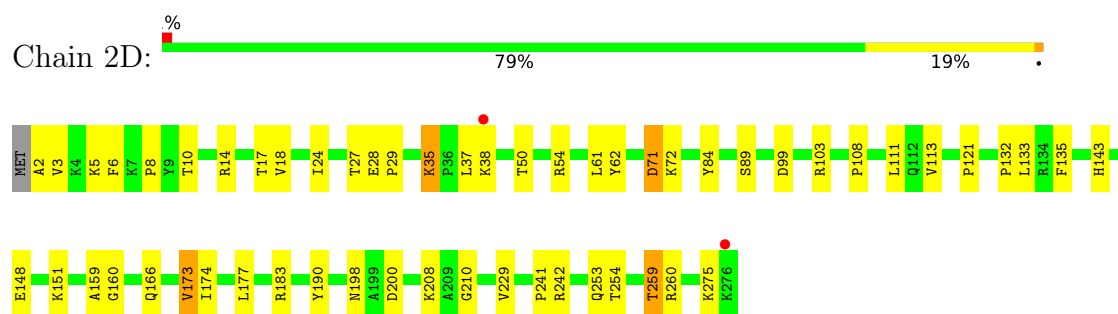


- Molecule 3: 50S ribosomal protein L2

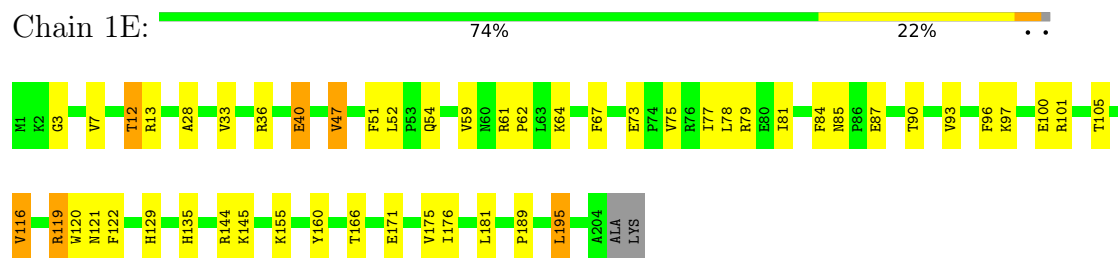
Chain 1D: 79% 19% .



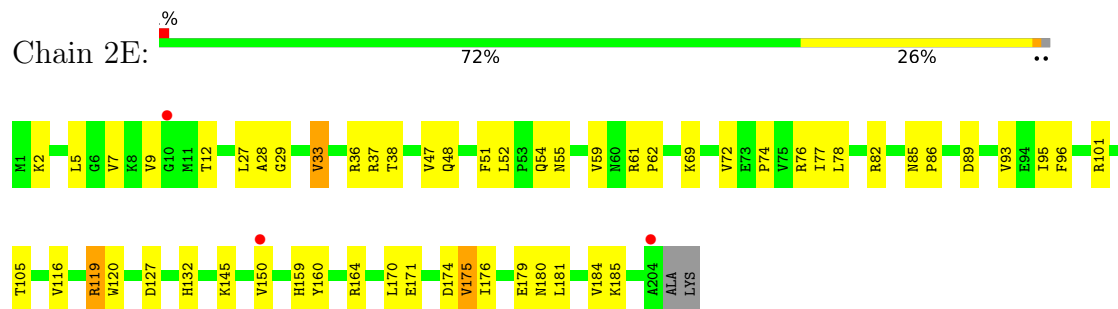
- Molecule 3: 50S ribosomal protein L2



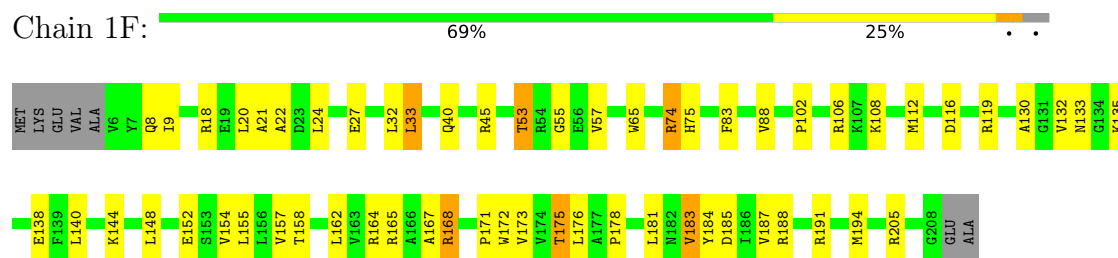
• Molecule 4: 50S ribosomal protein L3



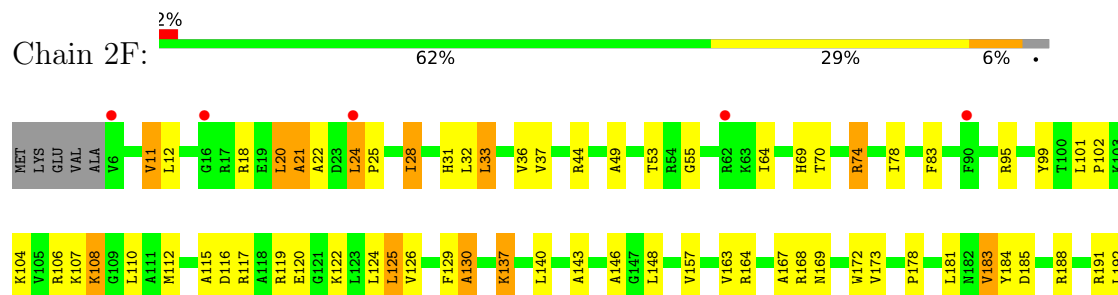
• Molecule 4: 50S ribosomal protein L3

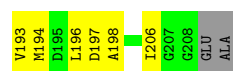


• Molecule 5: 50S ribosomal protein L4

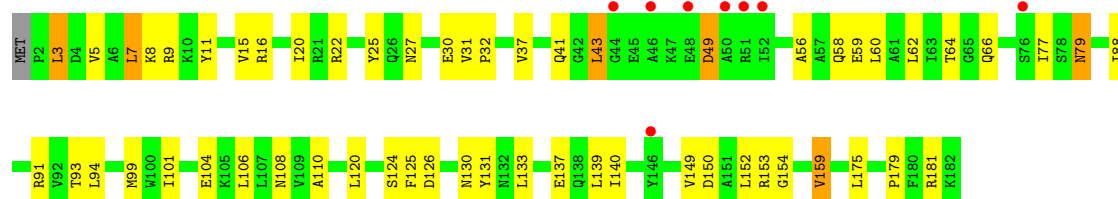


• Molecule 5: 50S ribosomal protein L4

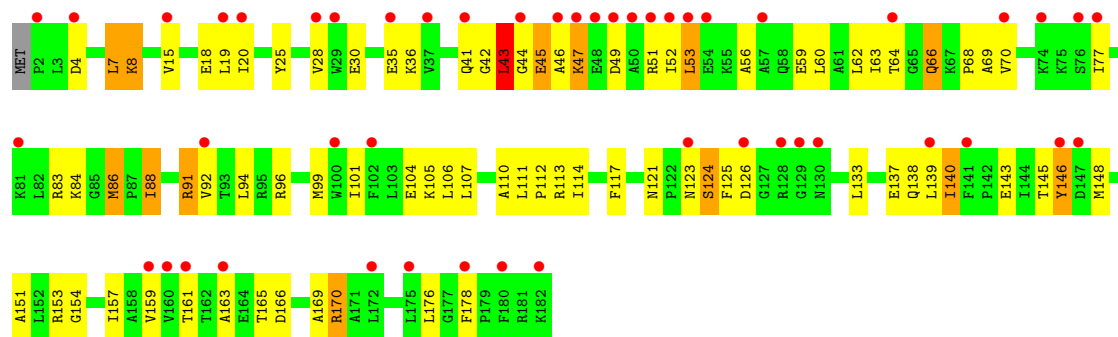




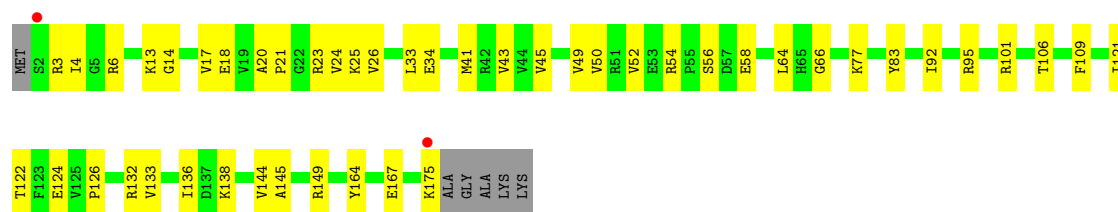
- Molecule 6: 50S ribosomal protein L5



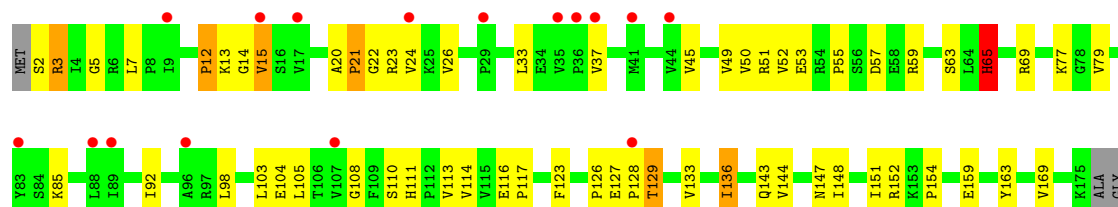
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



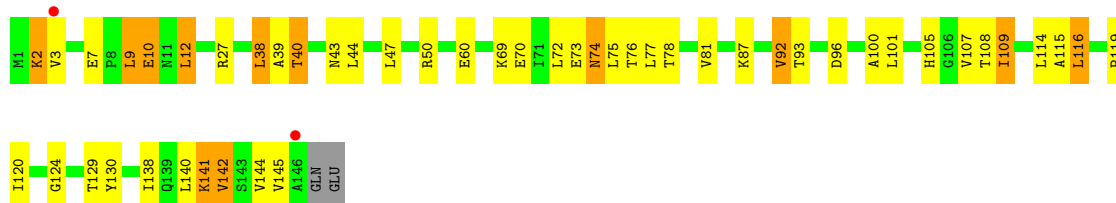
- Molecule 7: 50S ribosomal protein L6



ALA
LYS
LYS

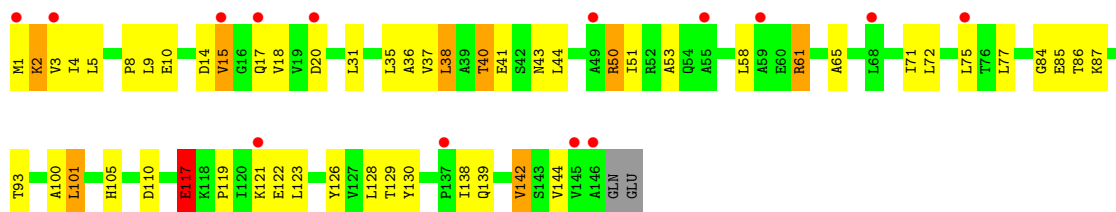
• Molecule 8: 50S ribosomal protein L9

Chain 1I: 



• Molecule 8: 50S ribosomal protein L9

Chain 2I: 



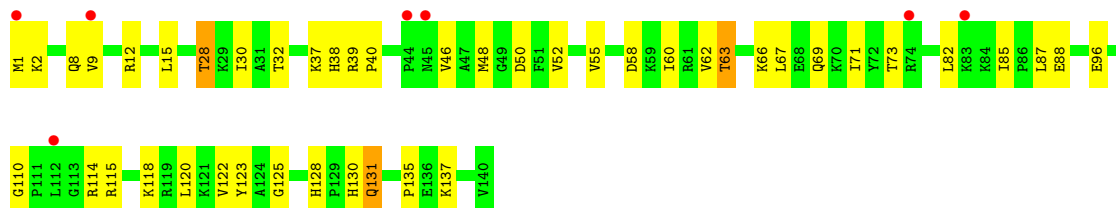
• Molecule 9: 50S ribosomal protein L13

Chain 1N: 



• Molecule 9: 50S ribosomal protein L13

Chain 2N: 



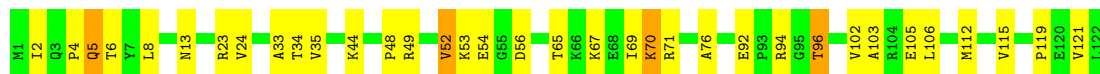
• Molecule 10: 50S ribosomal protein L14

Chain 1O: 



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  71% 25% .



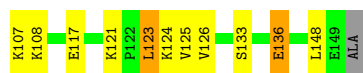
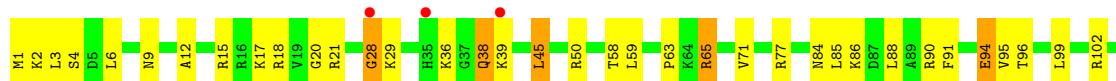
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  69% 26% . .



- Molecule 11: 50S ribosomal protein L15

Chain 2P:  2% 68% 27% 5% .



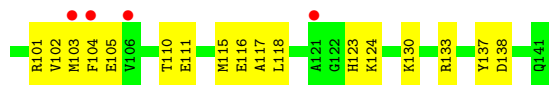
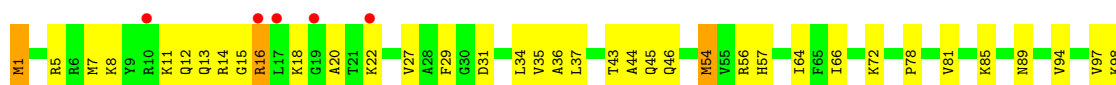
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  74% 21% .

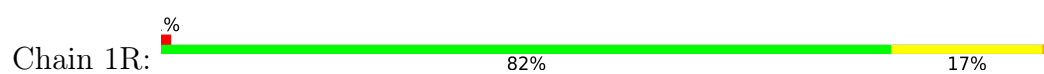


- Molecule 12: 50S ribosomal protein L16

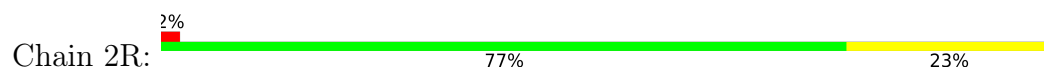
Chain 2Q:  6% 62% 36% .



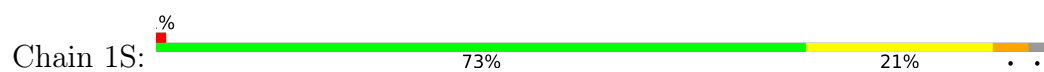
- Molecule 13: 50S ribosomal protein L17



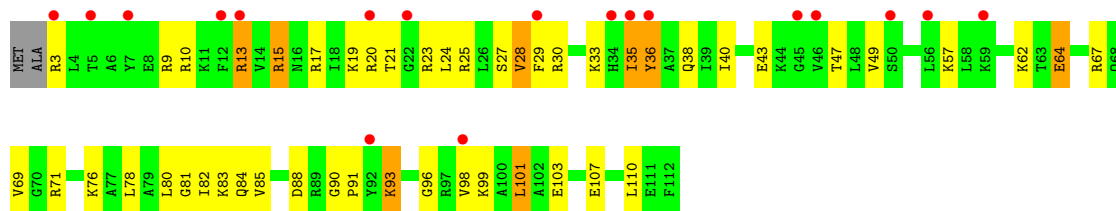
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18

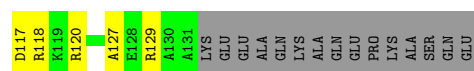


- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19





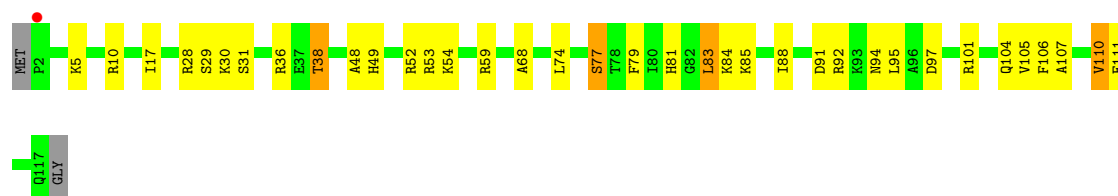
- Molecule 16: 50S ribosomal protein L20

Chain 1U: 81% 16% ..



- Molecule 16: 50S ribosomal protein L20

Chain 2U: 68% 27% ..



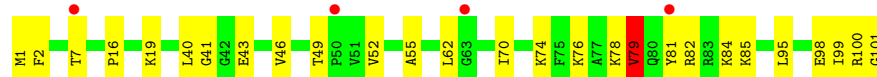
- Molecule 17: 50S ribosomal protein L21

Chain 1V: 86% 13% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V: 73% 26% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W: 83% 13% ..

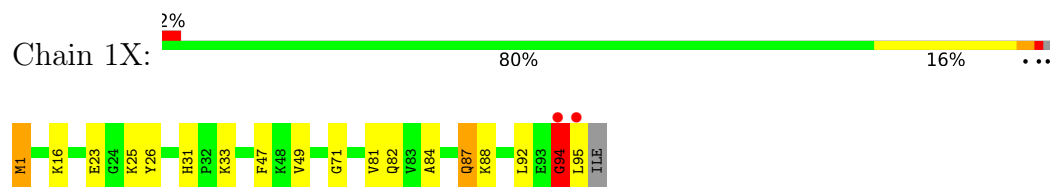


- Molecule 18: 50S ribosomal protein L22

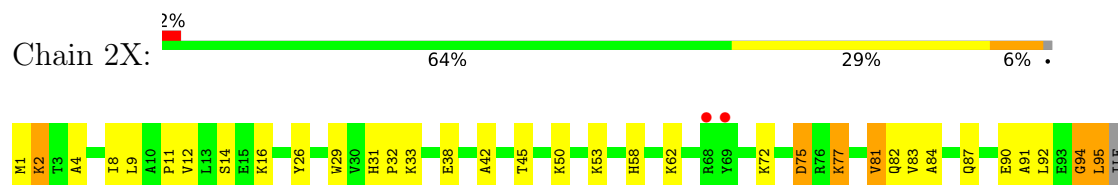
Chain 2W: 76% 21% ..



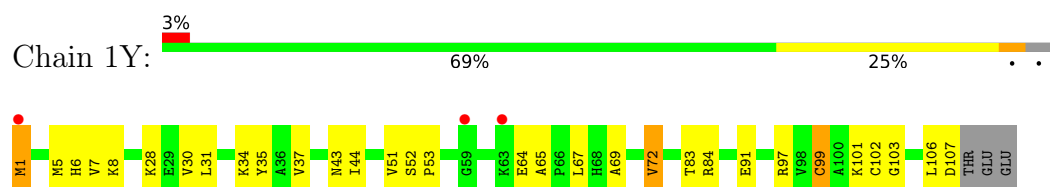
- Molecule 19: 50S ribosomal protein L23



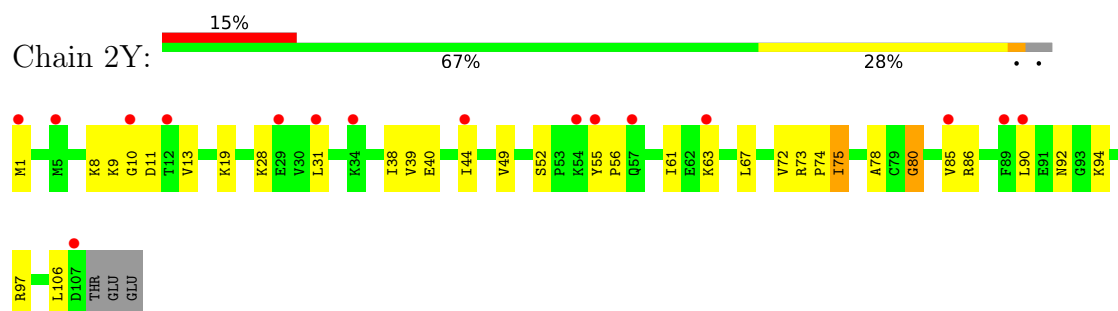
- Molecule 19: 50S ribosomal protein L23



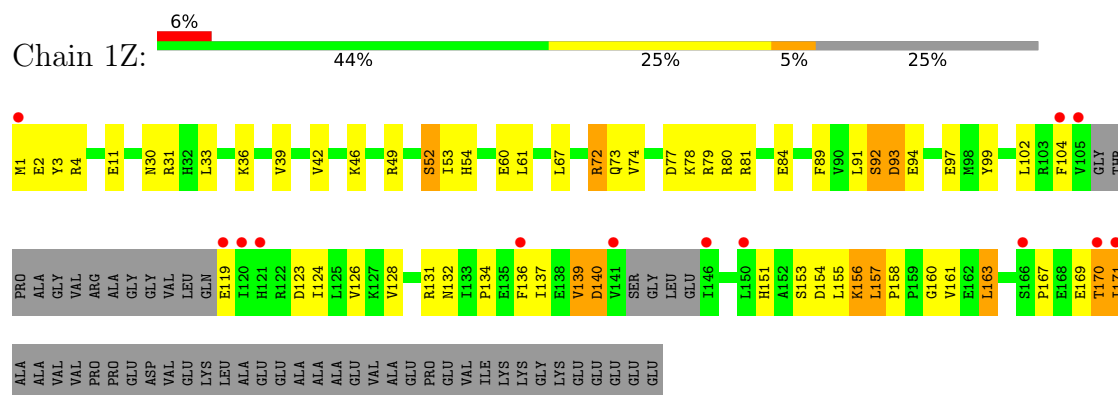
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

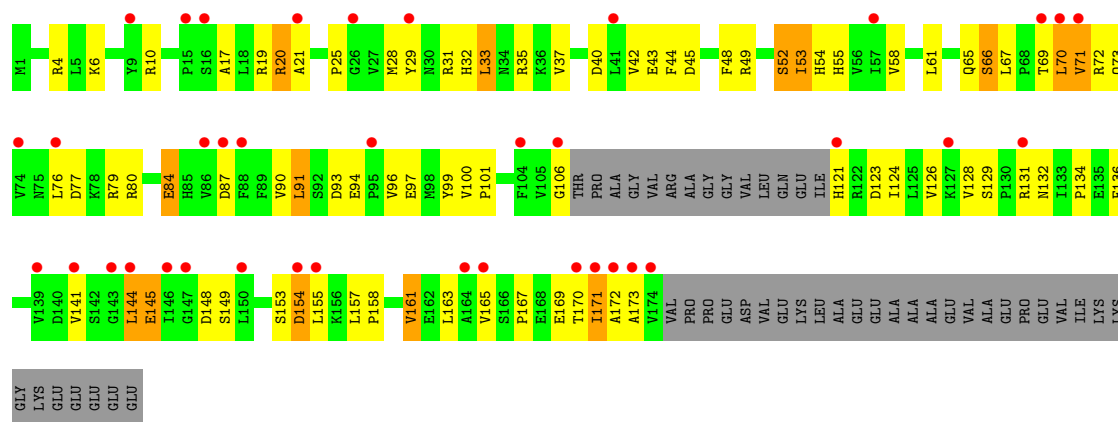


- Molecule 21: 50S ribosomal protein L25

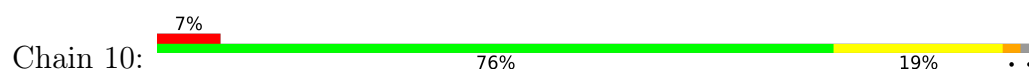


- Molecule 21: 50S ribosomal protein L25

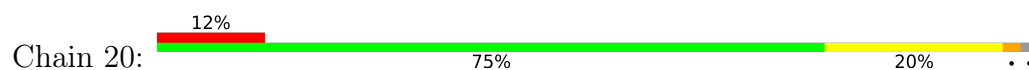




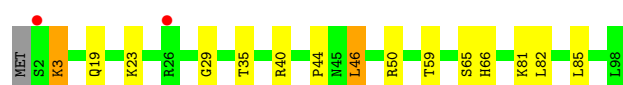
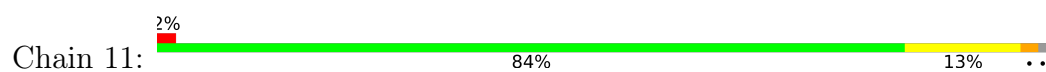
- Molecule 22: 50S ribosomal protein L27



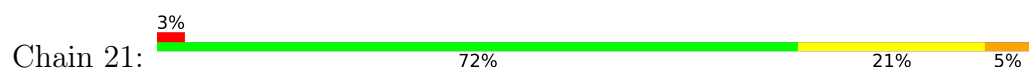
- Molecule 22: 50S ribosomal protein L27



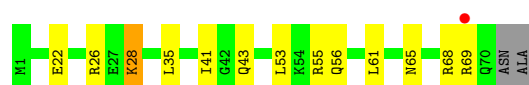
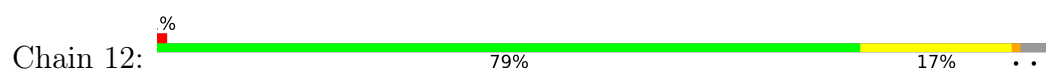
- Molecule 23: 50S ribosomal protein L28



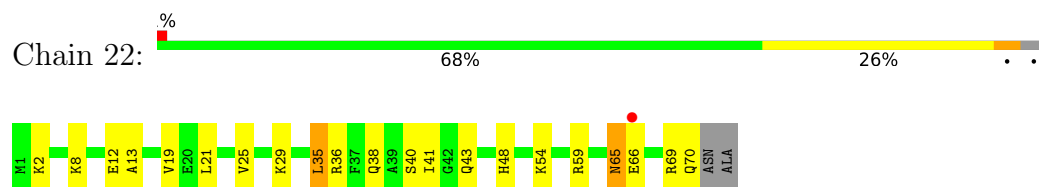
- Molecule 23: 50S ribosomal protein L28



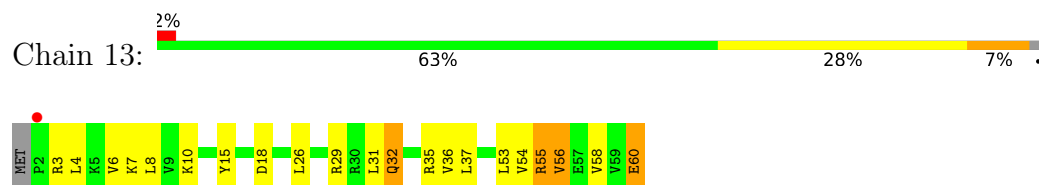
- Molecule 24: 50S ribosomal protein L29



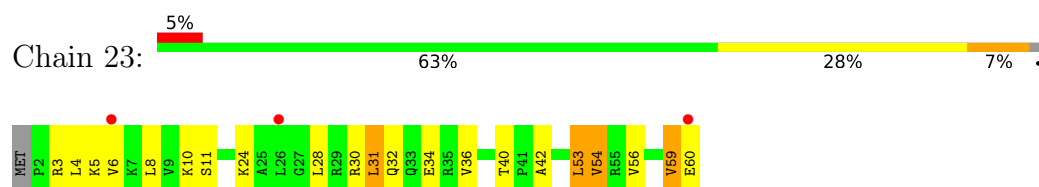
- Molecule 24: 50S ribosomal protein L29



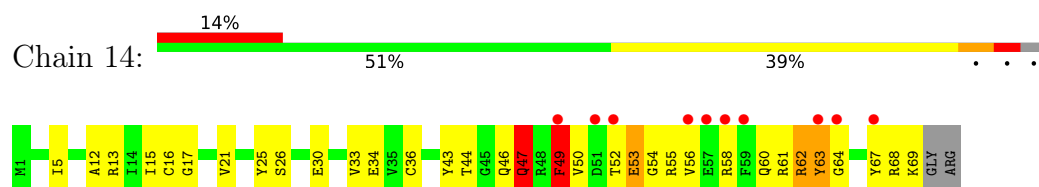
- Molecule 25: 50S ribosomal protein L30



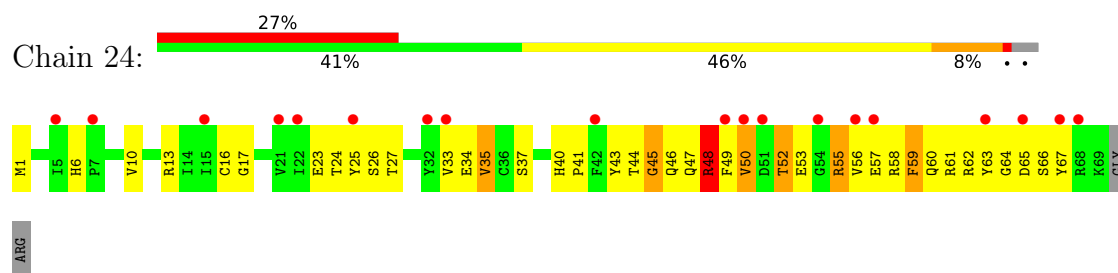
- Molecule 25: 50S ribosomal protein L30



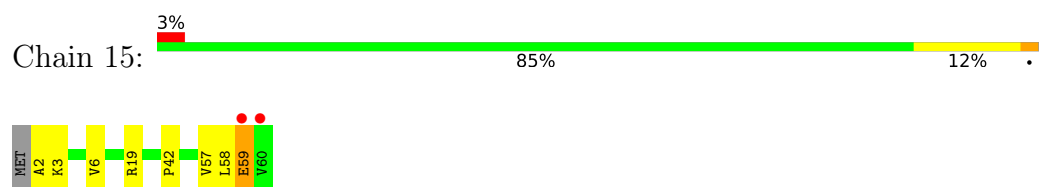
- Molecule 26: 50S ribosomal protein L31



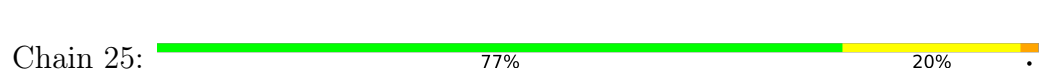
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

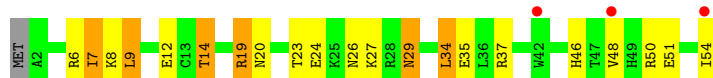




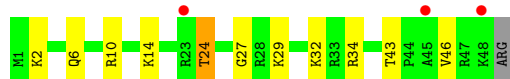
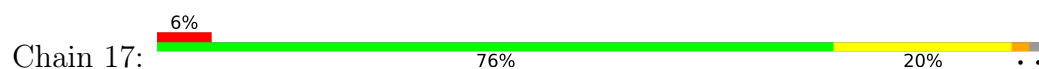
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



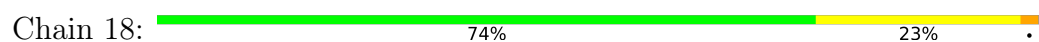
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



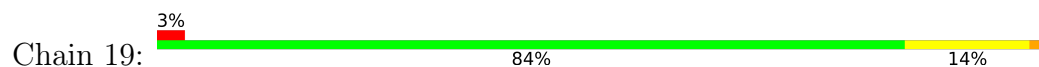
- Molecule 30: 50S ribosomal protein L35

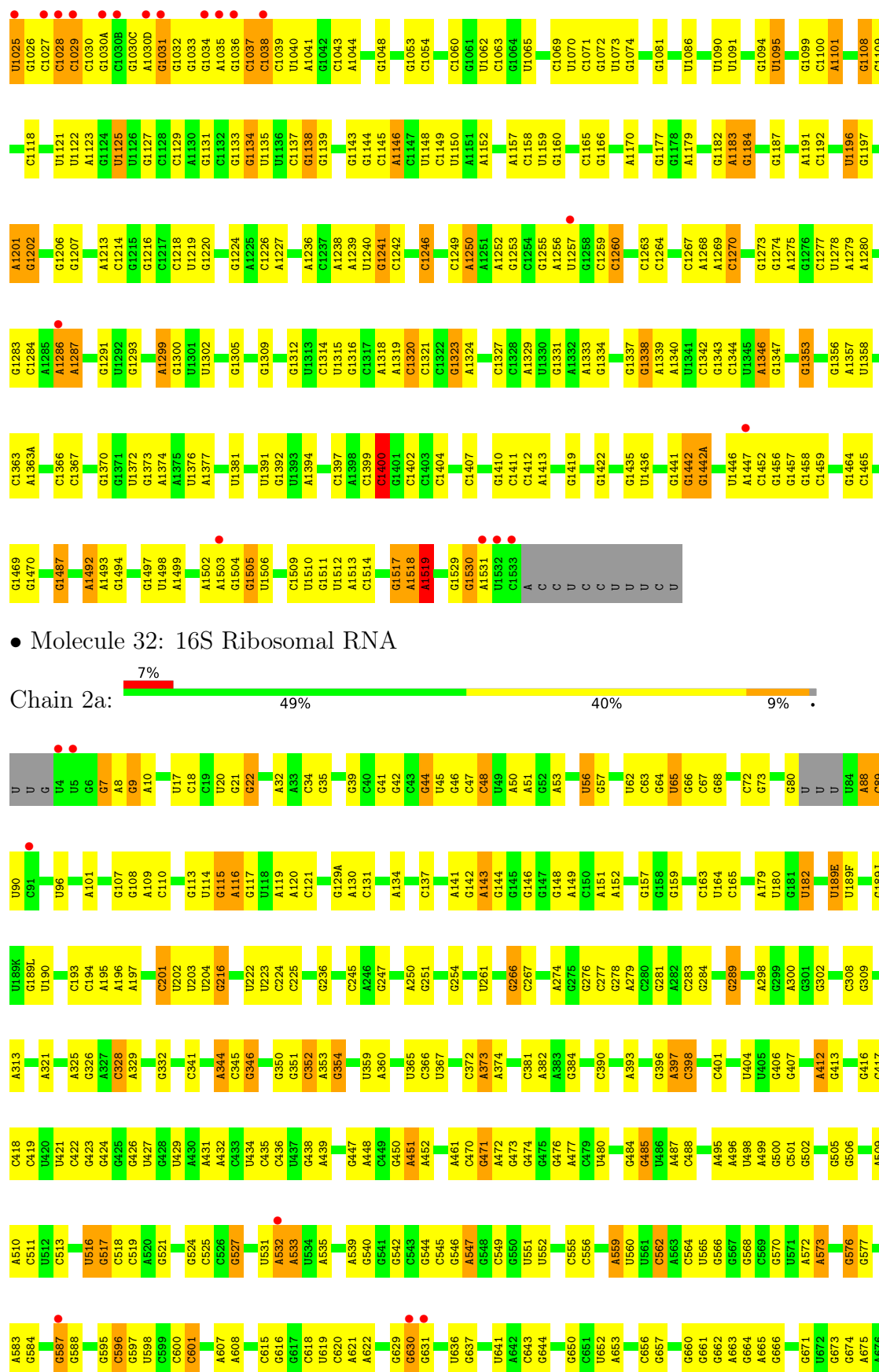


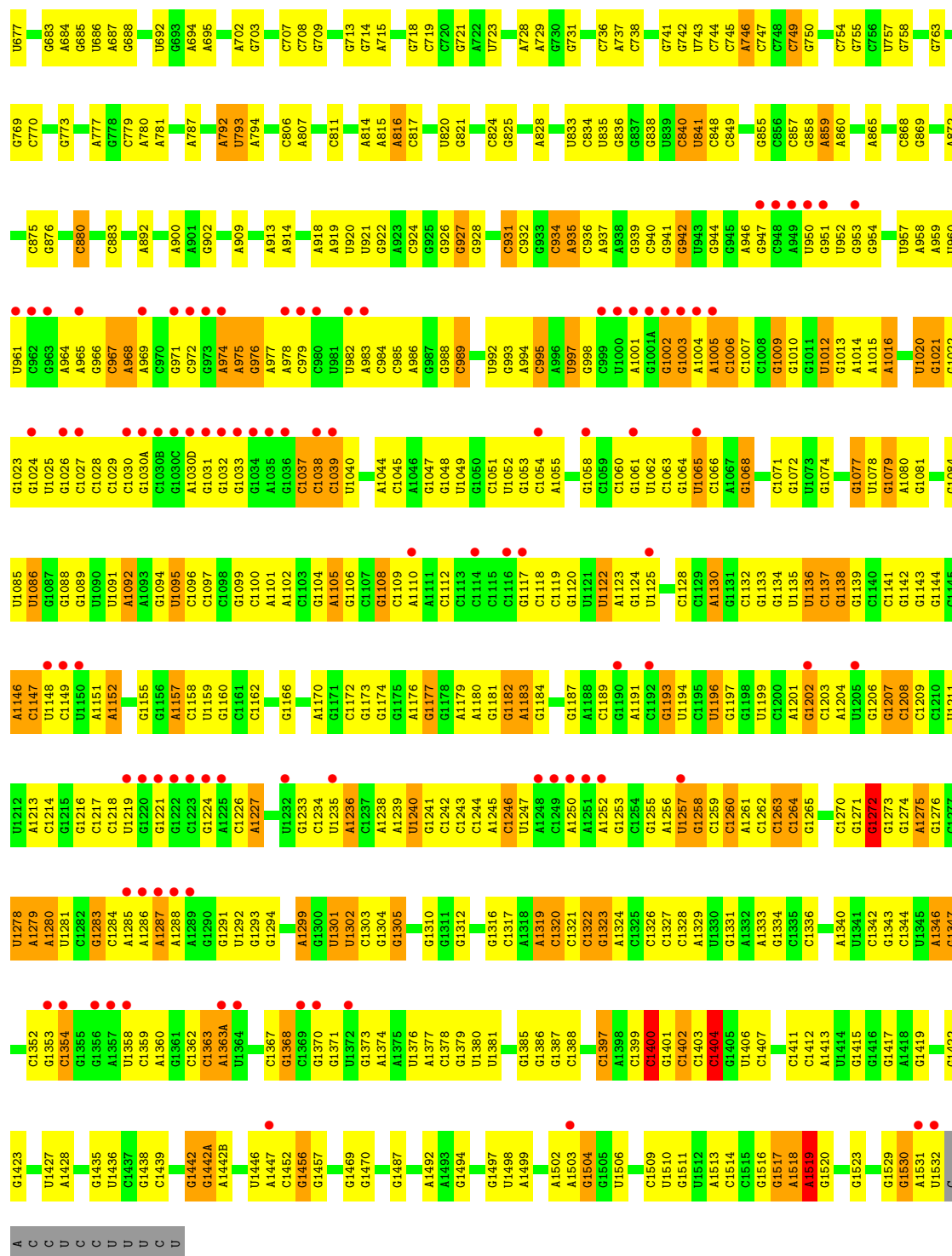
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

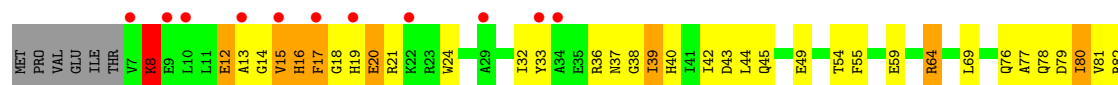


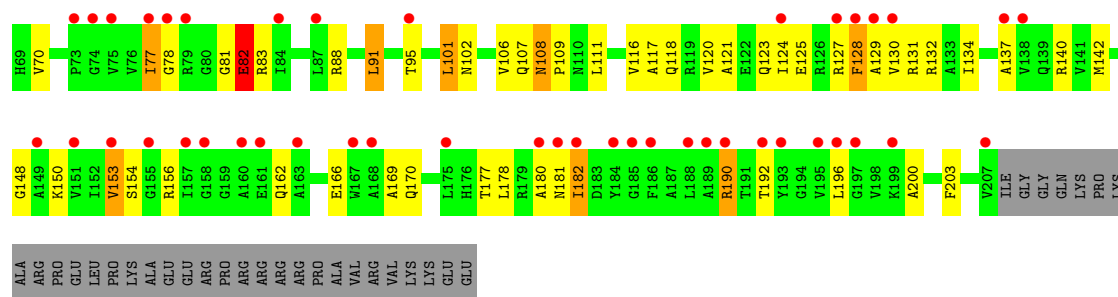




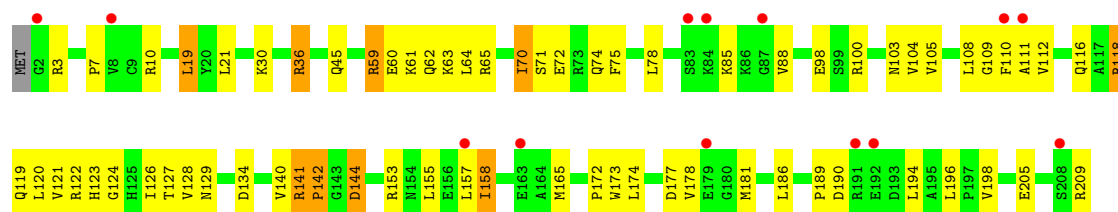
• Molecule 33: 30S ribosomal protein S2

Chain 1b: 11% 50% 33% 7% 10%

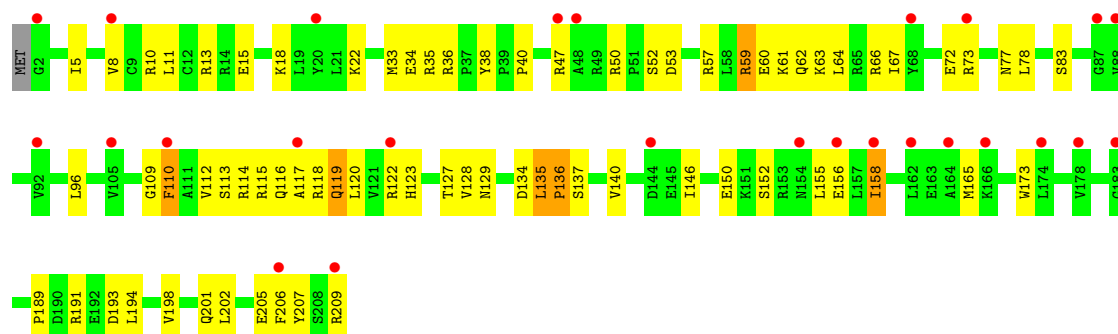




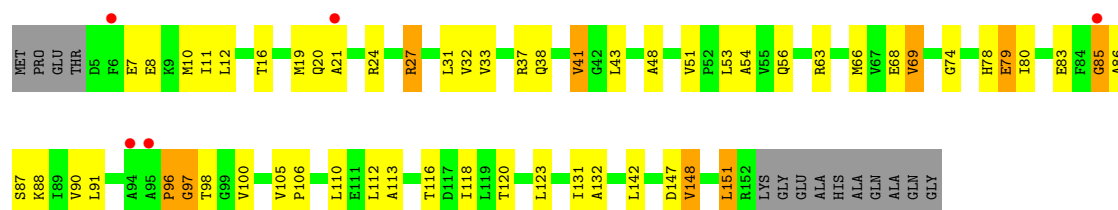
- Molecule 35: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S4

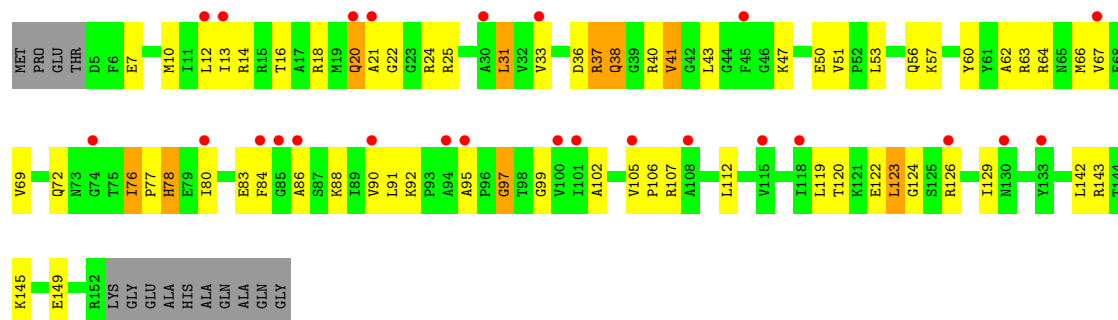


- Molecule 36: 30S ribosomal protein S5

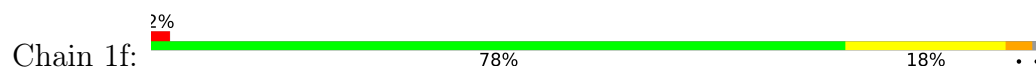


- Molecule 36: 30S ribosomal protein S5

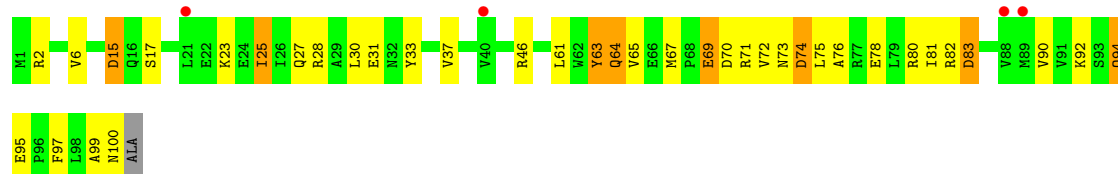




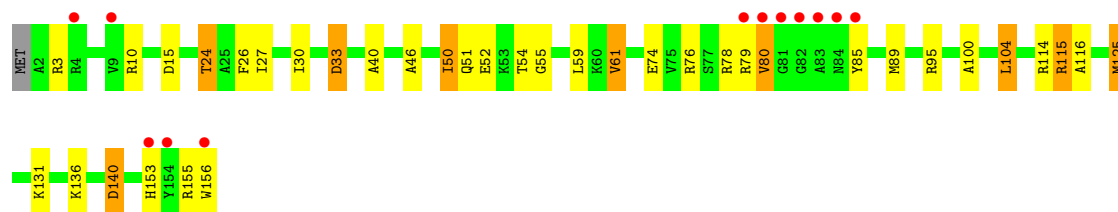
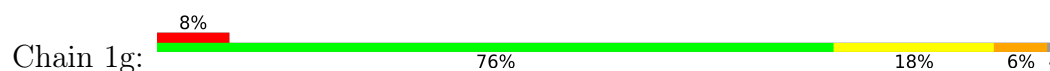
- Molecule 37: 30S ribosomal protein S6



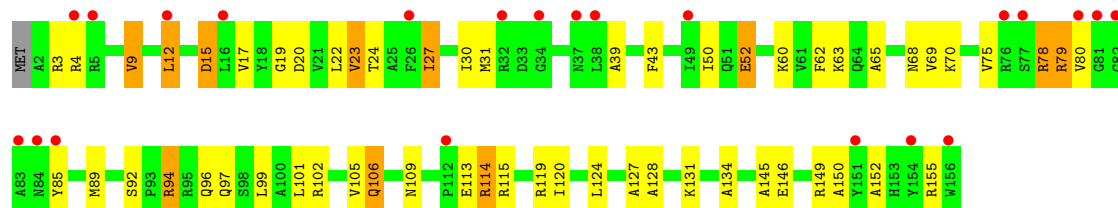
- Molecule 37: 30S ribosomal protein S6



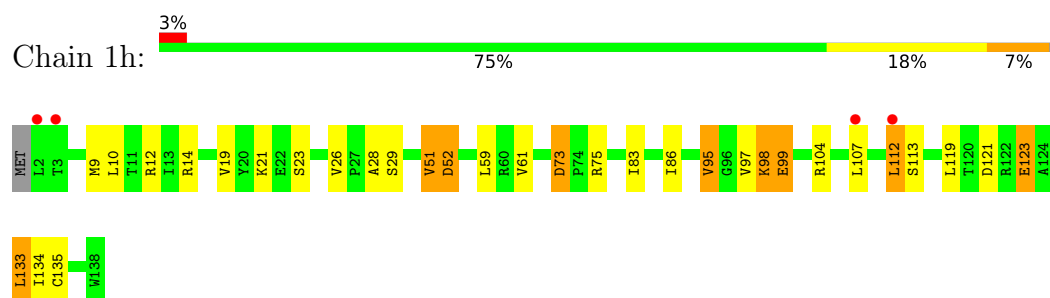
- Molecule 38: 30S ribosomal protein S7



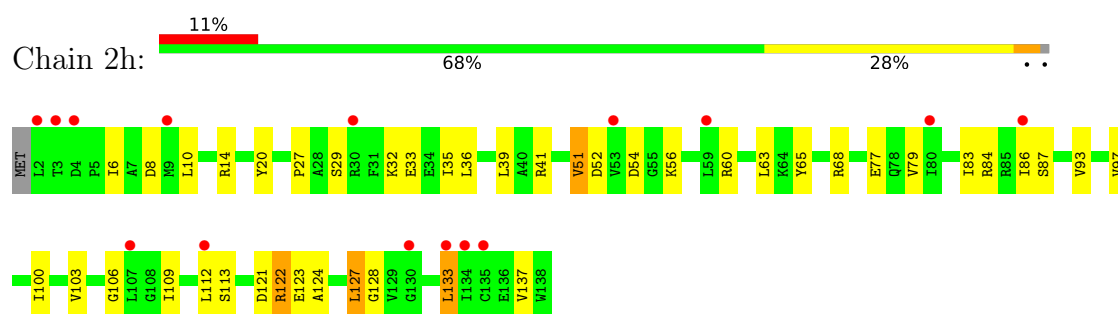
- Molecule 38: 30S ribosomal protein S7



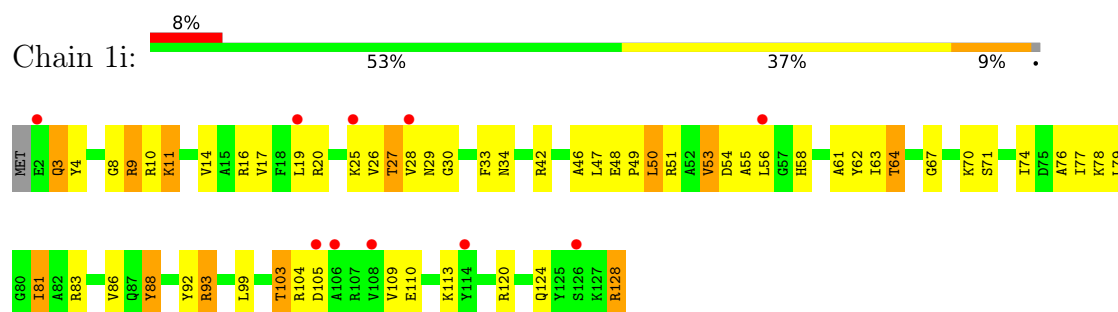
- Molecule 39: 30S ribosomal protein S8



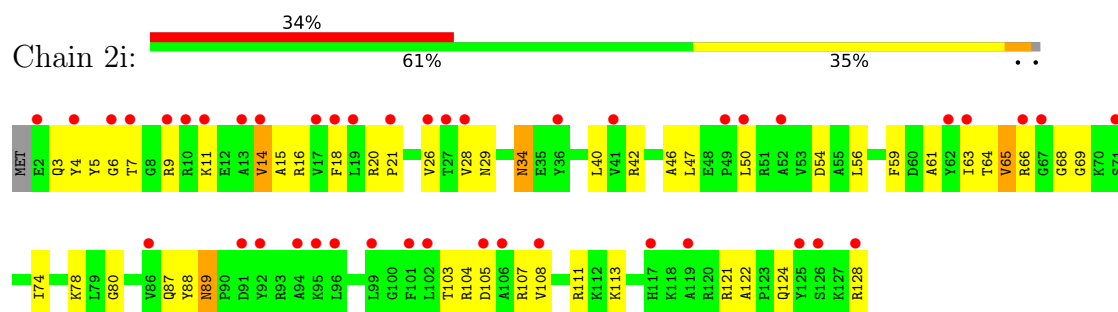
- Molecule 39: 30S ribosomal protein S8



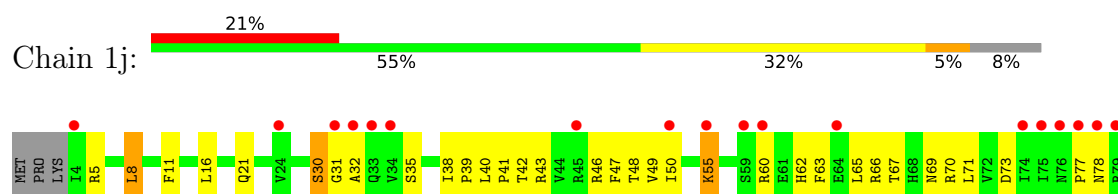
- Molecule 40: 30S ribosomal protein S9

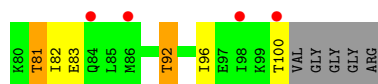


- Molecule 40: 30S ribosomal protein S9

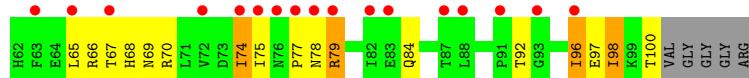
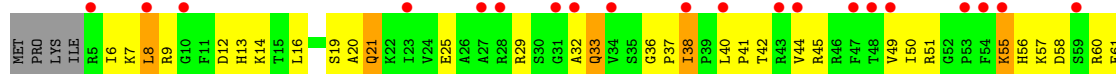
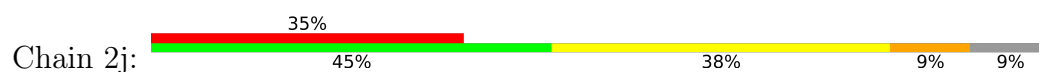


- Molecule 41: 30S ribosomal protein S10

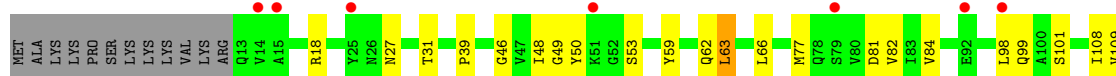




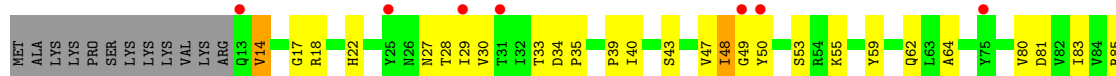
• Molecule 41: 30S ribosomal protein S10



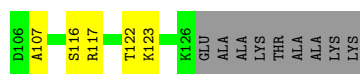
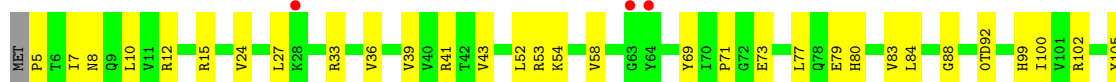
• Molecule 42: 30S ribosomal protein S11



• Molecule 42: 30S ribosomal protein S11

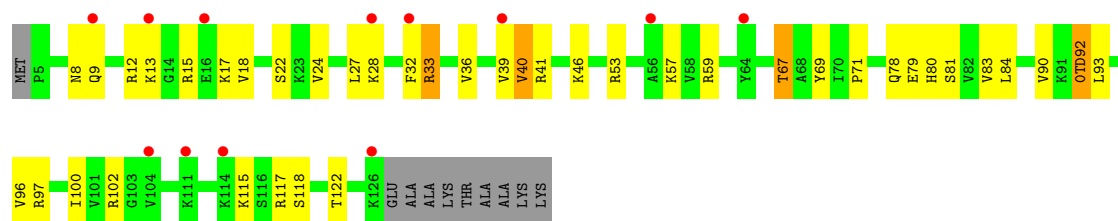


• Molecule 43: 30S ribosomal protein S12

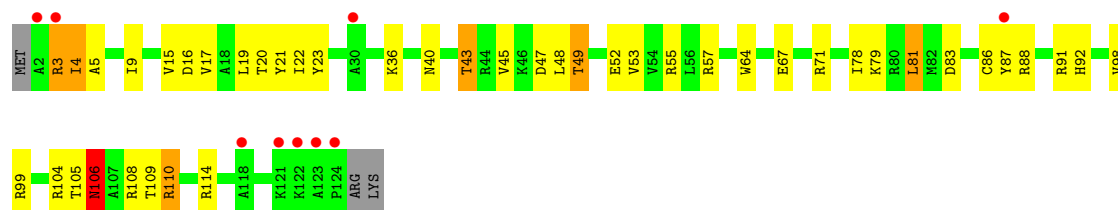


• Molecule 43: 30S ribosomal protein S12

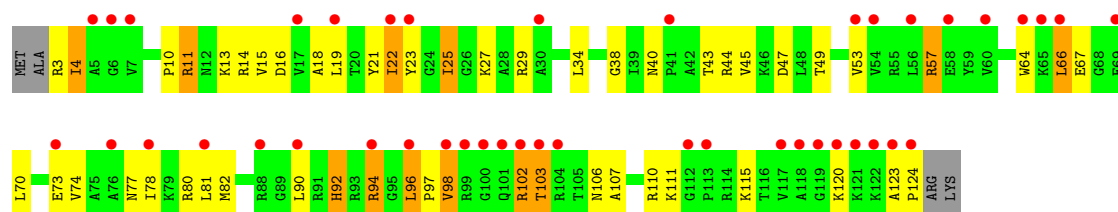




• Molecule 44: 30S ribosomal protein S13



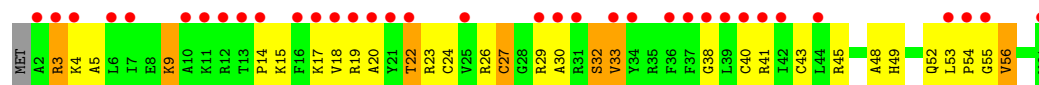
• Molecule 44: 30S ribosomal protein S13



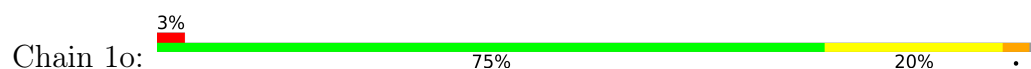
• Molecule 45: 30S ribosomal protein S14 type Z



• Molecule 45: 30S ribosomal protein S14 type Z

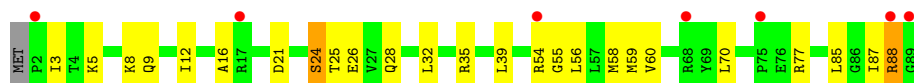
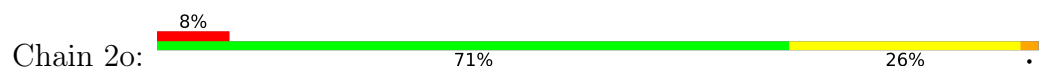


• Molecule 46: 30S ribosomal protein S15





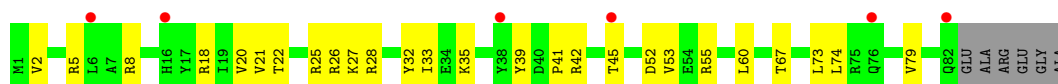
- Molecule 46: 30S ribosomal protein S15



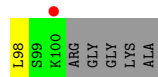
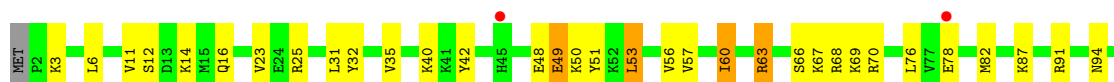
- Molecule 47: 30S ribosomal protein S16



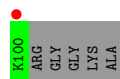
- Molecule 47: 30S ribosomal protein S16



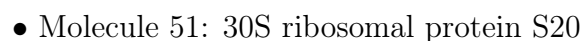
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18





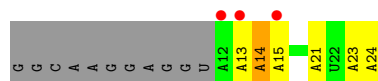
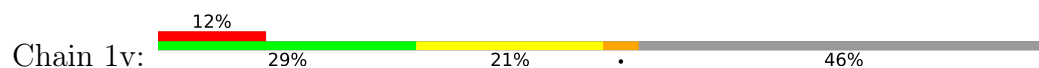
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



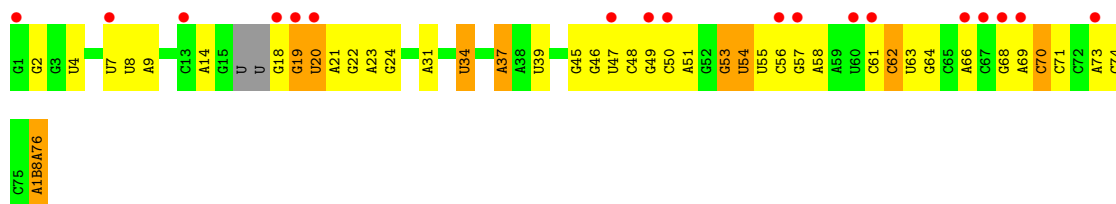
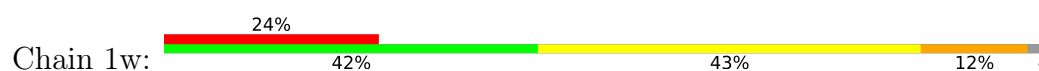
- Molecule 53: MET-LYS-mRNA



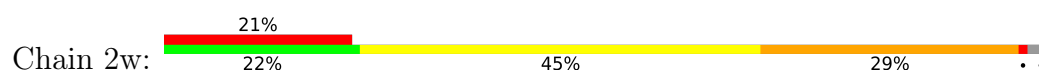
- Molecule 53: MET-LYS-mRNA

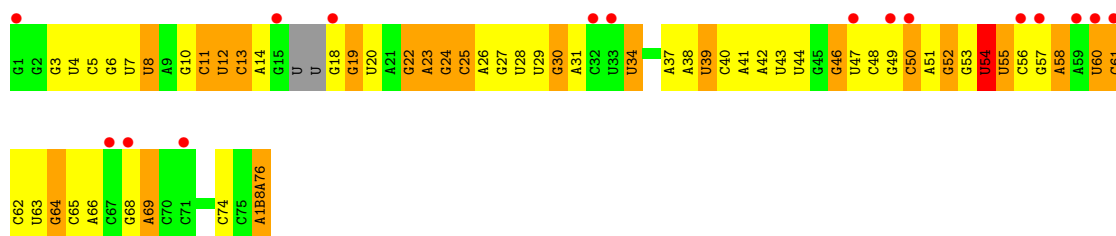


- Molecule 54: A-site Aminoacyl-tRNA Lys-tRNAlys



- Molecule 54: A-site Aminoacyl-tRNA Lys-tRNAlys





• Molecule 55: P-site Peptidyl-tRNA fMAC-tRNAcys RNA-part



• Molecule 55: P-site Peptidyl-tRNA fMAC-tRNAcys RNA-part



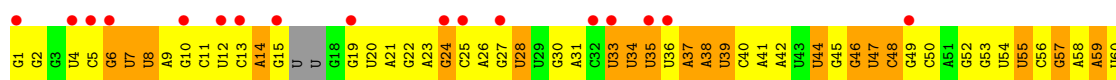
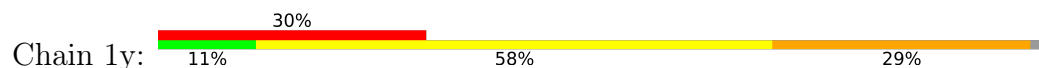
• Molecule 56: P-site Peptidyl-tRNA fMAC-tRNAcys Peptide-part



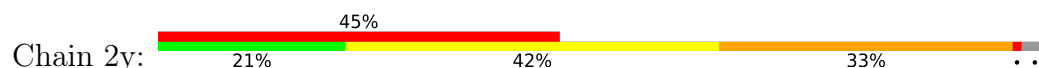
• Molecule 56: P-site Peptidyl-tRNA fMAC-tRNAcys Peptide-part

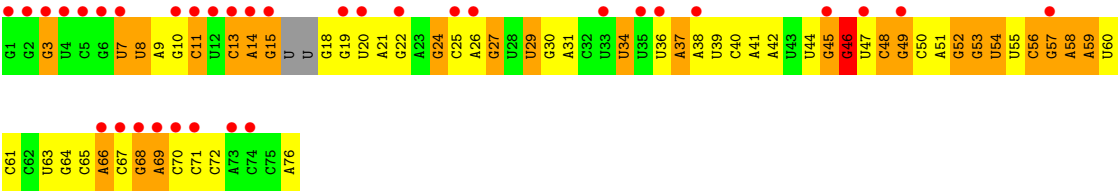


• Molecule 57: E-site Deacylated tRNAlys



• Molecule 57: E-site Deacylated tRNAlys





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.69Å 447.93Å 622.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.21 – 2.70 152.21 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (152.21-2.70) 99.5 (152.21-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.217 , 0.262 0.219 , 0.262	Depositor DCC
R_{free} test set	79068 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	298915	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 1.65% 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: UR3, 5MC, 2MA, ERY, OMU, 4SU, U8U, K, 8AN, MA6, FME, SF4, 5MU, ZN, M2G, OMG, PSU, 2MG, OMC, A1B8A, G7M, 0TD, T6A, MG, 4OC

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	1/69011 (0.0%)	0.44	2/107720 (0.0%)
1	2A	0.21	0/67295	0.39	1/105042 (0.0%)
2	1B	0.20	0/2882	0.38	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	0.47	0/2944
4	1E	0.25	0/1592	0.48	0/2149
4	2E	0.20	0/1592	0.44	0/2149
5	1F	0.24	0/1619	0.49	0/2193
5	2F	0.22	0/1615	0.47	2/2188 (0.1%)
6	1G	0.20	0/1448	0.44	0/1957
6	2G	0.20	0/1453	0.44	0/1963
7	1H	0.22	0/1356	0.43	0/1834
7	2H	0.20	0/1356	0.40	0/1834
8	1I	0.19	0/1112	0.40	0/1514
8	2I	0.17	0/1079	0.39	0/1475
9	1N	0.23	0/1144	0.44	0/1543
9	2N	0.18	0/1144	0.40	0/1543
10	1O	0.25	0/943	0.47	0/1269
10	2O	0.19	0/943	0.46	0/1269
11	1P	0.26	0/1152	0.52	0/1533
11	2P	0.20	0/1152	0.47	0/1533
12	1Q	0.26	0/1143	0.47	0/1527
12	2Q	0.20	0/1143	0.44	0/1527
13	1R	0.25	0/982	0.48	0/1312
13	2R	0.19	0/982	0.44	0/1312
14	1S	0.22	0/883	0.46	0/1176
14	2S	0.22	0/880	0.52	0/1172
15	1T	0.23	0/1105	0.45	0/1477
15	2T	0.20	0/1097	0.43	0/1468
16	1U	0.25	0/977	0.42	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.40	0/1301
17	1V	0.24	0/782	0.45	0/1049
17	2V	0.18	0/782	0.40	0/1049
18	1W	0.26	0/897	0.43	0/1205
18	2W	0.20	0/897	0.39	0/1205
19	1X	0.27	0/764	0.55	2/1025 (0.2%)
19	2X	0.22	0/764	0.57	2/1025 (0.2%)
20	1Y	0.22	0/819	0.45	0/1095
20	2Y	0.19	0/819	0.43	0/1095
21	1Z	0.22	0/1267	0.48	0/1717
21	2Z	0.22	0/1299	0.46	0/1763
22	10	0.24	0/662	0.45	0/881
22	20	0.20	0/662	0.44	0/881
23	11	0.26	0/762	0.45	0/1014
23	21	0.21	0/762	0.39	0/1014
24	12	0.26	0/590	0.47	0/781
24	22	0.18	0/590	0.36	0/781
25	13	0.24	0/474	0.44	0/635
25	23	0.17	0/469	0.39	0/630
26	14	0.26	0/565	0.65	0/761
26	24	0.23	0/545	0.53	0/737
27	15	0.25	0/469	0.44	0/635
27	25	0.21	0/469	0.44	0/635
28	16	0.26	0/460	0.43	0/613
28	26	0.22	0/456	0.46	0/608
29	17	0.30	0/426	0.54	0/561
29	27	0.24	0/426	0.50	0/561
30	18	0.27	0/525	0.50	0/691
30	28	0.20	0/525	0.42	0/691
31	19	0.24	0/310	0.57	0/407
31	29	0.19	0/310	0.41	0/407
32	1a	0.20	1/35795 (0.0%)	0.37	0/55864
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.21	0/1881	0.46	0/2542
33	2b	0.24	0/1860	0.55	0/2518
34	1c	0.19	0/1572	0.40	0/2126
34	2c	0.23	0/1566	0.48	0/2119
35	1d	0.19	0/1685	0.42	0/2262
35	2d	0.19	0/1704	0.43	0/2284
36	1e	0.20	0/1145	0.47	0/1543
36	2e	0.24	0/1149	0.51	0/1548
37	1f	0.19	0/823	0.40	0/1115
37	2f	0.19	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1250	0.40	0/1679
38	2g	0.23	0/1254	0.44	0/1683
39	1h	0.18	0/1108	0.40	0/1494
39	2h	0.21	0/1108	0.50	1/1494 (0.1%)
40	1i	0.19	0/1002	0.50	1/1346 (0.1%)
40	2i	0.26	0/997	0.55	0/1343
41	1j	0.20	0/722	0.51	1/982 (0.1%)
41	2j	0.33	1/727 (0.1%)	0.47	0/988
42	1k	0.20	0/844	0.41	0/1145
42	2k	0.22	0/848	0.41	0/1149
43	1l	0.20	0/937	0.41	0/1260
43	2l	0.21	0/937	0.42	0/1260
44	1m	0.21	0/969	0.56	1/1302 (0.1%)
44	2m	0.22	0/961	0.48	1/1291 (0.1%)
45	1n	0.20	0/501	0.46	0/664
45	2n	0.20	0/501	0.47	0/664
46	1o	0.19	0/739	0.40	0/985
46	2o	0.16	0/739	0.39	0/985
47	1p	0.19	0/697	0.49	0/939
47	2p	0.18	0/693	0.47	0/935
48	1q	0.20	0/836	0.46	0/1117
48	2q	0.18	0/836	0.44	0/1117
49	1r	0.20	0/560	0.40	0/746
49	2r	0.17	0/560	0.41	0/746
50	1s	0.19	0/667	0.47	0/900
50	2s	0.26	0/661	0.62	0/893
51	1t	0.20	0/730	0.49	0/965
51	2t	0.21	0/729	0.46	0/965
52	1u	0.17	0/203	0.43	0/266
52	2u	0.22	0/203	0.49	0/266
53	1v	0.22	0/319	0.35	0/495
53	2v	0.20	0/269	0.35	0/417
54	1w	0.31	1/1593 (0.1%)	0.41	0/2474
54	2w	0.35	2/1593 (0.1%)	0.50	0/2474
55	1x	0.26	0/1723	0.40	0/2684
55	2x	0.24	0/1723	0.40	0/2684
56	1z	0.34	0/10	0.32	0/12
56	2z	0.13	0/10	0.27	0/12
57	1y	0.31	0/1618	0.44	0/2513
57	2y	0.32	2/1618 (0.1%)	0.45	0/2513
All	All	0.22	8/316745 (0.0%)	0.42	17/474198 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	2j	79	ARG	CA-C	6.00	1.60	1.52
54	2w	46	G7M	O3'-P	5.49	1.61	1.56
57	2y	37	T6A	O3'-P	5.38	1.61	1.56
57	2y	46	G7M	O3'-P	5.19	1.61	1.56
54	1w	46	G7M	O3'-P	5.14	1.61	1.56
32	1a	527	G7M	O3'-P	5.06	1.61	1.56
54	2w	37	T6A	O3'-P	5.05	1.61	1.56
1	1A	2552	OMU	O3'-P	5.02	1.61	1.56

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	2h	79	VAL	N-CA-C	-9.78	103.18	112.96
41	1j	82	ILE	N-CA-C	-7.58	103.51	112.98
19	2X	94	GLY	CA-C-N	7.38	134.99	121.70
19	2X	94	GLY	C-N-CA	7.38	134.99	121.70
1	1A	1992	G	C2'-C3'-O3'	6.88	119.81	109.50
44	2m	107	ALA	N-CA-C	-6.77	104.92	112.57
44	1m	110	ARG	N-CA-C	-6.28	107.46	114.62
1	2A	1992	G	C2'-C3'-O3'	5.83	118.25	109.50
40	1i	88	TYR	N-CA-C	-5.72	107.54	114.75
5	2F	21	ALA	CA-C-N	5.49	131.58	121.70
5	2F	21	ALA	C-N-CA	5.49	131.58	121.70
32	2a	1272	G	N1-C2-N2	-5.45	99.85	116.20
32	2a	1263	C	N1-C2-O2	5.43	135.21	118.90
19	1X	94	GLY	CA-C-N	5.42	131.45	121.70
19	1X	94	GLY	C-N-CA	5.42	131.45	121.70
1	1A	1992	G	P-O3'-C3'	5.14	127.91	120.20
32	2a	1272	G	N3-C2-N2	5.14	135.33	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31197	555	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	60322	0	30427	641	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	37	0
3	1D	2136	0	2218	44	0
3	2D	2136	0	2218	35	0
4	1E	1559	0	1618	36	0
4	2E	1559	0	1618	37	0
5	1F	1584	0	1625	36	0
5	2F	1580	0	1619	56	0
6	1G	1423	0	1436	29	0
6	2G	1428	0	1438	48	0
7	1H	1330	0	1407	24	0
7	2H	1330	0	1407	33	0
8	1I	1097	0	1140	33	0
8	2I	1064	0	1082	26	0
9	1N	1117	0	1184	19	0
9	2N	1117	0	1184	24	0
10	1O	933	0	996	19	0
10	2O	933	0	996	23	0
11	1P	1135	0	1212	34	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	29	0
12	2Q	1122	0	1179	41	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	16	0
14	1S	873	0	927	15	0
14	2S	870	0	923	36	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	27	0
16	1U	959	0	1019	13	0
16	2U	959	0	1019	21	0
17	1V	771	0	830	8	0
17	2V	771	0	830	12	0
18	1W	886	0	940	10	0
18	2W	886	0	940	13	0
19	1X	750	0	814	12	0
19	2X	750	0	813	25	0
20	1Y	806	0	881	17	0
20	2Y	806	0	881	16	0
21	1Z	1240	0	1240	42	0
21	2Z	1271	0	1273	51	0
22	10	653	0	674	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	11	0
23	11	755	0	826	11	0
23	21	755	0	826	20	0
24	12	588	0	643	9	0
24	22	588	0	643	13	0
25	13	469	0	518	11	0
25	23	464	0	514	14	0
26	14	552	0	533	21	0
26	24	532	0	503	33	0
27	15	455	0	465	5	0
27	25	455	0	465	7	0
28	16	453	0	473	10	0
28	26	449	0	469	12	0
29	17	418	0	467	5	0
29	27	418	0	467	8	0
30	18	517	0	582	10	0
30	28	517	0	582	18	0
31	19	307	0	335	3	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	369	0
32	2a	32327	0	16338	487	0
33	1b	1846	0	1867	62	0
33	2b	1825	0	1828	82	0
34	1c	1548	0	1535	34	0
34	2c	1542	0	1517	65	0
35	1d	1655	0	1672	46	0
35	2d	1674	0	1714	51	0
36	1e	1129	0	1185	34	0
36	2e	1133	0	1191	39	0
37	1f	810	0	804	10	0
37	2f	816	0	808	26	0
38	1g	1231	0	1238	26	0
38	2g	1235	0	1249	41	0
39	1h	1088	0	1126	27	0
39	2h	1088	0	1126	25	0
40	1i	983	0	986	39	0
40	2i	978	0	966	34	0
41	1j	709	0	650	25	0
41	2j	714	0	672	29	0
42	1k	829	0	825	13	0
42	2k	833	0	835	21	0
43	1l	932	0	981	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	19	0
44	1m	958	0	1002	26	0
44	2m	950	0	988	43	0
45	1n	492	0	529	17	0
45	2n	492	0	529	38	0
46	1o	728	0	760	10	0
46	2o	728	0	760	17	0
47	1p	681	0	697	19	0
47	2p	677	0	686	15	0
48	1q	823	0	891	21	0
48	2q	823	0	891	20	0
49	1r	555	0	618	13	0
49	2r	555	0	618	19	0
50	1s	652	0	662	20	0
50	2s	646	0	644	36	0
51	1t	728	0	798	21	0
51	2t	727	0	796	11	0
52	1u	199	0	208	8	0
52	2u	199	0	208	6	0
53	1v	283	0	142	4	0
53	2v	239	0	119	7	0
54	1w	1599	0	801	17	0
54	2w	1599	0	800	51	0
55	1x	1646	0	839	11	0
55	2x	1646	0	838	25	0
56	1z	21	0	20	0	0
56	2z	21	0	20	0	0
57	1y	1577	0	799	42	0
57	2y	1577	0	798	31	0
58	10	9	0	0	0	0
58	11	4	0	0	0	0
58	12	2	0	0	0	0
58	13	3	0	0	0	0
58	14	1	0	0	0	0
58	15	4	0	0	0	0
58	16	1	0	0	0	0
58	17	5	0	0	0	0
58	18	7	0	0	0	0
58	19	1	0	0	0	0
58	1A	1096	0	0	0	0
58	1B	35	0	0	0	0
58	1D	11	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1E	13	0	0	0	0
58	1F	12	0	0	0	0
58	1G	4	0	0	0	0
58	1H	1	0	0	0	0
58	1I	1	0	0	0	0
58	1N	5	0	0	0	0
58	1O	5	0	0	0	0
58	1P	8	0	0	0	0
58	1Q	7	0	0	0	0
58	1R	6	0	0	0	0
58	1S	2	0	0	0	0
58	1T	2	0	0	0	0
58	1U	12	0	0	0	0
58	1V	7	0	0	0	0
58	1W	7	0	0	0	0
58	1X	5	0	0	0	0
58	1Y	4	0	0	0	0
58	1Z	2	0	0	0	0
58	1a	213	0	0	0	0
58	1b	1	0	0	0	0
58	1d	2	0	0	0	0
58	1e	2	0	0	0	0
58	1f	2	0	0	0	0
58	1k	1	0	0	0	0
58	1l	2	0	0	0	0
58	1m	1	0	0	0	0
58	1n	2	0	0	0	0
58	1p	1	0	0	0	0
58	1t	1	0	0	0	0
58	1v	1	0	0	0	0
58	1w	7	0	0	0	0
58	1x	11	0	0	0	0
58	20	3	0	0	0	0
58	23	3	0	0	0	0
58	25	4	0	0	0	0
58	27	2	0	0	0	0
58	28	1	0	0	0	0
58	2A	687	0	0	0	0
58	2B	15	0	0	0	0
58	2D	6	0	0	0	0
58	2E	7	0	0	0	0
58	2F	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2N	1	0	0	0	0
58	2O	1	0	0	0	0
58	2P	1	0	0	0	0
58	2Q	2	0	0	0	0
58	2R	3	0	0	0	0
58	2T	2	0	0	0	0
58	2V	1	0	0	0	0
58	2X	2	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	222	0	0	0	0
58	2d	2	0	0	0	0
58	2e	1	0	0	0	0
58	2f	2	0	0	0	0
58	2g	1	0	0	0	0
58	2j	1	0	0	0	0
58	2l	6	0	0	0	0
58	2q	2	0	0	0	0
58	2r	1	0	0	0	0
58	2t	1	0	0	0	0
58	2v	2	0	0	0	0
58	2w	1	0	0	0	0
58	2x	5	0	0	0	0
59	1A	1	0	0	0	0
59	2x	1	0	0	0	0
60	1A	51	0	67	1	0
60	2A	51	0	67	4	0
61	14	1	0	0	0	0
61	15	1	0	0	0	0
61	16	1	0	0	0	0
61	19	1	0	0	0	0
61	1Y	1	0	0	0	0
61	1n	1	0	0	0	0
61	24	1	0	0	0	0
61	25	1	0	0	0	0
61	26	1	0	0	0	0
61	29	1	0	0	0	0
61	2Y	1	0	0	0	0
61	2n	1	0	0	0	0
62	1d	8	0	0	0	0
62	2d	8	0	0	1	0
63	10	9	0	0	0	0
63	11	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	12	3	0	0	1	0
63	13	4	0	0	0	0
63	15	6	0	0	0	0
63	16	1	0	0	0	0
63	17	9	0	0	0	0
63	18	9	0	0	1	0
63	1A	1715	0	0	85	0
63	1B	53	0	0	2	0
63	1D	28	0	0	0	0
63	1E	25	0	0	1	0
63	1F	13	0	0	0	0
63	1G	3	0	0	1	0
63	1H	2	0	0	0	0
63	1N	3	0	0	1	0
63	1O	4	0	0	0	0
63	1P	17	0	0	1	0
63	1Q	6	0	0	0	0
63	1R	12	0	0	2	0
63	1S	5	0	0	0	0
63	1T	5	0	0	0	0
63	1U	9	0	0	1	0
63	1V	9	0	0	0	0
63	1W	8	0	0	0	0
63	1X	7	0	0	0	0
63	1Y	2	0	0	1	0
63	1Z	1	0	0	0	0
63	1a	284	0	0	23	0
63	1e	1	0	0	0	0
63	1f	1	0	0	0	0
63	1i	1	0	0	0	0
63	1l	5	0	0	0	0
63	1m	2	0	0	0	0
63	1o	1	0	0	0	0
63	1q	2	0	0	0	0
63	1u	1	0	0	1	0
63	1v	5	0	0	0	0
63	1w	7	0	0	0	0
63	1x	6	0	0	0	0
63	1y	1	0	0	0	0
63	1z	1	0	0	0	0
63	20	1	0	0	0	0
63	21	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	26	1	0	0	0	0
63	28	2	0	0	0	0
63	2A	624	0	0	49	0
63	2B	12	0	0	0	0
63	2D	14	0	0	2	0
63	2E	5	0	0	1	0
63	2F	9	0	0	0	0
63	2N	1	0	0	0	0
63	2O	1	0	0	0	0
63	2P	3	0	0	0	0
63	2Q	1	0	0	0	0
63	2R	1	0	0	0	0
63	2T	4	0	0	0	0
63	2U	1	0	0	1	0
63	2W	3	0	0	0	0
63	2Y	1	0	0	1	0
63	2a	161	0	0	13	0
63	2d	1	0	0	0	0
63	2e	2	0	0	0	0
63	2j	1	0	0	0	0
63	2l	4	0	0	0	0
63	2p	2	0	0	0	0
63	2v	1	0	0	0	0
63	2w	1	0	0	0	0
63	2x	2	0	0	0	0
All	All	298915	0	196861	4061	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 (4061) 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	1.43	1.14
54:2w:51:A:N6	54:2w:63:U:H3	1.45	1.13
54:2w:51:A:N6	54:2w:63:U:N3	2.04	0.99
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.48	0.95
12:1Q:12:GLN:HE21	12:1Q:73:PRO:HD2	1.32	0.93
54:2w:51:A:N1	54:2w:63:U:O4	2.03	0.91
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.52	0.89
1:1A:1082:U:O4	1:1A:1086:A:N1	2.06	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:10:10:THR:HG22	22:10:12:ASN:H	1.37	0.88
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.36	0.88
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.08	0.87
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.56	0.87
3:2D:8:PRO:HB3	3:2D:14:ARG:HB3	1.57	0.87
26:14:16:CYS:SG	26:14:17:GLY:N	2.42	0.86
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.58	0.85
29:17:24:THR:HG22	29:17:27:GLY:H	1.40	0.85
21:1Z:93:ASP:HB3	21:1Z:131:ARG:HH22	1.39	0.85
32:1a:664:G:H22	32:1a:741:G:H1	1.24	0.85
57:1y:25:C:N4	57:1y:45:G:N2	2.24	0.84
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.56	0.84
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.59	0.84
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.11	0.84
54:2w:51:A:H3'	54:2w:64:G:N2	1.90	0.84
33:2b:54:THR:HG22	33:2b:199:TYR:HB3	1.61	0.83
1:2A:2143:C:H42	1:2A:2148:G:H1	1.27	0.82
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.61	0.82
15:1T:77:PRO:HG2	15:1T:80:SER:HB2	1.61	0.82
54:1w:18:G:HO2'	54:1w:57:G:H1	1.28	0.82
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.62	0.82
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.45	0.81
1:2A:1604:C:OP1	63:2A:3702:HOH:O	1.97	0.81
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.63	0.81
1:1A:2140:C:H2'	1:1A:2141:G:H8	1.46	0.80
1:1A:1671:U:O4	63:1A:4102:HOH:O	1.99	0.80
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.15	0.80
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.14	0.79
32:1a:1505:G:OP2	63:1a:1902:HOH:O	1.99	0.79
32:1a:536:C:OP2	63:1a:1903:HOH:O	2.00	0.79
1:2A:2751:G:H8	7:2H:2:SER:HA	1.47	0.79
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.13	0.79
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.16	0.79
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.63	0.79
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.31	0.79
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.65	0.79
54:1w:20:U:H4'	54:1w:21:A:H5'	1.64	0.79
1:1A:1993:U:OP2	63:1A:4104:HOH:O	2.01	0.78
32:1a:975:A:H4'	32:1a:976:G:H5''	1.65	0.78
34:2c:137:ALA:HA	34:2c:140:ARG:HD3	1.65	0.78
1:1A:2499:C:OP1	63:1A:4103:HOH:O	2.00	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:42:SER:O	63:1P:301:HOH:O	2.01	0.78
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.65	0.78
1:2A:81:G:H21	20:2Y:1:MET:HE2	1.49	0.78
21:2Z:106:GLY:HA3	21:2Z:141:VAL:HB	1.66	0.78
52:1u:5:ASP:OD1	63:1u:101:HOH:O	2.01	0.78
1:1A:668:G:N7	63:1A:4132:HOH:O	2.16	0.77
1:1A:1865:G:OP1	63:1A:4106:HOH:O	2.03	0.77
48:1q:67:LYS:HA	48:1q:70:ARG:HH12	1.48	0.77
5:1F:155:LEU:HD11	5:1F:176:LEU:HD12	1.66	0.77
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.65	0.77
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.17	0.77
32:1a:557:G:OP1	63:1a:1904:HOH:O	2.03	0.77
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.30	0.77
4:1E:121:ASN:ND2	63:1E:401:HOH:O	2.18	0.76
10:1O:20:MET:HE3	10:1O:44:LYS:HE3	1.67	0.76
17:2V:55:ALA:HA	17:2V:101:GLY:HA2	1.67	0.76
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.66	0.76
1:2A:1204:A:H2	1:2A:1241:A:H62	1.30	0.76
4:2E:127:ASP:OD2	63:2E:401:HOH:O	2.03	0.76
32:2a:9:G:H2'	32:2a:10:A:H8	1.49	0.76
1:1A:2136:C:N3	1:1A:2155:G:C2	2.53	0.76
32:2a:1250:A:H4'	40:2i:68:GLY:H	1.49	0.76
1:1A:1315:C:OP2	63:1A:4105:HOH:O	2.02	0.76
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.18	0.76
2:2B:41:U:H5	6:2G:70:VAL:H	1.31	0.76
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.68	0.76
4:2E:119:ARG:HD3	4:2E:160:TYR:HB2	1.67	0.76
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.32	0.76
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.32	0.76
1:1A:604:G:OP2	11:1P:90:ARG:NH2	2.19	0.75
50:2s:33:THR:H	50:2s:57:HIS:HE1	1.32	0.75
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.18	0.75
57:1y:8:U:H4'	57:1y:48:C:H4'	1.68	0.75
1:2A:450:G:O6	63:2A:3704:HOH:O	2.04	0.75
1:2A:2154:G:N7	1:2A:2156:G:N2	2.34	0.75
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.18	0.75
1:2A:963:U:OP2	63:2A:3703:HOH:O	2.04	0.75
32:2a:974:A:OP2	45:2n:29:ARG:NH2	2.20	0.74
1:1A:1039:G:O6	1:1A:1116:C:N4	2.17	0.74
32:1a:36:C:OP1	43:1l:123:LYS:NZ	2.20	0.74
1:1A:1602:U:O4	63:1A:4107:HOH:O	2.04	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.69	0.74
48:2q:81:ARG:HH21	48:2q:84:LEU:HD21	1.52	0.74
1:1A:981:A:OP1	63:1A:4108:HOH:O	2.04	0.74
40:1i:53:VAL:O	40:1i:55:ALA:N	2.20	0.74
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.19	0.74
54:2w:18:G:O2'	54:2w:57:G:N2	2.20	0.74
1:1A:882:G:H1	1:1A:894:C:H42	1.34	0.73
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.20	0.73
1:2A:981:A:OP1	63:2A:3707:HOH:O	2.06	0.73
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.70	0.73
54:1w:54:5MU:O2	54:1w:58:A:N7	2.21	0.73
1:2A:1648:C:OP1	63:2A:3705:HOH:O	2.06	0.73
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.50	0.73
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.21	0.73
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	1.69	0.73
33:2b:48:MET:HA	33:2b:51:LEU:HB2	1.71	0.73
37:2f:99:ALA:HB3	49:2r:29:PHE:HE1	1.54	0.73
1:1A:1669:A:OP2	63:1A:4102:HOH:O	2.07	0.73
41:1j:5:ARG:NH2	41:1j:73:ASP:OD2	2.20	0.73
1:2A:882:G:H22	1:2A:894:C:H42	1.35	0.73
37:2f:2:ARG:HE	37:2f:69:GLU:HG2	1.53	0.73
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.53	0.73
1:1A:400:G:N7	63:1A:4160:HOH:O	2.22	0.73
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.36	0.73
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.70	0.73
1:2A:863:A:H2'	1:2A:864:G:H8	1.54	0.73
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.70	0.73
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.70	0.72
1:2A:731:C:OP2	63:2A:3706:HOH:O	2.06	0.72
1:2A:1689:A:H62	1:2A:1698:A:H2	1.36	0.72
1:1A:410:G:OP2	63:1A:4109:HOH:O	2.06	0.72
1:1A:1784:A:OP2	63:1A:4110:HOH:O	2.07	0.72
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.71	0.72
54:2w:63:U:H2'	54:2w:64:G:C8	2.25	0.72
32:1a:324:G:N7	63:1a:1920:HOH:O	2.22	0.72
36:2e:7:GLU:OE1	36:2e:37:ARG:NH2	2.21	0.72
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.54	0.72
21:2Z:70:LEU:HD12	21:2Z:71:VAL:H	1.55	0.72
32:1a:1499:A:OP2	63:1a:1902:HOH:O	2.08	0.72
18:2W:88:ARG:HB2	18:2W:92:ARG:HG2	1.72	0.72
36:1e:78:HIS:HD2	39:1h:104:ARG:HD2	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:78:ARG:HH21	38:1g:79:ARG:HH11	1.34	0.72
32:2a:130:A:H5'	48:2q:63:ARG:HE	1.54	0.72
21:1Z:153:SER:HA	21:1Z:167:PRO:HB3	1.70	0.72
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.23	0.72
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.53	0.72
32:2a:1108:G:O6	63:2a:1903:HOH:O	2.08	0.72
1:1A:2821:A:OP2	63:1R:301:HOH:O	2.07	0.71
63:1A:4131:HOH:O	4:1E:135:HIS:NE2	2.20	0.71
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.25	0.71
32:2a:770:C:OP1	63:2a:1902:HOH:O	2.07	0.71
1:1A:1014:U:OP2	63:1A:4112:HOH:O	2.08	0.71
4:1E:119:ARG:HD3	4:1E:160:TYR:HB2	1.71	0.71
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.23	0.71
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.55	0.71
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.70	0.71
1:1A:530:G:N1	1:1A:2023:G:OP1	2.21	0.71
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.23	0.71
41:2j:44:VAL:HG22	41:2j:66:ARG:HG2	1.72	0.71
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.71	0.71
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	1.73	0.71
1:1A:677:A:OP1	63:1A:4111:HOH:O	2.08	0.71
2:2B:104:U:HO2'	21:2Z:29:TYR:HH	1.37	0.71
36:1e:96:PRO:O	36:1e:98:THR:N	2.23	0.71
1:1A:2130:U:O2'	1:1A:2158:A:N1	2.23	0.70
32:1a:558:G:OP1	63:1a:1906:HOH:O	2.09	0.70
1:2A:2518:A:OP2	63:2A:3710:HOH:O	2.09	0.70
12:2Q:1:MET:HB3	12:2Q:44:ALA:HB1	1.74	0.70
1:1A:2140:C:H2'	1:1A:2141:G:C8	2.27	0.70
21:1Z:119:GLU:N	21:1Z:171:ILE:O	2.24	0.70
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.25	0.70
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.06	0.70
42:2k:48:ILE:O	42:2k:50:TYR:N	2.22	0.70
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.08	0.70
32:1a:1030(D):A:H3'	32:1a:1031:G:H4'	1.73	0.70
44:1m:49:THR:HB	44:1m:52:GLU:H	1.55	0.70
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.07	0.70
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.73	0.70
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.18	0.70
21:2Z:154:ASP:OD1	21:2Z:154:ASP:N	2.25	0.70
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.24	0.70
34:2c:47:LEU:HB3	34:2c:52:LEU:HB2	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:125:PHE:O	63:1G:301:HOH:O	2.10	0.70
32:1a:945:G:OP1	63:1a:1907:HOH:O	2.09	0.70
1:2A:854:G:H2'	1:2A:855:G:H8	1.57	0.70
34:2c:129:ALA:HB3	34:2c:132:ARG:HD2	1.74	0.70
54:2w:54:5MU:O2	54:2w:58:A:N7	2.24	0.70
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.24	0.69
6:1G:79:ASN:OD1	6:1G:79:ASN:N	2.25	0.69
1:2A:962:G:OP1	63:2A:3703:HOH:O	2.09	0.69
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.56	0.69
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.24	0.69
1:2A:948:G:OP1	63:2A:3703:HOH:O	2.10	0.69
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.11	0.69
32:2a:1196:U:H2'	54:2w:34:U8U:HA1	1.74	0.69
32:1a:352:C:OP2	63:1a:1908:HOH:O	2.11	0.69
1:1A:1055:G:H1	1:1A:1104:C:H42	1.41	0.69
6:1G:49:ASP:N	6:1G:49:ASP:OD1	2.25	0.69
57:2y:10:G:H1	57:2y:25:C:H42	1.40	0.69
21:1Z:102:LEU:HD11	21:1Z:124:ILE:HB	1.73	0.69
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.75	0.69
1:2A:975:C:OP1	63:2A:3709:HOH:O	2.09	0.69
1:2A:1902:C:OP2	63:2A:3712:HOH:O	2.10	0.69
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.26	0.69
32:2a:673:G:H2'	32:2a:674:G:C8	2.27	0.69
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	1.74	0.69
1:2A:568:U:O4	63:2A:3708:HOH:O	2.08	0.69
6:2G:35:GLU:HG2	6:2G:36:LYS:HG2	1.73	0.69
33:2b:92:TYR:N	33:2b:151:GLY:O	2.25	0.69
54:2w:5:C:H2'	54:2w:6:G:H8	1.57	0.69
1:1A:1271:G:OP2	63:1A:4114:HOH:O	2.11	0.69
1:2A:2394:C:N3	57:2y:76:A:O2'	2.25	0.69
32:2a:278:G:OP2	48:2q:41:LYS:NZ	2.25	0.69
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.75	0.69
34:2c:125:GLU:HB2	34:2c:190:ARG:HH21	1.58	0.69
57:2y:7:U:H2'	57:2y:49:G:C8	2.27	0.69
1:1A:1670:C:OP2	63:1A:4102:HOH:O	2.10	0.68
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.26	0.68
32:2a:944:G:OP1	63:2a:1905:HOH:O	2.12	0.68
36:2e:12:LEU:HB3	36:2e:31:LEU:HB2	1.74	0.68
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.24	0.68
2:1B:21:G:N7	63:1B:301:HOH:O	2.26	0.68
1:1A:1062:G:H1	1:1A:1077:A:H61	1.40	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2589:A:OP1	63:2A:3711:HOH:O	2.09	0.68
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.24	0.68
32:2a:953:G:H5'	32:2a:965:A:H61	1.59	0.68
1:1A:731:C:OP2	63:1A:4117:HOH:O	2.11	0.68
15:1T:16:ARG:NH1	15:1T:83:ILE:O	2.22	0.68
1:2A:601:C:O2'	5:2F:104:LYS:NZ	2.26	0.68
5:2F:117:ARG:HH12	11:2P:1:MET:H2	1.41	0.68
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.76	0.68
1:1A:1342:A:OP2	63:1A:4107:HOH:O	2.11	0.68
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.11	0.68
32:1a:560:U:O2'	32:1a:561:U:OP2	2.11	0.68
32:1a:1270:C:OP2	52:1u:24:ARG:NH2	2.27	0.68
1:1A:1418:G:OP2	63:1A:4118:HOH:O	2.12	0.68
32:1a:812:C:N3	63:1a:1925:HOH:O	2.26	0.68
1:1A:740:U:OP2	63:1A:4110:HOH:O	2.12	0.68
21:1Z:92:SER:O	21:1Z:94:GLU:N	2.26	0.68
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.73	0.68
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.76	0.68
54:2w:12:U:H3	54:2w:23:A:H61	1.41	0.68
11:1P:71:VAL:HG22	11:1P:72:PRO:HA	1.76	0.68
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.29	0.68
1:1A:818:G:OP2	63:1A:4113:HOH:O	2.11	0.68
14:1S:39:ILE:HB	14:1S:49:VAL:HG13	1.76	0.68
32:2a:596:C:OP2	63:2a:1904:HOH:O	2.11	0.68
1:1A:1971:A:OP1	63:1A:4115:HOH:O	2.11	0.68
32:2a:1002:G:H1	32:2a:1038:C:H42	1.41	0.68
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.59	0.68
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.27	0.68
1:1A:1890:A:OP2	63:1A:4119:HOH:O	2.12	0.67
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.76	0.67
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.76	0.67
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.57	0.67
53:1v:21:A:N1	54:1w:34:U8U:O4	2.27	0.67
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.27	0.67
26:24:53:GLU:HG2	26:24:55:ARG:H	1.58	0.67
1:1A:2243:U:OP1	63:1A:4120:HOH:O	2.13	0.67
6:1G:41:GLN:NE2	6:1G:154:GLY:O	2.28	0.67
1:1A:1082:U:N3	1:1A:1086:A:N6	2.17	0.67
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.27	0.67
1:2A:422:A:OP2	63:2A:3714:HOH:O	2.12	0.67
1:2A:2711:A:OP1	63:2A:3716:HOH:O	2.13	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:144:LEU:HD21	21:2Z:173:ALA:HB1	1.75	0.67
32:1a:1025:U:O2	32:1a:1036:G:O6	2.13	0.67
1:2A:749:C:OP2	63:2A:3717:HOH:O	2.13	0.67
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.58	0.67
33:2b:96:ARG:HG2	33:2b:98:LEU:HD12	1.75	0.67
1:1A:2136:C:N3	1:1A:2155:G:N2	2.43	0.67
32:1a:944:G:OP1	63:1a:1910:HOH:O	2.13	0.67
1:2A:2063:C:OP1	63:2A:3713:HOH:O	2.11	0.67
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.75	0.67
32:2a:67:C:H2'	32:2a:68:G:C8	2.29	0.67
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.76	0.67
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.27	0.67
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.43	0.67
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.76	0.67
33:2b:32:ILE:HG21	33:2b:40:HIS:HB3	1.76	0.67
53:1v:14:A:N6	57:1y:34:U8U:S2	2.68	0.67
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.76	0.67
32:2a:1122:U:H2'	32:2a:1123:A:H8	1.59	0.67
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.60	0.67
1:2A:852:G:H2'	1:2A:853:G:H8	1.61	0.66
1:2A:2504:U:OP2	63:2A:3719:HOH:O	2.13	0.66
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.28	0.66
57:2y:26:A:N6	57:2y:45:G:O6	2.27	0.66
32:1a:1224:G:OP1	63:1a:1909:HOH:O	2.12	0.66
30:28:33:ASN:OD1	30:28:36:LYS:NZ	2.27	0.66
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.76	0.66
1:1A:2208:A:N7	63:1A:4199:HOH:O	2.29	0.66
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.77	0.66
18:1W:12:ILE:HD13	18:1W:17:VAL:HG13	1.75	0.66
48:1q:3:LYS:HD3	48:1q:60:ILE:HD11	1.77	0.66
1:2A:2444:G:N7	63:2A:3767:HOH:O	2.28	0.66
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.77	0.66
54:2w:63:U:H2'	54:2w:64:G:H8	1.59	0.66
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.28	0.66
1:1A:1027:A:N3	63:1A:4202:HOH:O	2.29	0.66
33:1b:143:GLU:O	33:1b:147:LYS:N	2.27	0.66
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.30	0.66
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.76	0.66
54:2w:50:C:H2'	54:2w:51:A:H5''	1.78	0.66
2:2B:3:C:H2'	2:2B:4:C:C6	2.31	0.66
1:1A:1633:G:OP2	63:1A:4123:HOH:O	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:127:ALA:O	15:1T:129:ARG:N	2.23	0.66
1:1A:973:A:OP2	63:1A:4125:HOH:O	2.13	0.66
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.29	0.66
1:2A:987:G:OP2	63:2A:3718:HOH:O	2.13	0.66
1:2A:1226:A:OP1	17:2V:84:LYS:NZ	2.27	0.66
1:1A:303:U:O4	63:1A:4116:HOH:O	2.11	0.66
39:1h:121:ASP:HB2	39:1h:125:ARG:HH21	1.61	0.66
1:2A:2131:G:H22	1:2A:2158:A:H62	1.43	0.66
1:1A:154(A):C:H42	1:1A:171:G:H1	1.42	0.66
1:1A:1807:G:O2'	63:1A:4124:HOH:O	2.13	0.66
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.77	0.66
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.13	0.66
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.29	0.66
1:1A:2550:G:OP1	63:1A:4102:HOH:O	2.13	0.66
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.61	0.66
32:2a:1162:C:H42	32:2a:1174:G:H1	1.44	0.66
32:1a:903:G:OP1	63:1a:1911:HOH:O	2.14	0.65
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.78	0.65
32:1a:1441:G:H5''	32:1a:1442:G:H5'	1.78	0.65
1:2A:1025:G:O2'	63:2A:3720:HOH:O	2.13	0.65
32:1a:636:U:H2'	32:1a:637:G:H8	1.61	0.65
32:1a:955:U:O4	63:1a:1905:HOH:O	2.08	0.65
32:2a:393:A:OP1	63:2a:1906:HOH:O	2.14	0.65
32:1a:56:U:H2'	32:1a:57:G:C8	2.30	0.65
39:1h:98:LYS:H	39:1h:98:LYS:HE2	1.61	0.65
1:2A:994:C:OP2	16:2U:54:LYS:NZ	2.30	0.65
1:2A:2751:G:C8	7:2H:2:SER:HA	2.31	0.65
32:2a:1224:G:H1	32:2a:1363:C:H42	1.44	0.65
38:2g:9:VAL:HG23	38:2g:94:ARG:HH21	1.60	0.65
1:1A:773:U:OP1	63:1A:4121:HOH:O	2.13	0.65
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.31	0.65
1:1A:2504:U:OP2	63:1A:4122:HOH:O	2.13	0.65
1:2A:1394:U:OP1	63:2A:3702:HOH:O	2.15	0.65
27:25:41:PRO:O	27:25:44:THR:OG1	2.13	0.65
1:1A:1332:G:OP1	63:1A:4105:HOH:O	2.14	0.65
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.30	0.65
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.31	0.65
32:2a:1397:C:OP2	36:2e:24:ARG:NH2	2.30	0.65
1:1A:1139:G:OP2	9:1N:70:LYS:NZ	2.29	0.65
40:2i:46:ALA:HA	40:2i:78:LYS:HB2	1.79	0.65
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:752:A:H3'	29:27:1:MET:HE1	1.79	0.65
1:2A:783:A:OP2	63:2A:3711:HOH:O	2.14	0.65
1:2A:863:A:H2'	1:2A:864:G:C8	2.32	0.65
32:2a:276:G:O3'	48:2q:68:ARG:NH1	2.30	0.65
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.62	0.65
1:1A:2136:C:N4	1:1A:2155:G:N1	2.45	0.65
1:2A:2143:C:N4	1:2A:2148:G:H1	1.93	0.65
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.44	0.65
43:2l:46:LYS:HE3	43:2l:92:0TD:H8	1.78	0.65
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.61	0.65
19:2X:94:GLY:HA3	19:2X:95:LEU:HB2	1.78	0.65
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH22	1.61	0.65
25:23:40:THR:HG22	25:23:42:ALA:H	1.62	0.65
1:1A:365:C:OP2	63:1A:4126:HOH:O	2.14	0.65
32:2a:1193:G:O2'	36:2e:25:ARG:NH2	2.29	0.65
1:1A:279:C:H42	1:1A:361:G:H1	1.43	0.64
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.77	0.64
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	1.79	0.64
26:24:37:SER:HA	26:24:43:TYR:HD1	1.61	0.64
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.62	0.64
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.30	0.64
54:2w:51:A:H3'	54:2w:64:G:H21	1.60	0.64
1:1A:2006:C:OP1	63:1A:4127:HOH:O	2.15	0.64
1:2A:2843:G:N7	63:2A:3773:HOH:O	2.30	0.64
32:2a:289:G:OP2	63:2a:1907:HOH:O	2.14	0.64
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.30	0.64
7:1H:41:MET:HE3	7:1H:64:LEU:HB2	1.79	0.64
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.32	0.64
32:2a:1047:G:H5''	45:2n:4:LYS:HD3	1.79	0.64
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.62	0.64
1:1A:2706:G:N7	63:1A:4203:HOH:O	2.29	0.64
33:1b:84:GLU:OE1	33:1b:87:ARG:NH1	2.26	0.64
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.79	0.64
41:2j:8:LEU:HB3	41:2j:96:ILE:HG23	1.80	0.64
57:2y:11:C:H42	57:2y:24:G:H1	1.45	0.64
1:1A:2130:U:O2'	1:1A:2131:G:N2	2.30	0.64
1:2A:2006:C:OP2	63:2A:3722:HOH:O	2.15	0.64
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.30	0.64
32:2a:113:G:H1'	32:2a:354:G:H5'	1.79	0.64
33:2b:150:SER:OG	33:2b:151:GLY:N	2.28	0.64
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:664:G:H22	32:2a:741:G:H1	1.45	0.64
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	1.79	0.64
1:1A:1171:G:OP2	1:1A:1174:A:N6	2.31	0.64
14:1S:83:LYS:HB3	14:1S:111:GLU:HG3	1.79	0.64
38:1g:78:ARG:HG3	38:1g:79:ARG:H	1.63	0.64
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.27	0.64
40:2i:5:TYR:O	40:2i:87:GLN:NE2	2.31	0.64
1:1A:1658:C:OP1	63:1A:4131:HOH:O	2.15	0.64
32:1a:532:A:N6	32:1a:1206:G:O2'	2.31	0.64
32:1a:1135:U:O2'	32:1a:1138:G:O6	2.16	0.64
32:2a:598:U:O4	63:2a:1904:HOH:O	2.10	0.64
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.79	0.64
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.79	0.64
1:1A:1174:A:H4'	1:1A:1175:U:OP1	1.97	0.64
1:1A:1637:A:OP2	63:1A:4128:HOH:O	2.15	0.64
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.31	0.64
34:1c:19:GLU:O	34:1c:40:ARG:NH2	2.30	0.63
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.79	0.63
1:2A:882:G:H22	1:2A:894:C:N4	1.96	0.63
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.33	0.63
1:2A:2818:G:OP1	1:2A:2837:G:O2'	2.14	0.63
23:21:83:GLU:OE1	23:21:83:GLU:N	2.31	0.63
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.29	0.63
32:1a:677:U:H3	32:1a:713:G:H22	1.46	0.63
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.31	0.63
14:2S:69:VAL:HG13	14:2S:101:LEU:HD12	1.80	0.63
32:2a:1317:C:O2	50:2s:37:ARG:NH2	2.31	0.63
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.33	0.63
1:1A:2448:A:OP1	63:1A:4103:HOH:O	2.15	0.63
40:1i:16:ARG:HH11	40:1i:64:THR:HG21	1.62	0.63
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.64	0.63
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.33	0.63
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.28	0.63
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.79	0.63
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.46	0.63
32:2a:261:U:OP2	51:2t:79:ARG:NH2	2.32	0.63
32:2a:539:A:OP2	43:2l:115:LYS:NZ	2.27	0.63
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.34	0.63
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.80	0.63
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.81	0.63
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.79	0.63
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.33	0.63
1:1A:1673:U:OP1	63:1A:4129:HOH:O	2.15	0.63
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.31	0.63
32:1a:299:G:O6	63:1a:1906:HOH:O	2.09	0.63
5:2F:37:VAL:HG22	5:2F:183:VAL:HG23	1.81	0.63
1:2A:1324:G:O6	63:2A:3715:HOH:O	2.12	0.63
32:2a:976:G:P	45:2n:32:SER:H	2.22	0.63
32:2a:1130:A:H5''	40:2i:18:PHE:CE2	2.34	0.63
33:2b:178:ARG:HH22	39:2h:68:ARG:HH22	1.45	0.63
1:1A:2099:U:H3	1:1A:2190:G:H1	1.47	0.63
21:1Z:128:VAL:HG23	21:1Z:161:VAL:HG12	1.80	0.63
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.80	0.63
1:2A:249:C:O2	30:28:12:LYS:NZ	2.31	0.63
1:2A:2502:G:OP2	63:2A:3723:HOH:O	2.15	0.63
1:1A:2124:G:H1	1:1A:2174:C:H42	1.47	0.62
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.81	0.62
1:2A:2131:G:H4'	1:2A:2132:U:H3'	1.80	0.62
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.32	0.62
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.32	0.62
10:1O:104:ARG:CZ	15:1T:34:VAL:HG11	2.29	0.62
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.34	0.62
57:2y:18:G:H21	57:2y:58:A:H5'	1.64	0.62
51:1t:33:ILE:O	51:1t:37:SER:OG	2.16	0.62
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.65	0.62
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.35	0.62
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.32	0.62
1:1A:2379:G:O2'	14:1S:17:ARG:NH2	2.32	0.62
38:2g:97:GLN:HE21	38:2g:101:LEU:HD11	1.65	0.62
44:2m:25:ILE:HG12	44:2m:66:LEU:HD22	1.81	0.62
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.32	0.62
32:1a:426:G:OP1	35:1d:36:ARG:NH1	2.33	0.62
32:2a:975:A:H4'	32:2a:976:G:H5''	1.82	0.62
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.15	0.62
47:2p:21:VAL:HG23	47:2p:33:ILE:HB	1.81	0.62
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.34	0.62
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.14	0.62
57:1y:66:A:H2'	57:1y:67:C:C6	2.35	0.62
1:2A:2117:A:H61	1:2A:2166:G:H1	1.47	0.62
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.80	0.62
8:2I:77:LEU:HB3	8:2I:142:VAL:HG13	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.81	0.62
32:2a:1133:G:H1	32:2a:1141:C:H42	1.45	0.62
32:2a:1263:C:N3	32:2a:1272:G:O6	2.32	0.62
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.65	0.62
32:2a:951:G:N7	44:2m:102:ARG:NH2	2.48	0.62
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.82	0.62
12:1Q:78:PRO:HG2	12:1Q:81:VAL:HG11	1.80	0.62
32:1a:176:C:H2'	32:1a:177:C:H6	1.64	0.62
26:24:24:THR:OG1	26:24:25:TYR:N	2.33	0.62
26:24:40:HIS:HD2	26:24:41:PRO:HD2	1.65	0.62
38:2g:27:ILE:HG22	38:2g:39:ALA:HB1	1.81	0.62
1:2A:272:G:O2'	1:2A:421:U:OP2	2.14	0.62
1:2A:668:G:H5'	1:2A:669:G:OP2	2.00	0.62
18:2W:23:LEU:O	18:2W:27:LYS:NZ	2.32	0.62
34:2c:58:GLU:HB2	34:2c:65:ALA:HB3	1.82	0.62
1:1A:621:A:OP2	11:1P:108:LYS:NZ	2.32	0.61
1:1A:1968:G:OP1	63:1A:4134:HOH:O	2.16	0.61
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.82	0.61
6:1G:64:THR:HB	6:1G:94:LEU:HD11	1.80	0.61
16:1U:89:GLU:HG3	17:1V:50:PRO:HB3	1.80	0.61
20:1Y:34:LYS:NZ	63:1Y:301:HOH:O	2.33	0.61
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.33	0.61
37:1f:82:ARG:HB2	37:1f:85:VAL:HG23	1.80	0.61
32:2a:547:A:OP1	63:2a:1909:HOH:O	2.16	0.61
33:2b:18:GLY:HA2	33:2b:42:ILE:HG13	1.81	0.61
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.33	0.61
1:1A:249:C:O2	30:18:12:LYS:NZ	2.26	0.61
1:1A:1356:G:OP2	63:1A:4133:HOH:O	2.16	0.61
32:2a:254:G:OP1	48:2q:66:SER:OG	2.16	0.61
32:2a:501:C:H2'	32:2a:502:G:C8	2.35	0.61
21:1Z:156:LYS:HE2	21:1Z:158:PRO:HD3	1.82	0.61
32:1a:171:A:H2'	32:1a:172:A:C8	2.36	0.61
32:1a:953:G:H5'	32:1a:965:A:H61	1.66	0.61
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.83	0.61
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.35	0.61
32:2a:501:C:H2'	32:2a:502:G:H8	1.64	0.61
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.15	0.61
15:1T:51:ARG:HG3	15:1T:98:LYS:HD2	1.83	0.61
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.18	0.61
1:2A:1721:G:H8	1:2A:1741:A:H62	1.48	0.61
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.33	0.61
39:2h:106:GLY:O	39:2h:122:ARG:NH2	2.33	0.61
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.65	0.61
1:2A:2343:C:O2'	1:2A:2373:G:O2'	2.16	0.61
1:2A:2682:U:O2'	15:2T:58:ASN:ND2	2.33	0.61
15:2T:127:ALA:C	15:2T:129:ARG:H	2.09	0.61
32:2a:201:C:H42	32:2a:216:G:H1	1.48	0.61
32:2a:1245:A:H61	32:2a:1292:U:H3	1.48	0.61
11:1P:95:VAL:HB	11:1P:125:VAL:HG12	1.82	0.61
32:1a:1302:U:OP2	44:1m:21:TYR:OH	2.13	0.61
1:2A:567:A:OP2	11:2P:29:LYS:NZ	2.34	0.61
32:2a:236:G:OP1	48:2q:40:LYS:NZ	2.32	0.61
32:2a:407:G:H5''	35:2d:115:ARG:HB3	1.81	0.61
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.83	0.61
1:1A:271(K):U:H1'	8:1I:50:ARG:HD2	1.82	0.61
1:1A:881:G:C2	1:1A:882:G:H1'	2.36	0.61
1:1A:1054:A:H61	1:1A:1105:U:H3	1.49	0.61
1:2A:2124:G:O6	1:2A:2173:A:N6	2.34	0.61
33:2b:88:ALA:HA	33:2b:223:ILE:HD11	1.81	0.61
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.22	0.61
32:1a:865:A:H2	32:1a:918:A:H4'	1.66	0.61
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.64	0.61
1:2A:332:A:O2'	1:2A:334:C:OP2	2.16	0.61
11:2P:94:GLU:HG3	11:2P:124:LYS:HE3	1.81	0.61
15:2T:24:PRO:HA	15:2T:49:VAL:HG12	1.82	0.61
1:1A:2136:C:C2	1:1A:2155:G:N2	2.69	0.61
1:1A:2817:G:OP1	13:1R:42:LYS:NZ	2.34	0.61
1:2A:1237:A:OP1	63:2A:3725:HOH:O	2.16	0.61
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.28	0.61
32:2a:1271:G:N2	32:2a:1272:G:N7	2.49	0.61
34:2c:117:ALA:HB2	34:2c:200:ALA:HB2	1.82	0.61
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	1.82	0.61
39:1h:86:ILE:HD12	39:1h:133:LEU:HD22	1.83	0.61
32:2a:9:G:H2'	32:2a:10:A:C8	2.34	0.61
41:2j:8:LEU:HD11	41:2j:20:ALA:HB2	1.82	0.61
43:1l:117:ARG:HB3	43:1l:122:THR:HB	1.82	0.60
1:1A:602:G:O2'	1:1A:655:A:N6	2.33	0.60
32:2a:1274:G:N2	32:2a:1275:A:N7	2.49	0.60
34:2c:47:LEU:HD13	34:2c:52:LEU:HD13	1.81	0.60
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.83	0.60
42:2k:62:GLN:OE1	42:2k:93:GLN:NE2	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.01	0.60
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.34	0.60
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.33	0.60
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	1.84	0.60
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.34	0.60
32:1a:504:C:OP1	63:1a:1912:HOH:O	2.16	0.60
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.33	0.60
54:1w:34:U8U:O4	54:1w:34:U8U:N	2.35	0.60
1:2A:1434:A:H61	1:2A:1558:A:H62	1.48	0.60
32:2a:1530:G:OP1	32:2a:1530:G:H4'	2.01	0.60
33:2b:104:ASN:O	33:2b:107:THR:OG1	2.20	0.60
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.83	0.60
11:1P:39:LYS:HB2	11:1P:45:LEU:HD22	1.84	0.60
25:13:10:LYS:NZ	25:13:15:TYR:OH	2.33	0.60
32:1a:112:G:OP2	47:1p:27:LYS:NZ	2.35	0.60
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.01	0.60
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.17	0.60
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.19	0.60
1:2A:2138:C:N4	1:2A:2153:G:H1	2.00	0.60
44:2m:94:ARG:HB3	44:2m:96:LEU:HD12	1.84	0.60
45:2n:32:SER:O	45:2n:32:SER:OG	2.19	0.60
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.36	0.60
3:2D:2:ALA:N	3:2D:200:ASP:OD2	2.34	0.60
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.35	0.60
26:24:64:GLY:C	26:24:66:SER:H	2.10	0.60
32:2a:1275:A:H3'	32:2a:1276:G:H8	1.66	0.60
39:2h:54:ASP:HB3	39:2h:56:LYS:HD2	1.83	0.60
40:1i:3:GLN:HB3	40:1i:20:ARG:HG2	1.83	0.60
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.83	0.60
7:2H:51:ARG:NH1	7:2H:53:GLU:OE2	2.34	0.60
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.83	0.60
33:2b:70:PHE:HE2	33:2b:90:MET:HB2	1.66	0.60
33:2b:91:PRO:HG2	33:2b:155:LEU:HB2	1.84	0.60
33:2b:231:GLU:H	33:2b:232:PRO:HD2	1.67	0.60
37:2f:6:VAL:HG13	37:2f:90:VAL:HG22	1.82	0.60
44:1m:88:ARG:HG2	44:1m:98:VAL:HG13	1.83	0.60
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.82	0.60
38:2g:78:ARG:HE	38:2g:79:ARG:HE	1.49	0.60
1:1A:2096:U:H3	1:1A:2193:G:H1	1.50	0.60
2:1B:87:G:N2	2:1B:90:A:OP2	2.25	0.60
19:1X:94:GLY:H	19:1X:95:LEU:C	2.09	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1187:G:N3	45:1n:60:SER:OG	2.34	0.60
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.67	0.60
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.35	0.60
5:2F:12:LEU:HD12	5:2F:124:LEU:HD21	1.84	0.60
7:2H:12:PRO:HD2	7:2H:15:VAL:HG21	1.84	0.60
8:2I:1:MET:N	8:2I:20:ASP:OD1	2.23	0.60
33:2b:200:ILE:HG22	33:2b:202:PRO:HD3	1.84	0.60
37:2f:97:PHE:HE2	49:2r:62:GLU:HG2	1.66	0.60
40:2i:88:TYR:HD2	40:2i:89:ASN:HB2	1.66	0.60
51:2t:33:ILE:HG12	51:2t:63:ILE:HG12	1.84	0.60
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.84	0.60
54:1w:18:G:N2	54:1w:57:G:H2'	2.17	0.60
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.16	0.60
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.34	0.60
1:1A:1991:U:H2'	1:1A:1992:G:H5''	1.84	0.59
1:1A:2131:G:H5''	1:1A:2132:U:H3'	1.84	0.59
4:1E:105:THR:OG1	4:1E:166:THR:OG1	2.14	0.59
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.19	0.59
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.19	0.59
26:24:26:SER:OG	26:24:27:THR:N	2.35	0.59
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.19	0.59
32:1a:757:U:H2'	32:1a:758:G:O4'	2.02	0.59
1:2A:271(R):G:H5''	23:21:97:LEU:HD21	1.84	0.59
1:2A:1011:G:OP1	16:2U:77:SER:OG	2.20	0.59
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	1.84	0.59
32:2a:1279:A:O2'	32:2a:1281:U:OP2	2.19	0.59
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HD3	1.83	0.59
35:1d:108:LEU:HD21	35:1d:174:LEU:HD22	1.84	0.59
1:2A:578:A:OP2	63:2A:3724:HOH:O	2.16	0.59
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.17	0.59
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.66	0.59
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.84	0.59
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.37	0.59
1:2A:2524:G:N7	63:2A:3784:HOH:O	2.32	0.59
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.34	0.59
32:2a:1080:A:H5'	36:2e:14:ARG:HH21	1.67	0.59
51:2t:50:GLU:O	51:2t:100:ILE:HD11	2.03	0.59
54:2w:63:U:C2	54:2w:64:G:N7	2.70	0.59
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.29	0.59
26:14:54:GLY:N	26:14:55:ARG:HA	2.16	0.59
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.83	0.59
5:1F:8:GLN:HE22	5:1F:21:ALA:HB2	1.67	0.59
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.29	0.59
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.83	0.59
13:1R:38:VAL:HG12	13:1R:42:LYS:HD2	1.85	0.59
37:1f:45:LEU:HD12	37:1f:59:TYR:HD1	1.67	0.59
1:2A:810:U:OP1	63:2A:3727:HOH:O	2.17	0.59
5:2F:33:LEU:HB3	11:2P:6:LEU:HD21	1.85	0.59
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	1.85	0.59
4:1E:181:LEU:HD21	15:1T:6:LEU:HD22	1.85	0.59
32:1a:702:A:OP2	63:1a:1913:HOH:O	2.17	0.59
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.38	0.59
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.37	0.59
34:2c:180:ALA:HB1	34:2c:203:PHE:HE1	1.66	0.59
1:1A:2128:C:N4	1:1A:2160:G:H1	2.01	0.59
1:1A:2336:A:H61	22:10:43:THR:HG22	1.68	0.59
1:2A:1918:A:O2'	1:2A:1920:OMC:N4	2.36	0.59
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.83	0.59
1:1A:2422:A:O4'	57:1y:76:A:N6	2.36	0.59
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.84	0.59
1:2A:2248:C:OP2	63:2A:3729:HOH:O	2.17	0.59
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.32	0.59
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.84	0.59
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.35	0.59
25:13:3:ARG:NE	25:13:60:GLU:OE1	2.34	0.59
13:2R:33:ARG:NH2	13:2R:115:GLU:OE1	2.35	0.59
33:2b:27:LYS:HB3	33:2b:194:PRO:HD2	1.83	0.59
43:2l:40:VAL:HG21	43:2l:78:GLN:HA	1.83	0.59
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.83	0.58
13:1R:103:ARG:NH1	13:1R:108:GLY:O	2.34	0.58
21:1Z:77:ASP:OD2	21:1Z:80:ARG:NH1	2.36	0.58
32:1a:881:G:P	43:1l:12:ARG:HH22	2.26	0.58
40:1i:77:ILE:O	40:1i:81:ILE:HG22	2.03	0.58
34:2c:101:LEU:HD13	34:2c:102:ASN:H	1.67	0.58
54:2w:51:A:C8	54:2w:64:G:H2'	2.38	0.58
12:1Q:78:PRO:HD3	55:1x:1:C:N3	2.17	0.58
21:1Z:151:HIS:HB3	21:1Z:169:GLU:O	2.03	0.58
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.01	0.58
33:1b:80:ILE:HD12	33:1b:211:ILE:HG22	1.84	0.58
33:1b:82:ARG:NH1	33:1b:86:GLU:OE2	2.37	0.58
38:1g:50:ILE:HD11	38:1g:125:MET:HG3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.85	0.58
54:1w:63:U:H2'	54:1w:64:G:C8	2.38	0.58
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.30	0.58
1:2A:879:G:H3'	1:2A:880:G:H8	1.68	0.58
50:2s:12:ASP:O	50:2s:14:HIS:N	2.36	0.58
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.67	0.58
1:1A:2100:G:H1	1:1A:2189:U:H3	1.51	0.58
11:1P:38:GLN:O	11:1P:40:SER:N	2.36	0.58
28:16:13:CYS:SG	28:16:47:THR:HG21	2.43	0.58
32:1a:92:C:H2'	32:1a:93:G:C8	2.38	0.58
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.39	0.58
23:21:82:LEU:HA	23:21:85:LEU:HD12	1.85	0.58
34:2c:118:GLN:HA	34:2c:121:ALA:HB3	1.84	0.58
55:2x:40:C:H2'	55:2x:41:C:H6	1.67	0.58
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.36	0.58
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.85	0.58
9:2N:38:HIS:NE2	9:2N:39:ARG:HG3	2.18	0.58
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.37	0.58
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.17	0.58
38:2g:99:LEU:HD23	38:2g:102:ARG:HH12	1.67	0.58
50:2s:33:THR:HG21	50:2s:49:ILE:HD11	1.84	0.58
1:2A:2439:A:N6	55:2x:76:8AN:O1P	2.36	0.58
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.36	0.58
32:2a:984:C:H2'	32:2a:985:C:H6	1.68	0.58
3:1D:61:LEU:O	3:1D:63:ARG:NH1	2.37	0.58
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.36	0.58
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.35	0.58
33:2b:8:LYS:HB3	33:2b:217:ARG:HE	1.68	0.58
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.86	0.58
34:2c:6:HIS:HB3	45:2n:49:HIS:HD2	1.69	0.58
1:1A:588:U:H2'	1:1A:589:C:C6	2.38	0.58
9:1N:73:THR:HB	9:1N:82:LEU:HD11	1.84	0.58
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.83	0.58
39:1h:119:LEU:HB3	39:1h:123:GLU:HB3	1.84	0.58
1:2A:307:G:N1	1:2A:310:A:OP2	2.35	0.58
1:2A:854:G:H2'	1:2A:855:G:C8	2.37	0.58
32:2a:815:A:N7	32:2a:1509:C:O2'	2.37	0.58
32:2a:1240:U:N3	38:2g:30:ILE:O	2.26	0.58
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.39	0.58
34:2c:182:ILE:HG22	34:2c:203:PHE:HA	1.85	0.58
37:2f:25:ILE:HD12	37:2f:82:ARG:HD2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:40:ASN:HD22	44:2m:43:THR:HG23	1.68	0.58
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.38	0.58
21:1Z:52:SER:O	21:1Z:52:SER:OG	2.21	0.58
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.37	0.58
32:2a:1272:G:N2	32:2a:1273:G:C5	2.71	0.58
41:2j:13:HIS:HB3	41:2j:68:HIS:CE1	2.39	0.58
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.51	0.58
5:1F:164:ARG:HD2	5:1F:175:THR:HG23	1.85	0.58
1:2A:881:G:C2	1:2A:882:G:H1'	2.38	0.58
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.84	0.58
32:2a:1385:G:H2'	32:2a:1386:G:H8	1.68	0.58
34:2c:88:ARG:HA	34:2c:91:LEU:HD13	1.86	0.58
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	1.86	0.58
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.03	0.58
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.68	0.58
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.36	0.58
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.86	0.58
32:2a:64:G:H4'	32:2a:65:U:H3'	1.83	0.58
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.04	0.57
1:1A:2158:A:H1'	1:1A:2159:G:O4'	2.04	0.57
8:1I:70:GLU:O	8:1I:74:ASN:HB2	2.04	0.57
32:1a:1267:C:O2	52:1u:20:LYS:NZ	2.37	0.57
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.39	0.57
40:1i:33:PHE:HD2	40:1i:34:ASN:HD22	1.51	0.57
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.67	0.57
34:2c:125:GLU:O	34:2c:190:ARG:NH2	2.37	0.57
34:2c:127:ARG:HH22	34:2c:192:THR:H	1.52	0.57
38:2g:146:GLU:OE2	38:2g:149:ARG:NE	2.36	0.57
38:2g:152:ALA:O	38:2g:155:ARG:NH1	2.37	0.57
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.87	0.57
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.04	0.57
7:1H:25:LYS:HG3	7:1H:34:GLU:HG2	1.87	0.57
26:14:55:ARG:N	26:14:56:VAL:HA	2.19	0.57
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.38	0.57
1:2A:212:G:H2'	1:2A:213:A:O4'	2.03	0.57
1:1A:2336:A:H61	22:10:43:THR:CG2	2.17	0.57
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.68	0.57
7:1H:149:ARG:HH12	7:1H:167:GLU:CD	2.13	0.57
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.87	0.57
33:1b:189:ASP:HB3	33:1b:204:ASN:HA	1.86	0.57
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:852:G:H2'	1:2A:853:G:C8	2.38	0.57
1:2A:2722:G:H5'	13:2R:4:LEU:HD12	1.86	0.57
32:2a:662:G:O2'	32:2a:836:G:OP1	2.22	0.57
37:2f:74:ASP:N	37:2f:74:ASP:OD1	2.33	0.57
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.03	0.57
1:1A:2133:G:N1	1:1A:2157:G:H1'	2.19	0.57
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.33	0.57
32:1a:972:C:O2'	41:1j:55:LYS:O	2.22	0.57
1:2A:245:G:O6	30:28:8:LYS:NZ	2.32	0.57
6:2G:83:ARG:N	6:2G:86:MET:SD	2.65	0.57
1:1A:527:C:OP1	63:1A:4139:HOH:O	2.17	0.57
35:1d:129:ASN:HD21	35:1d:144:ASP:HB3	1.69	0.57
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.20	0.57
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.86	0.57
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.40	0.57
8:2I:37:VAL:HG12	8:2I:38:LEU:HD12	1.86	0.57
19:2X:31:HIS:HD2	19:2X:33:LYS:H	1.50	0.57
33:2b:112:VAL:HG23	33:2b:149:LEU:HD13	1.86	0.57
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.84	0.57
1:1A:363(A):A:H2'	1:1A:363(B):G:H8	1.69	0.57
26:14:15:ILE:O	26:14:33:VAL:N	2.33	0.57
35:1d:112:VAL:H	35:1d:116:GLN:NE2	2.03	0.57
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.39	0.57
2:2B:7:G:H21	14:2S:38:GLN:NE2	2.02	0.57
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.85	0.57
7:1H:17:VAL:HG22	7:1H:26:VAL:HG22	1.87	0.57
21:1Z:163:LEU:HD23	21:1Z:167:PRO:HG3	1.86	0.57
25:13:18:ASP:OD1	25:13:18:ASP:N	2.37	0.57
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.03	0.57
6:2G:145:THR:OG1	6:2G:146:TYR:N	2.38	0.57
18:2W:65:LEU:HD13	18:2W:68:ARG:HE	1.70	0.57
32:2a:957:U:O2'	32:2a:959:A:N7	2.34	0.57
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.05	0.57
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.37	0.57
1:1A:956:G:H5''	12:1Q:77:LYS:HD2	1.86	0.57
23:11:44:PRO:HB2	23:11:46:LEU:HD13	1.87	0.57
26:14:13:ARG:HB3	26:14:30:GLU:HG2	1.85	0.57
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.40	0.57
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.40	0.57
5:2F:110:LEU:HD21	5:2F:181:LEU:HD23	1.87	0.57
21:2Z:155:LEU:HB2	21:2Z:157:LEU:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:20:36:ILE:HD13	22:20:60:PHE:HB3	1.87	0.57
32:2a:931:C:H42	32:2a:1386:G:H1	1.52	0.57
1:1A:568:U:H5'	1:1A:945:A:N6	2.20	0.57
1:1A:2372:G:O6	63:1A:4130:HOH:O	2.15	0.57
40:2i:3:GLN:HG2	40:2i:20:ARG:HD2	1.87	0.57
32:1a:352:C:O2'	32:1a:354:G:OP1	2.19	0.56
57:1y:10:G:N2	57:1y:26:A:H1'	2.20	0.56
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.22	0.56
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.70	0.56
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.86	0.56
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.35	0.56
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.87	0.56
1:2A:495:G:N3	18:2W:61:ASN:ND2	2.53	0.56
5:2F:192:LEU:HD21	5:2F:194:MET:HE2	1.87	0.56
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.86	0.56
54:2w:51:A:N1	54:2w:63:U:C4	2.73	0.56
1:1A:1011:G:OP2	16:1U:66:ASN:ND2	2.24	0.56
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.87	0.56
32:1a:626:U:H2'	32:1a:627:G:C8	2.41	0.56
32:1a:674:G:H2'	32:1a:675:A:H8	1.69	0.56
32:1a:1202:G:H1'	45:1n:29:ARG:HD2	1.87	0.56
35:1d:59:ARG:HA	35:1d:59:ARG:NH1	2.20	0.56
35:1d:59:ARG:HH12	35:1d:62:GLN:HB2	1.71	0.56
41:1j:49:VAL:HG13	45:1n:41:ARG:HB2	1.85	0.56
43:1l:77:LEU:HD21	43:1l:107:ALA:HA	1.88	0.56
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.39	0.56
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.71	0.56
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.21	0.56
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.40	0.56
4:2E:119:ARG:HG2	4:2E:120:TRP:CD1	2.41	0.56
21:2Z:17:ALA:HA	21:2Z:20:ARG:HH11	1.70	0.56
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.38	0.56
32:2a:7:G:H5'	32:2a:298:A:O4'	2.04	0.56
35:2d:114:ARG:HA	35:2d:117:ALA:HB3	1.87	0.56
36:2e:31:LEU:HD11	36:2e:129:ILE:HA	1.88	0.56
43:2l:28:LYS:HB2	43:2l:33:ARG:HH21	1.69	0.56
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.19	0.56
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.70	0.56
28:16:35:GLU:OE1	28:16:50:ARG:NH1	2.36	0.56
32:1a:6:G:H1	36:1e:98:THR:HG21	1.70	0.56
36:1e:83:GLU:HG2	36:1e:88:LYS:HG3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.38	0.56
1:2A:2218:U:N3	23:21:55:GLY:O	2.39	0.56
12:2Q:137:TYR:HB3	21:2Z:76:LEU:HD21	1.86	0.56
30:28:62:LEU:HB3	30:28:65:GLU:HG3	1.87	0.56
32:2a:708:C:H2'	32:2a:709:G:H8	1.70	0.56
36:1e:78:HIS:HE1	36:1e:142:LEU:HA	1.70	0.56
1:2A:907:U:O2'	12:2Q:101:ARG:NH2	2.30	0.56
1:2A:2138:C:H42	1:2A:2153:G:H1	1.52	0.56
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.87	0.56
14:2S:28:VAL:HG21	14:2S:101:LEU:HD22	1.88	0.56
19:2X:72:LYS:NZ	19:2X:75:ASP:OD1	2.38	0.56
32:2a:1014:A:H1'	50:2s:34:TRP:HB2	1.88	0.56
34:2c:37:GLN:HE22	45:2n:52:GLN:HB3	1.70	0.56
1:1A:299:A:OP2	63:1A:4138:HOH:O	2.17	0.56
7:1H:3:ARG:HG2	7:1H:6:ARG:HG3	1.86	0.56
40:1i:19:LEU:HD21	40:1i:81:ILE:HG13	1.88	0.56
1:2A:2104:G:H1	1:2A:2185:C:H42	1.52	0.56
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.71	0.56
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.41	0.56
54:2w:7:U:H5'	54:2w:8:U:OP2	2.06	0.56
57:2y:48:C:H2'	57:2y:59:A:H1'	1.87	0.56
5:1F:178:PRO:O	5:1F:205:ARG:NH2	2.38	0.56
54:1w:62:C:H2'	54:1w:63:U:C6	2.41	0.56
37:2f:37:VAL:HA	37:2f:65:VAL:HG12	1.88	0.56
39:2h:29:SER:HB3	39:2h:32:LYS:HG3	1.87	0.56
1:1A:668:G:H5'	1:1A:669:G:OP2	2.06	0.56
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.40	0.56
34:1c:19:GLU:HB3	34:1c:40:ARG:HH21	1.71	0.56
1:2A:648:G:O2'	1:2A:2351:G:OP1	2.16	0.56
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.88	0.56
54:2w:18:G:H4'	54:2w:60:U:C6	2.41	0.56
7:2H:33:LEU:HD21	7:2H:136:ILE:HB	1.87	0.56
14:2S:23:ARG:HG3	14:2S:24:LEU:N	2.21	0.56
32:2a:56:U:H2'	32:2a:57:G:C8	2.41	0.56
1:1A:484:C:OP1	20:1Y:51:VAL:HG22	2.06	0.56
1:1A:859:G:O2'	1:1A:916:G:O6	2.20	0.56
32:1a:333:G:H4'	51:1t:16:HIS:CE1	2.40	0.56
32:1a:1399:C:H4'	32:1a:1400:5MC:H5''	1.88	0.56
40:1i:46:ALA:HA	40:1i:78:LYS:HB2	1.87	0.56
1:2A:892:G:H2'	1:2A:892:G:N3	2.21	0.56
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2295:C:H5	14:2S:13:ARG:HH22	1.54	0.56
6:2G:41:GLN:O	6:2G:43:LEU:N	2.39	0.56
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	1.88	0.56
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.88	0.56
14:2S:35:ILE:HD11	14:2S:101:LEU:HD13	1.88	0.56
38:2g:12:LEU:H	38:2g:12:LEU:HD12	1.70	0.56
57:1y:71:C:H2'	57:1y:72:C:C6	2.41	0.55
1:2A:1159:U:H2'	1:2A:1160:G:H8	1.70	0.55
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.31	0.55
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.88	0.55
1:2A:2255:G:OP2	63:2A:3728:HOH:O	2.17	0.55
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.34	0.55
9:2N:115:ARG:HA	9:2N:118:LYS:HE2	1.88	0.55
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.42	0.55
38:2g:15:ASP:OD1	38:2g:19:GLY:N	2.39	0.55
44:2m:78:ILE:HA	44:2m:81:LEU:HD12	1.88	0.55
3:1D:37:LEU:HD12	3:1D:62:TYR:HB2	1.87	0.55
32:1a:116:A:OP1	63:1a:1915:HOH:O	2.18	0.55
44:1m:105:THR:HG22	44:1m:106:ASN:H	1.71	0.55
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.40	0.55
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.88	0.55
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.36	0.55
1:2A:1782:C:O2	1:2A:2608:G:O2'	2.20	0.55
7:2H:127:GLU:C	7:2H:129:THR:H	2.14	0.55
26:24:59:PHE:HE2	50:2s:64:GLU:HB2	1.71	0.55
30:28:56:GLU:HA	30:28:59:LYS:HE3	1.87	0.55
32:2a:994:A:C5	32:2a:1216:G:H4'	2.41	0.55
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.33	0.55
1:1A:687:C:H5''	29:17:2:LYS:HE2	1.88	0.55
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.06	0.55
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.86	0.55
57:1y:10:G:N7	57:1y:45:G:O2'	2.39	0.55
1:2A:65:C:O2'	1:2A:456:C:N3	2.40	0.55
32:2a:45:U:H2'	32:2a:46:G:C8	2.42	0.55
32:2a:542:G:P	35:2d:10:ARG:HH22	2.30	0.55
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.89	0.55
1:1A:1448:G:O2'	1:1A:1528(A):A:N1	2.38	0.55
26:14:16:CYS:HB2	26:14:36:CYS:HB3	1.88	0.55
32:1a:695:A:OP2	42:1k:53:SER:N	2.39	0.55
47:1p:38:TYR:OH	47:1p:47:ASP:OD2	2.24	0.55
1:2A:958:U:O2	2:2B:90:A:O2'	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.07	0.55
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.06	0.55
33:2b:16:HIS:HE1	33:2b:42:ILE:HD12	1.70	0.55
1:1A:414:C:H2'	1:1A:415:A:C8	2.41	0.55
1:1A:639:U:H2'	1:1A:640:C:C6	2.42	0.55
1:1A:1054:A:N6	1:1A:1105:U:H3	2.05	0.55
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.06	0.55
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.55	0.55
34:1c:110:ASN:OD1	34:1c:110:ASN:N	2.32	0.55
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.07	0.55
1:2A:1851:U:O2'	57:2y:72:C:OP1	2.25	0.55
1:2A:2393:A:H5''	11:2P:63:PRO:HB3	1.89	0.55
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.42	0.55
14:2S:99:LYS:NZ	14:2S:103:GLU:OE2	2.39	0.55
32:2a:1009:G:H22	32:2a:1021:G:H1'	1.70	0.55
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	1.88	0.55
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.75	0.55
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.26	0.55
42:2k:14:VAL:HG11	42:2k:35:PRO:HD3	1.88	0.55
1:1A:1779:U:H2'	63:1A:4267:HOH:O	2.07	0.55
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.71	0.55
36:1e:27:ARG:HH11	36:1e:27:ARG:HB2	1.71	0.55
43:1l:52:LEU:O	43:1l:54:LYS:NZ	2.29	0.55
57:1y:63:U:H2'	57:1y:64:G:C8	2.41	0.55
5:2F:28:ILE:HG22	5:2F:112:MET:HB3	1.89	0.55
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.23	0.55
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.88	0.55
32:2a:116:A:H61	32:2a:313:A:H1'	1.72	0.55
37:2f:15:ASP:OD1	37:2f:17:SER:N	2.38	0.55
55:2x:55:PSU:N3	55:2x:58:A:OP2	2.36	0.55
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.30	0.55
51:1t:86:ARG:O	51:1t:90:GLN:NE2	2.40	0.55
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.52	0.55
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.42	0.55
1:2A:1876:A:H2'	1:2A:1877:A:C8	2.42	0.55
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.40	0.55
1:2A:2786:U:OP1	4:2E:69:LYS:NZ	2.32	0.55
2:2B:2:C:H2'	2:2B:3:C:H6	1.70	0.55
4:2E:27:LEU:HD22	15:2T:1:MET:SD	2.46	0.55
5:2F:124:LEU:HB3	5:2F:193:VAL:HG22	1.88	0.55
22:20:27:GLU:HB2	22:20:69:PHE:HD1	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.20	0.55
32:2a:1250:A:H4'	40:2i:68:GLY:N	2.21	0.55
32:2a:1263:C:C4	32:2a:1272:G:O6	2.59	0.55
34:2c:46:GLU:CD	34:2c:46:GLU:H	2.13	0.55
54:2w:18:G:HO2'	54:2w:57:G:N2	2.04	0.55
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.39	0.55
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.40	0.55
32:1a:848:C:H2'	32:1a:849:C:C6	2.41	0.55
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.19	0.55
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.41	0.55
32:2a:584:G:H5'	48:2q:91:ARG:HH22	1.71	0.55
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.88	0.55
44:2m:82:MET:HE2	44:2m:92:HIS:HB3	1.88	0.55
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.37	0.55
1:1A:1139:G:H5''	9:1N:70:LYS:HZ3	1.72	0.55
32:1a:1166:G:N2	32:1a:1170:A:OP2	2.40	0.55
39:1h:14:ARG:NH2	39:1h:83:ILE:O	2.34	0.55
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.07	0.55
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	1.89	0.55
23:21:35:THR:OG1	23:21:35:THR:O	2.24	0.55
32:2a:1071:C:H2'	32:2a:1072:G:C8	2.41	0.55
32:2a:1182:G:H4'	32:2a:1183:A:H5''	1.89	0.55
32:2a:1316:G:H5''	45:2n:17:LYS:HE3	1.89	0.55
34:2c:148:GLY:HA3	34:2c:203:PHE:HB3	1.89	0.55
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.89	0.55
36:2e:95:ALA:O	36:2e:97:GLY:N	2.38	0.55
1:1A:1045:A:H8	1:1A:1111:A:C6	2.25	0.55
1:1A:1077:A:H2'	1:1A:1078:U:H4'	1.88	0.55
1:1A:2186:G:H2'	1:1A:2187:G:H5'	1.89	0.55
41:1j:30:SER:HB3	41:1j:81:THR:HG23	1.89	0.55
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.06	0.55
32:2a:20:U:H2'	32:2a:21:G:O4'	2.07	0.55
32:2a:34:C:H2'	32:2a:35:G:H8	1.71	0.55
32:2a:524:G:H2'	32:2a:525:C:C6	2.42	0.55
32:2a:1240:U:OP2	38:2g:115:ARG:HA	2.07	0.55
38:2g:20:ASP:HB3	38:2g:23:VAL:HB	1.87	0.55
41:2j:12:ASP:OD1	41:2j:14:LYS:N	2.39	0.55
47:2p:39:TYR:CG	47:2p:73:LEU:HD21	2.42	0.55
33:1b:76:GLN:HG2	33:1b:206:ASP:O	2.07	0.54
35:1d:65:ARG:NH1	35:1d:72:GLU:OE1	2.40	0.54
38:1g:74:GLU:OE2	38:1g:95:ARG:NE	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.07	0.54
1:2A:2121:G:H1	1:2A:2177:C:H42	1.55	0.54
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.88	0.54
26:24:16:CYS:SG	26:24:17:GLY:N	2.81	0.54
7:1H:149:ARG:NH1	7:1H:167:GLU:OE1	2.39	0.54
32:1a:26:A:O2'	35:1d:209:ARG:NH2	2.40	0.54
32:1a:674:G:H2'	32:1a:675:A:C8	2.43	0.54
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.72	0.54
1:2A:2131:G:OP2	1:2A:2131:G:N2	2.40	0.54
20:2Y:52:SER:OG	20:2Y:55:TYR:HB2	2.07	0.54
21:2Z:144:LEU:HG	21:2Z:145:GLU:H	1.72	0.54
32:2a:17:U:H2'	32:2a:18:C:C6	2.42	0.54
32:2a:532:A:H2'	32:2a:532:A:N3	2.21	0.54
32:2a:1004:A:N6	32:2a:1037:C:O2	2.32	0.54
44:2m:80:ARG:HH21	50:2s:69:HIS:HE1	1.53	0.54
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.23	0.54
1:1A:1058:G:N1	1:1A:1080:C:N4	2.56	0.54
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.89	0.54
12:1Q:20:ALA:HB2	21:1Z:79:ARG:HG3	1.89	0.54
35:1d:122:ARG:NH1	35:1d:134:ASP:O	2.41	0.54
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.30	0.54
7:2H:3:ARG:NH2	7:2H:5:GLY:H	2.05	0.54
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.42	0.54
35:2d:110:PHE:HD1	35:2d:110:PHE:H	1.56	0.54
1:1A:1058:G:N2	1:1A:1080:C:N3	2.54	0.54
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	1.89	0.54
7:2H:159:GLU:HG2	7:2H:169:VAL:HG11	1.90	0.54
32:2a:542:G:OP1	35:2d:10:ARG:NH2	2.41	0.54
33:2b:76:GLN:HB2	33:2b:208:ILE:HG12	1.90	0.54
33:2b:180:LEU:HD12	33:2b:182:ILE:HD11	1.90	0.54
36:2e:145:LYS:O	36:2e:149:GLU:N	2.38	0.54
39:2h:51:VAL:HG22	39:2h:60:ARG:HB2	1.89	0.54
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.72	0.54
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.72	0.54
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.43	0.54
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.70	0.54
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.89	0.54
40:2i:34:ASN:HD22	40:2i:34:ASN:N	2.04	0.54
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.42	0.54
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.41	0.54
33:1b:12:GLU:C	33:1b:14:GLY:H	2.15	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:59:TYR:CE2	42:1k:63:LEU:HD11	2.43	0.54
38:2g:9:VAL:HG23	38:2g:94:ARG:NH2	2.22	0.54
41:2j:55:LYS:HG2	41:2j:56:HIS:N	2.23	0.54
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.90	0.54
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.43	0.54
1:1A:2608:G:N7	63:1A:4222:HOH:O	2.34	0.54
34:1c:152:ILE:HB	34:1c:199:LYS:HB2	1.90	0.54
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.89	0.54
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.90	0.54
32:2a:936:C:H2'	32:2a:937:A:O4'	2.08	0.54
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.40	0.54
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.21	0.54
32:2a:1385:G:H2'	32:2a:1386:G:C8	2.42	0.54
33:2b:12:GLU:HA	33:2b:213:LEU:HD11	1.89	0.54
41:2j:42:THR:HG23	41:2j:68:HIS:HA	1.89	0.54
1:1A:1359:A:H2	1:1A:1372:U:O4	1.89	0.54
1:1A:2406:U:H2'	1:1A:2406:U:OP2	2.08	0.54
25:13:26:LEU:O	25:13:35:ARG:NE	2.40	0.54
32:1a:1038:C:H2'	32:1a:1039:C:C6	2.43	0.54
38:1g:27:ILE:HD13	38:1g:40:ALA:HA	1.88	0.54
57:1y:69:A:H3'	57:1y:70:C:H5''	1.90	0.54
6:2G:123:ASN:C	6:2G:125:PHE:H	2.16	0.54
28:26:35:GLU:HG2	28:26:50:ARG:HD3	1.90	0.54
32:2a:1004:A:H5''	32:2a:1024:G:H22	1.71	0.54
32:2a:1134:G:C2	32:2a:1135:U:H1'	2.42	0.54
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.41	0.54
42:2k:18:ARG:HD2	42:2k:83:ILE:HD11	1.89	0.54
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.42	0.54
20:1Y:30:VAL:HG22	20:1Y:37:VAL:HG12	1.89	0.54
25:13:6:VAL:HG22	25:13:56:VAL:HG13	1.89	0.54
32:1a:376:G:H5''	47:1p:5:ARG:HG2	1.90	0.54
36:1e:69:VAL:HG11	36:1e:113:ALA:HB1	1.90	0.54
57:1y:26:A:H61	57:1y:44:U:H3	1.56	0.54
1:2A:829:A:N7	1:2A:2248:C:H5'	2.22	0.54
1:2A:2118:U:OP1	1:2A:2148:G:H4'	2.08	0.54
3:2D:241:PRO:O	63:2D:401:HOH:O	2.19	0.54
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.07	0.54
32:2a:222:U:H2'	32:2a:223:U:C6	2.43	0.54
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.42	0.54
21:1Z:1:MET:H2	21:1Z:3:TYR:HE2	1.56	0.54
32:1a:1255:G:N7	41:1j:43:ARG:NH2	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.90	0.54
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.89	0.54
35:1d:59:ARG:HA	35:1d:59:ARG:HH11	1.72	0.54
39:1h:112:LEU:HA	39:1h:134:ILE:HG12	1.91	0.54
1:2A:709:U:H2'	1:2A:710:G:C8	2.43	0.54
1:2A:1592:C:H2'	1:2A:1593:G:C8	2.42	0.54
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.23	0.54
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.90	0.54
43:2l:69:TYR:HB2	43:2l:96:VAL:HG11	1.90	0.54
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.06	0.53
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.41	0.53
1:1A:1823:G:OP1	3:1D:54:ARG:NH1	2.41	0.53
32:1a:731:G:H5'	32:1a:766:A:H4'	1.90	0.53
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.91	0.53
36:1e:20:GLN:NE2	36:1e:21:ALA:O	2.41	0.53
1:2A:800:A:H8	1:2A:800:A:OP1	1.92	0.53
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.41	0.53
32:2a:588:G:OP2	63:2a:1911:HOH:O	2.18	0.53
54:2w:23:A:H3'	54:2w:24:G:H8	1.73	0.53
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.08	0.53
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.43	0.53
1:1A:2037:G:O6	63:1A:4135:HOH:O	2.16	0.53
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	1.90	0.53
23:1i:23:LYS:HB2	57:1y:74:C:H4'	1.90	0.53
32:1a:1040:U:H2'	32:1a:1041:A:C8	2.44	0.53
33:1b:83:MET:HG3	33:1b:234:PRO:HG3	1.90	0.53
51:1t:34:LYS:HG2	51:1t:80:ARG:HH22	1.72	0.53
1:2A:2079:U:O3'	23:2i:35:THR:OG1	2.26	0.53
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.43	0.53
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.73	0.53
46:2o:32:LEU:HD22	46:2o:59:MET:HG2	1.89	0.53
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.08	0.53
9:1N:1:MET:O	9:1N:2:LYS:HB2	2.08	0.53
1:2A:796:C:H2'	1:2A:797:C:C6	2.42	0.53
1:2A:2131:G:N2	1:2A:2158:A:H62	2.06	0.53
32:2a:1278:U:H5'	32:2a:1279:A:OP1	2.07	0.53
63:1A:5124:HOH:O	11:1P:44:GLY:HA2	2.09	0.53
13:1R:20:LEU:HD21	13:1R:40:LYS:HD3	1.90	0.53
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.40	0.53
32:1a:673:G:H2'	32:1a:674:G:C8	2.43	0.53
35:1d:141:ARG:HD3	35:1d:142:PRO:HD2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:123:PHE:CD1	7:2H:133:VAL:HG12	2.44	0.53
32:2a:1203:C:H2'	32:2a:1204:A:C8	2.42	0.53
32:2a:1417:G:O6	63:2a:1908:HOH:O	2.15	0.53
35:2d:10:ARG:HB2	35:2d:40:PRO:HG3	1.91	0.53
49:2r:58:LEU:HD22	49:2r:62:GLU:HB3	1.90	0.53
1:1A:548:A:H1'	1:1A:549:G:OP1	2.08	0.53
1:1A:1075:C:H2'	1:1A:1076:C:H2'	1.89	0.53
4:1E:119:ARG:HG2	4:1E:120:TRP:CD1	2.44	0.53
32:1a:601:C:H2'	32:1a:602:A:H8	1.73	0.53
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.90	0.53
57:1y:71:C:H2'	57:1y:72:C:H6	1.73	0.53
1:2A:361:G:O2'	1:2A:362:U:H5'	2.09	0.53
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.08	0.53
1:2A:646:A:H2'	1:2A:647:G:O4'	2.09	0.53
1:2A:987:G:O2'	1:2A:1000:A:N3	2.40	0.53
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.26	0.53
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.43	0.53
32:2a:865:A:H5'	32:2a:1078:U:C5	2.44	0.53
32:2a:909:A:N3	32:2a:1413:A:O2'	2.38	0.53
44:2m:123:ALA:CB	54:2w:39:PSU:H4'	2.38	0.53
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.08	0.53
54:2w:23:A:H3'	54:2w:24:G:C8	2.43	0.53
1:1A:568:U:H5'	1:1A:945:A:H62	1.73	0.53
1:1A:2189:U:H2'	1:1A:2190:G:C8	2.44	0.53
1:1A:2250:G:OP1	12:1Q:85:LYS:NZ	2.34	0.53
32:1a:472:A:O2'	47:1p:82:GLN:N	2.42	0.53
32:1a:684:A:H1'	42:1k:39:PRO:HD2	1.91	0.53
32:1a:1007:C:H2'	32:1a:1008:C:C6	2.44	0.53
32:1a:1036:G:H5''	32:1a:1037:C:C5	2.44	0.53
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.90	0.53
44:1m:79:LYS:NZ	44:1m:83:ASP:OD2	2.39	0.53
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.44	0.53
1:2A:2572:A:N7	4:2E:145:LYS:HB2	2.24	0.53
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.90	0.53
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.91	0.53
33:2b:114:ARG:O	33:2b:118:LEU:HB2	2.07	0.53
34:2c:107:GLN:O	34:2c:108:ASN:HB2	2.07	0.53
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.90	0.53
55:2x:53:G:H3'	55:2x:54:5MU:H73	1.90	0.53
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.38	0.53
36:1e:88:LYS:HB3	36:1e:123:LEU:HB2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:637:A:OP1	11:2P:133:SER:OG	2.18	0.53
1:2A:2268:A:OP1	63:2A:3733:HOH:O	2.19	0.53
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.26	0.53
7:2H:22:GLY:C	7:2H:37:VAL:HB	2.32	0.53
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.07	0.53
1:1A:875:G:H1'	21:1Z:170:THR:HG21	1.91	0.53
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.44	0.53
32:1a:626:U:H2'	32:1a:627:G:H8	1.73	0.53
1:2A:571:A:N6	1:2A:2499:C:O3'	2.42	0.53
7:2H:105:LEU:HB2	7:2H:113:VAL:HB	1.89	0.53
12:2Q:54:MET:HB2	12:2Q:64:ILE:HD13	1.91	0.53
32:2a:920:U:H2'	32:2a:921:U:C6	2.43	0.53
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.44	0.53
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.44	0.53
1:1A:987:G:O2'	1:1A:1000:A:N3	2.40	0.53
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.44	0.53
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	1.90	0.53
57:1y:75:C:H5'	57:1y:76:A:H5'	1.90	0.53
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.44	0.53
21:2Z:4:ARG:NH2	21:2Z:66:SER:OG	2.40	0.53
23:21:50:ARG:HG2	23:21:59:THR:HG23	1.89	0.53
27:25:35:GLU:HG2	27:25:51:TYR:CG	2.44	0.53
41:2j:6:ILE:HG12	41:2j:98:ILE:HG22	1.89	0.53
1:1A:2605:PSU:O2	63:1A:4136:HOH:O	2.16	0.53
32:1a:404:U:OP1	35:1d:118:ARG:NH1	2.42	0.53
1:2A:848:G:H2'	1:2A:849:A:C8	2.44	0.53
1:2A:880:G:N2	1:2A:898:C:O2	2.42	0.53
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.09	0.53
2:2B:24:G:N3	2:2B:26:A:N6	2.57	0.53
5:2F:11:VAL:HG13	5:2F:125:LEU:HB2	1.90	0.53
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.90	0.53
14:2S:88:ASP:OD1	14:2S:90:GLY:N	2.41	0.53
32:2a:88:A:H5''	32:2a:89:C:C6	2.43	0.53
35:2d:15:GLU:OE2	35:2d:59:ARG:NH1	2.41	0.53
54:2w:43:U:H2'	54:2w:44:U:C6	2.44	0.53
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.45	0.52
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.91	0.52
9:1N:77:GLY:O	63:1N:301:HOH:O	2.18	0.52
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.40	0.52
12:1Q:136:ALA:HB1	21:1Z:52:SER:HB2	1.91	0.52
22:10:46:LYS:NZ	22:10:75:LEU:O	2.36	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:125:PRO:O	33:1b:127:ILE:N	2.42	0.52
40:1i:8:GLY:HA3	40:1i:76:ALA:O	2.09	0.52
1:2A:251:A:C5	1:2A:252:G:H1'	2.44	0.52
8:2I:5:LEU:HD23	8:2I:36:ALA:HB2	1.90	0.52
12:2Q:81:VAL:HG12	22:20:5:LYS:HD3	1.91	0.52
26:24:58:ARG:HE	50:2s:68:GLY:H	1.57	0.52
32:2a:707:C:H2'	32:2a:708:C:C6	2.44	0.52
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.44	0.52
41:2j:9:ARG:O	41:2j:16:LEU:HD21	2.09	0.52
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.44	0.52
1:1A:904:C:O2'	21:1Z:169:GLU:OE2	2.17	0.52
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.43	0.52
1:1A:2175:C:H2'	1:1A:2176:A:O4'	2.09	0.52
1:1A:2277:G:OP2	22:10:10:THR:HG21	2.09	0.52
32:1a:22:G:H4'	32:1a:885:G:C8	2.43	0.52
32:1a:186:C:H2'	32:1a:187:C:C6	2.44	0.52
45:1n:14:PRO:HG2	45:1n:16:PHE:O	2.09	0.52
1:2A:1271:G:OP2	63:2A:3705:HOH:O	2.18	0.52
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.90	0.52
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.09	0.52
1:2A:2689:U:OP2	1:2A:2719:G:N2	2.38	0.52
7:2H:7:LEU:HB3	7:2H:69:ARG:HH21	1.74	0.52
26:24:37:SER:HA	26:24:43:TYR:CD1	2.44	0.52
32:2a:1032:G:H2'	32:2a:1033:G:O4'	2.10	0.52
32:2a:1089:G:H1	32:2a:1096:C:H42	1.56	0.52
33:2b:28:PHE:CD2	33:2b:190:THR:HA	2.44	0.52
39:2h:36:LEU:HD23	39:2h:39:LEU:HD13	1.90	0.52
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.44	0.52
1:1A:2376:A:N3	14:1S:106:ARG:NH2	2.55	0.52
7:1H:124:GLU:HG2	7:1H:132:ARG:HB3	1.91	0.52
32:1a:848:C:H2'	32:1a:849:C:H6	1.73	0.52
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.44	0.52
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.57	0.52
17:2V:40:LEU:HB2	17:2V:46:VAL:HG12	1.90	0.52
25:23:6:VAL:HG12	25:23:28:LEU:HD11	1.91	0.52
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.24	0.52
32:2a:114:U:H2'	32:2a:115:G:C8	2.45	0.52
45:2n:29:ARG:HG3	45:2n:30:ALA:H	1.74	0.52
55:2x:66:C:H2'	55:2x:67:C:O4'	2.09	0.52
1:1A:528:A:O2'	1:1A:529:A:H5'	2.10	0.52
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.17	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.91	0.52
32:1a:405:U:H5''	32:1a:495:A:H2	1.74	0.52
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.92	0.52
55:1x:68:C:H2'	55:1x:69:C:C6	2.45	0.52
57:1y:1:G:H2'	57:1y:2:G:C8	2.45	0.52
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.41	0.52
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.42	0.52
24:22:41:ILE:HG13	24:22:43:GLN:HG2	1.91	0.52
32:2a:587:G:N1	32:2a:754:C:OP2	2.42	0.52
32:2a:947:G:H1	32:2a:1234:C:H42	1.55	0.52
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.41	0.52
46:2o:26:GLU:OE1	46:2o:77:ARG:NH2	2.41	0.52
1:1A:880:G:N2	1:1A:898:C:N3	2.57	0.52
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.41	0.52
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.82	0.52
42:1k:48:ILE:O	42:1k:50:TYR:N	2.40	0.52
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.44	0.52
1:2A:1604:C:OP2	63:2A:3732:HOH:O	2.19	0.52
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.44	0.52
7:2H:26:VAL:O	7:2H:79:VAL:HG11	2.09	0.52
40:2i:14:VAL:HG23	40:2i:66:ARG:O	2.09	0.52
54:2w:12:U:H3	54:2w:23:A:N6	2.08	0.52
57:2y:9:A:H5'	57:2y:46:G7M:N3	2.24	0.52
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.09	0.52
1:1A:2101:G:H2'	1:1A:2102:U:C6	2.45	0.52
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.91	0.52
32:1a:279:A:H4'	32:1a:280:C:H5''	1.91	0.52
32:1a:460:G:H21	32:1a:472:A:H62	1.56	0.52
32:1a:1179:A:O3'	40:1i:103:THR:HB	2.10	0.52
1:2A:479:A:H4'	1:2A:480:A:OP1	2.10	0.52
1:2A:774:A:H2'	1:2A:774:A:N3	2.25	0.52
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.43	0.52
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.10	0.52
8:2I:72:LEU:HD23	8:2I:75:LEU:HD12	1.92	0.52
41:2j:40:LEU:HB2	41:2j:69:ASN:HB3	1.91	0.52
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.09	0.52
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.45	0.52
32:1a:1273:G:H3'	32:1a:1274:G:H8	1.75	0.52
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.77	0.52
57:1y:48:C:C5	57:1y:59:A:H5'	2.45	0.52
1:2A:994:C:O2'	1:2A:996:A:OP1	2.26	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1301:A:H2	1:2A:1626:G:N3	2.08	0.52
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.90	0.52
32:2a:148:G:H2'	32:2a:149:A:H8	1.74	0.52
32:2a:662:G:H2'	32:2a:663:A:C8	2.44	0.52
32:2a:939:G:H1	32:2a:1344:C:H42	1.57	0.52
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.41	0.52
36:2e:92:LYS:HB3	36:2e:119:LEU:HB2	1.92	0.52
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.45	0.52
10:1O:16:ALA:HB2	10:1O:52:VAL:HG21	1.91	0.52
15:1T:84:GLN:HG2	15:1T:85:LYS:HG3	1.91	0.52
32:1a:973:G:H3'	32:1a:974:A:H5''	1.92	0.52
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.45	0.52
1:2A:2124:G:N7	1:2A:2125:G:N2	2.51	0.52
32:2a:67:C:H2'	32:2a:68:G:H8	1.71	0.52
32:2a:1133:G:H2'	32:2a:1134:G:H8	1.74	0.52
36:2e:41:VAL:O	36:2e:66:MET:HA	2.09	0.52
57:2y:66:A:H2'	57:2y:67:C:O4'	2.09	0.52
1:1A:81:G:H21	20:1Y:1:MET:HE2	1.74	0.52
1:1A:191:A:H2'	1:1A:192:C:C6	2.45	0.52
1:1A:271(K):U:O2	8:1I:50:ARG:NH2	2.38	0.52
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.91	0.52
32:1a:21:G:H2'	32:1a:22:G:C8	2.45	0.52
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.45	0.52
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.42	0.52
10:2O:49:ARG:NH2	32:2a:1423:G:OP1	2.40	0.52
35:2d:59:ARG:NH1	35:2d:59:ARG:HA	2.25	0.52
46:2o:55:GLY:HA2	46:2o:58:MET:HE3	1.91	0.52
53:2v:23:A:H4'	53:2v:24:A:H5'	1.91	0.52
1:1A:1062:G:O5'	1:1A:1070:A:O2'	2.27	0.52
1:1A:2163:C:OP2	1:1A:2164:C:N4	2.42	0.52
1:1A:2406:U:O4	11:1P:70:GLN:NE2	2.38	0.52
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.44	0.52
8:1I:2:LYS:HB2	8:1I:2:LYS:HZ2	1.75	0.52
32:1a:381:C:H2'	32:1a:382:A:O4'	2.09	0.52
32:1a:977:A:O2'	32:1a:979:C:OP2	2.25	0.52
33:1b:19:HIS:NE2	33:1b:206:ASP:HB2	2.25	0.52
39:1h:73:ASP:OD1	39:1h:75:ARG:NE	2.43	0.52
1:2A:2172:U:H3'	1:2A:2173:A:H5'	1.92	0.52
2:2B:7:G:H2'	2:2B:8:U:O4'	2.10	0.52
5:2F:117:ARG:HH12	11:2P:1:MET:N	2.06	0.52
7:2H:108:GLY:O	7:2H:152:ARG:NH2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.24	0.52
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.24	0.52
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.10	0.52
1:1A:890:A:H2'	1:1A:892:G:O4'	2.10	0.51
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.42	0.51
4:1E:120:TRP:CE3	4:1E:155:LYS:HD3	2.45	0.51
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.08	0.51
32:1a:461:A:O2'	32:1a:470:C:H5'	2.11	0.51
32:1a:689:C:OP1	42:1k:27:ASN:ND2	2.39	0.51
32:2a:757:U:H2'	32:2a:758:G:O4'	2.10	0.51
32:2a:1235:U:O2'	32:2a:1305:G:O5'	2.28	0.51
45:2n:22:THR:HB	45:2n:33:VAL:HG11	1.90	0.51
54:2w:51:A:H61	54:2w:63:U:H3	0.64	0.51
1:1A:2135:A:N6	1:1A:2156:G:O2'	2.44	0.51
5:1F:33:LEU:HB3	11:1P:6:LEU:HD21	1.92	0.51
15:1T:127:ALA:C	15:1T:129:ARG:H	2.14	0.51
32:1a:1037:C:H2'	32:1a:1038:C:C6	2.44	0.51
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.92	0.51
1:2A:2286:A:OP1	28:26:29:ASN:ND2	2.43	0.51
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.38	0.51
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.10	0.51
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.42	0.51
32:2a:620:C:C2	35:2d:135:LEU:HG	2.45	0.51
54:2w:19:G:C2	54:2w:56:C:N3	2.78	0.51
1:1A:1568:G:H5'	3:1D:60:ARG:HA	1.92	0.51
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.10	0.51
4:1E:176:ILE:HB	4:1E:181:LEU:HB2	1.93	0.51
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.93	0.51
13:1R:2:ARG:HA	13:1R:5:LYS:HD2	1.92	0.51
32:1a:964:A:OP1	63:1a:1916:HOH:O	2.19	0.51
1:2A:272(B):G:H2'	1:2A:272(C):G:H8	1.75	0.51
19:2X:32:PRO:O	19:2X:77:LYS:NZ	2.41	0.51
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.46	0.51
32:2a:1353:G:H2'	32:2a:1354:C:C6	2.46	0.51
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.09	0.51
34:2c:156:ARG:H	34:2c:196:LEU:HD22	1.75	0.51
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.10	0.51
5:1F:135:LYS:HB2	5:1F:138:GLU:HG3	1.92	0.51
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.40	0.51
26:14:44:THR:O	26:14:47:GLN:HB2	2.11	0.51
40:1i:4:TYR:CG	40:1i:88:TYR:HB2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1805:U:O2	3:2D:50:THR:HB	2.10	0.51
3:2D:5:LYS:HG2	3:2D:17:THR:HG22	1.92	0.51
7:2H:143:GLN:HE21	7:2H:147:ASN:HD21	1.58	0.51
8:2I:14:ASP:N	8:2I:17:GLN:OE1	2.34	0.51
19:2X:2:LYS:NZ	19:2X:38:GLU:OE2	2.39	0.51
19:2X:50:LYS:N	19:2X:87:GLN:OE1	2.37	0.51
32:2a:390:C:H4'	47:2p:28:ARG:HH21	1.75	0.51
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.93	0.51
57:2y:67:C:H2'	57:2y:68:G:C8	2.45	0.51
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.46	0.51
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.11	0.51
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.25	0.51
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.45	0.51
32:1a:503:C:OP2	43:1l:116:SER:OG	2.18	0.51
33:1b:111:ARG:HB3	33:1b:149:LEU:HD11	1.92	0.51
35:1d:88:VAL:HA	36:1e:97:GLY:HA3	1.92	0.51
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	1.93	0.51
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.93	0.51
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.28	0.51
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.91	0.51
33:2b:198:ASP:N	33:2b:198:ASP:OD1	2.43	0.51
34:2c:162:GLN:NE2	53:2v:24:A:O2'	2.43	0.51
44:2m:10:PRO:HD2	44:2m:18:ALA:HB1	1.93	0.51
46:2o:56:LEU:O	46:2o:60:VAL:HG23	2.10	0.51
1:1A:409:C:OP1	63:1A:4140:HOH:O	2.19	0.51
1:1A:512:G:N1	63:1A:4225:HOH:O	2.34	0.51
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.92	0.51
32:1a:399:G:H2'	32:1a:400:C:C6	2.45	0.51
32:1a:865:A:C2	32:1a:918:A:H4'	2.43	0.51
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.25	0.51
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.92	0.51
38:1g:15:ASP:HB3	38:1g:24:THR:HG23	1.91	0.51
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.45	0.51
19:2X:84:ALA:HB3	19:2X:87:GLN:HG3	1.92	0.51
32:2a:570:G:H1'	32:2a:820:U:C4	2.45	0.51
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.45	0.51
32:2a:1137:C:O2	32:2a:1138:G:N2	2.43	0.51
32:2a:1274:G:H2'	32:2a:1275:A:H5''	1.93	0.51
43:2l:24:VAL:HB	43:2l:27:LEU:HG	1.93	0.51
57:2y:68:G:H2'	57:2y:69:A:O4'	2.10	0.51
1:1A:832:G:OP1	63:1A:4142:HOH:O	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:880:G:H2'	1:1A:881:G:C8	2.46	0.51
1:1A:2843:G:N7	63:1A:4231:HOH:O	2.35	0.51
32:1a:222:U:H2'	32:1a:223:U:C6	2.45	0.51
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.46	0.51
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.92	0.51
5:2F:20:LEU:HD23	5:2F:125:LEU:HD13	1.91	0.51
6:2G:46:ALA:HB2	6:2G:53:LEU:HD23	1.92	0.51
14:2S:80:LEU:O	14:2S:82:ILE:N	2.43	0.51
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.92	0.51
32:2a:824:C:H2'	32:2a:825:G:C8	2.45	0.51
32:2a:857:C:H2'	32:2a:858:G:O4'	2.11	0.51
32:2a:1049:U:OP1	45:2n:3:ARG:HB2	2.11	0.51
32:2a:1329:A:H5'	44:2m:29:ARG:NE	2.26	0.51
33:2b:47:THR:O	33:2b:51:LEU:N	2.44	0.51
34:2c:91:LEU:HD21	34:2c:101:LEU:HD23	1.92	0.51
40:2i:9:ARG:O	40:2i:104:ARG:HG3	2.11	0.51
42:2k:98:LEU:O	42:2k:101:SER:OG	2.24	0.51
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.46	0.51
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.76	0.51
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.11	0.51
8:1I:75:LEU:O	8:1I:141:LYS:NZ	2.37	0.51
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.76	0.51
32:1a:1023:G:H3'	32:1a:1024:G:C8	2.46	0.51
35:1d:74:GLN:O	35:1d:78:LEU:HG	2.11	0.51
49:1r:31:LEU:HD23	49:1r:31:LEU:H	1.75	0.51
1:2A:106:C:H1'	20:2Y:1:MET:HG3	1.92	0.51
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.29	0.51
1:2A:1649:G:O2'	13:2R:107:ASP:OD2	2.27	0.51
1:2A:2557:G:H2'	1:2A:2558:C:H6	1.76	0.51
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.91	0.51
32:2a:48:C:OP1	63:2a:1910:HOH:O	2.18	0.51
32:2a:838:G:H1	32:2a:848:C:H42	1.59	0.51
32:2a:972:C:O2'	41:2j:55:LYS:O	2.28	0.51
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.40	0.51
32:2a:1271:G:C2	32:2a:1272:G:N7	2.78	0.51
32:2a:1316:G:H22	32:2a:1319:A:H5''	1.76	0.51
34:2c:34:LEU:HD11	34:2c:38:ARG:HH21	1.75	0.51
34:2c:124:ILE:HG21	34:2c:130:VAL:HG13	1.92	0.51
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.93	0.51
4:1E:67:PHE:HE1	4:1E:75:VAL:HG22	1.75	0.51
32:1a:672:U:O2'	32:1a:673:G:O5'	2.27	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1191:A:OP2	34:1c:3:ASN:ND2	2.44	0.51
16:2U:79:PHE:CZ	16:2U:83:LEU:HD11	2.46	0.51
32:2a:913:A:OP1	43:2l:46:LYS:NZ	2.43	0.51
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.46	0.51
35:2d:109:GLY:HA3	35:2d:165:MET:HG3	1.93	0.51
37:2f:83:ASP:N	37:2f:83:ASP:OD1	2.44	0.51
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.92	0.51
1:1A:1174:A:H1'	1:1A:1175:U:H5''	1.92	0.51
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.39	0.51
33:1b:64:ARG:HB2	33:1b:64:ARG:HH11	1.76	0.51
34:1c:172:ARG:NH2	34:1c:206:GLU:OE2	2.45	0.51
19:2X:94:GLY:CA	19:2X:95:LEU:HB2	2.41	0.51
32:2a:417:C:H2'	32:2a:418:C:C6	2.46	0.51
32:2a:1327:C:OP1	52:2u:12:LYS:NZ	2.39	0.51
34:2c:18:TRP:HB2	34:2c:21:ARG:HG2	1.93	0.51
48:2q:12:SER:HB3	48:2q:20:THR:HB	1.93	0.51
1:1A:184:C:H2'	1:1A:185:U:C6	2.46	0.50
1:1A:800:A:H8	1:1A:800:A:OP1	1.94	0.50
1:1A:1176:G:H4'	1:1A:1177:A:OP1	2.11	0.50
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.40	0.50
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.45	0.50
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.24	0.50
32:1a:1246:C:H42	32:1a:1291:G:H1	1.59	0.50
35:1d:65:ARG:HG3	35:1d:70:ILE:HG23	1.92	0.50
1:2A:30:G:H2'	1:2A:31:C:C6	2.46	0.50
1:2A:153:C:H2'	1:2A:154:G:O4'	2.10	0.50
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.46	0.50
1:2A:2320:A:H1'	1:2A:2321:G:C2	2.46	0.50
2:2B:24:G:H4'	2:2B:25:A:C8	2.46	0.50
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.92	0.50
32:2a:397:A:N7	32:2a:547:A:O2'	2.39	0.50
32:2a:1258:G:H2'	32:2a:1259:C:C6	2.46	0.50
33:2b:58:ILE:HA	33:2b:61:LEU:HB3	1.94	0.50
43:2l:117:ARG:HB3	43:2l:122:THR:HB	1.93	0.50
54:2w:13:C:N3	54:2w:22:G:O6	2.44	0.50
55:2x:40:C:H2'	55:2x:41:C:C6	2.46	0.50
1:1A:796:C:H2'	1:1A:797:C:C6	2.47	0.50
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.11	0.50
28:16:26:ASN:HD21	28:16:28:ARG:NH2	2.08	0.50
32:1a:1150:U:H4'	41:1j:41:PRO:HG3	1.94	0.50
36:1e:11:ILE:HB	36:1e:31:LEU:HD12	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1q:57:VAL:HG12	48:1q:76:LEU:HD12	1.93	0.50
49:1r:58:LEU:HB3	49:1r:62:GLU:HB2	1.93	0.50
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.10	0.50
1:2A:1815:A:OP2	3:2D:54:ARG:NH2	2.43	0.50
2:2B:15:A:OP2	2:2B:69:G:N2	2.44	0.50
38:2g:69:VAL:HG11	38:2g:134:ALA:HB1	1.93	0.50
42:2k:33:THR:HA	42:2k:39:PRO:HA	1.91	0.50
57:2y:26:A:H5'	57:2y:27:G:OP2	2.11	0.50
1:1A:248:G:OP1	63:1A:4141:HOH:O	2.19	0.50
1:1A:360:G:H2'	1:1A:361:G:O4'	2.11	0.50
1:1A:1062:G:C5'	1:1A:1070:A:HO2'	2.23	0.50
1:1A:1359:A:C2	1:1A:1372:U:O4	2.64	0.50
1:1A:2573:C:H3'	63:1A:4171:HOH:O	2.11	0.50
21:1Z:158:PRO:O	21:1Z:161:VAL:HG22	2.12	0.50
23:11:65:SER:OG	23:11:66:HIS:ND1	2.31	0.50
32:1a:1220:G:N2	50:1s:54:GLY:O	2.42	0.50
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.29	0.50
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.93	0.50
1:2A:574:C:OP1	63:2A:3731:HOH:O	2.18	0.50
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.33	0.50
6:2G:4:ASP:HA	6:2G:8:LYS:NZ	2.27	0.50
6:2G:112:PRO:HG3	26:24:43:TYR:HE1	1.75	0.50
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	1.93	0.50
11:2P:59:LEU:HD11	30:28:10:ALA:HA	1.93	0.50
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.47	0.50
32:2a:1244:C:H42	32:2a:1293:G:H1	1.59	0.50
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.93	0.50
47:2p:8:ARG:HB3	47:2p:28:ARG:NH1	2.27	0.50
19:1X:1:MET:HE1	24:12:26:ARG:NH2	2.25	0.50
32:1a:377:G:OP1	47:1p:5:ARG:HD2	2.12	0.50
32:1a:636:U:H2'	32:1a:637:G:C8	2.44	0.50
32:1a:1040:U:H2'	32:1a:1041:A:H8	1.76	0.50
32:1a:1086:U:H3	32:1a:1099:G:H22	1.58	0.50
32:1a:1226:C:H4'	50:1s:80:TYR:OH	2.12	0.50
33:1b:82:ARG:HD2	33:1b:92:TYR:OH	2.12	0.50
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.27	0.50
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.45	0.50
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.12	0.50
1:2A:2794:C:N4	1:2A:2802:G:O6	2.44	0.50
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.92	0.50
23:21:80:LEU:HD23	23:21:82:LEU:HD21	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:450:G:H4'	47:2p:41:PRO:HB2	1.94	0.50
32:2a:1064:G:OP1	32:2a:1386:G:H4'	2.12	0.50
32:2a:1316:G:H5'	32:2a:1360:A:H1'	1.94	0.50
32:2a:1403:C:H2'	32:2a:1404:5MC:HM53	1.92	0.50
1:1A:55:G:O2'	1:1A:127:A:N1	2.41	0.50
1:1A:1168:G:H1	1:1A:1181:C:H42	1.60	0.50
18:1W:97:LYS:HE2	18:1W:99:ARG:NH2	2.27	0.50
32:1a:159:G:O2'	32:1a:161:A:N7	2.32	0.50
32:1a:1309:G:OP2	44:1m:99:ARG:NH2	2.37	0.50
48:1q:66:SER:H	48:1q:69:LYS:HB3	1.77	0.50
1:2A:2130:U:H2'	1:2A:2158:A:N6	2.25	0.50
19:2X:90:GLU:C	19:2X:92:LEU:H	2.20	0.50
32:2a:142:G:H2'	32:2a:143:A:H8	1.77	0.50
32:2a:1095:U:P	32:2a:1108:G:H1	2.34	0.50
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.16	0.50
33:2b:95:GLN:HB3	33:2b:148:TYR:CD1	2.47	0.50
46:2o:87:ILE:O	46:2o:88:ARG:HB3	2.10	0.50
49:2r:48:GLY:O	49:2r:74:ARG:NH2	2.45	0.50
1:1A:764:A:H5''	3:1D:210:GLY:CA	2.41	0.50
12:1Q:10:ARG:HH12	12:1Q:90:VAL:H	1.60	0.50
32:1a:222:U:H2'	32:1a:223:U:H6	1.77	0.50
40:1i:33:PHE:CZ	40:1i:47:LEU:HD11	2.46	0.50
57:1y:15:G:H2'	57:1y:59:A:C2	2.46	0.50
57:1y:25:C:H42	57:1y:45:G:N2	2.04	0.50
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.12	0.50
2:2B:115:G:H2'	2:2B:116:G:O4'	2.11	0.50
7:2H:26:VAL:HG12	7:2H:79:VAL:HG21	1.92	0.50
12:2Q:43:THR:HG22	12:2Q:94:VAL:HG12	1.94	0.50
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.37	0.50
32:2a:419:C:OP1	32:2a:513:C:O2'	2.25	0.50
32:2a:532:A:N1	34:2c:156:ARG:NH1	2.56	0.50
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.46	0.50
2:1B:11:C:H3'	2:1B:12:C:C6	2.46	0.50
32:1a:15:G:H1'	36:1e:19:MET:HE2	1.93	0.50
32:1a:664:G:N2	32:1a:741:G:H1	2.01	0.50
32:1a:1025:U:C2	32:1a:1036:G:O6	2.65	0.50
33:1b:12:GLU:O	33:1b:14:GLY:N	2.39	0.50
1:2A:82:G:N1	1:2A:103:A:OP2	2.38	0.50
1:2A:272(B):G:H2'	1:2A:272(C):G:C8	2.46	0.50
1:2A:896:A:O2'	54:2w:56:C:H5'	2.12	0.50
1:2A:933:A:OP1	25:23:24:LYS:NZ	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:1:MET:H3	24:22:29:LYS:HE3	1.77	0.50
26:24:44:THR:O	26:24:46:GLN:N	2.44	0.50
35:2d:50:ARG:HH12	36:2e:10:MET:HE3	1.75	0.50
36:2e:78:HIS:CE1	36:2e:142:LEU:HD23	2.47	0.50
54:2w:54:5MU:HN3	54:2w:58:A:H8	1.59	0.50
1:1A:805:G:OP2	11:1P:41:ARG:HD2	2.11	0.50
3:1D:166:GLN:HB2	3:1D:174:ILE:HG22	1.93	0.50
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.93	0.50
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.12	0.50
32:1a:57:G:H2'	32:1a:58:C:C6	2.47	0.50
40:1i:50:LEU:HG	40:1i:81:ILE:HD11	1.93	0.50
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.12	0.50
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.28	0.50
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.41	0.50
32:2a:1172:C:H2'	32:2a:1173:G:C8	2.47	0.50
34:2c:6:HIS:HB3	45:2n:49:HIS:CD2	2.47	0.50
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.12	0.50
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.11	0.50
4:1E:77:ILE:HD13	4:1E:195:LEU:HD13	1.92	0.50
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.12	0.50
32:1a:555:C:H2'	32:1a:556:C:C6	2.47	0.50
32:1a:911:U:H2'	32:1a:912:C:C6	2.47	0.50
44:1m:20:THR:C	44:1m:22:ILE:H	2.19	0.50
57:1y:35:U:H2'	57:1y:36:U:C6	2.47	0.50
1:2A:288:C:H2'	1:2A:289:A:H8	1.76	0.50
26:24:45:GLY:C	26:24:47:GLN:H	2.19	0.50
32:2a:1347:G:HO2'	32:2a:1373:G:H1	1.59	0.50
33:2b:15:VAL:HG22	33:2b:209:ARG:HD2	1.94	0.50
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.12	0.50
7:1H:133:VAL:HG21	7:1H:145:ALA:HB2	1.93	0.49
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.47	0.49
32:1a:1273:G:C2	32:1a:1274:G:H1'	2.47	0.49
39:1h:95:VAL:HB	39:1h:99:GLU:HB2	1.94	0.49
57:1y:12:U:H2'	57:1y:13:C:O4'	2.12	0.49
1:2A:189:G:O6	1:2A:205:G:O2'	2.27	0.49
1:2A:2136:C:N3	1:2A:2155:G:N2	2.60	0.49
32:2a:1207:2MG:O2'	32:2a:1208:C:H5'	2.12	0.49
33:2b:55:PHE:CZ	33:2b:218:ALA:HA	2.47	0.49
36:2e:83:GLU:HA	36:2e:88:LYS:HA	1.93	0.49
51:2t:56:MET:HE3	51:2t:85:MET:HG2	1.93	0.49
1:1A:848:G:H2'	1:1A:849:A:C8	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.12	0.49
1:1A:2364:C:OP1	22:10:55:ARG:NH1	2.45	0.49
1:1A:2384:G:O6	63:1A:4137:HOH:O	2.17	0.49
5:1F:32:LEU:HB3	5:1F:112:MET:HE1	1.94	0.49
14:1S:15:ARG:HE	14:1S:88:ASP:CG	2.19	0.49
26:14:15:ILE:HG12	26:14:21:VAL:HG22	1.93	0.49
57:1y:52:G:H2'	57:1y:53:G:O4'	2.11	0.49
1:2A:335:C:H4'	20:2Y:73:ARG:HD2	1.95	0.49
1:2A:572:A:OP2	17:2V:78:LYS:NZ	2.45	0.49
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.45	0.49
28:26:23:THR:OG1	28:26:24:GLU:N	2.41	0.49
33:2b:16:HIS:O	33:2b:18:GLY:N	2.43	0.49
37:2f:28:ARG:HA	37:2f:31:GLU:HG2	1.94	0.49
54:2w:51:A:N7	54:2w:64:G:H2'	2.26	0.49
54:2w:54:5MU:H2'	54:2w:55:PSU:C6	2.47	0.49
1:1A:839:U:H2'	1:1A:840:C:C6	2.46	0.49
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.45	0.49
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.94	0.49
24:12:55:ARG:NH2	63:12:201:HOH:O	2.32	0.49
28:16:12:GLU:OE1	28:16:52:VAL:HG11	2.12	0.49
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.75	0.49
1:2A:455:C:N3	1:2A:472:A:H2'	2.28	0.49
1:2A:1927:A:H2'	1:2A:1928:A:C8	2.47	0.49
2:2B:92:C:H5''	21:2Z:79:ARG:HH22	1.77	0.49
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.41	0.49
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.12	0.49
6:2G:60:LEU:HD22	6:2G:68:PRO:HG3	1.93	0.49
25:23:6:VAL:HG13	25:23:54:VAL:HG13	1.95	0.49
36:2e:31:LEU:HD22	36:2e:43:LEU:HD11	1.95	0.49
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.46	0.49
57:2y:11:C:N4	57:2y:24:G:H1	2.10	0.49
1:1A:2572:A:N7	4:1E:145:LYS:HB2	2.27	0.49
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.12	0.49
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.93	0.49
8:1I:81:VAL:N	8:1I:145:VAL:O	2.32	0.49
15:1T:29:ARG:HG3	15:1T:46:GLU:HB3	1.93	0.49
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.46	0.49
1:2A:300:A:P	20:2Y:86:ARG:HH12	2.36	0.49
1:2A:302:C:OP2	20:2Y:73:ARG:NH1	2.45	0.49
1:2A:911:A:N6	12:2Q:11:LYS:O	2.41	0.49
1:2A:1359:A:H2	1:2A:1372:U:O4	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.47	0.49
7:2H:103:LEU:HD23	7:2H:123:PHE:CD2	2.47	0.49
10:2O:112:MET:N	10:2O:112:MET:SD	2.86	0.49
16:2U:81:HIS:HD2	16:2U:84:LYS:HD3	1.76	0.49
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.12	0.49
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.30	0.49
32:2a:142:G:H2'	32:2a:143:A:C8	2.47	0.49
32:2a:661:G:H1	32:2a:744:C:H42	1.61	0.49
32:2a:1320:C:H1'	50:2s:73:GLU:HG3	1.94	0.49
33:2b:51:LEU:HA	33:2b:54:THR:OG1	2.13	0.49
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.47	0.49
44:2m:25:ILE:HD11	44:2m:66:LEU:HD13	1.94	0.49
1:1A:207:A:H2'	1:1A:208:C:O4'	2.12	0.49
1:1A:784:A:OP2	63:1A:4143:HOH:O	2.20	0.49
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.76	0.49
2:1B:14:U:O2	2:1B:108:U:H4'	2.13	0.49
8:1I:101:LEU:HD22	8:1I:107:VAL:HB	1.94	0.49
15:1T:57:PHE:HA	15:1T:79:HIS:HD2	1.77	0.49
24:12:41:ILE:HG13	24:12:43:GLN:HG3	1.94	0.49
32:1a:110:C:O2'	47:1p:25:ARG:O	2.23	0.49
32:1a:1346:A:O2'	38:1g:10:ARG:NH2	2.46	0.49
1:2A:479:A:N3	1:2A:481:G:H5''	2.27	0.49
1:2A:877:U:O2'	1:2A:900:A:N6	2.45	0.49
1:2A:902:C:H2'	1:2A:903:C:C6	2.48	0.49
32:2a:1122:U:N3	32:2a:1123:A:N7	2.60	0.49
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.94	0.49
38:2g:23:VAL:HG13	38:2g:43:PHE:CE2	2.48	0.49
1:1A:226:G:H21	1:1A:228:A:H62	1.60	0.49
2:1B:11:C:H3'	2:1B:12:C:H6	1.78	0.49
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.95	0.49
32:1a:601:C:H2'	32:1a:602:A:C8	2.48	0.49
32:1a:1201:A:H4'	32:1a:1202:G:O5'	2.12	0.49
36:1e:85:GLY:O	36:1e:87:SER:N	2.45	0.49
38:1g:79:ARG:CZ	38:1g:80:VAL:HG22	2.43	0.49
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.78	0.49
57:1y:53:G:H1	57:1y:61:C:H42	1.61	0.49
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.12	0.49
1:2A:910:A:N1	1:2A:2277:G:H1'	2.28	0.49
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.47	0.49
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.48	0.49
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.27	0.49
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.48	0.49
2:2B:2:C:H2'	2:2B:3:C:C6	2.46	0.49
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.94	0.49
32:2a:865:A:H5'	32:2a:1078:U:H5	1.76	0.49
32:2a:986:A:N3	50:2s:52:TYR:OH	2.44	0.49
33:2b:79:ASP:O	33:2b:82:ARG:HG2	2.11	0.49
33:2b:175:ARG:HB3	33:2b:175:ARG:CZ	2.41	0.49
53:2v:22:U:H2'	53:2v:23:A:H8	1.78	0.49
1:1A:228:A:H8	1:1A:229:A:H5'	1.78	0.49
1:1A:579:G:H2'	1:1A:580:C:C6	2.48	0.49
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.94	0.49
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.37	0.49
32:1a:487:A:H2'	32:1a:488:C:O4'	2.12	0.49
33:1b:36:ARG:O	33:1b:38:GLY:N	2.46	0.49
35:1d:122:ARG:HD2	35:1d:122:ARG:HA	1.58	0.49
54:1w:53:G:H1	54:1w:61:C:H42	1.61	0.49
54:1w:61:C:H3'	54:1w:62:C:H5''	1.95	0.49
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.48	0.49
1:2A:2136:C:O2'	1:2A:2137:C:O4'	2.31	0.49
7:2H:116:GLU:HG3	7:2H:117:PRO:HD2	1.94	0.49
32:2a:660:G:H1	32:2a:745:C:H42	1.61	0.49
32:2a:953:G:H5'	32:2a:965:A:N6	2.26	0.49
32:2a:1135:U:H2'	32:2a:1137:C:N3	2.28	0.49
33:2b:73:THR:O	33:2b:73:THR:OG1	2.23	0.49
34:2c:190:ARG:NE	34:2c:190:ARG:O	2.46	0.49
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.46	0.49
37:2f:100:ASN:HD21	49:2r:23:LYS:HE3	1.76	0.49
40:2i:4:TYR:CZ	40:2i:88:TYR:HD1	2.31	0.49
50:2s:33:THR:H	50:2s:57:HIS:CE1	2.21	0.49
1:1A:1580:A:OP2	1:1A:1580:A:H8	1.95	0.49
7:1H:3:ARG:HH22	7:1H:66:GLY:HA3	1.77	0.49
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.46	0.49
46:1o:70:LEU:HD11	46:1o:77:ARG:HB3	1.94	0.49
49:1r:37:VAL:HG22	49:1r:78:LEU:HB3	1.94	0.49
1:2A:2299:G:N1	1:2A:2318:G:N7	2.60	0.49
28:26:14:THR:OG1	28:26:48:VAL:O	2.31	0.49
32:2a:533:A:O2'	32:2a:535:A:OP2	2.26	0.49
32:2a:1004:A:N3	32:2a:1038:C:C2	2.81	0.49
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.12	0.49
32:2a:1323:G:HO2'	32:2a:1362:C:HO2'	1.56	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:43:VAL:HG22	7:1H:52:VAL:HG22	1.94	0.49
32:1a:7:G:H5'	32:1a:298:A:O4'	2.12	0.49
32:1a:189(F):U:O2	48:1q:63:ARG:NH2	2.46	0.49
32:1a:1039:C:H2'	32:1a:1040:U:H6	1.76	0.49
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.95	0.49
54:1w:18:G:H21	54:1w:57:G:H2'	1.77	0.49
57:1y:47:U:H2'	57:1y:50:C:OP1	2.13	0.49
1:2A:99:U:H4'	1:2A:100:G:H5'	1.94	0.49
6:2G:44:GLY:N	6:2G:88:ILE:O	2.46	0.49
6:2G:166:ASP:O	6:2G:170:ARG:N	2.44	0.49
32:2a:1060:C:O2'	41:2j:56:HIS:ND1	2.42	0.49
32:2a:1071:C:H2'	32:2a:1072:G:H8	1.77	0.49
35:2d:201:GLN:HE21	36:2e:99:GLY:HA2	1.77	0.49
38:2g:105:VAL:O	38:2g:109:ASN:ND2	2.42	0.49
47:2p:26:ARG:HG3	47:2p:27:LYS:O	2.13	0.49
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.78	0.49
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.48	0.49
20:1Y:5:MET:HE3	20:1Y:30:VAL:HG13	1.94	0.49
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.48	0.49
41:1j:65:LEU:HB2	45:1n:56:VAL:HG13	1.93	0.49
1:2A:839:U:H2'	1:2A:840:C:C6	2.48	0.49
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.47	0.49
3:2D:71:ASP:CB	3:2D:103:ARG:HH12	2.26	0.49
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.46	0.49
6:2G:25:TYR:CD1	6:2G:30:GLU:HB3	2.48	0.49
8:2I:61:ARG:O	8:2I:65:ALA:N	2.44	0.49
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.48	0.49
32:2a:35:G:O2'	43:2l:118:SER:O	2.28	0.49
32:2a:736:C:H2'	32:2a:737:A:H8	1.77	0.49
33:2b:16:HIS:C	33:2b:18:GLY:H	2.20	0.49
38:2g:22:LEU:HG	38:2g:62:PHE:CE2	2.48	0.49
1:1A:760:G:OP1	63:1A:4147:HOH:O	2.20	0.48
1:1A:1038:C:H42	1:1A:1117:G:H1	1.61	0.48
1:1A:1070:A:N7	1:1A:1096:A:H2'	2.28	0.48
1:1A:2131:G:N2	1:1A:2158:A:N1	2.58	0.48
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.38	0.48
57:1y:25:C:N4	57:1y:45:G:H21	2.09	0.48
12:2Q:57:HIS:CE1	12:2Q:116:GLU:HG2	2.48	0.48
32:2a:412:A:O4'	35:2d:35:ARG:NH2	2.46	0.48
32:2a:1012:U:H2'	32:2a:1013:G:C8	2.48	0.48
32:2a:1015:A:H2'	32:2a:1016:A:C8	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.48	0.48
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.47	0.48
33:2b:16:HIS:CE1	33:2b:42:ILE:HD12	2.48	0.48
55:2x:23:C:H2'	55:2x:24:U:C6	2.48	0.48
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.48	0.48
1:1A:458:G:O2'	1:1A:469:G:O6	2.31	0.48
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.29	0.48
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.78	0.48
1:1A:2170:A:H8	1:1A:2170:A:O5'	1.96	0.48
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.48	0.48
1:1A:2765:A:OP2	63:1A:4145:HOH:O	2.20	0.48
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.12	0.48
15:1T:127:ALA:C	15:1T:129:ARG:N	2.71	0.48
26:14:58:ARG:HG2	50:1s:68:GLY:H	1.78	0.48
32:1a:67:C:H2'	32:1a:68:G:C8	2.48	0.48
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.13	0.48
37:1f:50:TYR:OH	49:1r:74:ARG:O	2.30	0.48
38:1g:46:ALA:O	38:1g:50:ILE:N	2.46	0.48
1:2A:80:G:H1	1:2A:106:C:H42	1.61	0.48
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.48	0.48
1:2A:2119:A:N1	1:2A:2170:A:H2'	2.28	0.48
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.96	0.48
1:2A:2319:G:N2	14:2S:3:ARG:HH11	2.06	0.48
1:2A:2320:A:H1'	1:2A:2321:G:N2	2.28	0.48
32:2a:595:G:H1'	32:2a:596:C:H5	1.77	0.48
32:2a:619:U:C4	35:2d:135:LEU:HD11	2.48	0.48
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.28	0.48
32:2a:1079:G:O3'	36:2e:14:ARG:NH2	2.46	0.48
41:2j:7:LYS:HG3	41:2j:70:ARG:O	2.13	0.48
41:2j:21:GLN:HE22	41:2j:25:GLU:HG2	1.78	0.48
44:2m:4:ILE:HG23	44:2m:22:ILE:HD11	1.94	0.48
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.48	0.48
48:2q:4:LYS:HE2	48:2q:6:LEU:HD21	1.95	0.48
54:2w:29:U:H2'	54:2w:30:G:C8	2.48	0.48
1:1A:2124:G:H1	1:1A:2174:C:N4	2.10	0.48
1:1A:2298:A:H2'	1:1A:2299:G:O4'	2.14	0.48
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.28	0.48
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.13	0.48
7:1H:45:VAL:HG22	7:1H:50:VAL:HG22	1.94	0.48
32:1a:559:A:H4'	32:1a:560:U:H5''	1.94	0.48
32:1a:584:G:H5'	48:1q:91:ARG:NH2	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.95	0.48
1:2A:2163:C:H3'	1:2A:2164:C:C6	2.48	0.48
2:2B:14:U:OP2	2:2B:70:C:O2'	2.28	0.48
6:2G:112:PRO:HG3	26:24:43:TYR:CE1	2.48	0.48
10:2O:71:ARG:NE	10:2O:105:GLU:OE2	2.45	0.48
32:2a:109:A:C6	32:2a:326:G:C6	3.02	0.48
32:2a:643:C:H2'	32:2a:644:G:H8	1.79	0.48
32:2a:1123:A:H4'	41:2j:37:PRO:HD2	1.95	0.48
39:2h:84:ARG:NH1	39:2h:86:ILE:HD13	2.28	0.48
43:2l:57:LYS:HG2	43:2l:67:THR:HB	1.94	0.48
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.95	0.48
32:1a:17:U:H2'	32:1a:18:C:C6	2.49	0.48
32:1a:616:G:O2'	32:1a:617:G:H5'	2.13	0.48
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.49	0.48
34:1c:44:GLU:HA	34:1c:52:LEU:HD23	1.95	0.48
4:2E:170:LEU:HD22	4:2E:185:LYS:O	2.13	0.48
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.14	0.48
25:23:59:VAL:HG12	25:23:60:GLU:H	1.78	0.48
32:2a:736:C:H2'	32:2a:737:A:C8	2.48	0.48
32:2a:859:A:H2'	32:2a:860:A:O4'	2.13	0.48
32:2a:1272:G:N2	32:2a:1273:G:C6	2.81	0.48
57:2y:14:A:H2'	57:2y:15:G:C8	2.48	0.48
57:2y:65:C:N3	57:2y:66:A:N6	2.61	0.48
1:1A:1720:U:H2'	1:1A:1721:G:O4'	2.13	0.48
1:1A:2118:U:H5	1:1A:2148:G:N3	2.11	0.48
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.48	0.48
32:1a:431:A:H2'	32:1a:432:A:O4'	2.13	0.48
32:1a:512:U:H2'	32:1a:513:C:C6	2.49	0.48
33:1b:160:ASP:OD1	33:1b:160:ASP:N	2.46	0.48
42:1k:48:ILE:HD12	42:1k:63:LEU:HB2	1.94	0.48
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.13	0.48
30:28:26:LYS:HD2	30:28:48:PHE:CD2	2.48	0.48
32:2a:107:G:H2'	32:2a:108:G:O4'	2.14	0.48
33:2b:120:ALA:O	33:2b:125:PRO:HG2	2.13	0.48
34:2c:9:GLY:N	45:2n:49:HIS:O	2.47	0.48
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	1.95	0.48
38:2g:78:ARG:HE	38:2g:79:ARG:NE	2.10	0.48
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.94	0.48
1:1A:1268:A:C2	1:1A:2013:A:C4	3.02	0.48
2:1B:78:A:C2	2:1B:100:A:C4	3.01	0.48
6:1G:66:GLN:NE2	6:1G:93:THR:O	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:103:ARG:HH12	13:1R:110:PRO:HD3	1.77	0.48
30:18:52:LYS:N	30:18:53:PRO:HD2	2.29	0.48
32:1a:148:G:H2'	32:1a:149:A:C8	2.48	0.48
32:1a:1118:C:H1'	32:1a:1179:A:C5	2.49	0.48
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.48	0.48
35:1d:121:VAL:HG22	35:1d:126:ILE:HG13	1.95	0.48
35:1d:124:GLY:C	35:1d:126:ILE:H	2.20	0.48
49:1r:52:PRO:HB2	49:1r:54:ARG:HG3	1.94	0.48
57:1y:71:C:O2'	57:1y:72:C:H5'	2.13	0.48
1:2A:288:C:H2'	1:2A:289:A:C8	2.49	0.48
1:2A:307:G:H21	1:2A:330:A:H62	1.61	0.48
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.14	0.48
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.49	0.48
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	1.97	0.48
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.13	0.48
12:2Q:37:LEU:HD11	12:2Q:130:LYS:HB2	1.95	0.48
32:2a:1261:A:H5'	32:2a:1283:G:O3'	2.13	0.48
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.48	0.48
37:2f:61:LEU:HB3	37:2f:63:TYR:CE2	2.43	0.48
37:2f:99:ALA:HB3	49:2r:29:PHE:CE1	2.41	0.48
1:1A:1069:A:H4'	1:1A:1070:A:H5''	1.96	0.48
32:1a:79:G:H1	32:1a:90:U:H3	1.60	0.48
32:1a:1239:A:H62	32:1a:1299:A:N6	2.12	0.48
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.14	0.48
57:1y:23:A:H2'	57:1y:24:G:C8	2.49	0.48
1:2A:614(B):G:N3	5:2F:44:ARG:HD2	2.29	0.48
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	1.95	0.48
26:24:59:PHE:CE2	50:2s:64:GLU:HB2	2.49	0.48
32:2a:555:C:H2'	32:2a:556:C:C6	2.49	0.48
32:2a:560:U:H5'	32:2a:566:G:N2	2.29	0.48
32:2a:1326:C:H2'	32:2a:1327:C:C6	2.49	0.48
50:2s:51:VAL:HB	50:2s:75:ALA:HB2	1.94	0.48
52:2u:6:ARG:HA	52:2u:11:GLY:HA3	1.95	0.48
6:1G:179:PRO:HG3	26:14:43:TYR:CZ	2.49	0.48
36:1e:85:GLY:C	36:1e:87:SER:H	2.21	0.48
37:1f:55:ASP:HB2	37:1f:86:ARG:HH12	1.79	0.48
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.78	0.48
48:1q:31:LEU:HD23	48:1q:32:TYR:CZ	2.49	0.48
1:2A:586:A:N1	1:2A:809:G:O2'	2.43	0.48
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.94	0.48
2:2B:86:G:H1	2:2B:91:C:H42	1.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:48:GLN:HE21	4:2E:78:LEU:HD22	1.79	0.48
10:2O:76:ALA:O	15:2T:74:ARG:HG3	2.14	0.48
26:24:1:MET:HE2	26:24:6:HIS:CD2	2.49	0.48
32:2a:539:A:H2'	32:2a:540:G:C8	2.48	0.48
35:2d:36:ARG:HD2	35:2d:38:TYR:OH	2.14	0.48
50:2s:30:LEU:HA	50:2s:48:THR:O	2.13	0.48
54:2w:19:G:N7	54:2w:57:G:N2	2.61	0.48
1:1A:2590:A:H2'	1:1A:2591:C:C6	2.48	0.48
21:1Z:54:HIS:HD2	21:1Z:99:TYR:O	1.97	0.48
21:1Z:156:LYS:O	21:1Z:157:LEU:HB2	2.14	0.48
32:1a:1035:A:N3	32:1a:1036:G:N2	2.62	0.48
1:2A:2390:U:P	30:28:35:GLN:HE22	2.36	0.48
2:2B:80:U:H2'	2:2B:81:G:C8	2.48	0.48
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.79	0.48
4:2E:29:GLY:H	4:2E:180:ASN:HB3	1.77	0.48
5:2F:11:VAL:HG22	5:2F:125:LEU:HD12	1.96	0.48
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.13	0.48
6:2G:15:VAL:HG21	6:2G:176:LEU:HD23	1.94	0.48
30:28:22:VAL:HG12	30:28:50:LEU:HD12	1.96	0.48
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.77	0.48
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.29	0.48
32:2a:1371:G:O3'	40:2i:69:GLY:HA3	2.13	0.48
41:2j:50:ILE:HD11	41:2j:57:LYS:HD2	1.94	0.48
49:2r:31:LEU:HD23	49:2r:31:LEU:H	1.79	0.48
51:2t:29:LYS:O	51:2t:33:ILE:HD12	2.13	0.48
55:2x:15:G:H2'	55:2x:59:A:N1	2.28	0.48
1:1A:1047:G:H2'	1:1A:1110:G:N1	2.28	0.48
1:1A:1342:A:O2'	1:1A:1344:G:OP2	2.22	0.48
32:1a:97:G:H2'	32:1a:98:G:O4'	2.13	0.48
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.96	0.48
51:1t:99:LEU:HA	51:1t:100:ILE:O	2.14	0.48
1:2A:652(A):A:H3'	1:2A:652(B):A:H5''	1.95	0.48
1:2A:2033:A:O2'	1:2A:2035:G:OP2	2.24	0.48
10:2O:119:PRO:HB2	15:2T:68:TYR:CE2	2.48	0.48
12:2Q:85:LYS:HB2	22:20:7:LEU:HD12	1.96	0.48
32:2a:328:C:H4'	32:2a:329:A:H5'	1.95	0.48
37:2f:67:MET:HE3	37:2f:72:VAL:HG22	1.94	0.48
43:2l:79:GLU:HG2	43:2l:80:HIS:CD2	2.49	0.48
1:1A:747:U:O2	1:1A:2014:A:H1'	2.14	0.47
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.29	0.47
1:1A:2028:U:H2'	1:1A:2029:G:O4'	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2335:A:C8	1:1A:2337:G:C5	3.02	0.47
2:1B:2:C:H2'	2:1B:3:C:C6	2.49	0.47
3:1D:141:VAL:HG13	3:1D:162:SER:HB2	1.96	0.47
4:1E:97:LYS:N	4:1E:100:GLU:OE2	2.26	0.47
22:10:18:ALA:HB3	22:10:20:ARG:NH1	2.29	0.47
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.30	0.47
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.47	0.47
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.49	0.47
6:2G:53:LEU:HD12	6:2G:56:ALA:H	1.78	0.47
8:2I:8:PRO:HD3	8:2I:15:VAL:HB	1.95	0.47
11:2P:2:LYS:HG2	11:2P:4:SER:H	1.78	0.47
21:2Z:91:LEU:HD12	21:2Z:96:VAL:HG21	1.95	0.47
32:2a:302:G:N3	32:2a:556:C:H4'	2.28	0.47
32:2a:978:A:O2'	32:2a:1322:C:N3	2.44	0.47
33:2b:77:ALA:O	33:2b:94:ASN:ND2	2.47	0.47
17:1V:24:LYS:HE2	17:1V:24:LYS:HB3	1.72	0.47
32:1a:625:G:H4'	47:1p:16:HIS:CG	2.49	0.47
32:1a:995:C:O2	45:1n:4:LYS:NZ	2.33	0.47
39:1h:19:VAL:HG23	39:1h:21:LYS:HG3	1.95	0.47
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.97	0.47
57:1y:72:C:H2'	57:1y:73:A:O4'	2.15	0.47
1:2A:959:A:N3	1:2A:2457:U:O2'	2.44	0.47
1:2A:1747(A):G:H2'	1:2A:1748:G:H8	1.79	0.47
1:2A:2070:G:H2'	1:2A:2071:A:H8	1.77	0.47
1:2A:2080:G:H5'	23:21:35:THR:O	2.13	0.47
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.79	0.47
8:2I:40:THR:OG1	8:2I:41:GLU:N	2.48	0.47
11:2P:95:VAL:HB	11:2P:125:VAL:HG12	1.96	0.47
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD11	1.96	0.47
21:2Z:126:VAL:HB	21:2Z:161:VAL:HG23	1.95	0.47
28:26:12:GLU:OE1	28:26:19:ARG:NH1	2.47	0.47
30:28:33:ASN:HA	30:28:36:LYS:HG3	1.95	0.47
32:2a:56:U:H2'	32:2a:57:G:H8	1.77	0.47
32:2a:473:G:H2'	32:2a:474:G:H8	1.79	0.47
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.97	0.47
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	1.95	0.47
57:2y:8:U:O4'	57:2y:48:C:O2'	2.25	0.47
1:1A:388:G:O2'	1:1A:389:G:N7	2.46	0.47
1:1A:857:C:N4	1:1A:858:U:O4	2.48	0.47
1:1A:1364:G:P	23:11:3:LYS:HG3	2.53	0.47
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:7:VAL:HG23	4:1E:51:PHE:HE2	1.79	0.47
5:1F:9:ILE:HD13	5:1F:22:ALA:HB3	1.95	0.47
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.48	0.47
24:12:28:LYS:NZ	24:12:56:GLN:OE1	2.30	0.47
32:1a:276:G:O2'	48:1q:68:ARG:NH1	2.47	0.47
1:2A:242:G:C8	30:28:5:LYS:HG2	2.49	0.47
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.74	0.47
24:22:8:LYS:O	24:22:12:GLU:HG2	2.14	0.47
26:24:34:GLU:CB	44:2m:57:ARG:HH21	2.26	0.47
32:2a:875:C:O2'	39:2h:14:ARG:HD2	2.14	0.47
33:2b:187:LEU:HD12	33:2b:201:ILE:HB	1.95	0.47
34:2c:67:THR:HG23	34:2c:102:ASN:HB3	1.96	0.47
44:2m:123:ALA:HB3	54:2w:39:PSU:H4'	1.96	0.47
50:2s:33:THR:N	50:2s:57:HIS:HE1	2.05	0.47
1:1A:861:A:N3	2:1B:79:C:O2'	2.43	0.47
1:1A:1227:G:OP2	16:1U:16:LYS:NZ	2.45	0.47
1:1A:2552:OMU:OP2	63:1A:4129:HOH:O	2.20	0.47
1:1A:2790:A:H5'	1:1A:2893:G:H21	1.79	0.47
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.50	0.47
8:1I:109:ILE:HA	8:1I:109:ILE:HD13	1.72	0.47
1:2A:222:A:H3'	1:2A:421:U:H5'	1.97	0.47
1:2A:247:G:H4'	1:2A:386:G:C5	2.49	0.47
1:2A:919:G:N2	1:2A:2269:A:OP2	2.45	0.47
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.40	0.47
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.49	0.47
6:2G:43:LEU:HD12	6:2G:45:GLU:HG3	1.97	0.47
13:2R:57:ARG:NH2	13:2R:59:ASP:OD1	2.46	0.47
20:2Y:94:LYS:NZ	63:2Y:601:HOH:O	2.41	0.47
26:24:48:ARG:NH1	26:24:52:THR:O	2.48	0.47
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.50	0.47
32:2a:1010:G:N2	32:2a:1020:U:H1'	2.29	0.47
32:2a:1316:G:N1	32:2a:1319:A:OP2	2.46	0.47
33:2b:187:LEU:HA	33:2b:201:ILE:O	2.14	0.47
35:2d:114:ARG:O	35:2d:118:ARG:N	2.47	0.47
39:2h:97:VAL:HA	39:2h:100:ILE:HD11	1.97	0.47
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.14	0.47
1:1A:1104:C:H2'	1:1A:1105:U:C6	2.50	0.47
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.49	0.47
32:1a:1015:A:O3'	45:1n:15:LYS:NZ	2.48	0.47
32:1a:1191:A:OP1	34:1c:4:LYS:NZ	2.37	0.47
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.24	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:90:VAL:O	36:1e:120:THR:HA	2.15	0.47
48:1q:87:LYS:HA	48:1q:87:LYS:HD3	1.70	0.47
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.27	0.47
5:2F:137:LYS:HA	5:2F:140:LEU:HD12	1.95	0.47
10:2O:76:ALA:HB3	15:2T:75:ILE:HB	1.95	0.47
21:2Z:171:ILE:H	21:2Z:171:ILE:HG13	1.42	0.47
32:2a:1162:C:N4	32:2a:1174:G:H1	2.10	0.47
33:2b:91:PRO:HG3	33:2b:154:LEU:HB2	1.96	0.47
35:2d:33:MET:HB2	62:2d:303:SF4:S2	2.55	0.47
42:2k:48:ILE:HD11	42:2k:64:ALA:HA	1.96	0.47
54:2w:76:A1B8A:N	55:2x:76:8AN:O2'	2.47	0.47
57:2y:10:G:H1	57:2y:25:C:N4	2.08	0.47
1:1A:534:U:H2'	1:1A:535:C:C6	2.50	0.47
1:1A:1080:C:H2'	1:1A:1081:U:O4'	2.14	0.47
6:1G:149:VAL:HG22	6:1G:150:ASP:H	1.78	0.47
18:1W:88:ARG:NH1	18:1W:94:ASP:OD2	2.46	0.47
21:1Z:30:ASN:HA	21:1Z:89:PHE:HE1	1.79	0.47
32:1a:834:C:H2'	32:1a:835:U:C6	2.49	0.47
32:1a:890:G:O2'	32:1a:906:G:O6	2.29	0.47
36:1e:148:VAL:HG11	39:1h:107:LEU:HB3	1.96	0.47
57:1y:7:U:O2'	57:1y:49:G:H5'	2.14	0.47
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.13	0.47
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.49	0.47
5:2F:184:TYR:O	5:2F:188:ARG:HG3	2.15	0.47
9:2N:67:LEU:HA	9:2N:87:LEU:HD23	1.97	0.47
19:2X:9:LEU:HA	24:22:36:ARG:HH21	1.79	0.47
26:24:13:ARG:HG2	26:24:23:GLU:HG2	1.97	0.47
32:2a:685:G:C2	32:2a:686:U:C4	3.03	0.47
32:2a:838:G:H1	32:2a:848:C:N4	2.13	0.47
32:2a:1224:G:N2	32:2a:1363:C:N3	2.61	0.47
32:2a:1399:C:H4'	32:2a:1400:5MC:H5''	1.97	0.47
50:2s:14:HIS:CE1	50:2s:15:LEU:HD13	2.50	0.47
1:1A:251:A:C5	1:1A:252:G:H1'	2.49	0.47
1:1A:740:U:H2'	1:1A:741:G:C8	2.50	0.47
1:1A:813:U:H2'	1:1A:814:C:C6	2.50	0.47
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.50	0.47
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.15	0.47
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.29	0.47
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.50	0.47
1:1A:2236:C:H2'	1:1A:2237:G:O4'	2.14	0.47
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:13:A:N1	2:1B:69:G:O2'	2.40	0.47
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.15	0.47
13:1R:86:ARG:NH1	63:1R:302:HOH:O	2.37	0.47
16:1U:82:GLY:HA3	16:1U:113:ALA:HB1	1.97	0.47
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.49	0.47
32:1a:341:C:H2'	32:1a:342:C:C6	2.49	0.47
32:1a:1239:A:H62	32:1a:1299:A:H62	1.63	0.47
32:1a:1302:U:C6	44:1m:17:VAL:HG11	2.49	0.47
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.30	0.47
33:1b:8:LYS:H	33:1b:8:LYS:HD3	1.80	0.47
34:1c:73:PRO:O	34:1c:77:ILE:HG13	2.14	0.47
43:1l:24:VAL:HB	43:1l:27:LEU:HD12	1.96	0.47
1:2A:141:A:C8	1:2A:1408:C:O2'	2.68	0.47
1:2A:602:G:O2'	1:2A:655:A:N6	2.48	0.47
1:2A:805:G:OP1	63:2A:3738:HOH:O	2.20	0.47
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.29	0.47
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.14	0.47
1:2A:1938:A:OP2	63:2A:3739:HOH:O	2.21	0.47
1:2A:1997:G:OP2	63:2A:3737:HOH:O	2.20	0.47
1:2A:2138:C:N3	1:2A:2153:G:N2	2.61	0.47
1:2A:2318:G:H21	14:2S:3:ARG:NE	2.12	0.47
1:2A:2499:C:OP2	63:2A:3735:HOH:O	2.20	0.47
6:2G:59:GLU:HA	6:2G:62:LEU:HD12	1.97	0.47
6:2G:69:ALA:HB3	6:2G:91:ARG:HH21	1.79	0.47
28:26:34:LEU:HB2	28:26:51:GLU:HB2	1.96	0.47
32:2a:80:G:N2	32:2a:90:U:H1'	2.30	0.47
32:2a:300:A:H1'	32:2a:565:U:O2	2.15	0.47
32:2a:438:G:H4'	35:2d:123:HIS:ND1	2.30	0.47
32:2a:677:U:H1'	42:2k:119:CYS:SG	2.55	0.47
32:2a:1002:G:H1	32:2a:1038:C:N4	2.09	0.47
32:2a:1265:G:C4	32:2a:1271:G:N2	2.83	0.47
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.41	0.47
35:2d:63:LYS:HD2	35:2d:198:VAL:HG22	1.97	0.47
35:2d:135:LEU:C	35:2d:137:SER:H	2.22	0.47
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.97	0.47
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.96	0.47
54:2w:51:A:N6	54:2w:63:U:C2	2.82	0.47
1:1A:72:U:H5'	24:12:61:LEU:HD12	1.95	0.47
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.15	0.47
1:1A:1637:A:H4'	1:1A:2711:A:O2'	2.15	0.47
1:1A:1970:A:OP1	63:1A:4115:HOH:O	2.20	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1W:24:ILE:HA	18:1W:27:LYS:HG3	1.97	0.47
32:1a:1216:G:OP1	45:1n:2:ALA:HA	2.15	0.47
55:1x:23:C:H2'	55:1x:24:U:C6	2.50	0.47
1:2A:521:G:H2'	1:2A:522:G:H8	1.79	0.47
1:2A:1019:U:O2'	1:2A:1021:A:H2	1.97	0.47
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.43	0.47
18:2W:86:LEU:HD13	18:2W:96:ILE:HD11	1.96	0.47
32:2a:134:A:H1'	32:2a:325:A:C5	2.50	0.47
36:2e:53:LEU:HA	36:2e:56:GLN:HB2	1.96	0.47
41:2j:36:GLY:O	41:2j:38:ILE:HD12	2.15	0.47
1:1A:1239:G:OP1	63:1A:4149:HOH:O	2.20	0.47
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.97	0.47
2:1B:24:G:N7	2:1B:56:G:H2'	2.30	0.47
4:1E:59:VAL:HG12	4:1E:64:LYS:HG3	1.95	0.47
9:1N:14:VAL:HB	9:1N:138:LEU:HG	1.97	0.47
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.49	0.47
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.97	0.47
23:11:19:GLN:O	23:11:35:THR:HG22	2.15	0.47
32:1a:270:A:H2'	32:1a:271:C:C6	2.50	0.47
32:1a:708:C:H2'	32:1a:709:G:H8	1.79	0.47
32:1a:864:A:OP1	63:1a:1917:HOH:O	2.20	0.47
33:1b:187:LEU:HD12	33:1b:201:ILE:O	2.15	0.47
40:1i:17:VAL:HG23	40:1i:63:ILE:HG12	1.97	0.47
41:1j:8:LEU:HB2	41:1j:16:LEU:HD11	1.97	0.47
42:1k:59:TYR:CZ	42:1k:63:LEU:HD21	2.50	0.47
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.40	0.47
1:2A:184:C:H2'	1:2A:185:U:C6	2.50	0.47
1:2A:375:C:H2'	1:2A:376:C:C6	2.50	0.47
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.50	0.47
1:2A:2592:G:OP1	63:2A:3736:HOH:O	2.20	0.47
32:2a:148:G:H2'	32:2a:149:A:C8	2.50	0.47
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.48	0.47
32:2a:1387:G:H2'	32:2a:1388:C:H6	1.79	0.47
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.50	0.47
37:2f:33:TYR:HE2	37:2f:78:GLU:HG2	1.80	0.47
38:2g:75:VAL:HG13	38:2g:145:ALA:HA	1.95	0.47
44:2m:40:ASN:HB3	44:2m:43:THR:HG23	1.97	0.47
1:1A:196:A:H2'	1:1A:196:A:N3	2.30	0.47
1:1A:2667:C:H1'	7:1H:109:PHE:CD1	2.49	0.47
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.73	0.47
22:10:46:LYS:NZ	22:10:78:TYR:OH	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:316:G:OP2	32:1a:351:G:O2'	2.28	0.47
32:1a:540:G:H2'	32:1a:541:G:O4'	2.14	0.47
38:1g:153:HIS:C	38:1g:155:ARG:H	2.23	0.47
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.50	0.47
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.50	0.47
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.80	0.47
1:2A:276:A:H5''	1:2A:277:C:H5'	1.97	0.47
1:2A:2117:A:N6	1:2A:2166:G:H1	2.11	0.47
1:2A:2807:G:C2	1:2A:2808:U:H1'	2.49	0.47
27:25:46:CYS:SG	27:25:48:GLU:HG2	2.54	0.47
32:2a:583:A:H2'	32:2a:584:G:O4'	2.14	0.47
32:2a:979:C:O2	45:2n:19:ARG:HG2	2.15	0.47
32:2a:1226:C:O2'	44:2m:111:LYS:NZ	2.34	0.47
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.49	0.47
34:2c:109:PRO:C	34:2c:111:LEU:H	2.22	0.47
35:2d:59:ARG:HH12	35:2d:62:GLN:HB2	1.80	0.47
35:2d:122:ARG:HA	35:2d:122:ARG:HD2	1.67	0.47
49:2r:53:ARG:HA	49:2r:56:THR:HG1	1.80	0.47
54:2w:11:C:H2'	54:2w:12:U:C6	2.49	0.47
1:1A:601:C:O2'	1:1A:605:C:OP1	2.26	0.46
1:1A:1062:G:P	1:1A:1070:A:H1'	2.55	0.46
1:1A:1065:U:H1'	1:1A:1074:G:C2	2.50	0.46
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.50	0.46
1:1A:1865:G:N2	1:1A:1877:A:OP2	2.47	0.46
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.50	0.46
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.68	0.46
8:1I:77:LEU:HD22	8:1I:101:LEU:HG	1.97	0.46
11:1P:8:PRO:HB2	11:1P:12:ALA:HB3	1.97	0.46
15:1T:2:ASN:O	15:1T:6:LEU:HD12	2.15	0.46
16:1U:50:ARG:HG2	16:1U:53:ARG:NH2	2.30	0.46
32:1a:148:G:H2'	32:1a:149:A:H8	1.79	0.46
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.97	0.46
57:1y:63:U:H2'	57:1y:64:G:H8	1.79	0.46
1:2A:1160:G:C6	1:2A:1161:C:C4	3.03	0.46
1:2A:1364:G:P	23:21:3:LYS:HG3	2.55	0.46
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.15	0.46
1:2A:2287:A:C8	1:2A:2289:G:C8	3.04	0.46
60:2A:3688:ERY:H321	60:2A:3688:ERY:H8	1.67	0.46
5:2F:137:LYS:NZ	5:2F:137:LYS:HB3	2.29	0.46
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.50	0.46
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:45:GLN:N	12:2Q:45:GLN:OE1	2.43	0.46
21:2Z:61:LEU:HB2	21:2Z:65:GLN:HB2	1.96	0.46
32:2a:352:C:H4'	32:2a:354:G:OP1	2.14	0.46
32:2a:1112:C:N3	34:2c:178:LEU:HD12	2.30	0.46
32:2a:1359:C:O2'	32:2a:1362:C:N4	2.48	0.46
44:2m:16:ASP:OD1	44:2m:16:ASP:N	2.48	0.46
47:2p:22:THR:HA	47:2p:33:ILE:HG13	1.97	0.46
57:2y:8:U:H2'	57:2y:46:G7M:H22	1.80	0.46
32:1a:299:G:H2'	32:1a:300:A:C8	2.50	0.46
32:1a:982:U:H4'	32:1a:983:A:O5'	2.14	0.46
43:1l:27:LEU:HD23	43:1l:33:ARG:HB2	1.98	0.46
1:2A:192:C:O2'	1:2A:802:A:N3	2.45	0.46
1:2A:582:G:H2'	1:2A:583:G:C8	2.50	0.46
1:2A:639:U:H2'	1:2A:640:C:C6	2.50	0.46
3:2D:253:GLN:HG3	63:2D:411:HOH:O	2.15	0.46
10:2O:2:ILE:HG21	10:2O:8:LEU:HD11	1.97	0.46
16:2U:29:SER:OG	16:2U:30:LYS:NZ	2.46	0.46
21:2Z:17:ALA:O	21:2Z:21:ALA:N	2.41	0.46
21:2Z:70:LEU:HD12	21:2Z:71:VAL:N	2.27	0.46
21:2Z:79:ARG:HD2	21:2Z:80:ARG:NH1	2.31	0.46
32:2a:397:A:H3'	32:2a:397:A:N3	2.31	0.46
32:2a:1207:2MG:C2'	32:2a:1208:C:H5'	2.45	0.46
32:2a:1239:A:H62	32:2a:1299:A:N6	2.12	0.46
32:2a:1401:G:OP1	53:2v:18:G:O2'	2.30	0.46
35:2d:122:ARG:NH1	35:2d:134:ASP:O	2.48	0.46
38:2g:120:ILE:O	38:2g:124:LEU:HB2	2.15	0.46
49:2r:66:LEU:O	49:2r:70:ILE:HG13	2.15	0.46
1:1A:1082:U:H3	1:1A:1086:A:H61	0.64	0.46
1:1A:1082:U:O4	1:1A:1086:A:C6	2.68	0.46
30:18:32:LEU:O	30:18:36:LYS:HE3	2.15	0.46
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.98	0.46
33:1b:24:TRP:H	33:1b:24:TRP:HD1	1.62	0.46
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.97	0.46
36:1e:78:HIS:CE1	36:1e:142:LEU:HA	2.50	0.46
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.43	0.46
1:2A:458:G:O2'	29:27:39:ARG:HD3	2.16	0.46
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.26	0.46
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.15	0.46
1:2A:1740:G:H2'	1:2A:1741:A:C8	2.51	0.46
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.50	0.46
1:2A:2391:G:O6	1:2A:2425:A:H8	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.80	0.46
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.48	0.46
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.48	0.46
21:2Z:54:HIS:O	21:2Z:55:HIS:ND1	2.48	0.46
21:2Z:129:SER:HB3	21:2Z:131:ARG:NH1	2.31	0.46
32:2a:728:A:H2'	32:2a:729:A:C8	2.50	0.46
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.15	0.46
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.96	0.46
36:2e:102:ALA:HB2	36:2e:120:THR:HG21	1.98	0.46
39:2h:35:ILE:O	39:2h:39:LEU:HD12	2.16	0.46
1:1A:287:C:H2'	1:1A:288:C:H6	1.80	0.46
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.14	0.46
7:1H:95:ARG:HE	7:1H:95:ARG:HB2	1.59	0.46
11:1P:2:LYS:HE2	11:1P:4:SER:HB3	1.98	0.46
12:1Q:12:GLN:NE2	12:1Q:73:PRO:HD2	2.15	0.46
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.97	0.46
32:1a:300:A:H2'	32:1a:301:G:O4'	2.16	0.46
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.57	0.46
34:1c:131:ARG:NH1	34:1c:166:GLU:HG3	2.29	0.46
1:2A:478:A:N1	1:2A:500:G:H4'	2.30	0.46
1:2A:2250:G:O2'	1:2A:2496:C:OP1	2.32	0.46
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.30	0.46
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.16	0.46
6:2G:41:GLN:O	6:2G:43:LEU:HD22	2.16	0.46
8:2I:2:LYS:HA	8:2I:20:ASP:HA	1.97	0.46
19:2X:92:LEU:C	19:2X:94:GLY:H	2.23	0.46
21:2Z:53:ILE:HA	21:2Z:71:VAL:HG23	1.98	0.46
32:2a:72:C:H2'	32:2a:73:G:C8	2.51	0.46
32:2a:417:C:H2'	32:2a:418:C:H6	1.79	0.46
32:2a:685:G:N1	32:2a:686:U:O4	2.48	0.46
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.49	0.46
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.15	0.46
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.30	0.46
33:2b:178:ARG:NH2	39:2h:68:ARG:HH22	2.10	0.46
36:2e:36:ASP:C	36:2e:38:GLN:H	2.23	0.46
38:2g:114:ARG:HG3	38:2g:115:ARG:NH2	2.31	0.46
1:1A:1903:G:OP1	3:1D:241:PRO:HB2	2.15	0.46
1:1A:2111:C:O2	1:1A:2118:U:H5'	2.15	0.46
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.51	0.46
32:1a:406:G:H21	35:1d:119:GLN:HE22	1.63	0.46
32:1a:647:C:H2'	32:1a:648:A:C8	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:82:ARG:HD2	33:1b:92:TYR:CZ	2.50	0.46
49:1r:59:SER:H	49:1r:62:GLU:HB2	1.81	0.46
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.97	0.46
1:2A:468:G:N7	29:27:39:ARG:NH2	2.60	0.46
8:2I:43:ASN:ND2	23:21:75:GLU:OE2	2.49	0.46
14:2S:71:ARG:NH1	14:2S:107:GLU:OE1	2.49	0.46
32:2a:742:G:P	46:2o:35:ARG:HH22	2.39	0.46
32:2a:1060:C:H2'	32:2a:1061:G:H8	1.80	0.46
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.15	0.46
57:2y:18:G:O2'	57:2y:57:G:O6	2.18	0.46
1:1A:1919:A:O2'	32:1a:1517:G:N3	2.45	0.46
1:1A:2125:G:H1	1:1A:2172:U:P	2.38	0.46
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.33	0.46
4:1E:47:VAL:HG22	4:1E:84:PHE:O	2.15	0.46
8:1I:3:VAL:HA	8:1I:39:ALA:H	1.81	0.46
16:1U:10:ARG:NH2	63:1U:301:HOH:O	2.48	0.46
20:1Y:83:THR:HB	20:1Y:101:LYS:HG2	1.97	0.46
25:13:10:LYS:HB3	25:13:53:LEU:HA	1.98	0.46
32:1a:826:C:H5'	39:1h:12:ARG:NH2	2.30	0.46
32:1a:1305:G:H5''	52:1u:4:GLY:HA3	1.97	0.46
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.62	0.46
34:1c:22:TRP:CE2	45:1n:54:PRO:HG2	2.51	0.46
44:1m:15:VAL:O	44:1m:19:LEU:HG	2.16	0.46
54:1w:70:C:H2'	54:1w:71:C:O4'	2.16	0.46
57:1y:55:PSU:C4	57:1y:57:G:H5'	2.51	0.46
1:2A:864:G:H1'	1:2A:914:C:N4	2.31	0.46
17:2V:2:PHE:CZ	17:2V:41:GLY:HA3	2.49	0.46
20:2Y:90:LEU:HB3	20:2Y:92:ASN:H	1.81	0.46
32:2a:576:G:O6	32:2a:880:C:O2'	2.22	0.46
32:2a:636:U:H2'	32:2a:637:G:C8	2.51	0.46
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.51	0.46
33:2b:180:LEU:O	33:2b:181:PHE:HB2	2.16	0.46
35:2d:128:VAL:HG12	35:2d:129:ASN:HD22	1.81	0.46
36:2e:78:HIS:HE1	36:2e:142:LEU:HD23	1.80	0.46
37:2f:46:ARG:HA	37:2f:46:ARG:HD2	1.72	0.46
55:2x:43:A:H2'	55:2x:44:A:C8	2.51	0.46
1:1A:1055:G:H1	1:1A:1104:C:N4	2.08	0.46
1:1A:2469:A:O2'	12:1Q:56:ARG:HD3	2.15	0.46
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.80	0.46
11:1P:119:GLU:OE2	25:23:3:ARG:NH1	2.48	0.46
12:1Q:138:ASP:OD2	21:1Z:81:ARG:NH1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1q:50:LYS:HE2	48:1q:51:TYR:CE2	2.51	0.46
1:2A:581:C:H2'	1:2A:582:G:C8	2.51	0.46
1:2A:1021:A:H62	1:2A:1141:U:H3	1.63	0.46
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.30	0.46
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.16	0.46
6:2G:112:PRO:HA	26:24:40:HIS:CE1	2.51	0.46
12:2Q:29:PHE:HB2	12:2Q:105:GLU:OE1	2.16	0.46
30:28:26:LYS:HB2	30:28:44:LYS:O	2.16	0.46
32:2a:224:C:H2'	32:2a:225:C:C6	2.51	0.46
32:2a:516:PSU:O2'	32:2a:519:C:N3	2.46	0.46
33:2b:55:PHE:O	33:2b:59:GLU:HB2	2.16	0.46
34:2c:47:LEU:O	34:2c:51:GLY:N	2.42	0.46
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.98	0.46
44:2m:34:LEU:O	44:2m:38:GLY:N	2.48	0.46
45:2n:32:SER:O	45:2n:40:CYS:HA	2.16	0.46
1:1A:41:C:H2'	1:1A:42:G:O4'	2.16	0.46
1:1A:918:A:H5''	2:1B:98:G:O2'	2.16	0.46
1:1A:2106:G:H2'	1:1A:2107:C:O4'	2.16	0.46
1:1A:2697:G:OP1	63:1A:4146:HOH:O	2.20	0.46
32:1a:920:U:H2'	32:1a:921:U:C6	2.51	0.46
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.51	0.46
32:1a:1131:G:P	40:1i:20:ARG:HH22	2.39	0.46
32:1a:1412:C:H2'	32:1a:1413:A:H8	1.79	0.46
32:1a:1459:C:OP1	51:1t:31:SER:OG	2.30	0.46
33:1b:130:ARG:O	33:1b:131:PRO:C	2.58	0.46
57:1y:38:A:H2'	57:1y:39:PSU:O4'	2.15	0.46
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.51	0.46
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.97	0.46
3:2D:121:PRO:HB3	3:2D:135:PHE:CE2	2.51	0.46
6:2G:96:ARG:H	6:2G:99:MET:HE2	1.81	0.46
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.15	0.46
7:2H:53:GLU:HA	7:2H:65:HIS:HE2	1.80	0.46
11:2P:99:LEU:HA	11:2P:102:ARG:HH21	1.80	0.46
36:2e:62:ALA:C	36:2e:64:ARG:H	2.24	0.46
1:1A:1047:G:H2'	1:1A:1110:G:H1	1.81	0.46
1:1A:1512:U:H2'	1:1A:1513:C:C6	2.51	0.46
1:1A:1655:A:H3'	1:1A:1656:C:H6	1.81	0.46
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.30	0.46
1:1A:2612:C:OP2	27:15:2:ALA:N	2.48	0.46
4:1E:119:ARG:HG2	4:1E:120:TRP:NE1	2.31	0.46
32:1a:130:A:O2'	32:1a:131:C:O5'	2.32	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1342:C:O2'	40:1i:124:GLN:HG3	2.15	0.46
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.51	0.46
32:1a:1366:C:H2'	32:1a:1367:C:H6	1.81	0.46
35:1d:109:GLY:HA3	35:1d:165:MET:SD	2.56	0.46
37:1f:9:VAL:HB	37:1f:87:ARG:HB2	1.98	0.46
57:1y:36:U:C2	57:1y:37:T6A:H1'	2.51	0.46
1:2A:27:G:O2'	1:2A:28:A:OP2	2.30	0.46
1:2A:262:A:H2'	1:2A:263:C:O4'	2.16	0.46
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.98	0.46
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.97	0.46
10:2O:4:PRO:O	10:2O:5:GLN:HB2	2.16	0.46
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.49	0.46
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB2	1.97	0.46
32:2a:499:A:H4'	32:2a:500:G:OP1	2.15	0.46
32:2a:743:U:H2'	32:2a:744:C:C6	2.51	0.46
32:2a:833:U:H2'	32:2a:834:C:H6	1.81	0.46
32:2a:848:C:H2'	32:2a:849:C:O4'	2.15	0.46
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.51	0.46
32:2a:1227:A:O3'	44:2m:115:LYS:HE2	2.15	0.46
45:2n:27:CYS:SG	45:2n:29:ARG:HB2	2.56	0.46
55:2x:21:A:H61	55:2x:46:G:H2'	1.80	0.46
1:1A:1114:G:H2'	1:1A:1115:G:O4'	2.16	0.46
1:1A:1405:U:H2'	1:1A:1406:U:H6	1.77	0.46
11:1P:81:GLN:NE2	11:1P:105:LEU:O	2.49	0.46
32:1a:584:G:H5'	48:1q:91:ARG:HH22	1.81	0.46
32:1a:828:A:H2'	32:1a:829:G:O4'	2.16	0.46
32:1a:1327:C:OP2	52:1u:12:LYS:NZ	2.47	0.46
33:1b:15:VAL:HB	33:1b:209:ARG:HG3	1.97	0.46
33:1b:55:PHE:CE1	33:1b:218:ALA:HA	2.51	0.46
1:2A:895:U:H2'	1:2A:897:C:OP2	2.15	0.46
1:2A:927:G:H2'	1:2A:928:G:O4'	2.15	0.46
1:2A:1036:G:P	7:2H:59:ARG:HD2	2.56	0.46
9:2N:120:LEU:HG	9:2N:122:VAL:HG23	1.98	0.46
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.55	0.46
21:2Z:10:ARG:NE	21:2Z:37:VAL:O	2.45	0.46
32:2a:544:G:OP1	35:2d:59:ARG:NH2	2.49	0.46
32:2a:950:U:OP2	44:2m:102:ARG:HD3	2.16	0.46
32:2a:1216:G:H5''	45:2n:5:ALA:HB2	1.97	0.46
40:2i:14:VAL:HG23	40:2i:66:ARG:HG3	1.98	0.46
55:2x:50:U:H3	55:2x:64:G:H1	1.63	0.46
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:880:G:H2'	1:1A:881:G:H8	1.81	0.45
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.51	0.45
2:1B:8:U:H5''	14:1S:15:ARG:HH22	1.80	0.45
32:1a:265:G:H2'	32:1a:267:C:H5	1.79	0.45
36:1e:10:MET:HA	36:1e:32:VAL:HG22	1.97	0.45
57:1y:30:G:H2'	57:1y:31:A:H8	1.81	0.45
1:2A:236:C:H2'	1:2A:237:C:H6	1.81	0.45
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.49	0.45
1:2A:903:C:H2'	1:2A:904:C:C6	2.51	0.45
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.51	0.45
5:2F:126:VAL:HG21	5:2F:129:PHE:CE1	2.51	0.45
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.16	0.45
32:2a:1133:G:H1	32:2a:1141:C:N4	2.12	0.45
32:2a:1259:C:C4	32:2a:1260:C:H1'	2.51	0.45
36:2e:143:ARG:NE	39:2h:77:GLU:OE2	2.40	0.45
39:2h:87:SER:HB2	39:2h:93:VAL:H	1.81	0.45
1:1A:414:C:H2'	1:1A:415:A:H8	1.80	0.45
1:1A:764:A:H5''	3:1D:210:GLY:HA3	1.98	0.45
1:1A:1111:A:N3	1:1A:1112:G:H1'	2.30	0.45
1:1A:1156:A:OP2	63:1A:4148:HOH:O	2.20	0.45
1:1A:1406:U:H2'	1:1A:1407:C:H6	1.80	0.45
1:1A:2118:U:H4'	1:1A:2119:A:OP1	2.15	0.45
1:1A:2134:A:N3	1:1A:2159:G:O2'	2.45	0.45
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.51	0.45
32:1a:192:U:H4'	51:1t:57:ARG:HD3	1.98	0.45
32:1a:256:U:H2'	32:1a:257:G:O4'	2.17	0.45
32:1a:521:G:H4'	43:1l:73:GLU:HG3	1.98	0.45
32:1a:1048:G:OP1	45:1n:3:ARG:HB3	2.16	0.45
32:1a:1316:G:N2	32:1a:1318:A:H3'	2.32	0.45
33:1b:131:PRO:O	33:1b:134:GLU:N	2.49	0.45
33:1b:143:GLU:H	33:1b:143:GLU:HG2	1.38	0.45
35:1d:129:ASN:ND2	35:1d:144:ASP:HB3	2.31	0.45
35:1d:196:LEU:O	35:1d:198:VAL:N	2.47	0.45
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.98	0.45
1:2A:1359:A:H2'	1:2A:1360:A:H5'	1.97	0.45
6:2G:138:GLN:OE1	6:2G:153:ARG:N	2.42	0.45
8:2I:77:LEU:HD21	8:2I:100:ALA:HB3	1.97	0.45
9:2N:73:THR:HB	9:2N:82:LEU:HD11	1.98	0.45
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.16	0.45
21:2Z:100:VAL:HG21	21:2Z:134:PRO:HG2	1.97	0.45
25:23:4:LEU:O	25:23:36:VAL:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:714:G:H2'	32:2a:715:A:C8	2.52	0.45
32:2a:1118:C:H1'	32:2a:1179:A:C5	2.52	0.45
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.51	0.45
42:2k:43:SER:HA	42:2k:47:VAL:HG21	1.97	0.45
57:2y:29:U:H3	57:2y:41:A:H61	1.63	0.45
1:1A:831:G:N2	11:1P:53:GLY:O	2.49	0.45
15:1T:73:GLU:OE2	15:1T:103:ARG:NE	2.46	0.45
32:1a:244:U:O2	63:1a:1919:HOH:O	2.20	0.45
32:1a:667:G:H4'	46:1o:51:HIS:ND1	2.30	0.45
32:1a:1100:C:OP2	33:1b:96:ARG:HD2	2.17	0.45
35:1d:70:ILE:HG12	35:1d:71:SER:N	2.31	0.45
36:1e:147:ASP:O	36:1e:151:LEU:HD12	2.16	0.45
57:1y:14:A:C6	57:1y:22:G:C2	3.04	0.45
1:2A:601:C:OP1	5:2F:108:LYS:HE2	2.16	0.45
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.16	0.45
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.47	0.45
1:2A:2115:G:C8	1:2A:2117:A:H8	2.34	0.45
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.31	0.45
3:2D:71:ASP:HB3	3:2D:72:LYS:HG3	1.99	0.45
32:2a:677:U:H3	32:2a:713:G:H22	1.64	0.45
32:2a:1002:G:C6	32:2a:1003:G:H8	2.35	0.45
32:2a:1264:C:H42	32:2a:1271:G:H1	1.64	0.45
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.98	0.45
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.97	0.45
50:2s:15:LEU:HA	50:2s:15:LEU:HD12	1.81	0.45
54:2w:19:G:N2	54:2w:56:C:N3	2.64	0.45
57:2y:56:C:H2'	57:2y:57:G:H8	1.81	0.45
1:1A:862:G:H2'	1:1A:863:A:O4'	2.17	0.45
1:1A:2785:C:H2'	1:1A:2786:U:O4'	2.16	0.45
4:1E:67:PHE:CE1	4:1E:75:VAL:HG22	2.52	0.45
19:1X:94:GLY:N	19:1X:95:LEU:HB2	2.32	0.45
26:14:49:PHE:HB3	26:14:50:VAL:H	1.44	0.45
32:1a:460:G:N2	32:1a:472:A:H62	2.15	0.45
32:1a:1095:U:P	32:1a:1108:G:H1	2.39	0.45
37:1f:70:ASP:OD1	37:1f:70:ASP:N	2.46	0.45
41:1j:31:GLY:HA3	41:1j:32:ALA:HA	1.49	0.45
1:2A:875:G:C2	1:2A:903:C:C2	3.04	0.45
1:2A:994:C:H3'	16:2U:54:LYS:HE3	1.99	0.45
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.17	0.45
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.51	0.45
1:2A:2841:C:H2'	1:2A:2842:G:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:105:THR:HG21	4:2E:164:ARG:CZ	2.46	0.45
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	1.98	0.45
12:2Q:89:ASN:HB2	55:2x:1:C:N3	2.30	0.45
19:2X:92:LEU:HD23	19:2X:92:LEU:HA	1.71	0.45
34:2c:123:GLN:O	34:2c:128:PHE:HB2	2.17	0.45
37:2f:94:GLN:OE1	49:2r:32:ARG:HD3	2.17	0.45
1:1A:278:A:H61	1:1A:362:U:H3	1.62	0.45
1:1A:1655:A:H3'	1:1A:1656:C:C6	2.51	0.45
1:1A:2404:C:O3'	11:1P:77:ARG:NH2	2.50	0.45
2:1B:33:G:C2	2:1B:50:G:C2	3.04	0.45
21:1Z:126:VAL:HG12	21:1Z:128:VAL:HB	1.98	0.45
30:18:28:GLY:O	30:18:36:LYS:NZ	2.46	0.45
1:2A:902:C:H2'	1:2A:903:C:H6	1.81	0.45
1:2A:1816:G:H8	3:2D:62:TYR:CZ	2.35	0.45
6:2G:41:GLN:HG2	6:2G:154:GLY:O	2.16	0.45
14:2S:93:LYS:NZ	14:2S:93:LYS:HB2	2.32	0.45
19:2X:14:SER:C	19:2X:16:LYS:H	2.22	0.45
32:2a:448:A:P	32:2a:485:G:H22	2.39	0.45
32:2a:934:C:OP1	63:2a:1914:HOH:O	2.21	0.45
32:2a:984:C:H2'	32:2a:985:C:C6	2.50	0.45
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.30	0.45
32:2a:1312:G:H5'	50:2s:5:LEU:HD11	1.98	0.45
35:2d:119:GLN:HG3	35:2d:123:HIS:CD2	2.52	0.45
38:2g:150:ALA:HA	42:2k:59:TYR:HB3	1.99	0.45
57:2y:37:T6A:H2'	57:2y:38:A:O4'	2.16	0.45
1:1A:1045:A:H8	1:1A:1111:A:N6	2.15	0.45
1:1A:2163:C:OP1	1:1A:2171:A:O2'	2.34	0.45
1:1A:2718:G:O2'	1:1A:2847:U:OP1	2.31	0.45
3:1D:183:ARG:NH2	3:1D:266:SER:HB2	2.31	0.45
3:1D:223:GLY:HA3	3:1D:231:HIS:CE1	2.52	0.45
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.49	0.45
4:1E:40:GLU:CD	4:1E:40:GLU:H	2.25	0.45
6:1G:126:ASP:OD2	6:1G:130:ASN:ND2	2.40	0.45
12:1Q:59:ARG:C	12:1Q:61:GLY:H	2.25	0.45
19:1X:84:ALA:HB3	19:1X:87:GLN:OE1	2.17	0.45
21:1Z:99:TYR:HA	21:1Z:124:ILE:O	2.15	0.45
32:1a:167:G:H2'	32:1a:168:G:H8	1.81	0.45
39:1h:112:LEU:HB3	39:1h:133:LEU:HA	1.99	0.45
51:1t:56:MET:HE3	51:1t:85:MET:HG2	1.99	0.45
1:2A:1001:A:H2'	1:2A:1002:G:O4'	2.17	0.45
32:2a:1141:C:H2'	32:2a:1142:G:O4'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1208:C:H2'	32:2a:1209:C:C6	2.51	0.45
37:2f:64:GLN:HE21	37:2f:64:GLN:HB3	1.56	0.45
48:2q:76:LEU:HD12	48:2q:77:VAL:N	2.32	0.45
57:2y:63:U:H2'	57:2y:64:G:C8	2.51	0.45
1:1A:466:A:OP1	29:17:34:ARG:NH1	2.50	0.45
1:1A:876:C:H2'	1:1A:877:U:O4'	2.17	0.45
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.31	0.45
5:1F:172:TRP:CD1	5:1F:172:TRP:H	2.35	0.45
15:1T:50:ILE:HD13	15:1T:64:ARG:HB2	1.99	0.45
15:1T:57:PHE:HA	15:1T:79:HIS:CD2	2.51	0.45
32:1a:1413:A:H2	32:1a:1487:G:H22	1.63	0.45
39:1h:98:LYS:H	39:1h:98:LYS:CE	2.29	0.45
40:1i:9:ARG:HD2	40:1i:104:ARG:NH1	2.31	0.45
42:1k:82:VAL:HB	42:1k:108:ILE:HG12	1.98	0.45
1:2A:918:A:C5	1:2A:919:G:H1'	2.52	0.45
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.51	0.45
12:2Q:12:GLN:HE21	12:2Q:72:LYS:HG3	1.82	0.45
15:2T:23:ARG:HD3	15:2T:120:ARG:CZ	2.46	0.45
16:2U:10:ARG:NH2	63:2U:201:HOH:O	2.50	0.45
21:2Z:31:ARG:HG3	21:2Z:32:HIS:CD2	2.52	0.45
32:2a:44:G:H2'	32:2a:45:U:O4'	2.17	0.45
32:2a:737:A:H2'	32:2a:738:C:C6	2.51	0.45
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.52	0.45
33:2b:95:GLN:HG3	33:2b:147:LYS:O	2.17	0.45
34:2c:36:ASP:HA	34:2c:39:ILE:HD12	1.98	0.45
43:2l:41:ARG:HH12	43:2l:57:LYS:NZ	2.15	0.45
53:2v:22:U:H2'	53:2v:23:A:C8	2.52	0.45
54:2w:52:G:OP2	54:2w:64:G:N2	2.49	0.45
54:2w:58:A:O2'	54:2w:61:C:N4	2.50	0.45
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.17	0.45
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.46	0.45
5:1F:33:LEU:HD13	5:1F:112:MET:HE2	1.99	0.45
11:1P:2:LYS:HG3	11:1P:4:SER:H	1.82	0.45
20:1Y:106:LEU:O	20:1Y:107:ASP:HB2	2.15	0.45
22:10:38:VAL:HG12	22:10:40:GLN:HG2	1.99	0.45
32:1a:1144:G:N2	32:1a:1146:A:H62	2.14	0.45
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.17	0.45
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.52	0.45
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.17	0.45
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.98	0.45
34:1c:121:ALA:O	34:1c:125:GLU:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:588:U:H2'	1:2A:589:C:C6	2.51	0.45
1:2A:1487:G:H2'	1:2A:1488:G:O4'	2.16	0.45
1:2A:2128:C:H6	1:2A:2128:C:O5'	2.00	0.45
1:2A:2162:G:H5''	1:2A:2172:U:H2'	1.99	0.45
4:2E:119:ARG:HG2	4:2E:120:TRP:NE1	2.32	0.45
19:2X:9:LEU:HA	24:22:36:ARG:NH2	2.31	0.45
32:2a:34:C:H2'	32:2a:35:G:C8	2.49	0.45
32:2a:448:A:OP2	32:2a:485:G:N1	2.29	0.45
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.17	0.45
34:2c:180:ALA:HB1	34:2c:203:PHE:CE1	2.50	0.45
50:2s:32:LYS:HD2	50:2s:34:TRP:CH2	2.51	0.45
21:1Z:137:ILE:HA	21:1Z:156:LYS:HZ1	1.82	0.45
22:10:70:GLN:HG2	22:10:72:ARG:HG3	1.99	0.45
28:16:28:ARG:NH1	28:16:29:ASN:OD1	2.50	0.45
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.51	0.45
2:2B:17:C:H2'	2:2B:18:G:O4'	2.16	0.45
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.97	0.45
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.63	0.45
8:2I:50:ARG:HA	8:2I:53:ALA:HB3	1.99	0.45
9:2N:12:ARG:HB3	9:2N:50:ASP:OD1	2.17	0.45
14:2S:38:GLN:HB3	14:2S:47:THR:HG23	1.99	0.45
29:27:47:ARG:O	29:27:48:LYS:HB2	2.17	0.45
32:2a:73:G:H1	32:2a:96:U:H3	1.65	0.45
32:2a:600:C:H2'	32:2a:601:C:C6	2.52	0.45
32:2a:995:C:O2	45:2n:4:LYS:NZ	2.36	0.45
32:2a:1097:C:H1'	32:2a:1170:A:H1'	1.99	0.45
36:2e:57:LYS:HE3	36:2e:57:LYS:HB2	1.76	0.45
41:2j:74:ILE:HD12	41:2j:74:ILE:HA	1.80	0.45
45:2n:18:VAL:C	45:2n:20:ALA:H	2.25	0.45
1:1A:287:C:H2'	1:1A:288:C:C6	2.52	0.45
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.17	0.45
2:1B:66:A:H61	2:1B:108:U:H2'	1.82	0.45
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.30	0.45
9:1N:8:GLN:HE21	9:1N:8:GLN:HB3	1.53	0.45
21:1Z:153:SER:CA	21:1Z:167:PRO:HB3	2.42	0.45
32:1a:328:C:H4'	32:1a:329:A:H5''	1.98	0.45
33:1b:208:ILE:HD13	33:1b:208:ILE:H	1.81	0.45
39:1h:9:MET:HG3	39:1h:26:VAL:HG21	1.98	0.45
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.81	0.45
47:1p:53:VAL:O	47:1p:57:ARG:HG2	2.17	0.45
1:2A:1260:G:C6	1:2A:1261:C:C4	3.04	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2786:U:O2'	4:2E:62:PRO:O	2.32	0.45
6:2G:68:PRO:HA	6:2G:92:VAL:HB	1.99	0.45
21:2Z:149:SER:HA	21:2Z:173:ALA:CB	2.47	0.45
32:2a:8:A:N6	35:2d:209:ARG:HB2	2.31	0.45
32:2a:277:C:P	48:2q:68:ARG:HH12	2.39	0.45
32:2a:1104:G:H4'	33:2b:111:ARG:NE	2.32	0.45
40:2i:6:GLY:HA3	40:2i:80:GLY:O	2.17	0.45
45:2n:4:LYS:HE2	45:2n:4:LYS:HB3	1.76	0.45
1:1A:84:A:H5'	20:1Y:8:LYS:HG2	1.98	0.44
1:1A:880:G:H8	1:1A:880:G:OP2	2.01	0.44
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.50	0.44
1:1A:2166:G:H2'	1:1A:2167:U:C6	2.52	0.44
3:1D:62:TYR:HA	3:1D:87:ASN:OD1	2.17	0.44
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.35	0.44
6:1G:37:VAL:HG23	6:1G:99:MET:HG3	1.99	0.44
11:1P:121:LYS:O	11:1P:123:LEU:N	2.49	0.44
32:1a:642:A:N3	39:1h:113:SER:OG	2.36	0.44
33:1b:102:LEU:HB3	33:1b:180:LEU:CD1	2.47	0.44
34:1c:8:ILE:HD13	34:1c:184:TYR:HB3	1.99	0.44
35:1d:172:PRO:C	35:1d:174:LEU:H	2.25	0.44
39:1h:28:ALA:HA	39:1h:59:LEU:HG	1.99	0.44
46:1o:87:ILE:O	46:1o:88:ARG:HB3	2.16	0.44
1:2A:171:G:H2'	1:2A:172:C:C6	2.51	0.44
1:2A:1354:A:H5''	3:2D:38:LYS:HD3	1.97	0.44
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.18	0.44
6:2G:63:ILE:HD13	6:2G:143:GLU:HB2	1.98	0.44
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.50	0.44
26:24:34:GLU:HG3	26:24:35:VAL:HG23	1.99	0.44
32:2a:719:C:H42	49:2r:71:LYS:HE2	1.82	0.44
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.45	0.44
36:2e:40:ARG:HD3	36:2e:67:VAL:O	2.16	0.44
42:2k:87:THR:HA	42:2k:91:ARG:CZ	2.47	0.44
44:2m:90:LEU:HD21	44:2m:94:ARG:HH11	1.82	0.44
46:2o:85:LEU:HD23	46:2o:85:LEU:HA	1.80	0.44
1:1A:1058:G:H4'	1:1A:1058:G:OP1	2.17	0.44
1:1A:1540:U:H2'	1:1A:1541:G:O4'	2.17	0.44
1:1A:1698:A:OP2	63:1A:4152:HOH:O	2.21	0.44
3:1D:34:VAL:HG12	3:1D:63:ARG:HG3	1.99	0.44
4:1E:78:LEU:O	4:1E:79:ARG:NH1	2.49	0.44
32:1a:8:A:N6	35:1d:205:GLU:O	2.50	0.44
32:1a:1249:C:O4'	40:1i:70:LYS:HE2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.46	0.44
46:1o:18:PHE:CE2	46:1o:21:ASP:HB2	2.53	0.44
1:2A:981:A:N1	1:2A:2027:G:O2'	2.41	0.44
1:2A:1510:G:C2	1:2A:1511:C:C2	3.05	0.44
2:2B:90:A:C5	2:2B:91:C:H1'	2.51	0.44
6:2G:59:GLU:OE2	6:2G:138:GLN:NE2	2.51	0.44
7:2H:7:LEU:HB3	7:2H:69:ARG:NH2	2.31	0.44
12:2Q:54:MET:HB2	12:2Q:64:ILE:CD1	2.47	0.44
24:22:66:GLU:HA	24:22:69:ARG:NH1	2.32	0.44
32:2a:396:G:O2'	32:2a:398:C:OP1	2.30	0.44
32:2a:674:G:H2'	32:2a:675:A:H8	1.82	0.44
32:2a:1246:C:H2'	32:2a:1247:U:O4'	2.17	0.44
36:2e:76:ILE:HD12	36:2e:142:LEU:HD21	2.00	0.44
38:2g:31:MET:HB2	38:2g:39:ALA:HB2	2.00	0.44
44:2m:92:HIS:CD2	44:2m:98:VAL:HG21	2.53	0.44
44:2m:123:ALA:HB1	44:2m:124:PRO:HD2	1.99	0.44
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.53	0.44
1:1A:2165:G:N2	1:1A:2171:A:O2'	2.50	0.44
4:1E:7:VAL:HG23	4:1E:51:PHE:CE2	2.52	0.44
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.47	0.44
12:1Q:10:ARG:NH1	12:1Q:90:VAL:H	2.15	0.44
44:1m:4:ILE:HD12	44:1m:57:ARG:HA	1.99	0.44
1:2A:645:C:H5''	1:2A:646:A:OP2	2.18	0.44
1:2A:2847:U:OP1	15:2T:98:LYS:NZ	2.50	0.44
60:2A:3688:ERY:H71	60:2A:3688:ERY:H4	1.93	0.44
3:2D:27:THR:O	3:2D:28:GLU:HG2	2.18	0.44
9:2N:69:GLN:O	9:2N:71:ILE:HG13	2.17	0.44
10:2O:13:ASN:HD21	10:2O:96:THR:HG22	1.81	0.44
32:2a:189(L):G:H2'	32:2a:190:U:H6	1.82	0.44
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.17	0.44
32:2a:1092:A:H5''	38:2g:4:ARG:NH2	2.32	0.44
34:2c:33:LEU:HD13	45:2n:54:PRO:HD3	1.99	0.44
1:1A:502:A:OP1	63:1A:4153:HOH:O	2.21	0.44
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.35	0.44
1:1A:1058:G:N2	1:1A:1081:U:O2	2.50	0.44
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.16	0.44
1:1A:1411:C:H2'	1:1A:1412:A:C8	2.53	0.44
1:1A:1648:C:OP1	63:1A:4114:HOH:O	2.21	0.44
2:1B:76:G:N7	63:1B:303:HOH:O	2.36	0.44
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.99	0.44
5:1F:183:VAL:O	5:1F:187:VAL:HG23	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.52	0.44
6:1G:137:GLU:HG2	6:1G:152:LEU:HD22	1.99	0.44
32:1a:236:G:H5'	48:1q:42:TYR:OH	2.17	0.44
32:1a:269:C:H2'	32:1a:270:A:C8	2.53	0.44
33:1b:84:GLU:O	33:1b:219:VAL:HG21	2.17	0.44
33:1b:183:PRO:HA	33:1b:198:ASP:OD2	2.17	0.44
38:1g:78:ARG:HD3	38:1g:156:TRP:HZ3	1.82	0.44
44:1m:45:VAL:C	44:1m:47:ASP:H	2.26	0.44
1:2A:311:A:C6	1:2A:328:U:C4	3.06	0.44
1:2A:372:G:H8	23:21:65:SER:O	2.01	0.44
1:2A:801:G:O6	5:2F:53:THR:OG1	2.36	0.44
1:2A:829:A:N7	1:2A:2247:A:O2'	2.41	0.44
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.53	0.44
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.53	0.44
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.16	0.44
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.99	0.44
32:2a:620:C:H2'	32:2a:621:A:O4'	2.18	0.44
32:2a:1038:C:H2'	32:2a:1039:C:C6	2.52	0.44
33:2b:105:PHE:C	33:2b:107:THR:H	2.23	0.44
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.29	0.44
34:2c:101:LEU:HD13	34:2c:102:ASN:N	2.33	0.44
36:2e:102:ALA:O	36:2e:107:ARG:NH2	2.50	0.44
44:2m:3:ARG:HH22	44:2m:11:ARG:NE	2.15	0.44
1:1A:30:G:OP2	16:1U:5:LYS:NZ	2.47	0.44
1:1A:2168:G:N2	1:1A:2171:A:N7	2.66	0.44
12:1Q:81:VAL:HB	22:10:7:LEU:HD21	2.00	0.44
23:11:82:LEU:HA	23:11:85:LEU:HD12	1.99	0.44
32:1a:78:G:H8	32:1a:78:G:OP2	2.01	0.44
32:1a:118:U:O4	63:1a:1918:HOH:O	2.20	0.44
32:1a:933:G:OP2	38:1g:3:ARG:HB2	2.18	0.44
34:1c:148:GLY:HA2	34:1c:171:GLY:HA3	1.99	0.44
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.47	0.44
51:1t:9:ASN:O	51:1t:10:LEU:HB2	2.17	0.44
1:2A:657:U:H2'	1:2A:658:C:C6	2.52	0.44
1:2A:740:U:H2'	1:2A:741:G:C8	2.53	0.44
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.53	0.44
15:2T:61:PHE:CE2	15:2T:76:PHE:HB2	2.53	0.44
32:2a:53:A:OP2	63:2a:1913:HOH:O	2.21	0.44
32:2a:551:U:H2'	32:2a:552:U:C6	2.53	0.44
39:2h:41:ARG:NH2	39:2h:123:GLU:OE1	2.50	0.44
39:2h:127:LEU:HA	39:2h:127:LEU:HD13	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:14:ARG:HA	44:2m:44:ARG:HA	1.99	0.44
49:2r:37:VAL:HG22	49:2r:78:LEU:HB3	2.00	0.44
1:1A:1800:C:OP2	3:1D:183:ARG:NH2	2.50	0.44
26:14:34:GLU:H	26:14:34:GLU:CD	2.26	0.44
32:1a:437:U:H5'	35:1d:155:LEU:HD11	1.99	0.44
32:1a:688:G:H5'	42:1k:46:GLY:C	2.42	0.44
32:1a:738:C:H2'	32:1a:739:C:C6	2.53	0.44
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.53	0.44
36:1e:43:LEU:HD21	36:1e:132:ALA:HB1	2.00	0.44
43:1l:7:ILE:HD13	43:1l:10:LEU:HD12	1.99	0.44
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.53	0.44
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.81	0.44
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.53	0.44
11:2P:20:GLY:HA2	11:2P:28:GLY:O	2.16	0.44
32:2a:21:G:H2'	32:2a:22:G:C8	2.53	0.44
32:2a:80:G:H22	32:2a:90:U:H1'	1.82	0.44
32:2a:1063:C:H3'	32:2a:1064:G:H2'	1.98	0.44
38:2g:131:LYS:HB3	38:2g:131:LYS:HE2	1.82	0.44
55:2x:17:C:OP2	55:2x:18:G:H5'	2.17	0.44
1:1A:2053:G:OP1	4:1E:144:ARG:HG3	2.18	0.44
1:1A:2059:A:OP2	63:1A:4150:HOH:O	2.20	0.44
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	1.99	0.44
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.83	0.44
19:1X:47:PHE:O	19:1X:49:VAL:HG13	2.18	0.44
24:12:35:LEU:HD12	24:12:53:LEU:HD12	1.99	0.44
32:1a:56:U:H2'	32:1a:57:G:H8	1.80	0.44
32:1a:134:A:H1'	32:1a:325:A:C5	2.52	0.44
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.53	0.44
32:1a:872:A:C8	32:1a:874:G:C8	3.06	0.44
32:1a:1337:G:N7	63:1a:1934:HOH:O	2.36	0.44
38:1g:27:ILE:HA	38:1g:30:ILE:HD12	1.99	0.44
42:1k:98:LEU:O	42:1k:101:SER:OG	2.32	0.44
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.79	0.44
6:2G:45:GLU:H	6:2G:45:GLU:HG2	1.37	0.44
6:2G:66:GLN:HA	26:24:6:HIS:ND1	2.33	0.44
8:2I:71:ILE:O	8:2I:75:LEU:HG	2.17	0.44
8:2I:101:LEU:O	8:2I:105:HIS:N	2.40	0.44
23:21:77:ALA:HB2	23:21:94:LEU:HD21	1.99	0.44
32:2a:109:A:H2'	32:2a:326:G:N2	2.33	0.44
32:2a:266:G:H2'	32:2a:266:G:N3	2.32	0.44
32:2a:935:A:H2'	32:2a:936:C:C6	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.83	0.44
33:2b:139:LYS:HB2	33:2b:139:LYS:HE3	1.80	0.44
37:2f:63:TYR:N	37:2f:63:TYR:CD2	2.86	0.44
42:2k:48:ILE:C	42:2k:50:TYR:H	2.20	0.44
48:2q:57:VAL:HG12	48:2q:76:LEU:HA	1.99	0.44
1:1A:45:C:OP2	1:1A:215:G:H2'	2.17	0.44
1:1A:305:U:H2'	1:1A:306:U:C6	2.52	0.44
1:1A:858:U:P	22:10:77:ARG:HH22	2.41	0.44
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.53	0.44
1:1A:1394:U:H2'	1:1A:1395:A:O4'	2.18	0.44
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.99	0.44
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.18	0.44
4:1E:101:ARG:NH2	4:1E:171:GLU:HB2	2.32	0.44
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.99	0.44
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.69	0.44
32:1a:184:G:H2'	32:1a:185:A:H8	1.82	0.44
32:1a:539:A:H2'	32:1a:540:G:C8	2.52	0.44
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.46	0.44
32:1a:864:A:H2'	32:1a:865:A:C8	2.53	0.44
38:1g:33:ASP:OD1	38:1g:33:ASP:N	2.48	0.44
46:1o:57:LEU:HD23	46:1o:57:LEU:HA	1.79	0.44
1:2A:660:G:H5'	5:2F:99:TYR:CE1	2.53	0.44
1:2A:1600:C:OP1	19:2X:58:HIS:NE2	2.39	0.44
1:2A:2469:A:H2'	1:2A:2470:G:O4'	2.18	0.44
4:2E:2:LYS:NZ	4:2E:95:ILE:O	2.36	0.44
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.48	0.44
6:2G:123:ASN:O	6:2G:125:PHE:N	2.51	0.44
11:2P:6:LEU:HD23	11:2P:6:LEU:HA	1.85	0.44
12:2Q:54:MET:HE1	12:2Q:104:PHE:HB3	2.00	0.44
15:2T:59:THR:HG23	15:2T:78:LEU:HB3	2.00	0.44
32:2a:193:C:H2'	32:2a:194:C:H6	1.82	0.44
32:2a:975:A:H5''	32:2a:1363(A):A:N6	2.33	0.44
32:2a:976:G:OP1	45:2n:32:SER:N	2.50	0.44
32:2a:1058:G:H1	32:2a:1199:U:H3	1.66	0.44
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.17	0.44
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.42	0.44
32:2a:1304:G:C6	32:2a:1305:G:N1	2.86	0.44
1:1A:142(A):C:H2'	1:1A:143:G:O4'	2.18	0.44
1:1A:2865:U:OP2	15:1T:119:LYS:NZ	2.47	0.44
2:1B:88:C:H2'	2:1B:89:G:O4'	2.18	0.44
8:1I:9:LEU:HD13	8:1I:10:GLU:HG3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:18:8:LYS:O	30:18:12:LYS:HG3	2.18	0.44
32:1a:715:A:H2'	32:1a:716:A:C8	2.53	0.44
33:1b:45:GLN:O	33:1b:49:GLU:HG3	2.17	0.44
39:1h:121:ASP:OD1	39:1h:121:ASP:N	2.50	0.44
55:1x:19:G:H5''	55:1x:60:U:O4	2.17	0.44
1:2A:29:U:H2'	1:2A:30:G:C8	2.53	0.44
1:2A:97:C:O3'	24:22:2:LYS:HA	2.18	0.44
1:2A:538:G:H2'	1:2A:539:G:H8	1.82	0.44
1:2A:947:G:H2'	1:2A:948:G:C8	2.53	0.44
1:2A:987:G:H2'	1:2A:988:A:O4'	2.18	0.44
1:2A:1179:C:H2'	1:2A:1180:C:C6	2.53	0.44
1:2A:1257:C:H4'	5:2F:83:PHE:CD1	2.53	0.44
3:2D:166:GLN:HB2	3:2D:174:ILE:HG22	1.99	0.44
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	2.00	0.44
14:2S:67:ARG:NH2	14:2S:103:GLU:OE1	2.51	0.44
20:2Y:75:ILE:HD13	20:2Y:75:ILE:HA	1.83	0.44
28:26:7:ILE:HD13	28:26:27:LYS:HB3	1.98	0.44
32:2a:792:A:H4'	32:2a:793:U:H5''	2.00	0.44
32:2a:1264:C:C4	32:2a:1272:G:O6	2.71	0.44
32:2a:1367:C:H5'	41:2j:60:ARG:HH12	1.82	0.44
35:2d:61:LYS:HD3	35:2d:206:PHE:CE2	2.53	0.44
48:2q:13:ASP:C	48:2q:15:MET:H	2.26	0.44
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.17	0.44
54:2w:39:PSU:H2'	54:2w:40:C:C6	2.53	0.44
1:1A:1021:A:H3'	1:1A:1021:A:N3	2.33	0.43
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.52	0.43
32:1a:396:G:O2'	32:1a:398:C:OP1	2.24	0.43
32:1a:719:C:O2'	49:1r:49:LYS:HB3	2.18	0.43
40:1i:79:LEU:O	40:1i:83:ARG:HG3	2.18	0.43
55:1x:47:U:H5'	55:1x:48:C:H5'	2.00	0.43
1:2A:1962:5MC:O2'	1:2A:1964:G:OP2	2.33	0.43
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.83	0.43
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.99	0.43
15:2T:106:SER:N	15:2T:109:GLU:OE1	2.45	0.43
18:2W:68:ARG:HB2	18:2W:109:GLU:HG2	2.00	0.43
28:26:9:LEU:HA	28:26:54:ILE:HB	2.00	0.43
32:2a:565:U:OP2	32:2a:566:G:O2'	2.33	0.43
32:2a:989:C:H1'	32:2a:1016:A:H2	1.83	0.43
32:2a:1065:U:H3	32:2a:1109:C:H5''	1.83	0.43
32:2a:1134:G:N2	32:2a:1136:U:O4	2.51	0.43
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.53	0.43
55:2x:19:G:H5''	55:2x:60:U:O4	2.18	0.43
1:1A:484:C:H2'	1:1A:485:C:C6	2.53	0.43
1:1A:1053:C:H42	1:1A:1106:G:H1	1.66	0.43
1:1A:2135:A:H61	1:1A:2156:G:H4'	1.83	0.43
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.18	0.43
1:1A:2721:A:H5''	63:1A:4204:HOH:O	2.18	0.43
5:1F:167:ALA:HB1	5:1F:173:VAL:HG11	2.00	0.43
9:1N:66:LYS:O	9:1N:70:LYS:HB3	2.18	0.43
12:1Q:16:ARG:HG2	12:1Q:18:LYS:HG3	1.99	0.43
40:1i:56:LEU:HD23	40:1i:56:LEU:H	1.82	0.43
47:1p:53:VAL:HG13	47:1p:79:VAL:HG22	2.00	0.43
1:2A:133:C:H42	1:2A:146:G:H1	1.66	0.43
1:2A:271(U):G:N7	63:2A:3797:HOH:O	2.36	0.43
1:2A:299:A:N1	1:2A:322:A:O2'	2.45	0.43
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.18	0.43
1:2A:2108:C:H2'	1:2A:2109:U:C6	2.53	0.43
1:2A:2371:G:O2'	28:26:46:HIS:ND1	2.43	0.43
32:2a:345:C:H4'	32:2a:346:G:O5'	2.18	0.43
32:2a:1144:G:H21	32:2a:1146:A:H62	1.65	0.43
32:2a:1380:U:C4	38:2g:3:ARG:HG2	2.52	0.43
32:2a:1502:A:H5'	32:2a:1504:G:N7	2.34	0.43
57:2y:13:C:N3	57:2y:22:G:O6	2.50	0.43
1:1A:700:G:H2'	1:1A:701:G:O4'	2.18	0.43
1:1A:724:U:H2'	1:1A:725:G:O4'	2.18	0.43
1:1A:1054:A:C6	1:1A:1055:G:C6	3.07	0.43
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	2.00	0.43
7:1H:83:TYR:CZ	7:1H:138:LYS:HD2	2.53	0.43
30:18:42:ARG:HD2	63:18:201:HOH:O	2.18	0.43
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.53	0.43
33:1b:8:LYS:O	33:1b:217:ARG:NH1	2.51	0.43
33:1b:93:VAL:HG11	33:1b:97:TRP:CD1	2.53	0.43
34:1c:109:PRO:HG2	34:1c:110:ASN:OD1	2.18	0.43
40:1i:55:ALA:HA	40:1i:58:HIS:CD2	2.53	0.43
50:1s:50:ALA:HA	50:1s:58:VAL:O	2.18	0.43
51:1t:39:LYS:HG2	51:1t:55:ILE:HG21	2.00	0.43
1:2A:330:A:H2	1:2A:1210:A:H2'	1.83	0.43
1:2A:528:A:N1	1:2A:2042:A:H2'	2.33	0.43
1:2A:879:G:H3'	1:2A:880:G:C8	2.51	0.43
1:2A:1423:G:H2'	1:2A:1424:G:H8	1.83	0.43
1:2A:1782:C:O2'	1:2A:2609:U:H5''	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:69:ALA:HB3	6:2G:91:ARG:NH2	2.34	0.43
8:2I:41:GLU:HA	8:2I:44:LEU:HB3	1.99	0.43
14:2S:29:PHE:O	14:2S:35:ILE:HA	2.18	0.43
26:24:16:CYS:HA	26:24:33:VAL:HG12	1.98	0.43
32:2a:1079:G:H2'	32:2a:1080:A:C8	2.53	0.43
32:2a:1134:G:N1	32:2a:1135:U:H1'	2.34	0.43
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.67	0.43
32:2a:1328:C:O2'	44:2m:29:ARG:NH2	2.40	0.43
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.53	0.43
41:2j:12:ASP:OD1	41:2j:13:HIS:N	2.51	0.43
45:2n:29:ARG:HG3	45:2n:30:ALA:N	2.34	0.43
1:1A:1174:A:H1'	1:1A:1175:U:C5'	2.48	0.43
1:1A:1614:A:P	1:1A:1614:A:H8	2.41	0.43
1:1A:2701:C:H2'	1:1A:2702:U:H2'	2.01	0.43
1:1A:2804:C:H2'	1:1A:2805:G:H8	1.83	0.43
7:1H:101:ARG:NH2	7:1H:122:THR:HG22	2.32	0.43
11:1P:63:PRO:HD3	30:18:27:THR:HG22	2.01	0.43
15:1T:1:MET:HE2	15:1T:3:ARG:HG3	1.99	0.43
16:1U:50:ARG:HG2	16:1U:53:ARG:HH22	1.82	0.43
41:1j:48:THR:OG1	41:1j:62:HIS:ND1	2.51	0.43
1:2A:90:U:H1'	1:2A:92:A:C8	2.53	0.43
1:2A:236:C:H2'	1:2A:237:C:C6	2.54	0.43
1:2A:287:C:H2'	1:2A:288:C:H6	1.84	0.43
1:2A:1341:U:OP2	1:2A:1394:U:O2'	2.22	0.43
1:2A:1991:U:H2'	1:2A:1992:G:H5''	2.01	0.43
1:2A:2224:G:H4'	1:2A:2226:C:C2	2.53	0.43
1:2A:2544:G:H1'	1:2A:2646:C:H4'	1.99	0.43
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.34	0.43
9:2N:55:VAL:HB	9:2N:125:GLY:O	2.18	0.43
12:2Q:57:HIS:NE2	12:2Q:116:GLU:HG2	2.33	0.43
12:2Q:97:VAL:HG11	12:2Q:103:MET:HE3	2.00	0.43
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.18	0.43
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.83	0.43
31:29:27:CYS:SG	31:29:28:GLU:N	2.91	0.43
32:2a:1130:A:H5''	40:2i:18:PHE:HE2	1.79	0.43
35:2d:73:ARG:HD2	35:2d:73:ARG:HA	1.78	0.43
36:2e:77:PRO:HD2	36:2e:142:LEU:HD22	1.99	0.43
41:2j:65:LEU:HB2	45:2n:56:VAL:HG13	2.01	0.43
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.33	0.43
55:2x:72:A:H2'	55:2x:73:A:C8	2.53	0.43
57:2y:9:A:H1'	57:2y:45:G:H21	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:443:A:C5	5:1F:45:ARG:HD2	2.53	0.43
1:1A:1006:C:C2	1:1A:1138:G:N2	2.86	0.43
1:1A:1833:U:O2'	1:1A:1969:A:N1	2.40	0.43
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.53	0.43
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.51	0.43
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.54	0.43
33:1b:122:PHE:HE2	33:1b:139:LYS:HB2	1.82	0.43
33:1b:174:VAL:O	33:1b:178:ARG:HG3	2.18	0.43
34:1c:62:ASP:O	34:1c:97:LYS:HB3	2.18	0.43
35:1d:112:VAL:H	35:1d:116:GLN:HE21	1.65	0.43
38:1g:100:ALA:O	38:1g:104:LEU:HB2	2.18	0.43
47:1p:20:VAL:HG23	47:1p:35:LYS:HA	2.01	0.43
47:1p:40:ASP:HB3	47:1p:48:TRP:HB2	2.00	0.43
47:1p:49:LEU:HD13	47:1p:50:LYS:N	2.32	0.43
49:1r:40:LEU:HD22	49:1r:70:ILE:HG12	2.00	0.43
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.32	0.43
54:1w:7:U:H6	54:1w:7:U:H2'	1.70	0.43
57:1y:28:U:H3	57:1y:42:A:H61	1.65	0.43
1:2A:764:A:H5''	3:2D:210:GLY:CA	2.48	0.43
1:2A:828:U:H4'	1:2A:831:G:N1	2.34	0.43
1:2A:895:U:O3'	1:2A:896:A:H3'	2.19	0.43
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.54	0.43
1:2A:1181:C:H2'	1:2A:1182:A:C8	2.54	0.43
4:2E:33:VAL:HG12	4:2E:89:ASP:O	2.19	0.43
16:2U:88:ILE:HG12	17:2V:49:THR:HG22	2.00	0.43
21:2Z:54:HIS:HB3	21:2Z:101:PRO:HD3	2.00	0.43
32:2a:114:U:O2'	32:2a:115:G:H5'	2.18	0.43
32:2a:473:G:C2	32:2a:474:G:C5	3.06	0.43
32:2a:918:A:H2'	32:2a:919:A:C8	2.53	0.43
32:2a:964:A:O2'	41:2j:55:LYS:NZ	2.50	0.43
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	2.01	0.43
35:2d:119:GLN:HG3	35:2d:123:HIS:HD2	1.83	0.43
54:2w:26:A:H2'	54:2w:27:G:C8	2.52	0.43
1:1A:529:A:OP2	9:1N:114:ARG:NH2	2.47	0.43
1:1A:730:C:H3'	63:1A:4117:HOH:O	2.18	0.43
1:1A:764:A:H5''	3:1D:210:GLY:HA2	2.00	0.43
1:1A:1143:A:OP2	63:1A:4154:HOH:O	2.21	0.43
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.18	0.43
1:1A:2477:C:N4	31:19:10:ILE:HG23	2.34	0.43
20:1Y:43:ASN:HB3	20:1Y:65:ALA:HB3	1.99	0.43
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:62:ARG:C	26:14:63:TYR:CG	2.96	0.43
32:1a:45:U:H2'	32:1a:46:G:C8	2.53	0.43
32:1a:262:A:C6	32:1a:263:A:C6	3.06	0.43
32:1a:1458:G:H5''	51:1t:31:SER:HB2	1.99	0.43
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.53	0.43
50:1s:39:THR:HG22	50:1s:40:ILE:O	2.17	0.43
57:1y:4:U:H2'	57:1y:5:C:O4'	2.18	0.43
1:2A:196:A:N3	1:2A:196:A:H2'	2.34	0.43
1:2A:275:G:H2'	1:2A:276:A:O4'	2.18	0.43
1:2A:879:G:H2'	1:2A:879:G:N3	2.34	0.43
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.54	0.43
1:2A:2075:U:OP2	1:2A:2238:G:O2'	2.34	0.43
1:2A:2330:G:O2'	22:20:41:ARG:O	2.32	0.43
1:2A:2749:A:H1'	7:2H:63:SER:OG	2.19	0.43
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.34	0.43
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.83	0.43
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.51	0.43
24:22:35:LEU:HD22	24:22:35:LEU:HA	1.91	0.43
26:24:67:TYR:HD2	50:2s:9:VAL:HB	1.83	0.43
32:2a:1279:A:H5''	32:2a:1280:A:OP1	2.19	0.43
33:2b:15:VAL:HG13	33:2b:209:ARG:HB3	2.00	0.43
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.18	0.43
54:2w:4:U:H3	54:2w:69:A:H61	1.67	0.43
1:1A:411:G:H3'	63:1A:4429:HOH:O	2.17	0.43
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.54	0.43
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	2.01	0.43
63:1A:5431:HOH:O	10:1O:20:MET:HE2	2.18	0.43
7:1H:3:ARG:NE	7:1H:3:ARG:HA	2.34	0.43
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.84	0.43
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	2.01	0.43
19:1X:26:TYR:HB3	19:1X:92:LEU:HD22	2.00	0.43
31:19:17:ILE:HD13	31:19:24:TYR:HB2	2.01	0.43
32:1a:834:C:H2'	32:1a:835:U:H6	1.84	0.43
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.19	0.43
32:1a:1131:G:OP1	40:1i:20:ARG:NH2	2.42	0.43
32:1a:1157:A:H4'	32:1a:1158:C:O5'	2.19	0.43
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.51	0.43
40:1i:49:PRO:HG2	40:1i:81:ILE:HG23	2.01	0.43
47:1p:6:LEU:HB3	47:1p:17:TYR:CD1	2.54	0.43
54:1w:37:T6A:N11	54:1w:37:T6A:N1	2.57	0.43
1:2A:492:A:H2'	1:2A:493:G:O4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.47	0.43
1:2A:887:A:H4'	1:2A:888:C:H5	1.83	0.43
1:2A:1359:A:C2	1:2A:1372:U:O4	2.71	0.43
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.18	0.43
1:2A:1372:U:H2'	1:2A:1373:A:O4'	2.18	0.43
1:2A:2135:A:C8	1:2A:2136:C:H5	2.36	0.43
1:2A:2697:G:H2'	1:2A:2698:U:O4'	2.19	0.43
7:2H:92:ILE:H	7:2H:92:ILE:HD12	1.83	0.43
15:2T:113:LYS:HD3	15:2T:113:LYS:HA	1.88	0.43
15:2T:127:ALA:C	15:2T:129:ARG:N	2.75	0.43
16:2U:97:ASP:OD1	16:2U:101:ARG:HD2	2.18	0.43
22:20:53:MET:HG2	22:20:57:PHE:HA	1.99	0.43
24:22:38:GLN:HE21	24:22:38:GLN:HB3	1.69	0.43
25:23:11:SER:HA	25:23:31:LEU:HD21	2.00	0.43
32:2a:431:A:H2'	32:2a:432:A:O4'	2.18	0.43
32:2a:718:G:H5'	42:2k:117:ASN:OD1	2.18	0.43
32:2a:988:G:H2'	32:2a:989:C:O4'	2.18	0.43
35:2d:112:VAL:H	35:2d:116:GLN:NE2	2.17	0.43
45:2n:23:ARG:HH12	45:2n:30:ALA:HB2	1.84	0.43
55:2x:10:G:N2	55:2x:26:G:H1'	2.34	0.43
1:1A:828:U:H4'	1:1A:831:G:N1	2.33	0.43
1:1A:1060:U:N3	1:1A:1088:A:C8	2.83	0.43
1:1A:1062:G:H22	1:1A:1077:A:H61	1.66	0.43
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.83	0.43
1:1A:2189:U:H2'	1:1A:2190:G:H8	1.81	0.43
1:1A:2252:G:OP2	63:1A:4151:HOH:O	2.21	0.43
2:1B:31:C:N4	14:1S:32:LEU:HD22	2.34	0.43
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.19	0.43
14:1S:36:TYR:CD1	14:1S:52:SER:HB3	2.54	0.43
21:1Z:151:HIS:HA	21:1Z:171:ILE:HG23	1.99	0.43
25:13:4:LEU:O	25:13:36:VAL:HA	2.18	0.43
32:1a:356:A:N3	32:1a:368:U:O2'	2.44	0.43
32:1a:714:G:H2'	32:1a:715:A:C8	2.54	0.43
32:1a:1179:A:H4'	40:1i:103:THR:HA	2.01	0.43
35:1d:60:GLU:OE2	35:1d:63:LYS:NZ	2.33	0.43
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.99	0.43
39:1h:97:VAL:HG13	39:1h:98:LYS:HG3	2.01	0.43
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	2.01	0.43
51:1t:43:LEU:HD22	51:1t:51:GLU:HB3	2.01	0.43
55:1x:13:C:H2'	55:1x:14:A:H5''	2.01	0.43
1:2A:340:A:H2'	1:2A:341:G:O4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:656:G:H2'	1:2A:657:U:O4'	2.18	0.43
1:2A:676:A:H1'	1:2A:2443:C:H1'	2.01	0.43
1:2A:1662:C:O2'	1:2A:2687:U:OP1	2.35	0.43
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.21	0.43
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.18	0.43
2:2B:40:U:H1'	2:2B:45:A:H61	1.84	0.43
5:2F:28:ILE:H	5:2F:28:ILE:HG13	1.71	0.43
7:2H:20:ALA:O	7:2H:22:GLY:N	2.52	0.43
9:2N:96:GLU:OE1	9:2N:96:GLU:N	2.39	0.43
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.59	0.43
23:21:72:GLU:O	23:21:76:ARG:HG2	2.19	0.43
32:2a:46:G:H2'	32:2a:366:C:C5	2.54	0.43
32:2a:447:G:O6	32:2a:485:G:O2'	2.21	0.43
32:2a:942:G:C2	32:2a:1342:C:C2	3.07	0.43
32:2a:1239:A:H4'	32:2a:1240:U:H5'	2.01	0.43
32:2a:1245:A:N6	32:2a:1292:U:H3	2.15	0.43
42:2k:17:GLY:O	42:2k:80:VAL:HA	2.19	0.43
54:2w:54:5MU:H2'	54:2w:55:PSU:O4'	2.19	0.43
1:1A:107:C:H2'	1:1A:108:U:H6	1.82	0.43
1:1A:1339:G:H5''	19:1X:16:LYS:HD3	2.01	0.43
1:1A:2784:C:H2'	1:1A:2785:C:C6	2.53	0.43
8:1I:72:LEU:HB3	8:1I:140:LEU:HD13	2.00	0.43
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.54	0.43
32:1a:580:U:H2'	32:1a:581:G:O4'	2.19	0.43
33:1b:32:ILE:HD13	33:1b:40:HIS:CD2	2.54	0.43
38:1g:115:ARG:HE	38:1g:115:ARG:H	1.67	0.43
45:1n:29:ARG:HD3	45:1n:40:CYS:SG	2.58	0.43
48:1q:56:VAL:HB	48:1q:78:GLU:HB3	2.01	0.43
1:2A:459:U:H4'	29:27:40:TRP:CZ3	2.53	0.43
1:2A:600:G:H5'	5:2F:32:LEU:HD12	2.00	0.43
1:2A:761:A:OP1	63:2A:3706:HOH:O	2.21	0.43
1:2A:1275:A:N1	1:2A:1295:C:O2'	2.40	0.43
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.36	0.43
1:2A:2591:C:H2'	1:2A:2592:G:C8	2.54	0.43
5:2F:126:VAL:O	5:2F:196:LEU:HG	2.19	0.43
12:2Q:20:ALA:HB2	21:2Z:79:ARG:HG3	2.01	0.43
21:2Z:149:SER:HA	21:2Z:173:ALA:HB2	2.00	0.43
30:28:26:LYS:HG2	30:28:46:ARG:O	2.19	0.43
32:2a:62:U:H2'	32:2a:63:C:C6	2.54	0.43
32:2a:373:A:O2'	32:2a:451:A:N7	2.52	0.43
32:2a:1226:C:H6	44:2m:103:THR:HB	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:71:VAL:HB	33:2b:164:VAL:HG13	2.01	0.43
34:2c:120:VAL:HA	34:2c:123:GLN:HB2	2.00	0.43
39:2h:63:LEU:HD12	39:2h:65:TYR:OH	2.19	0.43
46:2o:8:LYS:O	46:2o:12:ILE:HG13	2.18	0.43
1:1A:185:U:H2'	1:1A:186:G:H8	1.84	0.43
1:1A:784:A:C5	3:1D:229:VAL:HG21	2.54	0.43
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.53	0.43
1:1A:2816:C:O3'	13:1R:99:LYS:NZ	2.52	0.43
9:1N:91:LEU:O	9:1N:95:PRO:HB3	2.19	0.43
11:1P:81:GLN:NE2	11:1P:106:LEU:HA	2.34	0.43
32:1a:815:A:N7	32:1a:1509:C:O2'	2.50	0.43
32:1a:964:A:N3	32:1a:969:A:O2'	2.48	0.43
32:1a:1252:A:H2'	32:1a:1253:G:O4'	2.19	0.43
34:1c:58:GLU:HB3	41:1j:92:THR:HG21	2.00	0.43
48:1q:94:ASN:O	48:1q:98:LEU:HD13	2.19	0.43
57:1y:33:U:H2'	57:1y:35:U:OP2	2.19	0.43
1:2A:570:G:H2'	1:2A:2030:A:C5	2.54	0.43
1:2A:878:A:C6	1:2A:900:A:C8	3.07	0.43
1:2A:2206:G:H3'	1:2A:2207:G:N7	2.34	0.43
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.18	0.43
1:2A:2705:A:O2'	1:2A:2852:G:OP1	2.37	0.43
1:2A:2788:C:C5'	4:2E:61:ARG:HH21	2.32	0.43
23:21:4:VAL:HG21	23:21:11:ARG:HH21	1.82	0.43
26:24:58:ARG:O	26:24:61:ARG:HB2	2.19	0.43
32:2a:72:C:H2'	32:2a:73:G:H8	1.83	0.43
32:2a:141:A:H1'	32:2a:182:U:O2	2.19	0.43
32:2a:451:A:N6	32:2a:480:U:H2'	2.34	0.43
32:2a:629:G:H2'	32:2a:630:G:O4'	2.19	0.43
32:2a:814:A:N7	32:2a:816:A:C4	2.87	0.43
32:2a:942:G:H21	40:2i:124:GLN:CD	2.25	0.43
33:2b:105:PHE:O	33:2b:107:THR:N	2.45	0.43
33:2b:187:LEU:HD11	33:2b:214:ILE:HG21	2.01	0.43
35:2d:119:GLN:HE21	35:2d:119:GLN:HB2	1.58	0.43
55:2x:7:G:H5''	55:2x:8:4SU:H5	2.01	0.43
55:2x:21:A:N6	55:2x:46:G:H2'	2.33	0.43
55:2x:64:G:H2'	55:2x:65:C:C6	2.54	0.43
1:1A:686:G:H8	29:17:6:GLN:O	2.02	0.42
1:1A:774:A:N3	1:1A:774:A:H2'	2.34	0.42
1:1A:1495:A:C6	1:1A:1496:A:C6	3.07	0.42
1:1A:2163:C:H5''	1:1A:2164:C:OP2	2.19	0.42
1:1A:2763:G:OP2	63:1A:4155:HOH:O	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:35:VAL:HG21	10:1O:69:ILE:HD13	1.99	0.42
10:1O:53:LYS:HE3	10:1O:56:ASP:OD1	2.18	0.42
11:1P:45:LEU:HA	11:1P:45:LEU:HD12	1.79	0.42
32:1a:953:G:N7	44:1m:104:ARG:NH2	2.67	0.42
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.54	0.42
34:1c:11:ARG:NH2	34:1c:177:THR:O	2.48	0.42
40:1i:27:THR:HG23	40:1i:62:TYR:HA	2.01	0.42
42:1k:99:GLN:HE21	42:1k:108:ILE:HD11	1.84	0.42
44:1m:23:TYR:CE2	44:1m:71:ARG:HG3	2.54	0.42
54:1w:19:G:H4'	54:1w:20:U:OP1	2.19	0.42
1:2A:35:G:H1'	1:2A:454:A:C4	2.54	0.42
1:2A:603:A:O4'	1:2A:655:A:N6	2.52	0.42
1:2A:792:G:N3	1:2A:2072:G:O2'	2.43	0.42
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.54	0.42
1:2A:1537:G:H2'	1:2A:1538:G:H8	1.83	0.42
1:2A:1800:C:OP1	3:2D:260:ARG:NH2	2.52	0.42
1:2A:2118:U:C4	1:2A:2149:G:H1'	2.53	0.42
1:2A:2732:G:H3'	1:2A:2733:A:O4'	2.19	0.42
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.54	0.42
4:2E:96:PHE:O	4:2E:175:VAL:HG21	2.19	0.42
5:2F:36:VAL:HB	5:2F:183:VAL:HG21	2.01	0.42
14:2S:10:ARG:NH2	14:2S:91:PRO:O	2.37	0.42
14:2S:64:GLU:H	14:2S:64:GLU:HG3	1.63	0.42
15:2T:41:ARG:NH1	32:2a:346:G:OP1	2.52	0.42
28:26:34:LEU:H	28:26:51:GLU:HB3	1.83	0.42
32:2a:89:C:H2'	32:2a:90:U:O4'	2.18	0.42
32:2a:151:A:H2'	32:2a:152:A:O4'	2.18	0.42
32:2a:806:C:H2'	32:2a:807:A:C8	2.54	0.42
32:2a:920:U:H2'	32:2a:921:U:H6	1.84	0.42
32:2a:1151:A:O2'	32:2a:1152:A:H8	2.01	0.42
32:2a:1235:U:H2'	32:2a:1236:A:O4'	2.19	0.42
32:2a:1252:A:H2'	32:2a:1253:G:O4'	2.19	0.42
33:2b:153:ARG:C	33:2b:155:LEU:H	2.26	0.42
35:2d:13:ARG:HB3	35:2d:38:TYR:O	2.19	0.42
35:2d:110:PHE:N	35:2d:110:PHE:CD1	2.87	0.42
40:2i:21:PRO:HA	40:2i:59:PHE:HA	2.01	0.42
1:1A:322:A:OP1	5:1F:168:ARG:HD3	2.19	0.42
1:1A:601:C:OP1	5:1F:108:LYS:HE3	2.18	0.42
1:1A:882:G:H4'	54:1w:19:G:O6	2.19	0.42
1:1A:1657:C:H2'	1:1A:1658:C:C6	2.54	0.42
1:1A:2601:C:H2'	1:1A:2603:G:C8	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.84	0.42
6:1G:58:GLN:O	6:1G:62:LEU:HG	2.19	0.42
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	2.01	0.42
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.54	0.42
18:1W:65:LEU:HD12	18:1W:68:ARG:HE	1.83	0.42
32:1a:254:G:O2'	48:1q:16:GLN:O	2.31	0.42
32:1a:629:G:H2'	32:1a:630:G:C8	2.54	0.42
35:1d:19:LEU:HB3	35:1d:21:LEU:HD21	2.01	0.42
38:1g:78:ARG:HH12	38:1g:155:ARG:C	2.26	0.42
51:1t:90:GLN:N	51:1t:90:GLN:HE21	2.17	0.42
53:1v:23:A:H4'	53:1v:24:A:H5'	2.01	0.42
57:1y:10:G:H2'	57:1y:10:G:N3	2.33	0.42
1:2A:71:A:H5''	1:2A:73:A:C8	2.54	0.42
1:2A:265:A:H1'	1:2A:266:G:O4'	2.19	0.42
1:2A:320:A:O2'	1:2A:322:A:OP2	2.34	0.42
1:2A:446:G:OP2	63:2A:3743:HOH:O	2.22	0.42
1:2A:484:C:H2'	1:2A:485:C:H6	1.84	0.42
1:2A:851:U:O2'	25:23:42:ALA:O	2.32	0.42
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.18	0.42
1:2A:2808:U:H5''	1:2A:2891:G:O6	2.19	0.42
2:2B:105:A:H5'	2:2B:106:G:OP2	2.19	0.42
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	2.01	0.42
7:2H:20:ALA:HB3	7:2H:23:ARG:HB2	2.01	0.42
11:2P:84:ASN:HB3	11:2P:86:LYS:HG2	2.00	0.42
32:2a:119:A:H4'	32:2a:120:A:C8	2.54	0.42
32:2a:179:A:H2'	32:2a:180:U:C6	2.54	0.42
32:2a:946:A:H2'	32:2a:947:G:C8	2.54	0.42
38:2g:113:GLU:CG	38:2g:119:ARG:HG2	2.48	0.42
1:1A:721:C:H2'	1:1A:722:A:C8	2.54	0.42
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.54	0.42
8:1I:9:LEU:HB3	8:1I:12:LEU:HB3	2.00	0.42
12:1Q:12:GLN:NE2	12:1Q:72:LYS:HA	2.35	0.42
18:1W:12:ILE:O	18:1W:101:SER:OG	2.37	0.42
27:15:58:LEU:HG	27:15:59:GLU:H	1.84	0.42
32:1a:946:A:H2'	32:1a:947:G:C8	2.55	0.42
33:1b:59:GLU:HG2	33:1b:225:ALA:HB2	2.01	0.42
33:1b:230:VAL:HG12	33:1b:231:GLU:H	1.83	0.42
34:1c:77:ILE:O	34:1c:84:ILE:N	2.52	0.42
57:1y:1:G:H2'	57:1y:2:G:H8	1.84	0.42
1:2A:93:G:H2'	1:2A:94:C:C6	2.54	0.42
1:2A:872:A:OP1	12:2Q:5:ARG:NH2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1913:A:N6	54:2w:38:A:H5'	2.33	0.42
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.20	0.42
2:2B:43:C:H5''	26:24:1:MET:HG2	2.01	0.42
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	2.01	0.42
12:2Q:18:LYS:HE3	12:2Q:18:LYS:HB2	1.68	0.42
19:2X:11:PRO:CB	19:2X:92:LEU:HD21	2.50	0.42
21:2Z:53:ILE:HD12	21:2Z:99:TYR:HB2	2.00	0.42
32:2a:664:G:P	49:2r:64:ARG:HH21	2.42	0.42
32:2a:746:A:H2'	32:2a:747:C:C6	2.54	0.42
32:2a:1004:A:H5''	32:2a:1024:G:N2	2.35	0.42
34:2c:125:GLU:HB2	34:2c:190:ARG:NH2	2.29	0.42
35:2d:64:LEU:HB2	35:2d:198:VAL:HG11	2.01	0.42
40:2i:11:LYS:HA	40:2i:108:VAL:HG12	2.01	0.42
40:2i:47:LEU:HB3	40:2i:50:LEU:HD21	2.01	0.42
41:2j:42:THR:HG22	41:2j:66:ARG:HB3	2.01	0.42
44:2m:97:PRO:N	44:2m:110:ARG:HG2	2.34	0.42
55:2x:8:4SU:O5'	55:2x:8:4SU:H6	2.19	0.42
1:1A:644:A:H4'	1:1A:645:C:H5	1.85	0.42
1:1A:1064:C:H2'	1:1A:1065:U:H5'	2.01	0.42
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.45	0.42
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.19	0.42
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.54	0.42
26:14:61:ARG:HD3	50:1s:67:VAL:HG12	2.01	0.42
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.73	0.42
31:19:8:LYS:O	31:19:34:GLN:NE2	2.42	0.42
32:1a:184:G:H2'	32:1a:185:A:C8	2.54	0.42
32:1a:738:C:H2'	32:1a:739:C:H6	1.84	0.42
33:1b:160:ASP:O	33:1b:183:PRO:HD2	2.18	0.42
1:2A:1158:C:H4'	25:23:32:GLN:HB2	2.02	0.42
3:2D:5:LYS:HE3	3:2D:5:LYS:HB3	1.74	0.42
6:2G:111:LEU:HD23	6:2G:117:PHE:CZ	2.54	0.42
6:2G:166:ASP:HA	6:2G:169:ALA:HB3	2.01	0.42
7:2H:45:VAL:HG22	7:2H:50:VAL:HB	2.01	0.42
32:2a:42:G:O2'	32:2a:622:A:N1	2.49	0.42
33:2b:100:GLY:H	33:2b:176:GLU:CD	2.27	0.42
34:2c:125:GLU:HB2	34:2c:190:ARG:HE	1.83	0.42
35:2d:18:LYS:HG3	35:2d:33:MET:HG2	2.01	0.42
36:2e:80:ILE:HG22	36:2e:91:LEU:HB2	2.00	0.42
38:2g:99:LEU:HD23	38:2g:102:ARG:NH1	2.33	0.42
42:2k:86:GLY:O	42:2k:91:ARG:NH1	2.53	0.42
44:2m:10:PRO:HG2	44:2m:21:TYR:CE1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2p:25:ARG:HE	47:2p:25:ARG:HB2	1.73	0.42
49:2r:26:LEU:HD22	49:2r:29:PHE:CD2	2.55	0.42
1:1A:8:A:H2'	1:1A:9:U:H6	1.85	0.42
1:1A:264:C:O2'	1:1A:265:A:H2'	2.19	0.42
1:1A:1041:C:H42	1:1A:1114:G:H1	1.67	0.42
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.34	0.42
1:1A:1414:G:C6	1:1A:1415:U:C4	3.08	0.42
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.55	0.42
32:1a:60:A:N1	32:1a:107:G:O2'	2.51	0.42
32:1a:186:C:H2'	32:1a:187:C:H6	1.83	0.42
32:1a:203:U:O2	32:1a:216:G:N1	2.52	0.42
32:1a:925:G:H1'	32:1a:1502:A:C4	2.53	0.42
49:1r:47:THR:O	49:1r:83:GLU:N	2.49	0.42
1:2A:514:A:N3	1:2A:581:C:O2'	2.49	0.42
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.19	0.42
1:2A:1462:C:H4'	1:2A:2703:C:H5'	2.02	0.42
1:2A:1791:A:N6	1:2A:1828:G:O2'	2.50	0.42
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.20	0.42
1:2A:2023:G:H5'	1:2A:2617:C:H4'	2.01	0.42
1:2A:2726:U:O2'	1:2A:2727:G:H8	2.03	0.42
22:20:11:ARG:O	22:20:14:ARG:NH2	2.41	0.42
32:2a:781:A:OP1	32:2a:1523:G:H5'	2.19	0.42
32:2a:868:C:H2'	32:2a:869:G:O4'	2.18	0.42
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.55	0.42
32:2a:1438:G:H2'	32:2a:1439:C:C6	2.53	0.42
34:2c:6:HIS:CD2	34:2c:8:ILE:H	2.37	0.42
34:2c:35:GLU:O	34:2c:39:ILE:HG13	2.19	0.42
35:2d:202:LEU:HD23	35:2d:202:LEU:HA	1.86	0.42
47:2p:52:ASP:CG	47:2p:55:ARG:HG2	2.45	0.42
51:2t:16:HIS:O	51:2t:19:SER:OG	2.31	0.42
1:1A:11:G:N7	63:1A:4248:HOH:O	2.37	0.42
1:1A:1295:C:H2'	1:1A:1296:G:H8	1.83	0.42
1:1A:1509:C:H6	1:1A:1509:C:H2'	1.61	0.42
1:1A:2161:C:O2'	1:1A:2162:G:H8	2.03	0.42
8:1I:9:LEU:HD12	8:1I:12:LEU:HB2	2.02	0.42
10:1O:35:VAL:HG11	10:1O:103:ALA:CB	2.49	0.42
26:14:62:ARG:HB3	26:14:63:TYR:H	1.69	0.42
32:1a:728:A:H2'	32:1a:729:A:C8	2.55	0.42
32:1a:954:G:C6	32:1a:955:U:C4	3.08	0.42
40:1i:33:PHE:HD2	40:1i:34:ASN:ND2	2.15	0.42
41:1j:50:ILE:HA	41:1j:60:ARG:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1l:79:GLU:HG2	43:1l:80:HIS:CE1	2.54	0.42
57:1y:30:G:H2'	57:1y:31:A:C8	2.54	0.42
1:2A:881:G:H3'	1:2A:882:G:C8	2.55	0.42
1:2A:984:A:H5''	1:2A:985:C:H5	1.84	0.42
2:2B:88:C:H2'	2:2B:89:G:O4'	2.19	0.42
3:2D:6:PHE:HE2	3:2D:18:VAL:HG13	1.83	0.42
5:2F:33:LEU:HD12	5:2F:33:LEU:HA	1.83	0.42
16:2U:28:ARG:HH11	16:2U:38:THR:HG23	1.84	0.42
20:2Y:28:LYS:NZ	20:2Y:40:GLU:HG3	2.35	0.42
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	2.01	0.42
21:2Z:153:SER:HB2	21:2Z:167:PRO:HB3	2.00	0.42
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.54	0.42
34:2c:153:VAL:HG23	34:2c:166:GLU:O	2.18	0.42
42:2k:53:SER:C	42:2k:55:LYS:H	2.27	0.42
1:1A:586:A:N1	1:1A:809:G:O2'	2.47	0.42
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	2.01	0.42
2:1B:101:G:H2'	2:1B:102:A:O4'	2.20	0.42
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	2.01	0.42
7:1H:121:ILE:HG21	7:1H:144:VAL:HG11	2.01	0.42
12:1Q:1:MET:HB2	12:1Q:1:MET:HE3	1.74	0.42
21:1Z:31:ARG:NE	21:1Z:94:GLU:OE2	2.50	0.42
21:1Z:151:HIS:CD2	21:1Z:170:THR:HA	2.54	0.42
32:1a:141:A:H1'	32:1a:182:U:C2	2.55	0.42
32:1a:219:C:H2'	32:1a:220:G:O4'	2.20	0.42
32:1a:383:A:C5	32:1a:384:G:H1'	2.54	0.42
32:1a:502:G:H2'	32:1a:503:C:O4'	2.19	0.42
32:1a:911:U:H2'	32:1a:912:C:H6	1.84	0.42
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.20	0.42
32:1a:1273:G:H3'	32:1a:1274:G:C8	2.53	0.42
32:1a:1309:G:OP1	44:1m:92:HIS:HE1	2.02	0.42
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.20	0.42
38:1g:50:ILE:HD12	38:1g:61:VAL:HG11	2.00	0.42
40:1i:99:LEU:HD23	40:1i:99:LEU:HA	1.86	0.42
44:1m:108:ARG:C	44:1m:110:ARG:H	2.28	0.42
1:2A:530:G:N3	1:2A:530:G:O4'	2.53	0.42
1:2A:667:U:O2	30:28:2:PRO:HD2	2.20	0.42
1:2A:1186:G:C2	1:2A:1187:G:H1'	2.54	0.42
1:2A:1777:U:H2'	1:2A:1778:U:H6	1.85	0.42
1:2A:1910:G:H2'	1:2A:1911:PSU:H6	1.84	0.42
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.35	0.42
2:2B:21:G:H2'	2:2B:22:U:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:5:LEU:HD12	4:2E:51:PHE:HB2	2.00	0.42
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.20	0.42
32:2a:157:G:H1	32:2a:164:U:H3	1.67	0.42
32:2a:427:U:OP2	35:2d:36:ARG:NH2	2.53	0.42
32:2a:1135:U:H4'	32:2a:1136:U:H5	1.84	0.42
32:2a:1260:C:P	32:2a:1284:C:H4'	2.60	0.42
34:2c:30:ARG:CZ	45:2n:38:GLY:HA2	2.50	0.42
35:2d:57:ARG:NH1	35:2d:205:GLU:HB3	2.34	0.42
38:2g:22:LEU:HG	38:2g:62:PHE:HE2	1.84	0.42
38:2g:23:VAL:HG13	38:2g:43:PHE:HE2	1.85	0.42
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.19	0.42
46:2o:5:LYS:H	46:2o:5:LYS:HG3	1.72	0.42
54:2w:55:PSU:O2'	54:2w:57:G:N7	2.46	0.42
1:1A:576:U:H2'	1:1A:577:G:C8	2.55	0.42
1:1A:709:U:H2'	1:1A:710:G:C8	2.55	0.42
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.81	0.42
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.20	0.42
1:1A:1579:A:H2'	1:1A:1580:A:C8	2.55	0.42
1:1A:1782:C:O2	1:1A:2608:G:O2'	2.37	0.42
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.20	0.42
8:1I:77:LEU:HD21	8:1I:100:ALA:HB3	2.01	0.42
8:1I:114:LEU:HD12	8:1I:115:ALA:H	1.84	0.42
12:1Q:89:ASN:HB2	55:1x:1:C:N3	2.35	0.42
32:1a:401:C:H2'	32:1a:402:G:C8	2.54	0.42
32:1a:562:C:H1'	43:1l:15:ARG:HB3	2.02	0.42
32:1a:721:G:H4'	32:1a:722:A:O4'	2.20	0.42
32:1a:947:G:H4'	44:1m:109:THR:HG23	2.00	0.42
32:1a:963:G:H5'	63:1a:1992:HOH:O	2.19	0.42
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.37	0.42
32:1a:1372:U:H2'	32:1a:1373:G:O4'	2.19	0.42
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.55	0.42
32:1a:1492:A:H2'	32:1a:1493:A:C8	2.54	0.42
33:1b:19:HIS:HA	33:1b:39:ILE:HG23	2.02	0.42
36:1e:80:ILE:HG22	36:1e:91:LEU:HB2	2.02	0.42
39:1h:127:LEU:HD13	39:1h:127:LEU:HA	1.94	0.42
1:2A:383:U:H2'	1:2A:385:C:H5	1.85	0.42
1:2A:1249:U:O4	11:2P:18:ARG:HD2	2.20	0.42
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.84	0.42
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.34	0.42
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.19	0.42
8:2I:9:LEU:HD21	8:2I:35:LEU:HD13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:39:LYS:HG3	11:2P:45:LEU:HD22	2.01	0.42
22:20:46:LYS:HG2	22:20:77:ARG:O	2.19	0.42
32:2a:359:U:H2'	32:2a:360:A:C8	2.54	0.42
32:2a:749:C:H2'	32:2a:750:G:H8	1.85	0.42
45:2n:3:ARG:HA	45:2n:3:ARG:HD3	1.52	0.42
48:2q:76:LEU:HD12	48:2q:77:VAL:H	1.85	0.42
51:2t:87:LYS:O	51:2t:91:LEU:HG	2.20	0.42
54:2w:25:C:H2'	54:2w:26:A:H8	1.84	0.42
1:1A:411:G:C5	11:1P:72:PRO:HB3	2.55	0.42
1:1A:1028:A:N3	1:1A:2486:G:O2'	2.50	0.42
1:1A:2788:C:P	4:1E:61:ARG:HH21	2.42	0.42
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	2.01	0.42
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	2.02	0.42
6:1G:56:ALA:HA	6:1G:59:GLU:HG2	2.01	0.42
8:1I:124:GLY:H	8:1I:144:VAL:HG23	1.85	0.42
12:1Q:7:MET:HE2	12:1Q:7:MET:HB3	1.72	0.42
21:1Z:139:VAL:HG12	21:1Z:140:ASP:H	1.84	0.42
26:14:63:TYR:N	26:14:64:GLY:HA2	2.34	0.42
32:1a:167:G:H2'	32:1a:168:G:C8	2.54	0.42
32:1a:938:A:C6	32:1a:939:G:C5	3.08	0.42
33:1b:19:HIS:HA	33:1b:39:ILE:CG2	2.50	0.42
48:1q:6:LEU:HD22	48:1q:23:VAL:HG11	2.02	0.42
1:2A:26:G:C6	1:2A:27:G:N1	2.87	0.42
1:2A:608:A:H2'	1:2A:609:A:C8	2.55	0.42
1:2A:992:C:OP1	17:2V:74:LYS:NZ	2.50	0.42
1:2A:1444:G:H2'	1:2A:1445(A):C:C5	2.55	0.42
1:2A:2100:G:H1	1:2A:2189:U:H3	1.67	0.42
1:2A:2611:U:C5	60:2A:3688:ERY:H312	2.55	0.42
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	2.02	0.42
6:2G:107:LEU:HD21	6:2G:178:PHE:CE2	2.55	0.42
10:2O:53:LYS:N	10:2O:56:ASP:OD2	2.33	0.42
11:2P:121:LYS:O	11:2P:123:LEU:N	2.53	0.42
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.53	0.42
19:2X:32:PRO:HA	19:2X:77:LYS:HB2	2.02	0.42
24:22:13:ALA:HB1	24:22:21:LEU:HD21	2.02	0.42
24:22:65:ASN:O	24:22:69:ARG:HB2	2.20	0.42
32:2a:779:C:H2'	32:2a:780:A:O4'	2.20	0.42
32:2a:940:C:H2'	32:2a:941:G:C8	2.54	0.42
32:2a:954:G:H5''	44:2m:120:LYS:HD2	2.01	0.42
33:2b:20:GLU:HB2	33:2b:190:THR:OG1	2.20	0.42
33:2b:133:LYS:HA	33:2b:136:VAL:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:23:LYS:O	37:2f:27:GLN:N	2.49	0.42
44:2m:64:TRP:HB2	44:2m:66:LEU:HD21	2.02	0.42
46:2o:39:LEU:HD12	46:2o:39:LEU:HA	1.86	0.42
50:2s:40:ILE:HB	50:2s:67:VAL:O	2.20	0.42
54:2w:27:G:H1	54:2w:43:U:H3	1.67	0.42
57:2y:51:A:H2'	57:2y:52:G:O4'	2.19	0.42
1:1A:224:G:H2'	1:1A:225:A:O4'	2.20	0.42
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.19	0.42
1:1A:1882:C:H2'	1:1A:1883:G:O4'	2.20	0.42
14:1S:74:ALA:HB2	14:1S:110:LEU:HD22	2.02	0.42
32:1a:1182:G:H4'	32:1a:1183:A:H5''	2.01	0.42
33:1b:80:ILE:O	33:1b:84:GLU:HG2	2.19	0.42
38:1g:78:ARG:HD3	38:1g:156:TRP:CZ3	2.55	0.42
43:1l:5:PRO:HG2	43:1l:10:LEU:HD21	2.01	0.42
1:2A:55:G:O2'	1:2A:127:A:N1	2.43	0.42
1:2A:631:A:H2'	1:2A:632:A:O4'	2.20	0.42
1:2A:1003:G:N2	1:2A:1153:C:C2	2.88	0.42
1:2A:1786:A:C4	1:2A:1938:A:C6	3.08	0.42
2:2B:42:C:C4	2:2B:43:C:C4	3.08	0.42
2:2B:48:A:OP1	14:2S:30:ARG:NH2	2.53	0.42
2:2B:51:G:N7	14:2S:62:LYS:NZ	2.66	0.42
2:2B:52:A:N6	14:2S:33:LYS:HG2	2.35	0.42
5:2F:33:LEU:O	5:2F:37:VAL:HG23	2.19	0.42
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.54	0.42
14:2S:76:LYS:HE3	14:2S:76:LYS:HB2	1.94	0.42
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	2.00	0.42
34:2c:18:TRP:HE3	34:2c:18:TRP:H	1.66	0.42
34:2c:134:ILE:HD11	34:2c:153:VAL:HG22	2.00	0.42
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.37	0.42
50:2s:38:SER:O	50:2s:71:LEU:HG	2.20	0.42
54:2w:38:A:H2'	54:2w:39:PSU:O4'	2.20	0.42
1:1A:8:A:H2'	1:1A:9:U:C6	2.55	0.41
1:1A:295:G:OP1	20:1Y:1:MET:HB2	2.20	0.41
1:1A:1011:G:OP1	16:1U:77:SER:OG	2.36	0.41
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.20	0.41
4:1E:54:GLN:HG2	4:1E:59:VAL:HG23	2.02	0.41
5:1F:148:LEU:HD22	5:1F:154:VAL:HG21	2.01	0.41
8:1I:9:LEU:HD22	8:1I:9:LEU:HA	1.91	0.41
15:1T:45:PHE:CE1	15:1T:65:LYS:HD3	2.55	0.41
32:1a:691:G:H2'	32:1a:692:U:C6	2.55	0.41
32:1a:1004:A:H5''	32:1a:1025:U:H5	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1442:G:O2'	32:1a:1442(A):G:H5'	2.20	0.41
39:1h:121:ASP:HB2	39:1h:125:ARG:NH2	2.32	0.41
44:1m:81:LEU:HD23	44:1m:86:CYS:SG	2.60	0.41
45:1n:6:LEU:HB3	45:1n:23:ARG:NH2	2.36	0.41
1:2A:17:G:H2'	1:2A:18:C:C6	2.55	0.41
1:2A:271(H):G:H5'	23:21:81:LYS:NZ	2.35	0.41
1:2A:1357:U:H2'	1:2A:1358:G:O4'	2.19	0.41
1:2A:1455:G:O2'	1:2A:2853:C:OP1	2.27	0.41
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	2.02	0.41
1:2A:2094:G:C2	1:2A:2196:C:C2	3.08	0.41
1:2A:2104:G:H1	1:2A:2185:C:N4	2.18	0.41
1:2A:2397:G:N2	1:2A:2420:C:H1'	2.36	0.41
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.55	0.41
1:2A:2615:U:C2	27:25:7:PRO:HA	2.54	0.41
1:2A:2671:A:H2'	1:2A:2672:G:O4'	2.20	0.41
25:23:10:LYS:HB3	25:23:53:LEU:HA	2.02	0.41
32:2a:997:U:H3	32:2a:1044:A:H61	1.67	0.41
32:2a:1144:G:N2	32:2a:1146:A:H62	2.18	0.41
32:2a:1271:G:N2	32:2a:1272:G:C8	2.88	0.41
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.50	0.41
33:2b:212:GLN:CD	33:2b:235:SER:HB3	2.44	0.41
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	2.02	0.41
40:2i:88:TYR:CD2	40:2i:89:ASN:HB2	2.51	0.41
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.86	0.41
44:2m:18:ALA:HB3	44:2m:45:VAL:HG21	2.01	0.41
44:2m:70:LEU:O	44:2m:74:VAL:HG23	2.20	0.41
53:2v:14:A:N6	57:2y:34:U8U:S2	2.92	0.41
1:1A:383:U:H2'	1:1A:385:C:H5	1.85	0.41
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.55	0.41
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.55	0.41
5:1F:152:GLU:OE1	5:1F:191:ARG:HD2	2.20	0.41
12:1Q:4:PRO:HD3	12:1Q:70:PRO:O	2.20	0.41
21:1Z:67:LEU:HD23	21:1Z:67:LEU:HA	1.84	0.41
26:14:61:ARG:HG3	26:14:61:ARG:O	2.20	0.41
29:17:10:ARG:NH2	29:17:14:LYS:HE3	2.35	0.41
32:1a:742:G:OP1	46:1o:59:MET:HE2	2.20	0.41
32:1a:909:A:H2'	32:1a:910:C:O4'	2.20	0.41
32:1a:975:A:H5'	32:1a:975:A:H8	1.85	0.41
32:1a:985:C:H2'	32:1a:986:A:H8	1.85	0.41
32:1a:1001(A):G:H2'	32:1a:1002:G:O4'	2.21	0.41
32:1a:1072:G:C6	32:1a:1073:U:C4	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1314:C:H2'	32:1a:1315:U:C6	2.55	0.41
32:1a:1366:C:H2'	32:1a:1367:C:C6	2.55	0.41
32:1a:1530:G:OP1	32:1a:1530:G:H4'	2.20	0.41
36:1e:83:GLU:HA	36:1e:87:SER:O	2.20	0.41
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	2.01	0.41
53:1v:23:A:H4'	53:1v:24:A:C5'	2.51	0.41
1:2A:244:A:H2'	1:2A:245:G:O4'	2.19	0.41
1:2A:629:G:H5''	1:2A:650:C:O2'	2.20	0.41
1:2A:1923:U:OP1	55:2x:24:U:O2'	2.31	0.41
1:2A:2168:G:OP2	1:2A:2168:G:N2	2.50	0.41
1:2A:2245:U:O2'	1:2A:2436:G:OP2	2.33	0.41
60:2A:3688:ERY:H312	60:2A:3688:ERY:H2	1.83	0.41
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.53	0.41
2:2B:91:C:OP1	12:2Q:16:ARG:HD2	2.20	0.41
4:2E:170:LEU:HB3	4:2E:184:VAL:HG22	2.01	0.41
6:2G:121:ASN:HD22	6:2G:124:SER:HB2	1.84	0.41
7:2H:98:LEU:HD23	7:2H:103:LEU:HB3	2.03	0.41
7:2H:98:LEU:HA	7:2H:103:LEU:HA	2.03	0.41
8:2I:117:GLU:H	8:2I:117:GLU:HG3	1.42	0.41
10:2O:49:ARG:HH22	32:2a:1423:G:P	2.42	0.41
14:2S:80:LEU:HA	14:2S:80:LEU:HD23	1.79	0.41
20:2Y:78:ALA:C	20:2Y:80:GLY:H	2.28	0.41
21:2Z:101:PRO:HA	21:2Z:123:ASP:HA	2.02	0.41
30:28:62:LEU:HB3	30:28:65:GLU:CG	2.49	0.41
32:2a:344:A:H4'	32:2a:345:C:OP2	2.20	0.41
32:2a:573:A:N3	32:2a:883:C:O2'	2.52	0.41
32:2a:892:A:O2'	32:2a:1415:G:H4'	2.20	0.41
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.38	0.41
32:2a:1077:G:N2	32:2a:1080:A:OP2	2.48	0.41
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	2.02	0.41
32:2a:1516:G:N1	32:2a:1519:MA6:OP2	2.54	0.41
34:2c:88:ARG:O	34:2c:91:LEU:HB2	2.20	0.41
36:2e:84:PHE:O	36:2e:86:ALA:N	2.52	0.41
38:2g:115:ARG:O	38:2g:119:ARG:HG3	2.20	0.41
40:2i:40:LEU:HD23	40:2i:42:ARG:H	1.85	0.41
46:2o:21:ASP:OD1	46:2o:24:SER:HB3	2.20	0.41
1:1A:26:G:H1'	1:1A:515:A:H61	1.85	0.41
1:1A:428:A:H8	1:1A:428:A:OP2	2.02	0.41
1:1A:555:U:O2'	1:1A:556:G:N7	2.46	0.41
1:1A:1055:G:H2'	1:1A:1056:G:O4'	2.20	0.41
1:1A:1258:C:H2'	1:1A:1259:G:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.21	0.41
1:1A:2097:C:H2'	1:1A:2098:U:O4'	2.20	0.41
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.55	0.41
1:1A:2347:C:OP1	28:16:38:LYS:NZ	2.49	0.41
1:1A:2406:U:H2'	1:1A:2406:U:H6	1.68	0.41
1:1A:2815:C:O2'	27:15:42:PRO:HG2	2.20	0.41
3:1D:147:LEU:HD22	3:1D:155:LEU:HD21	2.01	0.41
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.45	0.41
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.35	0.41
32:1a:708:C:H2'	32:1a:709:G:C8	2.54	0.41
32:1a:1090:U:H2'	32:1a:1091:U:H6	1.85	0.41
32:1a:1464:G:H2'	32:1a:1465:C:C6	2.55	0.41
35:1d:153:ARG:O	35:1d:181:MET:HE1	2.20	0.41
41:1j:49:VAL:HG11	45:1n:41:ARG:O	2.21	0.41
50:1s:27:GLU:HB2	50:1s:28:LYS:CA	2.49	0.41
51:1t:92:LEU:O	51:1t:96:GLY:HA2	2.20	0.41
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.20	0.41
1:2A:330:A:H2	1:2A:1210:A:O2'	2.04	0.41
1:2A:511:U:O4	1:2A:512:G:N1	2.53	0.41
1:2A:569:U:C4	1:2A:570:G:C6	3.08	0.41
1:2A:658:C:H2'	1:2A:659:C:C6	2.55	0.41
1:2A:827:U:O2'	1:2A:2068:U:C2	2.69	0.41
1:2A:860:U:C2	1:2A:2268:A:C8	3.08	0.41
1:2A:1192:G:OP2	11:2P:17:LYS:NZ	2.47	0.41
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.20	0.41
1:2A:1639:U:H5''	63:2A:4254:HOH:O	2.21	0.41
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.56	0.41
1:2A:2100:G:H2'	1:2A:2101:G:H8	1.85	0.41
1:2A:2275:C:O2	12:2Q:85:LYS:HD2	2.20	0.41
1:2A:2542:A:H4'	1:2A:2543:G:C8	2.54	0.41
1:2A:2735:G:H2'	1:2A:2736:G:H8	1.84	0.41
9:2N:38:HIS:CD2	9:2N:39:ARG:HG3	2.54	0.41
14:2S:19:LYS:O	14:2S:21:THR:N	2.54	0.41
14:2S:25:ARG:HB3	14:2S:40:ILE:HB	2.02	0.41
16:2U:48:ALA:O	16:2U:52:ARG:HG3	2.20	0.41
16:2U:85:LYS:HE2	16:2U:85:LYS:HB3	1.93	0.41
25:23:8:LEU:HD23	25:23:30:ARG:O	2.20	0.41
32:2a:21:G:C2	32:2a:22:G:C5	3.07	0.41
32:2a:630:G:H2'	32:2a:631:G:H8	1.86	0.41
32:2a:707:C:H2'	32:2a:708:C:H6	1.85	0.41
32:2a:1224:G:H1	32:2a:1363:C:N4	2.14	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:149:LEU:HD23	33:2b:149:LEU:HA	1.91	0.41
34:2c:77:ILE:HG13	34:2c:78:GLY:H	1.84	0.41
34:2c:106:VAL:C	34:2c:108:ASN:H	2.28	0.41
35:2d:134:ASP:O	35:2d:136:PRO:HD3	2.21	0.41
44:2m:10:PRO:HG2	44:2m:21:TYR:CD1	2.56	0.41
48:2q:67:LYS:O	48:2q:68:ARG:HB2	2.20	0.41
50:2s:32:LYS:HD2	50:2s:34:TRP:CZ3	2.54	0.41
55:2x:61:C:H2'	55:2x:62:C:C6	2.55	0.41
57:2y:3:G:N2	57:2y:71:C:H1'	2.35	0.41
57:2y:53:G:H3'	57:2y:54:5MU:H73	2.01	0.41
1:1A:69:C:O2'	1:1A:70:G:H5'	2.20	0.41
1:1A:376:C:H2'	1:1A:377:C:C6	2.55	0.41
1:1A:886:C:OP1	1:1A:886:C:H4'	2.14	0.41
1:1A:956:G:H2'	1:1A:957:A:H2'	2.02	0.41
1:1A:1179:C:H2'	1:1A:1180:C:H6	1.85	0.41
1:1A:1914:C:H2'	1:1A:1915:5MU:O4'	2.20	0.41
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.20	0.41
1:1A:2136:C:N4	1:1A:2155:G:C6	2.84	0.41
1:1A:2749:A:OP2	1:1A:2750:A:O2'	2.30	0.41
3:1D:20:ASP:N	3:1D:20:ASP:OD1	2.53	0.41
4:1E:59:VAL:O	4:1E:64:LYS:HE3	2.20	0.41
11:1P:37:GLY:C	11:1P:38:GLN:O	2.64	0.41
21:1Z:104:PHE:HA	21:1Z:139:VAL:HB	2.02	0.41
32:1a:600:C:H2'	32:1a:601:C:C6	2.55	0.41
32:1a:734:G:H21	49:1r:75:ILE:HD11	1.85	0.41
32:1a:841:U:H3'	32:1a:848:C:O4'	2.20	0.41
32:1a:1165:C:N4	32:1a:1166:G:O6	2.53	0.41
34:1c:130:VAL:HG21	34:1c:157:ILE:HG23	2.03	0.41
41:1j:47:PHE:HB2	41:1j:63:PHE:HB2	2.03	0.41
57:1y:6:G:C2'	57:1y:7:U:H5'	2.50	0.41
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.55	0.41
1:2A:251:A:C4	1:2A:252:G:H1'	2.56	0.41
1:2A:634:C:H2'	1:2A:635:C:C6	2.56	0.41
1:2A:956:G:OP2	12:2Q:14:ARG:NH1	2.52	0.41
1:2A:2165:G:H1	1:2A:2171:A:H8	1.67	0.41
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.21	0.41
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.20	0.41
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	2.01	0.41
32:2a:1005:A:H3'	32:2a:1006:C:H6	1.86	0.41
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.21	0.41
33:2b:31:TYR:CE2	33:2b:200:ILE:HG21	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:82:GLU:HB3	34:2c:83:ARG:H	1.76	0.41
35:2d:11:LEU:HD23	35:2d:66:ARG:HB3	2.02	0.41
35:2d:191:ARG:NH1	35:2d:194:LEU:O	2.53	0.41
37:2f:76:ALA:O	37:2f:80:ARG:HG3	2.21	0.41
44:2m:94:ARG:NH2	50:2s:81:ARG:HA	2.34	0.41
50:2s:36:ARG:HD3	50:2s:52:TYR:O	2.21	0.41
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.21	0.41
1:1A:2572:A:OP1	1:1A:2574:G:O2'	2.35	0.41
3:1D:206:LEU:HD23	3:1D:206:LEU:HA	1.71	0.41
8:1I:96:ASP:OD1	8:1I:96:ASP:N	2.54	0.41
32:1a:34:C:H2'	32:1a:35:G:C8	2.56	0.41
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.28	0.41
32:1a:1320:C:H2'	32:1a:1321:C:O4'	2.19	0.41
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.20	0.41
34:1c:180:ALA:HB1	34:1c:203:PHE:CE1	2.55	0.41
44:1m:86:CYS:HB2	50:1s:73:GLU:HB3	2.03	0.41
54:1w:76:A1B8A:N	55:1x:76:8AN:O2'	2.54	0.41
1:2A:19:C:H2'	1:2A:20:C:H6	1.85	0.41
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.55	0.41
1:2A:1431:U:H2'	1:2A:1432:C:C6	2.55	0.41
19:2X:26:TYR:O	19:2X:81:VAL:HG23	2.19	0.41
32:2a:189(L):G:H2'	32:2a:190:U:C6	2.56	0.41
32:2a:1074:G:H4'	33:2b:103:THR:O	2.20	0.41
32:2a:1086:U:H3	32:2a:1099:G:H22	1.67	0.41
32:2a:1128:C:O2'	32:2a:1147:C:N3	2.37	0.41
34:2c:42:LEU:O	34:2c:43:LEU:HD23	2.21	0.41
34:2c:54:ARG:HA	34:2c:54:ARG:HD2	1.89	0.41
1:1A:1257:C:H4'	5:1F:83:PHE:CD1	2.55	0.41
1:1A:1670:C:O2	4:1E:129:HIS:NE2	2.52	0.41
1:1A:2680:C:H5'	4:1E:189:PRO:HA	2.03	0.41
12:1Q:12:GLN:HE21	12:1Q:72:LYS:HA	1.85	0.41
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.55	0.41
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.46	0.41
26:14:12:ALA:HB2	26:14:26:SER:HB3	2.02	0.41
28:16:17:LYS:HE3	28:16:17:LYS:HB3	1.89	0.41
32:1a:439:A:C8	32:1a:496:A:C6	3.09	0.41
33:1b:200:ILE:HG22	33:1b:202:PRO:HD3	2.03	0.41
36:1e:112:LEU:HD23	36:1e:112:LEU:HA	1.88	0.41
40:1i:10:ARG:O	40:1i:11:LYS:C	2.63	0.41
40:1i:53:VAL:HG11	40:1i:92:TYR:CE1	2.56	0.41
48:1q:48:GLU:O	48:1q:49:GLU:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1t:92:LEU:HA	51:1t:92:LEU:HD23	1.81	0.41
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	2.02	0.41
1:2A:522:G:H2'	1:2A:523:C:C6	2.56	0.41
1:2A:723:G:H2'	1:2A:724:U:O4'	2.21	0.41
1:2A:760:G:H2'	1:2A:761:A:O4'	2.19	0.41
1:2A:893:C:H5'	1:2A:894:C:C5	2.55	0.41
1:2A:1853:A:N1	1:2A:2087:G:H1'	2.36	0.41
1:2A:1952:A:OP1	10:2O:44:LYS:NZ	2.44	0.41
1:2A:2070:G:C2	1:2A:2442:C:C2	3.09	0.41
1:2A:2110:G:C2	1:2A:2120:G:H1'	2.55	0.41
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.35	0.41
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.55	0.41
1:2A:2370:G:C6	1:2A:2371:G:C6	3.09	0.41
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.55	0.41
1:2A:2752:C:H2'	1:2A:2753:A:O4'	2.20	0.41
2:2B:95:C:H2'	2:2B:96:U:C6	2.56	0.41
8:2I:3:VAL:O	8:2I:18:VAL:HA	2.21	0.41
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	2.02	0.41
32:2a:607:A:H2'	32:2a:608:A:O4'	2.21	0.41
32:2a:1206:G:C6	32:2a:1207:2MG:C5	3.09	0.41
38:2g:102:ARG:O	38:2g:106:GLN:HG3	2.20	0.41
43:2l:53:ARG:HD2	43:2l:93:LEU:HD11	2.03	0.41
44:2m:15:VAL:O	44:2m:19:LEU:HG	2.20	0.41
48:2q:27:PHE:CE1	48:2q:36:ILE:HD11	2.56	0.41
1:1A:127:A:H5''	1:1A:128:C:C6	2.56	0.41
1:1A:995:C:OP2	16:1U:54:LYS:NZ	2.54	0.41
1:1A:1541:G:H3'	1:1A:1542:A:H2'	2.02	0.41
1:1A:1957:C:H2'	1:1A:1958:C:C6	2.56	0.41
1:1A:2166:G:H2'	1:1A:2167:U:H6	1.84	0.41
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.55	0.41
1:1A:2295:C:OP1	14:1S:10:ARG:NH1	2.53	0.41
1:1A:2361:A:OP1	30:18:27:THR:OG1	2.29	0.41
2:1B:32:C:C2	2:1B:51:G:N2	2.89	0.41
3:1D:16:MET:HE2	3:1D:16:MET:HB2	1.88	0.41
5:1F:181:LEU:HD12	5:1F:181:LEU:HA	1.95	0.41
20:1Y:8:LYS:HD3	20:1Y:97:ARG:NH1	2.36	0.41
32:1a:955:U:O2'	50:1s:83:HIS:HD2	2.04	0.41
32:1a:1069:C:O2'	32:1a:1192:C:H1'	2.20	0.41
32:1a:1129:C:H42	32:1a:1143:G:H1	1.69	0.41
32:1a:1250:A:O3'	40:1i:67:GLY:HA2	2.21	0.41
35:1d:158:ILE:H	35:1d:158:ILE:HG13	1.43	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:1x:15:G:H21	55:1x:21:A:H1'	1.85	0.41
1:2A:74:A:H4'	1:2A:75:G:O5'	2.21	0.41
1:2A:921:G:C2	1:2A:922:U:C2	3.09	0.41
1:2A:921:G:C6	1:2A:922:U:C4	3.08	0.41
1:2A:1638:C:H2'	1:2A:1639:U:O4'	2.21	0.41
1:2A:1830:C:H2'	1:2A:1831:G:H8	1.84	0.41
1:2A:1876:A:H2'	1:2A:1877:A:H8	1.84	0.41
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	2.03	0.41
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.20	0.41
1:2A:2618:G:H21	4:2E:150:VAL:HG21	1.85	0.41
4:2E:176:ILE:HB	4:2E:181:LEU:HB2	2.03	0.41
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	2.02	0.41
11:2P:88:LEU:HA	11:2P:91:PHE:HD2	1.86	0.41
20:2Y:55:TYR:N	20:2Y:56:PRO:HD3	2.35	0.41
32:2a:983:A:H3'	32:2a:983:A:N3	2.36	0.41
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.20	0.41
1:1A:27:G:O2'	1:1A:28:A:OP2	2.34	0.41
1:1A:505:A:OP2	63:1A:4158:HOH:O	2.22	0.41
1:1A:725:G:C6	1:1A:726:G:N1	2.89	0.41
1:1A:919:G:N2	1:1A:2269:A:OP2	2.53	0.41
1:1A:1614:A:C2	18:1W:93:ALA:HB2	2.56	0.41
1:1A:1762:A:H2'	63:1A:5472:HOH:O	2.19	0.41
1:1A:2065:C:OP2	63:1A:4156:HOH:O	2.22	0.41
1:1A:2319:G:C2	14:1S:3:ARG:HA	2.56	0.41
6:1G:101:ILE:HD13	26:14:25:TYR:HB2	2.03	0.41
30:18:4:MET:HE3	30:18:63:PRO:HG3	2.02	0.41
32:1a:857:C:H2'	32:1a:858:G:O4'	2.21	0.41
32:1a:918:A:H2'	32:1a:919:A:O4'	2.21	0.41
32:1a:958:A:C2	50:1s:55:LYS:HB2	2.56	0.41
32:1a:1121:U:H2'	32:1a:1122:U:C6	2.56	0.41
32:1a:1259:C:O2'	32:1a:1283:G:N3	2.48	0.41
32:1a:1457:G:H2'	32:1a:1458:G:C8	2.56	0.41
35:1d:64:LEU:HD13	35:1d:198:VAL:HG11	2.03	0.41
36:1e:41:VAL:O	36:1e:66:MET:HA	2.21	0.41
1:2A:176:G:O2'	1:2A:177:G:H5'	2.21	0.41
1:2A:1183:G:H5''	25:23:30:ARG:HH22	1.86	0.41
1:2A:1470:G:O6	63:2A:3742:HOH:O	2.21	0.41
1:2A:1777:U:H2'	1:2A:1778:U:C6	2.56	0.41
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.36	0.41
1:2A:2038:G:H2'	1:2A:2039:C:O4'	2.20	0.41
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:106:G:OP1	21:2Z:31:ARG:HB3	2.21	0.41
4:2E:54:GLN:OE1	4:2E:55:ASN:N	2.54	0.41
4:2E:181:LEU:HD23	4:2E:181:LEU:HA	1.84	0.41
5:2F:116:ASP:O	5:2F:120:GLU:HG2	2.21	0.41
10:2O:52:VAL:HG12	10:2O:94:ARG:NH2	2.36	0.41
13:2R:38:VAL:HB	13:2R:39:PRO:HD3	2.03	0.41
21:2Z:19:ARG:HG3	21:2Z:25:PRO:HD3	2.01	0.41
21:2Z:44:PHE:O	21:2Z:48:PHE:HB3	2.21	0.41
32:2a:164:U:H2'	32:2a:165:C:C6	2.55	0.41
32:2a:615:C:H2'	32:2a:616:G:O4'	2.20	0.41
32:2a:957:U:H2'	32:2a:959:A:OP2	2.21	0.41
32:2a:1243:C:H42	32:2a:1294:G:H1	1.68	0.41
43:2l:69:TYR:CD1	43:2l:90:VAL:HG21	2.56	0.41
48:2q:92:ARG:O	48:2q:95:TYR:HB2	2.21	0.41
50:2s:37:ARG:O	50:2s:37:ARG:HD3	2.21	0.41
57:2y:30:G:H2'	57:2y:31:A:H8	1.86	0.41
1:1A:548:A:N6	17:1V:19:LYS:H	2.18	0.41
1:1A:662:G:H5''	11:1P:16:ARG:HG2	2.03	0.41
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.55	0.41
1:1A:2317:C:H2'	1:1A:2318:G:O4'	2.21	0.41
4:1E:96:PHE:O	4:1E:175:VAL:HG21	2.21	0.41
6:1G:7:LEU:HD12	6:1G:104:GLU:N	2.36	0.41
6:1G:120:LEU:HD23	6:1G:120:LEU:HA	1.90	0.41
8:1I:38:LEU:HD23	8:1I:38:LEU:N	2.35	0.41
8:1I:69:LYS:HE2	8:1I:73:GLU:OE2	2.21	0.41
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.21	0.41
10:1O:107:ARG:NH2	15:1T:36:GLU:HG2	2.36	0.41
14:1S:34:HIS:O	14:1S:97:ARG:NH2	2.53	0.41
32:1a:452:A:H4'	47:1p:72:ARG:CZ	2.50	0.41
32:1a:458:C:H2'	32:1a:460:G:O4'	2.21	0.41
32:1a:1033:G:H3'	32:1a:1034:G:H8	1.85	0.41
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.36	0.41
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.56	0.41
33:1b:84:GLU:HA	33:1b:87:ARG:HD3	2.02	0.41
34:1c:12:LEU:O	45:1n:57:ARG:HD3	2.20	0.41
36:1e:48:ALA:HB3	36:1e:54:ALA:HB2	2.03	0.41
36:1e:79:GLU:HG2	39:1h:104:ARG:HD3	2.03	0.41
37:1f:22:GLU:O	37:1f:26:ILE:HG13	2.21	0.41
38:1g:78:ARG:HG3	38:1g:80:VAL:HG23	2.02	0.41
39:1h:23:SER:HA	39:1h:61:VAL:O	2.21	0.41
39:1h:86:ILE:HG13	39:1h:135:CYS:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:49:VAL:HG12	41:1j:50:ILE:O	2.20	0.41
41:1j:81:THR:C	41:1j:83:GLU:H	2.29	0.41
44:1m:53:VAL:HG12	44:1m:57:ARG:HH12	1.86	0.41
51:1t:89:ARG:HH12	51:1t:103:GLY:HA3	1.86	0.41
57:1y:6:G:O6	57:1y:66:A:N6	2.54	0.41
1:2A:8:A:H2'	1:2A:9:U:C6	2.56	0.41
1:2A:1027:A:C6	1:2A:1126:A:C4	3.09	0.41
1:2A:1127:A:N7	1:2A:2488:A:O2'	2.51	0.41
1:2A:1983:C:H4'	1:2A:2606:C:H4'	2.02	0.41
1:2A:2097:C:H2'	1:2A:2098:U:O4'	2.20	0.41
1:2A:2274:A:C5	1:2A:2276:G:C8	3.08	0.41
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.56	0.41
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.21	0.41
4:2E:9:VAL:HG13	15:2T:3:ARG:HG2	2.02	0.41
14:2S:36:TYR:CD2	14:2S:36:TYR:N	2.89	0.41
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.39	0.41
32:2a:46:G:O2'	32:2a:365:U:H1'	2.20	0.41
32:2a:193:C:H2'	32:2a:194:C:C6	2.56	0.41
32:2a:435:C:H2'	32:2a:436:C:H6	1.86	0.41
32:2a:838:G:OP2	32:2a:840:C:N4	2.54	0.41
32:2a:1217:C:H2'	32:2a:1218:C:C6	2.56	0.41
32:2a:1221:G:H4'	50:2s:53:ASN:O	2.20	0.41
32:2a:1327:C:P	52:2u:12:LYS:HZ1	2.44	0.41
32:2a:1378:C:N3	32:2a:1379:G:H1'	2.36	0.41
33:2b:25:ASN:OD1	33:2b:27:LYS:HB2	2.21	0.41
33:2b:55:PHE:HZ	33:2b:218:ALA:HA	1.84	0.41
33:2b:77:ALA:HA	33:2b:80:ILE:HG23	2.02	0.41
36:2e:123:LEU:HD23	36:2e:123:LEU:HA	1.74	0.41
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.86	0.41
39:2h:33:GLU:O	39:2h:36:LEU:N	2.54	0.41
45:2n:24:CYS:C	45:2n:26:ARG:H	2.28	0.41
49:2r:63:GLN:HE21	49:2r:63:GLN:HB2	1.61	0.41
53:2v:14:A:N3	53:2v:14:A:H2'	2.34	0.41
54:2w:50:C:H2'	54:2w:50:C:O2	2.21	0.41
54:2w:63:U:C2	54:2w:64:G:C8	3.08	0.41
1:1A:848:G:O6	1:1A:928:G:H2'	2.21	0.41
1:1A:1062:G:H2'	1:1A:1063:G:C8	2.55	0.41
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.56	0.41
1:1A:2128:C:N3	1:1A:2160:G:N2	2.62	0.41
1:1A:2251:OMG:H1'	1:1A:2251:OMG:HM23	1.88	0.41
63:1A:4865:HOH:O	5:1F:74:ARG:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:154:VAL:HG22	5:1F:191:ARG:HB2	2.03	0.41
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	2.02	0.41
7:1H:56:SER:OG	7:1H:58:GLU:HG2	2.19	0.41
10:1O:104:ARG:NH2	15:1T:36:GLU:OE2	2.49	0.41
12:1Q:63:LYS:HG2	12:1Q:65:PHE:CZ	2.56	0.41
25:13:55:ARG:HE	25:13:55:ARG:C	2.29	0.41
26:14:56:VAL:HB	26:14:60:GLN:HG3	2.02	0.41
32:1a:23:C:OP2	32:1a:561:U:N3	2.42	0.41
32:1a:66:G:O4'	32:1a:173:U:C4	2.74	0.41
32:1a:411:A:O2'	32:1a:413:G:H5'	2.21	0.41
32:1a:880:C:OP1	43:1l:8:ASN:ND2	2.53	0.41
32:1a:1054:C:C4	32:1a:1196:U:H5	2.39	0.41
32:1a:1109:C:OP2	34:1c:176:HIS:ND1	2.54	0.41
32:1a:1226:C:H4'	50:1s:80:TYR:CZ	2.57	0.41
34:1c:58:GLU:HB2	34:1c:65:ALA:HB3	2.03	0.41
36:1e:7:GLU:OE2	36:1e:37:ARG:NH2	2.54	0.41
38:1g:89:MET:HG3	38:1g:156:TRP:CZ2	2.56	0.41
42:1k:62:GLN:O	42:1k:66:LEU:HG	2.21	0.41
1:2A:747:U:O2	1:2A:2014:A:H1'	2.21	0.41
1:2A:861:A:N3	2:2B:79:C:O2'	2.50	0.41
1:2A:2748:A:H2'	1:2A:2749:A:O4'	2.21	0.41
6:2G:53:LEU:HA	6:2G:53:LEU:HD13	1.76	0.41
6:2G:133:LEU:HG	6:2G:157:ILE:HB	2.03	0.41
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CE1	2.56	0.41
21:2Z:144:LEU:CG	21:2Z:145:GLU:H	2.31	0.41
23:21:76:ARG:HB2	23:21:97:LEU:HD13	2.03	0.41
26:24:61:ARG:HG2	50:2s:42:PRO:HG3	2.03	0.41
32:2a:109:A:H5'	32:2a:110:C:C5	2.56	0.41
32:2a:381:C:H2'	32:2a:382:A:O4'	2.21	0.41
32:2a:416:G:C5	32:2a:417:C:C4	3.08	0.41
32:2a:471:G:H2'	32:2a:472:A:H8	1.85	0.41
32:2a:811:C:H4'	32:2a:900:A:N6	2.35	0.41
32:2a:1014:A:H5'	50:2s:14:HIS:CE1	2.56	0.41
32:2a:1191:A:O5'	32:2a:1191:A:H8	2.04	0.41
32:2a:1236:A:O2'	32:2a:1304:G:H4'	2.20	0.41
35:2d:152:SER:O	35:2d:158:ILE:HD11	2.20	0.41
39:2h:124:ALA:O	39:2h:128:GLY:N	2.54	0.41
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.54	0.41
46:2o:39:LEU:HD23	46:2o:56:LEU:HB2	2.03	0.41
1:1A:185:U:H2'	1:1A:186:G:C8	2.57	0.40
1:1A:536:A:H2'	1:1A:537: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:1005:C:H5''	63:1A:4497:HOH:O	2.20	0.40
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.56	0.40
1:1A:1697:G:OP2	1:1A:1698:A:O2'	2.32	0.40
1:1A:1858:G:N2	1:1A:1883:G:H2'	2.36	0.40
1:1A:2314:C:H2'	1:1A:2315:G:C8	2.57	0.40
1:1A:2590:A:H2'	1:1A:2591:C:H6	1.87	0.40
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.20	0.40
11:1P:100:LEU:HD23	11:1P:100:LEU:HA	1.87	0.40
16:1U:43:GLY:HA3	17:1V:73:SER:OG	2.22	0.40
32:1a:161:A:H2'	32:1a:162:A:C8	2.56	0.40
34:1c:22:TRP:HB3	34:1c:59:ARG:HB3	2.02	0.40
42:1k:18:ARG:HA	42:1k:81:ASP:H	1.86	0.40
44:1m:16:ASP:N	44:1m:16:ASP:OD1	2.54	0.40
44:1m:108:ARG:HA	44:1m:108:ARG:HD3	1.85	0.40
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.56	0.40
1:2A:614(B):G:H5''	1:2A:614(C):A:OP1	2.21	0.40
1:2A:764:A:H5''	3:2D:210:GLY:HA2	2.03	0.40
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.21	0.40
1:2A:1717:G:H2'	1:2A:1718:G:H8	1.85	0.40
1:2A:1970:A:OP1	63:2A:3744:HOH:O	2.22	0.40
1:2A:2136:C:N4	1:2A:2155:G:N1	2.69	0.40
1:2A:2168:G:H2'	1:2A:2170:A:N7	2.36	0.40
1:2A:2344:U:H3'	28:26:37:ARG:O	2.21	0.40
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.20	0.40
2:2B:29:A:H2'	2:2B:30:C:C6	2.56	0.40
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	2.03	0.40
5:2F:129:PHE:O	5:2F:130:ALA:C	2.64	0.40
6:2G:96:ARG:N	6:2G:99:MET:HE2	2.35	0.40
12:2Q:27:VAL:O	12:2Q:138:ASP:HB3	2.21	0.40
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.21	0.40
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	2.04	0.40
26:24:60:GLN:O	26:24:62:ARG:NH2	2.54	0.40
26:24:67:TYR:CD2	50:2s:9:VAL:HB	2.56	0.40
32:2a:1010:G:C2	32:2a:1020:U:H1'	2.56	0.40
32:2a:1099:G:OP2	33:2b:144:ARG:NH2	2.41	0.40
32:2a:1100:C:C2	32:2a:1102:A:H5'	2.56	0.40
32:2a:1273:G:C6	32:2a:1274:G:C4	3.09	0.40
37:2f:63:TYR:N	37:2f:63:TYR:HD2	2.19	0.40
38:2g:70:LYS:HG2	38:2g:96:GLN:HB3	2.03	0.40
38:2g:152:ALA:O	38:2g:155:ARG:HD3	2.21	0.40
39:2h:51:VAL:CG2	39:2h:60:ARG:HB2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:49:THR:O	44:2m:53:VAL:HG13	2.21	0.40
48:2q:66:SER:HB3	48:2q:69:LYS:HB2	2.02	0.40
1:1A:84:A:H5'	20:1Y:8:LYS:HE3	2.02	0.40
1:1A:1567:A:OP2	3:1D:84:TYR:OH	2.33	0.40
1:1A:1676:A:H2'	1:1A:1677:A:O4'	2.21	0.40
1:1A:2178:C:H2'	1:1A:2179:C:C6	2.56	0.40
8:1I:109:ILE:HD12	8:1I:130:TYR:OH	2.22	0.40
11:1P:21:ARG:HD3	11:1P:21:ARG:HA	1.91	0.40
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	2.05	0.40
32:1a:110:C:H2'	32:1a:111:G:O4'	2.19	0.40
32:1a:524:G:H2'	32:1a:525:C:C6	2.56	0.40
32:1a:606:G:H1'	32:1a:632:A:H61	1.86	0.40
32:1a:685:G:O2'	32:1a:686:U:H5'	2.20	0.40
32:1a:769:G:H4'	32:1a:1513:A:H4'	2.02	0.40
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.54	0.40
35:1d:64:LEU:HD23	35:1d:75:PHE:HZ	1.87	0.40
37:1f:37:VAL:HA	37:1f:65:VAL:HG12	2.03	0.40
47:1p:72:ARG:HA	47:1p:75:ARG:HB3	2.02	0.40
49:1r:52:PRO:O	49:1r:56:THR:HG23	2.21	0.40
50:1s:11:VAL:C	50:1s:13:ASP:H	2.29	0.40
1:2A:21:A:H2'	1:2A:22:C:O4'	2.21	0.40
1:2A:315:G:H2'	1:2A:316:C:C6	2.57	0.40
1:2A:885:C:H2'	1:2A:886:C:O4'	2.21	0.40
1:2A:2448:A:OP1	63:2A:3741:HOH:O	2.21	0.40
1:2A:2774:C:H2'	1:2A:2775:A:O4'	2.22	0.40
13:2R:59:ASP:OD2	13:2R:61:HIS:HB3	2.21	0.40
14:2S:24:LEU:HD23	14:2S:24:LEU:HA	1.94	0.40
18:2W:1:MET:HE3	18:2W:62:HIS:HB3	2.03	0.40
26:24:61:ARG:HG2	50:2s:42:PRO:CG	2.50	0.40
29:27:26:GLY:O	29:27:30:VAL:HG23	2.22	0.40
32:2a:283:C:H2'	32:2a:284:G:O4'	2.21	0.40
32:2a:683:G:H2'	32:2a:684:A:C8	2.56	0.40
32:2a:1048:G:OP1	45:2n:3:ARG:HB3	2.21	0.40
38:2g:27:ILE:HA	38:2g:30:ILE:HD12	2.04	0.40
38:2g:92:SER:O	38:2g:96:GLN:HG3	2.21	0.40
1:1A:570:G:H2'	1:1A:2030:A:N7	2.37	0.40
1:1A:1308:A:H2'	1:1A:1309:G:O4'	2.22	0.40
1:1A:1365:A:OP2	23:11:3:LYS:HG2	2.22	0.40
1:1A:1453:U:OP1	13:1R:77:ARG:HD3	2.21	0.40
1:1A:2142:C:H2'	1:1A:2143:C:C6	2.56	0.40
3:1D:5:LYS:HE3	3:1D:5:LYS:HB3	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.45	0.40
32:1a:600:C:H2'	32:1a:601:C:H6	1.85	0.40
32:1a:692:U:O2'	32:1a:694:A:N7	2.46	0.40
32:1a:993:G:H2'	32:1a:995:C:H41	1.87	0.40
33:1b:16:HIS:HD2	33:1b:204:ASN:H	1.68	0.40
33:1b:231:GLU:HB3	33:1b:232:PRO:HD3	2.03	0.40
34:1c:157:ILE:HD13	34:1c:166:GLU:HB2	2.04	0.40
35:1d:186:LEU:HD13	35:1d:186:LEU:HA	1.91	0.40
37:1f:44:GLY:HA2	37:1f:59:TYR:CZ	2.56	0.40
40:1i:86:VAL:C	40:1i:88:TYR:H	2.29	0.40
43:1l:84:LEU:HB2	43:1l:105:TYR:CE2	2.56	0.40
1:2A:752:A:P	29:27:3:ARG:HH22	2.43	0.40
1:2A:817:C:H2'	1:2A:818:G:O4'	2.20	0.40
1:2A:1355:G:C6	1:2A:1356:G:C5	3.09	0.40
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.56	0.40
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.85	0.40
2:2B:28:C:H2'	2:2B:29:A:O4'	2.21	0.40
4:2E:54:GLN:HB2	4:2E:76:ARG:HG2	2.02	0.40
13:2R:36:THR:HG22	13:2R:37:THR:H	1.85	0.40
21:2Z:97:GLU:HA	21:2Z:126:VAL:O	2.21	0.40
26:24:34:GLU:HB3	44:2m:57:ARG:HH21	1.87	0.40
27:25:38:ALA:HB3	27:25:48:GLU:HG3	2.03	0.40
32:2a:308:C:H2'	32:2a:309:G:C8	2.56	0.40
32:2a:516:PSU:C2	32:2a:517:G:C6	3.10	0.40
32:2a:692:U:H2'	32:2a:694:A:OP2	2.22	0.40
32:2a:841:U:C4	32:2a:848:C:H1'	2.57	0.40
32:2a:952:U:H4'	32:2a:964:A:N1	2.37	0.40
32:2a:1051:C:H2'	32:2a:1052:U:H6	1.87	0.40
32:2a:1122:U:C2	32:2a:1123:A:C8	3.09	0.40
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.56	0.40
33:2b:163:PHE:HA	33:2b:185:ILE:HG12	2.03	0.40
43:2l:9:GLN:O	43:2l:13:LYS:N	2.44	0.40
49:2r:67:ALA:HA	49:2r:70:ILE:HD12	2.04	0.40
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.56	0.40
1:1A:1396:U:H6	1:1A:1396:U:H2'	1.73	0.40
1:1A:2239:G:H5'	3:1D:251:GLY:HA3	2.03	0.40
1:1A:2266:A:H4'	1:1A:2267:A:C4	2.56	0.40
1:1A:2497:A:H5''	63:1A:4365:HOH:O	2.21	0.40
1:1A:2848:G:H3'	15:1T:95:ARG:O	2.21	0.40
60:1A:4098:ERY:H71	60:1A:4098:ERY:H4	1.80	0.40
6:1G:41:GLN:HG3	6:1G:60:LEU:HD22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:91:LEU:HD23	21:1Z:91:LEU:HA	1.91	0.40
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.76	0.40
32:1a:1183:A:O2'	32:1a:1184:G:H5''	2.21	0.40
33:1b:196:LEU:HD12	33:1b:196:LEU:HA	1.93	0.40
38:1g:51:GLN:O	38:1g:55:GLY:HA2	2.22	0.40
38:1g:136:LYS:O	38:1g:140:ASP:HB2	2.21	0.40
47:1p:53:VAL:HG13	47:1p:79:VAL:HG13	2.03	0.40
50:1s:20:LEU:HD23	50:1s:20:LEU:HA	1.88	0.40
1:2A:171:G:H2'	1:2A:172:C:H6	1.86	0.40
1:2A:271(S):G:C6	1:2A:271(T):C:C4	3.09	0.40
1:2A:1190:G:O2'	1:2A:1191:G:H5'	2.22	0.40
1:2A:1545:A:H2'	1:2A:1546:C:O4'	2.22	0.40
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.56	0.40
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.21	0.40
5:2F:122:LYS:HA	5:2F:191:ARG:NH1	2.37	0.40
9:2N:40:PRO:HB3	16:2U:68:ALA:HB2	2.02	0.40
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.57	0.40
21:2Z:77:ASP:OD2	21:2Z:80:ARG:HD2	2.22	0.40
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.54	0.40
32:2a:434:U:H2'	32:2a:435:C:C6	2.56	0.40
32:2a:487:A:H2'	32:2a:488:C:O4'	2.20	0.40
32:2a:927:G:H2'	32:2a:928:G:O4'	2.21	0.40
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.56	0.40
33:2b:48:MET:HA	33:2b:51:LEU:HD12	2.04	0.40
36:2e:60:TYR:CD1	36:2e:60:TYR:C	3.00	0.40
38:2g:60:LYS:HA	38:2g:63:LYS:HE3	2.02	0.40
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.21	0.40
1:1A:573:G:O2'	1:1A:574:C:H3'	2.21	0.40
1:1A:1069:A:H5'	1:1A:1070:A:O5'	2.21	0.40
1:1A:1142(A):A:C4	1:1A:1144:G:N7	2.89	0.40
1:1A:1813:G:H4'	3:1D:43:ARG:O	2.21	0.40
1:1A:1952:A:C6	1:1A:1953:A:N1	2.90	0.40
1:1A:2002:G:OP2	13:1R:9:LYS:NZ	2.53	0.40
6:1G:153:ARG:HE	6:1G:153:ARG:HB2	1.61	0.40
7:1H:6:ARG:NH2	7:1H:54:ARG:HH22	2.19	0.40
8:1I:81:VAL:HG22	8:1I:145:VAL:O	2.21	0.40
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.45	0.40
19:1X:25:LYS:NZ	19:1X:82:GLN:HE21	2.20	0.40
28:16:47:THR:HG22	28:16:48:VAL:O	2.22	0.40
32:1a:26:A:H1'	35:1d:209:ARG:HH22	1.85	0.40
32:1a:612:C:O2	32:1a:629:G:N2	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:936:C:H2'	32:1a:937:A:O4'	2.21	0.40
32:1a:1338:G:H2'	32:1a:1339:A:C8	2.56	0.40
33:1b:158:LEU:HD23	33:1b:158:LEU:HA	1.91	0.40
33:1b:158:LEU:HA	33:1b:159:PRO:HD3	1.93	0.40
34:1c:71:ALA:O	34:1c:73:PRO:HD3	2.21	0.40
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.81	0.40
1:2A:390:A:C6	11:2P:71:VAL:HG11	2.56	0.40
1:2A:444:C:H4'	5:2F:49:ALA:HB2	2.02	0.40
1:2A:471:A:H2'	1:2A:472:A:O4'	2.21	0.40
1:2A:881:G:H3'	1:2A:882:G:H8	1.85	0.40
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.22	0.40
1:2A:1512:U:H2'	1:2A:1513:C:C6	2.57	0.40
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.57	0.40
3:2D:133:LEU:HB3	3:2D:173:VAL:HG11	2.04	0.40
6:2G:151:ALA:HB3	6:2G:153:ARG:NH1	2.37	0.40
8:2I:84:GLY:O	8:2I:86:THR:N	2.54	0.40
10:2O:102:VAL:HB	10:2O:106:LEU:HD12	2.02	0.40
18:2W:7:ALA:HB2	18:2W:50:VAL:HG22	2.04	0.40
26:24:50:VAL:HG11	44:2m:64:TRP:O	2.21	0.40
26:24:57:GLU:HA	26:24:58:ARG:HA	1.84	0.40
32:2a:142:G:N3	32:2a:196:A:H2	2.19	0.40
32:2a:374:A:O2'	32:2a:451:A:OP2	2.37	0.40
32:2a:545:C:H2'	32:2a:546:G:O4'	2.21	0.40
32:2a:1202:G:C1'	45:2n:29:ARG:HH11	2.35	0.40
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.36	0.40
32:2a:1406:U:O2	32:2a:1517:G:N2	2.53	0.40
34:2c:18:TRP:CD1	45:2n:55:GLY:H	2.40	0.40
35:2d:63:LYS:O	35:2d:67:ILE:HG13	2.22	0.40
37:2f:67:MET:HE1	37:2f:75:LEU:HD23	2.03	0.40
38:2g:89:MET:HE3	38:2g:89:MET:HB3	1.98	0.40
39:2h:27:PRO:O	39:2h:32:LYS:HD2	2.22	0.40
42:2k:85:ARG:HD3	42:2k:113:PRO:HD3	2.03	0.40
47:2p:21:VAL:O	47:2p:32:TYR:HB2	2.21	0.40
47:2p:39:TYR:CD2	47:2p:73:LEU:HD21	2.57	0.40
51:2t:54:LYS:HA	51:2t:57:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	255 (93%)	16 (6%)	2 (1%)	18	41
3	2D	273/276 (99%)	250 (92%)	20 (7%)	3 (1%)	11	29
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	24	48
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	48
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	48
5	2F	201/210 (96%)	182 (90%)	15 (8%)	4 (2%)	6	16
6	1G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	11	29
6	2G	179/182 (98%)	149 (83%)	22 (12%)	8 (4%)	2	4
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	21	44
7	2H	172/180 (96%)	145 (84%)	20 (12%)	7 (4%)	2	5
8	1I	144/148 (97%)	125 (87%)	18 (12%)	1 (1%)	18	41
8	2I	144/148 (97%)	123 (85%)	17 (12%)	4 (3%)	4	9
9	1N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	41
9	2N	138/140 (99%)	128 (93%)	7 (5%)	3 (2%)	5	14
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	107 (89%)	11 (9%)	2 (2%)	7	19
11	1P	147/150 (98%)	131 (89%)	12 (8%)	4 (3%)	4	10
11	2P	147/150 (98%)	123 (84%)	17 (12%)	7 (5%)	2	3
12	1Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	18	41
12	2Q	139/141 (99%)	126 (91%)	10 (7%)	3 (2%)	5	14
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	94 (87%)	9 (8%)	5 (5%)	2	4
15	1T	129/146 (88%)	121 (94%)	4 (3%)	4 (3%)	3	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	2T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6	16
17	2V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6	16
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	11	29
19	2X	93/96 (97%)	84 (90%)	7 (8%)	2 (2%)	5	14
20	1Y	105/110 (96%)	95 (90%)	9 (9%)	1 (1%)	12	32
20	2Y	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	12	32
21	1Z	148/206 (72%)	130 (88%)	12 (8%)	6 (4%)	2	5
21	2Z	156/206 (76%)	119 (76%)	32 (20%)	5 (3%)	3	7
22	10	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
22	20	81/85 (95%)	74 (91%)	7 (9%)	0	100	100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	29
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	29
24	12	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
24	22	68/72 (94%)	62 (91%)	6 (9%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	2
26	24	67/71 (94%)	50 (75%)	13 (19%)	4 (6%)	1	2
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	19	35/37 (95%)	34 (97%)	0	1 (3%)	3	9
31	29	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
33	1b	229/256 (90%)	187 (82%)	28 (12%)	14 (6%)	1	2
33	2b	229/256 (90%)	178 (78%)	39 (17%)	12 (5%)	1	3
34	1c	204/239 (85%)	185 (91%)	17 (8%)	2 (1%)	12	32
34	2c	204/239 (85%)	157 (77%)	38 (19%)	9 (4%)	2	4
35	1d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	24	48
35	2d	206/209 (99%)	187 (91%)	18 (9%)	1 (0%)	24	48
36	1e	146/162 (90%)	131 (90%)	10 (7%)	5 (3%)	3	7
36	2e	146/162 (90%)	119 (82%)	21 (14%)	6 (4%)	2	5
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/156 (98%)	134 (88%)	17 (11%)	2 (1%)	9	25
38	2g	153/156 (98%)	130 (85%)	19 (12%)	4 (3%)	4	11
39	1h	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	18	41
39	2h	135/138 (98%)	119 (88%)	16 (12%)	0	100	100
40	1i	125/128 (98%)	105 (84%)	15 (12%)	5 (4%)	2	5
40	2i	125/128 (98%)	106 (85%)	19 (15%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	7
41	2j	94/105 (90%)	77 (82%)	12 (13%)	5 (5%)	1	3
42	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	35
42	2k	112/129 (87%)	94 (84%)	16 (14%)	2 (2%)	6	18
43	1l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
43	2l	119/132 (90%)	100 (84%)	17 (14%)	2 (2%)	7	19
44	1m	121/126 (96%)	101 (84%)	17 (14%)	3 (2%)	4	11
44	2m	120/126 (95%)	100 (83%)	18 (15%)	2 (2%)	7	19
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/61 (95%)	47 (81%)	9 (16%)	2 (3%)	3	7
46	1o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	10	27
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	27
47	1p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	9	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	12	32
48	2q	97/105 (92%)	84 (87%)	11 (11%)	2 (2%)	5	15
49	1r	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	22
50	1s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	10	27
50	2s	81/93 (87%)	62 (76%)	16 (20%)	3 (4%)	2	6
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	1	3
51	2t	94/106 (89%)	83 (88%)	6 (6%)	5 (5%)	1	3
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	17 (81%)	3 (14%)	1 (5%)	2	3
56	1z	1/3 (33%)	1 (100%)	0	0	100	100
56	2z	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11372/12134 (94%)	10199 (90%)	973 (9%)	200 (2%)	6	18

All (200) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
11	1P	38	GLN
21	1Z	93	ASP
26	14	47	GLN
26	14	49	PHE
33	1b	17	PHE
33	1b	126	GLU
36	1e	96	PRO
40	1i	54	ASP
44	1m	106	ASN
51	1t	100	ILE
5	2F	130	ALA
7	2H	126	PRO
8	2I	10	GLU
11	2P	117	GLU
14	2S	81	GLY
21	2Z	165	VAL
26	24	45	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	17	PHE
33	2b	105	PHE
33	2b	119	GLU
33	2b	123	ALA
33	2b	126	GLU
34	2c	108	ASN
36	2e	124	GLY
42	2k	125	PHE
45	2n	14	PRO
51	2t	100	ILE
15	1T	37	GLY
17	1V	100	ARG
31	19	12	ASP
33	1b	13	ALA
33	1b	20	GLU
34	1c	107	GLN
36	1e	85	GLY
36	1e	97	GLY
40	1i	11	LYS
40	1i	93	ARG
44	1m	36	LYS
44	1m	67	GLU
47	1p	81	ARG
5	2F	146	ALA
6	2G	42	GLY
6	2G	47	LYS
6	2G	84	LYS
6	2G	124	SER
6	2G	126	ASP
10	2O	5	GLN
11	2P	36	LYS
12	2Q	16	ARG
12	2Q	22	LYS
14	2S	96	GLY
17	2V	79	VAL
17	2V	100	ARG
21	2Z	144	LEU
26	24	48	ARG
26	24	55	ARG
33	2b	204	ASN
34	2c	82	GLU
34	2c	95	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	181	ASN
38	2g	52	GLU
42	2k	49	GLY
43	2l	22	SER
45	2n	27	CYS
48	2q	68	ARG
3	1D	262	ARG
4	1E	52	LEU
6	1G	43	LEU
8	1I	40	THR
15	1T	127	ALA
17	1V	79	VAL
19	1X	94	GLY
21	1Z	53	ILE
21	1Z	134	PRO
21	1Z	156	LYS
23	1l	3	LYS
26	14	53	GLU
26	14	68	ARG
33	1b	8	LYS
33	1b	16	HIS
33	1b	129	GLU
33	1b	231	GLU
41	1j	30	SER
51	1t	102	GLY
4	2E	52	LEU
6	2G	146	TYR
8	2I	40	THR
8	2I	85	GLU
8	2I	117	GLU
9	2N	2	LYS
9	2N	8	GLN
11	2P	12	ALA
12	2Q	15	GLY
14	2S	84	GLN
21	2Z	52	SER
23	2l	3	LYS
33	2b	106	LYS
36	2e	97	GLY
36	2e	123	LEU
41	2j	77	PRO
43	2l	17	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	2o	88	ARG
6	1G	181	ARG
11	1P	29	LYS
12	1Q	60	ARG
15	1T	128	GLU
33	1b	78	GLN
33	1b	124	SER
33	1b	127	ILE
36	1e	86	ALA
41	1j	77	PRO
50	1s	27	GLU
51	1t	10	LEU
51	1t	47	GLY
7	2H	12	PRO
7	2H	21	PRO
10	2O	54	GLU
11	2P	38	GLN
19	2X	91	ALA
21	2Z	158	PRO
34	2c	22	TRP
34	2c	91	LEU
36	2e	37	ARG
44	2m	23	TYR
44	2m	106	ASN
48	2q	99	SER
50	2s	9	VAL
50	2s	11	VAL
51	2t	9	ASN
51	2t	99	LEU
9	1N	2	LYS
11	1P	45	LEU
21	1Z	163	LEU
33	1b	37	ASN
36	1e	69	VAL
38	1g	52	GLU
38	1g	54	THR
39	1h	73	ASP
40	1i	29	ASN
41	1j	78	ASN
48	1q	49	GLU
51	1t	95	ALA
3	2D	275	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	2F	18	ARG
6	2G	43	LEU
7	2H	65	HIS
11	2P	45	LEU
11	2P	136	GLU
14	2S	20	ARG
14	2S	57	LYS
26	24	65	ASP
33	2b	16	HIS
33	2b	122	PHE
33	2b	188	ALA
34	2c	54	ARG
34	2c	60	ALA
36	2e	63	ARG
41	2j	75	ILE
41	2j	79	ARG
49	2r	59	SER
50	2s	81	ARG
51	2t	95	ALA
11	1P	122	PRO
15	1T	129	ARG
33	1b	227	GLY
3	2D	29	PRO
7	2H	110	SER
9	2N	9	VAL
11	2P	28	GLY
19	2X	2	LYS
21	2Z	66	SER
33	2b	231	GLU
35	2d	136	PRO
36	2e	69	VAL
41	2j	78	ASN
20	1Y	53	PRO
34	1c	109	PRO
46	1o	23	GLY
51	2t	47	GLY
52	2u	23	PRO
21	1Z	157	LEU
35	1d	142	PRO
42	1k	49	GLY
3	2D	160	GLY
38	2g	80	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1D	125	ILE
7	2H	55	PRO
7	2H	128	PRO
20	2Y	80	GLY
34	2c	81	GLY
41	2j	41	PRO
33	1b	131	PRO
40	1i	30	GLY
5	2F	206	ILE
38	2g	17	VAL
38	2g	50	ILE
6	2G	52	ILE
33	2b	72	GLY

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	55
3	2D	215/218 (99%)	201 (94%)	14 (6%)	15	37
4	1E	164/166 (99%)	154 (94%)	10 (6%)	17	40
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19	45
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5	13
5	2F	159/166 (96%)	143 (90%)	16 (10%)	7	18
6	1G	143/156 (92%)	127 (89%)	16 (11%)	6	15
6	2G	143/156 (92%)	120 (84%)	23 (16%)	2	6
7	1H	144/148 (97%)	136 (94%)	8 (6%)	19	44
7	2H	144/148 (97%)	130 (90%)	14 (10%)	8	20
8	1I	113/124 (91%)	92 (81%)	21 (19%)	1	4
8	2I	105/124 (85%)	87 (83%)	18 (17%)	2	6
9	1N	118/119 (99%)	110 (93%)	8 (7%)	14	35
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68	86
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	41
11	1P	115/116 (99%)	103 (90%)	12 (10%)	7	17
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	29
12	1Q	111/111 (100%)	101 (91%)	10 (9%)	9	23
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	39
13	1R	101/101 (100%)	95 (94%)	6 (6%)	18	42
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28	56
14	1S	86/88 (98%)	74 (86%)	12 (14%)	3	9
14	2S	85/88 (97%)	70 (82%)	15 (18%)	2	5
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	47
15	2T	113/127 (89%)	105 (93%)	8 (7%)	13	33
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12	31
16	2U	93/94 (99%)	82 (88%)	11 (12%)	5	13
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	48
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5	14
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	44
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	23
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15	37
19	2X	77/78 (99%)	70 (91%)	7 (9%)	9	22
20	1Y	85/91 (93%)	74 (87%)	11 (13%)	4	10
20	2Y	85/91 (93%)	72 (85%)	13 (15%)	3	7
21	1Z	135/179 (75%)	115 (85%)	20 (15%)	3	8
21	2Z	137/179 (76%)	112 (82%)	25 (18%)	2	5
22	10	65/67 (97%)	60 (92%)	5 (8%)	12	30
22	20	65/67 (97%)	58 (89%)	7 (11%)	6	16
23	11	80/83 (96%)	77 (96%)	3 (4%)	29	58
23	21	80/83 (96%)	71 (89%)	9 (11%)	5	14
24	12	65/67 (97%)	64 (98%)	1 (2%)	57	81
24	22	65/67 (97%)	57 (88%)	8 (12%)	4	12
25	13	51/52 (98%)	43 (84%)	8 (16%)	2	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	19
26	14	59/63 (94%)	49 (83%)	10 (17%)	2	6
26	24	53/63 (84%)	44 (83%)	9 (17%)	2	6
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	41
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	28
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	19
28	26	50/52 (96%)	42 (84%)	8 (16%)	2	6
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	12
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	12
30	18	54/55 (98%)	49 (91%)	5 (9%)	8	21
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	59
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	67
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	23
33	1b	192/220 (87%)	161 (84%)	31 (16%)	2	6
33	2b	187/220 (85%)	141 (75%)	46 (25%)	1	2
34	1c	142/188 (76%)	128 (90%)	14 (10%)	7	19
34	2c	140/188 (74%)	125 (89%)	15 (11%)	6	16
35	1d	169/181 (93%)	148 (88%)	21 (12%)	4	11
35	2d	173/181 (96%)	151 (87%)	22 (13%)	4	11
36	1e	113/123 (92%)	98 (87%)	15 (13%)	4	10
36	2e	114/123 (93%)	101 (89%)	13 (11%)	5	14
37	1f	84/90 (93%)	76 (90%)	8 (10%)	8	20
37	2f	85/90 (94%)	72 (85%)	13 (15%)	3	7
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5	13
38	2g	120/127 (94%)	107 (89%)	13 (11%)	6	16
39	1h	114/119 (96%)	105 (92%)	9 (8%)	11	28
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	20
40	1i	90/99 (91%)	76 (84%)	14 (16%)	2	7
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	18
41	1j	66/92 (72%)	57 (86%)	9 (14%)	3	9
41	2j	69/92 (75%)	53 (77%)	16 (23%)	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	25
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	16
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21	47
43	2l	96/108 (89%)	85 (88%)	11 (12%)	5	14
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5	13
44	2m	92/101 (91%)	76 (83%)	16 (17%)	2	5
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	12
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3	8
46	1o	78/80 (98%)	69 (88%)	9 (12%)	5	14
46	2o	78/80 (98%)	76 (97%)	2 (3%)	40	70
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	18
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	18
48	1q	94/97 (97%)	86 (92%)	8 (8%)	10	25
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	32
49	1r	59/77 (77%)	49 (83%)	10 (17%)	2	6
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5	13
50	1s	69/80 (86%)	66 (96%)	3 (4%)	26	54
50	2s	67/80 (84%)	55 (82%)	12 (18%)	2	5
51	1t	70/82 (85%)	61 (87%)	9 (13%)	4	10
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4	10
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	44
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	15
56	1z	1/1 (100%)	1 (100%)	0	100	100
56	2z	1/1 (100%)	1 (100%)	0	100	100
All	All	9305/10066 (92%)	8326 (90%)	979 (10%)	6	17

All (979) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	14	ARG
3	1D	15	PHE
3	1D	32	SER
3	1D	38	LYS
3	1D	174	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1D	229	VAL
3	1D	242	ARG
3	1D	253	GLN
3	1D	273	ARG
4	1E	12	THR
4	1E	33	VAL
4	1E	40	GLU
4	1E	47	VAL
4	1E	73	GLU
4	1E	87	GLU
4	1E	90	THR
4	1E	116	VAL
4	1E	119	ARG
4	1E	195	LEU
5	1F	18	ARG
5	1F	20	LEU
5	1F	24	LEU
5	1F	27	GLU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	133	ASN
5	1F	140	LEU
5	1F	144	LYS
5	1F	158	THR
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	9	ARG
6	1G	22	ARG
6	1G	31	VAL
6	1G	43	LEU
6	1G	49	ASP
6	1G	77	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	1G	79	ASN
6	1G	91	ARG
6	1G	108	ASN
6	1G	133	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	159	VAL
7	1H	18	GLU
7	1H	23	ARG
7	1H	24	VAL
7	1H	49	VAL
7	1H	77	LYS
7	1H	92	ILE
7	1H	106	THR
7	1H	175	LYS
8	1I	2	LYS
8	1I	7	GLU
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	27	ARG
8	1I	38	LEU
8	1I	43	ASN
8	1I	47	LEU
8	1I	60	GLU
8	1I	74	ASN
8	1I	76	THR
8	1I	78	THR
8	1I	87	LYS
8	1I	92	VAL
8	1I	108	THR
8	1I	109	ILE
8	1I	116	LEU
8	1I	129	THR
8	1I	141	LYS
8	1I	142	VAL
9	1N	8	GLN
9	1N	9	VAL
9	1N	10	GLU
9	1N	28	THR
9	1N	46	VAL
9	1N	62	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	1N	65	LYS
9	1N	68	GLU
10	1O	35	VAL
11	1P	2	LYS
11	1P	3	LEU
11	1P	45	LEU
11	1P	65	ARG
11	1P	71	VAL
11	1P	86	LYS
11	1P	90	ARG
11	1P	94	GLU
11	1P	96	THR
11	1P	99	LEU
11	1P	101	VAL
11	1P	135	LEU
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	16	ARG
12	1Q	56	ARG
12	1Q	81	VAL
12	1Q	98	LYS
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	127	ILE
12	1Q	133	ARG
13	1R	6	SER
13	1R	36	THR
13	1R	48	VAL
13	1R	102	GLU
13	1R	114	VAL
13	1R	117	VAL
14	1S	14	VAL
14	1S	17	ARG
14	1S	46	VAL
14	1S	49	VAL
14	1S	50	SER
14	1S	52	SER
14	1S	68	GLN
14	1S	69	VAL
14	1S	78	LEU
14	1S	85	VAL
14	1S	107	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	1S	110	LEU
15	1T	17	THR
15	1T	23	ARG
15	1T	28	VAL
15	1T	36	GLU
15	1T	67	SER
15	1T	96	ARG
16	1U	31	SER
16	1U	59	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	78	THR
16	1U	95	LEU
16	1U	100	VAL
17	1V	46	VAL
17	1V	61	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	37	ARG
18	1W	101	SER
19	1X	1	MET
19	1X	23	GLU
19	1X	81	VAL
19	1X	87	GLN
19	1X	88	LYS
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	28	LYS
20	1Y	31	LEU
20	1Y	44	ILE
20	1Y	52	SER
20	1Y	64	GLU
20	1Y	67	LEU
20	1Y	72	VAL
20	1Y	91	GLU
20	1Y	99	CYS
21	1Z	33	LEU
21	1Z	39	VAL
21	1Z	42	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	46	LYS
21	1Z	49	ARG
21	1Z	52	SER
21	1Z	61	LEU
21	1Z	72	ARG
21	1Z	74	VAL
21	1Z	78	LYS
21	1Z	84	GLU
21	1Z	92	SER
21	1Z	123	ASP
21	1Z	136	PHE
21	1Z	139	VAL
21	1Z	140	ASP
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	11	ARG
22	10	46	LYS
22	10	53	MET
22	10	55	ARG
22	10	74	ARG
23	11	40	ARG
23	11	46	LEU
23	11	81	LYS
24	12	28	LYS
25	13	29	ARG
25	13	32	GLN
25	13	37	LEU
25	13	54	VAL
25	13	55	ARG
25	13	56	VAL
25	13	58	VAL
25	13	60	GLU
26	14	5	ILE
26	14	46	GLN
26	14	47	GLN
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	62	ARG
26	14	63	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	67	TYR
26	14	69	LYS
27	15	6	VAL
27	15	57	VAL
27	15	59	GLU
28	16	5	VAL
28	16	7	ILE
28	16	14	THR
28	16	19	ARG
28	16	44	ARG
29	17	24	THR
29	17	29	LYS
29	17	32	LYS
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
30	18	52	LYS
30	18	58	ILE
31	19	17	ILE
33	1b	8	LYS
33	1b	12	GLU
33	1b	15	VAL
33	1b	20	GLU
33	1b	21	ARG
33	1b	39	ILE
33	1b	44	LEU
33	1b	54	THR
33	1b	64	ARG
33	1b	79	ASP
33	1b	80	ILE
33	1b	81	VAL
33	1b	95	GLN
33	1b	112	VAL
33	1b	121	LEU
33	1b	128	GLU
33	1b	133	LYS
33	1b	142	LEU
33	1b	143	GLU
33	1b	157	ARG
33	1b	160	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	170	GLU
33	1b	185	ILE
33	1b	196	LEU
33	1b	208	ILE
33	1b	212	GLN
33	1b	219	VAL
33	1b	229	VAL
33	1b	230	VAL
33	1b	233	SER
33	1b	236	TYR
34	1c	3	ASN
34	1c	15	THR
34	1c	58	GLU
34	1c	64	VAL
34	1c	70	VAL
34	1c	77	ILE
34	1c	89	GLU
34	1c	103	VAL
34	1c	105	GLU
34	1c	110	ASN
34	1c	112	SER
34	1c	119	ARG
34	1c	190	ARG
34	1c	207	VAL
35	1d	3	ARG
35	1d	19	LEU
35	1d	36	ARG
35	1d	45	GLN
35	1d	59	ARG
35	1d	70	ILE
35	1d	85	LYS
35	1d	100	ARG
35	1d	104	VAL
35	1d	118	ARG
35	1d	127	THR
35	1d	128	VAL
35	1d	140	VAL
35	1d	141	ARG
35	1d	144	ASP
35	1d	157	LEU
35	1d	158	ILE
35	1d	177	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	178	VAL
35	1d	190	ASP
35	1d	194	LEU
36	1e	12	LEU
36	1e	16	THR
36	1e	24	ARG
36	1e	27	ARG
36	1e	38	GLN
36	1e	41	VAL
36	1e	51	VAL
36	1e	53	LEU
36	1e	56	GLN
36	1e	68	GLU
36	1e	79	GLU
36	1e	100	VAL
36	1e	131	ILE
36	1e	148	VAL
36	1e	151	LEU
37	1f	19	LEU
37	1f	46	ARG
37	1f	55	ASP
37	1f	64	GLN
37	1f	70	ASP
37	1f	72	VAL
37	1f	75	LEU
37	1f	85	VAL
38	1g	24	THR
38	1g	33	ASP
38	1g	50	ILE
38	1g	59	LEU
38	1g	61	VAL
38	1g	76	ARG
38	1g	80	VAL
38	1g	85	TYR
38	1g	104	LEU
38	1g	114	ARG
38	1g	115	ARG
38	1g	125	MET
38	1g	131	LYS
38	1g	140	ASP
39	1h	29	SER
39	1h	51	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	1h	52	ASP
39	1h	95	VAL
39	1h	98	LYS
39	1h	99	GLU
39	1h	112	LEU
39	1h	123	GLU
39	1h	133	LEU
40	1i	3	GLN
40	1i	9	ARG
40	1i	14	VAL
40	1i	25	LYS
40	1i	27	THR
40	1i	50	LEU
40	1i	53	VAL
40	1i	64	THR
40	1i	81	ILE
40	1i	93	ARG
40	1i	103	THR
40	1i	105	ASP
40	1i	109	VAL
40	1i	128	ARG
41	1j	8	LEU
41	1j	21	GLN
41	1j	42	THR
41	1j	46	ARG
41	1j	55	LYS
41	1j	66	ARG
41	1j	81	THR
41	1j	92	THR
41	1j	100	THR
42	1k	31	THR
42	1k	63	LEU
42	1k	77	MET
42	1k	84	VAL
42	1k	109	VAL
42	1k	114	VAL
42	1k	122	LYS
43	1l	36	VAL
43	1l	43	VAL
43	1l	58	VAL
43	1l	83	VAL
43	1l	100	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	1m	3	ARG
44	1m	4	ILE
44	1m	43	THR
44	1m	48	LEU
44	1m	49	THR
44	1m	55	ARG
44	1m	64	TRP
44	1m	78	ILE
44	1m	81	LEU
44	1m	106	ASN
44	1m	114	ARG
45	1n	9	LYS
45	1n	15	LYS
45	1n	22	THR
45	1n	33	VAL
45	1n	50	LYS
45	1n	56	VAL
46	1o	3	ILE
46	1o	5	LYS
46	1o	21	ASP
46	1o	27	VAL
46	1o	45	VAL
46	1o	57	LEU
46	1o	76	GLU
46	1o	84	LYS
46	1o	87	ILE
47	1p	20	VAL
47	1p	21	VAL
47	1p	27	LYS
47	1p	43	LYS
47	1p	45	THR
47	1p	60	LEU
47	1p	62	VAL
48	1q	11	VAL
48	1q	12	SER
48	1q	14	LYS
48	1q	25	ARG
48	1q	35	VAL
48	1q	53	LEU
48	1q	60	ILE
48	1q	63	ARG
49	1r	31	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	1r	35	ARG
49	1r	36	ASN
49	1r	49	LYS
49	1r	63	GLN
49	1r	66	LEU
49	1r	69	THR
49	1r	76	LEU
49	1r	86	VAL
49	1r	87	ARG
50	1s	41	VAL
50	1s	62	ILE
50	1s	79	THR
51	1t	10	LEU
51	1t	11	SER
51	1t	13	LEU
51	1t	24	LEU
51	1t	38	LYS
51	1t	42	GLN
51	1t	71	THR
51	1t	90	GLN
51	1t	100	ILE
52	1u	20	LYS
3	2D	3	VAL
3	2D	10	THR
3	2D	35	LYS
3	2D	37	LEU
3	2D	61	LEU
3	2D	71	ASP
3	2D	89	SER
3	2D	99	ASP
3	2D	113	VAL
3	2D	173	VAL
3	2D	177	LEU
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	7	VAL
4	2E	12	THR
4	2E	33	VAL
4	2E	38	THR
4	2E	72	VAL
4	2E	77	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	116	VAL
4	2E	119	ARG
4	2E	175	VAL
5	2F	11	VAL
5	2F	20	LEU
5	2F	24	LEU
5	2F	28	ILE
5	2F	33	LEU
5	2F	70	THR
5	2F	74	ARG
5	2F	95	ARG
5	2F	107	LYS
5	2F	108	LYS
5	2F	119	ARG
5	2F	125	LEU
5	2F	137	LYS
5	2F	157	VAL
5	2F	183	VAL
5	2F	197	ASP
6	2G	7	LEU
6	2G	8	LYS
6	2G	18	GLU
6	2G	19	LEU
6	2G	20	ILE
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	66	GLN
6	2G	77	ILE
6	2G	86	MET
6	2G	88	ILE
6	2G	91	ARG
6	2G	137	GLU
6	2G	140	ILE
6	2G	148	MET
6	2G	159	VAL
6	2G	165	THR
6	2G	170	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	2H	3	ARG
7	2H	15	VAL
7	2H	24	VAL
7	2H	49	VAL
7	2H	52	VAL
7	2H	57	ASP
7	2H	65	HIS
7	2H	77	LYS
7	2H	85	LYS
7	2H	104	GLU
7	2H	111	HIS
7	2H	114	VAL
7	2H	129	THR
7	2H	136	ILE
8	2I	2	LYS
8	2I	4	ILE
8	2I	15	VAL
8	2I	38	LEU
8	2I	50	ARG
8	2I	51	ILE
8	2I	58	LEU
8	2I	61	ARG
8	2I	87	LYS
8	2I	101	LEU
8	2I	117	GLU
8	2I	121	LYS
8	2I	123	LEU
8	2I	128	LEU
8	2I	129	THR
8	2I	139	GLN
8	2I	142	VAL
8	2I	144	VAL
9	2N	28	THR
9	2N	46	VAL
9	2N	48	MET
9	2N	60	ILE
9	2N	62	VAL
9	2N	63	THR
9	2N	85	ILE
9	2N	131	GLN
9	2N	137	LYS
10	2O	52	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	2O	65	THR
10	2O	69	ILE
10	2O	70	LYS
10	2O	92	GLU
10	2O	96	THR
11	2P	3	LEU
11	2P	15	ARG
11	2P	58	THR
11	2P	65	ARG
11	2P	90	ARG
11	2P	94	GLU
11	2P	96	THR
11	2P	123	LEU
11	2P	136	GLU
12	2Q	1	MET
12	2Q	7	MET
12	2Q	31	ASP
12	2Q	46	GLN
12	2Q	54	MET
12	2Q	56	ARG
12	2Q	110	THR
13	2R	15	SER
13	2R	24	GLN
13	2R	95	THR
13	2R	114	VAL
14	2S	13	ARG
14	2S	15	ARG
14	2S	28	VAL
14	2S	35	ILE
14	2S	36	TYR
14	2S	43	GLU
14	2S	49	VAL
14	2S	64	GLU
14	2S	78	LEU
14	2S	83	LYS
14	2S	85	VAL
14	2S	93	LYS
14	2S	98	VAL
14	2S	101	LEU
14	2S	110	LEU
15	2T	9	LEU
15	2T	23	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	2T	31	SER
15	2T	39	ARG
15	2T	49	VAL
15	2T	63	VAL
15	2T	89	VAL
15	2T	96	ARG
16	2U	5	LYS
16	2U	17	ILE
16	2U	31	SER
16	2U	36	ARG
16	2U	38	THR
16	2U	59	ARG
16	2U	74	LEU
16	2U	77	SER
16	2U	83	LEU
16	2U	95	LEU
16	2U	110	VAL
17	2V	1	MET
17	2V	7	THR
17	2V	19	LYS
17	2V	52	VAL
17	2V	70	ILE
17	2V	79	VAL
17	2V	82	ARG
17	2V	85	LYS
17	2V	98	GLU
18	2W	2	GLU
18	2W	11	ARG
18	2W	17	VAL
18	2W	39	THR
18	2W	59	VAL
18	2W	67	ASP
18	2W	92	ARG
18	2W	103	ILE
19	2X	45	THR
19	2X	62	LYS
19	2X	75	ASP
19	2X	77	LYS
19	2X	81	VAL
19	2X	83	VAL
19	2X	95	LEU
20	2Y	11	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	2Y	19	LYS
20	2Y	31	LEU
20	2Y	38	ILE
20	2Y	39	VAL
20	2Y	49	VAL
20	2Y	61	ILE
20	2Y	67	LEU
20	2Y	72	VAL
20	2Y	75	ILE
20	2Y	85	VAL
20	2Y	97	ARG
20	2Y	106	LEU
21	2Z	6	LYS
21	2Z	20	ARG
21	2Z	33	LEU
21	2Z	35	ARG
21	2Z	42	VAL
21	2Z	53	ILE
21	2Z	67	LEU
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	84	GLU
21	2Z	91	LEU
21	2Z	94	GLU
21	2Z	121	HIS
21	2Z	128	VAL
21	2Z	132	ASN
21	2Z	136	PHE
21	2Z	145	GLU
21	2Z	148	ASP
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	163	LEU
21	2Z	169	GLU
21	2Z	170	THR
21	2Z	171	ILE
22	20	7	LEU
22	20	10	THR
22	20	46	LYS
22	20	63	VAL
22	20	64	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	20	67	VAL
22	20	68	GLU
23	21	6	GLU
23	21	11	ARG
23	21	35	THR
23	21	38	SER
23	21	40	ARG
23	21	46	LEU
23	21	78	LYS
23	21	80	LEU
23	21	81	LYS
24	22	19	VAL
24	22	25	VAL
24	22	35	LEU
24	22	40	SER
24	22	54	LYS
24	22	59	ARG
24	22	65	ASN
24	22	70	GLN
25	23	31	LEU
25	23	53	LEU
25	23	54	VAL
25	23	56	VAL
25	23	59	VAL
26	24	10	VAL
26	24	35	VAL
26	24	48	ARG
26	24	49	PHE
26	24	50	VAL
26	24	52	THR
26	24	56	VAL
26	24	59	PHE
26	24	63	TYR
27	25	6	VAL
27	25	48	GLU
27	25	57	VAL
27	25	58	LEU
28	26	7	ILE
28	26	8	LYS
28	26	9	LEU
28	26	14	THR
28	26	19	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	26	20	ASN
28	26	29	ASN
28	26	34	LEU
29	27	1	MET
29	27	4	THR
29	27	24	THR
29	27	41	ARG
29	27	43	THR
30	28	14	VAL
30	28	41	ILE
31	29	10	ILE
31	29	12	ASP
31	29	18	ARG
33	2b	8	LYS
33	2b	11	LEU
33	2b	16	HIS
33	2b	27	LYS
33	2b	32	ILE
33	2b	44	LEU
33	2b	47	THR
33	2b	48	MET
33	2b	56	ARG
33	2b	58	ILE
33	2b	67	THR
33	2b	68	ILE
33	2b	71	VAL
33	2b	73	THR
33	2b	76	GLN
33	2b	80	ILE
33	2b	83	MET
33	2b	93	VAL
33	2b	94	ASN
33	2b	96	ARG
33	2b	102	LEU
33	2b	107	THR
33	2b	112	VAL
33	2b	117	GLU
33	2b	118	LEU
33	2b	126	GLU
33	2b	127	ILE
33	2b	141	GLU
33	2b	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	158	LEU
33	2b	164	VAL
33	2b	169	LYS
33	2b	175	ARG
33	2b	179	LYS
33	2b	182	ILE
33	2b	185	ILE
33	2b	189	ASP
33	2b	191	ASP
33	2b	195	ASP
33	2b	196	LEU
33	2b	198	ASP
33	2b	201	ILE
33	2b	208	ILE
33	2b	214	ILE
33	2b	224	GLN
33	2b	230	VAL
34	2c	32	LEU
34	2c	45	LYS
34	2c	47	LEU
34	2c	55	VAL
34	2c	68	VAL
34	2c	70	VAL
34	2c	77	ILE
34	2c	82	GLU
34	2c	101	LEU
34	2c	116	VAL
34	2c	128	PHE
34	2c	153	VAL
34	2c	154	SER
34	2c	182	ILE
34	2c	190	ARG
35	2d	5	ILE
35	2d	8	VAL
35	2d	34	GLU
35	2d	47	ARG
35	2d	52	SER
35	2d	53	ASP
35	2d	59	ARG
35	2d	60	GLU
35	2d	77	ASN
35	2d	78	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	83	SER
35	2d	96	LEU
35	2d	110	PHE
35	2d	119	GLN
35	2d	120	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	158	ILE
35	2d	193	ASP
36	2e	13	ILE
36	2e	16	THR
36	2e	18	ARG
36	2e	20	GLN
36	2e	31	LEU
36	2e	38	GLN
36	2e	41	VAL
36	2e	47	LYS
36	2e	51	VAL
36	2e	72	GLN
36	2e	76	ILE
36	2e	78	HIS
36	2e	90	VAL
37	2f	15	ASP
37	2f	25	ILE
37	2f	63	TYR
37	2f	64	GLN
37	2f	69	GLU
37	2f	70	ASP
37	2f	71	ARG
37	2f	74	ASP
37	2f	81	ILE
37	2f	83	ASP
37	2f	92	LYS
37	2f	94	GLN
37	2f	95	GLU
38	2g	9	VAL
38	2g	12	LEU
38	2g	15	ASP
38	2g	23	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	2g	24	THR
38	2g	27	ILE
38	2g	52	GLU
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	94	ARG
38	2g	106	GLN
38	2g	114	ARG
39	2h	8	ASP
39	2h	51	VAL
39	2h	52	ASP
39	2h	103	VAL
39	2h	109	ILE
39	2h	112	LEU
39	2h	113	SER
39	2h	122	ARG
39	2h	127	LEU
39	2h	133	LEU
39	2h	137	VAL
40	2i	7	THR
40	2i	14	VAL
40	2i	29	ASN
40	2i	34	ASN
40	2i	54	ASP
40	2i	65	VAL
40	2i	89	ASN
40	2i	103	THR
40	2i	113	LYS
41	2j	8	LEU
41	2j	19	SER
41	2j	21	GLN
41	2j	29	ARG
41	2j	33	GLN
41	2j	38	ILE
41	2j	55	LYS
41	2j	58	ASP
41	2j	61	GLU
41	2j	67	THR
41	2j	74	ILE
41	2j	84	GLN
41	2j	96	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	97	GLU
41	2j	98	ILE
41	2j	100	THR
42	2k	14	VAL
42	2k	30	VAL
42	2k	48	ILE
42	2k	81	ASP
42	2k	95	ILE
42	2k	105	VAL
42	2k	114	VAL
42	2k	123	LYS
42	2k	126	ARG
43	2l	18	VAL
43	2l	33	ARG
43	2l	36	VAL
43	2l	39	VAL
43	2l	40	VAL
43	2l	59	ARG
43	2l	67	THR
43	2l	81	SER
43	2l	83	VAL
43	2l	97	ARG
43	2l	100	ILE
44	2m	4	ILE
44	2m	11	ARG
44	2m	22	ILE
44	2m	25	ILE
44	2m	27	LYS
44	2m	47	ASP
44	2m	57	ARG
44	2m	66	LEU
44	2m	67	GLU
44	2m	73	GLU
44	2m	92	HIS
44	2m	94	ARG
44	2m	96	LEU
44	2m	98	VAL
44	2m	102	ARG
44	2m	103	THR
45	2n	3	ARG
45	2n	9	LYS
45	2n	15	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	2n	22	THR
45	2n	32	SER
45	2n	33	VAL
45	2n	56	VAL
46	2o	3	ILE
46	2o	24	SER
47	2p	2	VAL
47	2p	20	VAL
47	2p	42	ARG
47	2p	45	THR
47	2p	60	LEU
47	2p	67	THR
47	2p	74	LEU
48	2q	34	LYS
48	2q	43	LEU
48	2q	60	ILE
48	2q	63	ARG
48	2q	66	SER
48	2q	67	LYS
48	2q	77	VAL
49	2r	26	LEU
49	2r	29	PHE
49	2r	31	LEU
49	2r	35	ARG
49	2r	46	GLU
49	2r	65	ILE
49	2r	84	LYS
50	2s	14	HIS
50	2s	15	LEU
50	2s	27	GLU
50	2s	33	THR
50	2s	37	ARG
50	2s	43	GLU
50	2s	45	VAL
50	2s	48	THR
50	2s	49	ILE
50	2s	51	VAL
50	2s	57	HIS
50	2s	77	THR
51	2t	9	ASN
51	2t	30	LYS
51	2t	33	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	2t	45	GLN
51	2t	46	GLU
51	2t	62	LEU
51	2t	70	SER
51	2t	71	THR
51	2t	100	ILE
52	2u	7	ARG
52	2u	13	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	201	HIS
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
5	1F	204	ASN
6	1G	26	GLN
6	1G	108	ASN
8	1I	105	HIS
9	1N	8	GLN
11	1P	84	ASN
12	1Q	12	GLN
12	1Q	57	HIS
12	1Q	123	HIS
13	1R	71	GLN
15	1T	79	HIS
15	1T	90	GLN
16	1U	117	GLN
18	1W	60	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	34	ASN
21	1Z	54	HIS
21	1Z	73	GLN
21	1Z	132	ASN
21	1Z	151	HIS
24	12	38	GLN
25	13	32	GLN
33	1b	40	HIS
33	1b	78	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	110	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	69	HIS
34	1c	108	ASN
34	1c	123	GLN
34	1c	162	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
36	1e	20	GLN
36	1e	38	GLN
36	1e	73	ASN
36	1e	78	HIS
36	1e	141	GLN
37	1f	13	ASN
37	1f	18	GLN
37	1f	57	GLN
37	1f	100	ASN
38	1g	28	ASN
38	1g	64	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
42	1k	104	GLN
42	1k	116	HIS
43	1l	99	HIS
44	1m	12	ASN
44	1m	77	ASN
44	1m	92	HIS
46	1o	9	GLN
47	1p	13	HIS
47	1p	76	GLN
50	1s	23	ASN
50	1s	57	HIS
50	1s	83	HIS
51	1t	9	ASN
51	1t	16	HIS
51	1t	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2D	87	ASN
4	2E	48	GLN
4	2E	121	ASN
4	2E	169	ASN
5	2F	69	HIS
6	2G	26	GLN
6	2G	121	ASN
6	2G	123	ASN
7	2H	111	HIS
7	2H	143	GLN
9	2N	8	GLN
9	2N	94	HIS
10	2O	5	GLN
11	2P	27	HIS
11	2P	81	GLN
12	2Q	12	GLN
12	2Q	13	GLN
12	2Q	46	GLN
12	2Q	57	HIS
12	2Q	123	HIS
14	2S	38	GLN
15	2T	38	ASN
15	2T	43	GLN
15	2T	58	ASN
15	2T	84	GLN
15	2T	90	GLN
16	2U	94	ASN
18	2W	62	HIS
19	2X	31	HIS
21	2Z	73	GLN
24	22	38	GLN
24	22	70	GLN
26	24	40	HIS
26	24	46	GLN
28	26	20	ASN
30	28	35	GLN
31	29	20	HIS
33	2b	76	GLN
33	2b	95	GLN
33	2b	135	GLN
34	2c	6	HIS
34	2c	28	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	37	GLN
34	2c	98	ASN
34	2c	162	GLN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	129	ASN
35	2d	201	GLN
36	2e	72	GLN
37	2f	64	GLN
37	2f	73	ASN
37	2f	100	ASN
38	2g	97	GLN
38	2g	148	ASN
39	2h	78	GLN
40	2i	31	GLN
40	2i	34	ASN
40	2i	58	HIS
40	2i	117	HIS
42	2k	22	HIS
42	2k	104	GLN
42	2k	116	HIS
42	2k	117	ASN
43	2l	75	HIS
43	2l	99	HIS
44	2m	40	ASN
44	2m	62	ASN
44	2m	77	ASN
44	2m	92	HIS
47	2p	16	HIS
48	2q	16	GLN
49	2r	63	GLN
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	42	GLN
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	454 (15%)	22 (0%)
1	2A	2791/2915 (95%)	478 (17%)	29 (1%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	118/121 (97%)	31 (26%)	0
32	1a	1497/1521 (98%)	259 (17%)	0
32	2a	1501/1521 (98%)	323 (21%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	10/24 (41%)	2 (20%)	0
54	1w	71/76 (93%)	26 (36%)	0
54	2w	71/76 (93%)	36 (50%)	0
55	1x	75/77 (97%)	11 (14%)	0
55	2x	75/77 (97%)	12 (16%)	0
57	1y	72/76 (94%)	30 (41%)	0
57	2y	72/76 (94%)	35 (48%)	0
All	All	9348/9620 (97%)	1713 (18%)	51 (0%)

All (1713) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	92	A
1	1A	93	G
1	1A	95	G
1	1A	102	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	154	G
1	1A	154(A)	C
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	225	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	250	G
1	1A	271(B)	C
1	1A	271(C)	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
1	1A	271(R)	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	329	G
1	1A	330	A
1	1A	333	G
1	1A	345	A
1	1A	352	G
1	1A	362	U
1	1A	363	G
1	1A	372	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	491	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	568	U
1	1A	573	G
1	1A	575	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	614(C)	A
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(F)	G
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	762	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	811	U
1	1A	812	C
1	1A	819	A
1	1A	827	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	828	U
1	1A	830	G
1	1A	855	G
1	1A	859	G
1	1A	866	A
1	1A	880	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	889	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	910	A
1	1A	915	C
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	963	U
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	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1039	G
1	1A	1042	G
1	1A	1043	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1063	G
1	1A	1068	G
1	1A	1069	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1083	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	1099	G
1	1A	1101	U
1	1A	1104	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1117	G
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G
1	1A	1141	U
1	1A	1149	G
1	1A	1156	A
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1220	A
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1379	A
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	1461	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1539	G
1	1A	1540	U
1	1A	1543	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1554	A
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	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1627	G
1	1A	1633	G
1	1A	1648	C
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	1746	G
1	1A	1756	G
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	1858	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1919	A
1	1A	1929	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1930	G
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
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	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2049	G
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2097	C
1	1A	2098	U
1	1A	2101	G
1	1A	2108	C
1	1A	2110	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2117	A
1	1A	2119	A
1	1A	2120	G
1	1A	2121	G
1	1A	2122	U
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2137	C
1	1A	2138	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
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	2162	G
1	1A	2164	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2168	G
1	1A	2169	A
1	1A	2170	A
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2175	C
1	1A	2181	G
1	1A	2183	C
1	1A	2184	G
1	1A	2187	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2219	G
1	1A	2225	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2238	G
1	1A	2239	G
1	1A	2240	C
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2423	U
1	1A	2424	C
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	2440	C
1	1A	2441	C
1	1A	2448	A
1	1A	2469	A
1	1A	2470	G
1	1A	2476	A
1	1A	2478	A
1	1A	2487	G
1	1A	2491	U
1	1A	2494	G
1	1A	2498	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2535	G
1	1A	2554	U
1	1A	2555	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2673	G
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2732	G
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2804	C
1	1A	2807	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2893	G
1	1A	2894	G
1	1A	2897	U
2	1B	13	A
2	1B	15	A
2	1B	25	A
2	1B	32	C
2	1B	35	U
2	1B	42	C
2	1B	52	A
2	1B	56	G
2	1B	63	G
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	110	G
32	1a	5	U
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	77	G
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	111	G
32	1a	116	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	143	A
32	1a	144	G
32	1a	151	A
32	1a	163	C
32	1a	174	C
32	1a	181	G
32	1a	182	U
32	1a	189(F)	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	200	G
32	1a	203	U
32	1a	204	U
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	280	C
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	342	C
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	392	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	536	C
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	617	G
32	1a	630	G
32	1a	639	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	653	A
32	1a	665	A
32	1a	671	G
32	1a	673	G
32	1a	686	U
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	759	A
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	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	885	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	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	983	A
32	1a	991	U
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	997	U
32	1a	999	C
32	1a	1000	U
32	1a	1001	A
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
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	1037	C
32	1a	1038	C
32	1a	1043	C
32	1a	1044	A
32	1a	1053	G
32	1a	1065	U
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	1125	U
32	1a	1127	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1133	G
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1160	G
32	1a	1177	G
32	1a	1183	A
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
32	1a	1238	A
32	1a	1241	G
32	1a	1246	C
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1268	A
32	1a	1269	A
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1293	G
32	1a	1299	A
32	1a	1300	G
32	1a	1312	G
32	1a	1319	A
32	1a	1320	C
32	1a	1323	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1370	G
32	1a	1394	A
32	1a	1397	C
32	1a	1400	5MC
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	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	14	A
53	1v	15	A
54	1w	2	G
54	1w	4	U
54	1w	8	U
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	22	G
54	1w	23	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1w	24	G
54	1w	31	A
54	1w	45	G
54	1w	47	U
54	1w	48	C
54	1w	49	G
54	1w	50	C
54	1w	51	A
54	1w	53	G
54	1w	56	C
54	1w	62	C
54	1w	66	A
54	1w	68	G
54	1w	69	A
54	1w	70	C
54	1w	73	A
54	1w	74	C
55	1x	2	G
55	1x	4	G
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	31	G
55	1x	61	C
55	1x	69	C
57	1y	6	G
57	1y	7	U
57	1y	8	U
57	1y	9	A
57	1y	11	C
57	1y	14	A
57	1y	19	G
57	1y	20	U
57	1y	21	A
57	1y	24	G
57	1y	27	G
57	1y	28	U
57	1y	33	U
57	1y	35	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	1y	38	A
57	1y	40	C
57	1y	41	A
57	1y	44	U
57	1y	46	G7M
57	1y	47	U
57	1y	48	C
57	1y	56	C
57	1y	57	G
57	1y	58	A
57	1y	59	A
57	1y	60	U
57	1y	65	C
57	1y	67	C
57	1y	70	C
57	1y	72	C
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
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
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	154	G
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	197	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	266	G
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	271(O)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	317	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	342	G
1	2A	346	A
1	2A	352	G
1	2A	354	G
1	2A	372	G
1	2A	386	G
1	2A	389	G
1	2A	396	G
1	2A	404	C
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	434	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	442	G
1	2A	444	C
1	2A	451	C
1	2A	455	C
1	2A	457	A
1	2A	480	A
1	2A	481	G
1	2A	505	A
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	715	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	753	C
1	2A	771	G
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	793	A
1	2A	794	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	833	U
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	872	A
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	881	G
1	2A	882	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	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	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1115	G
1	2A	1117	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1171	G
1	2A	1181	C
1	2A	1188	U
1	2A	1195	G
1	2A	1205	U
1	2A	1210	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1221	C
1	2A	1229	G
1	2A	1237	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1288	U
1	2A	1292	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1306	C
1	2A	1314	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	1379	A
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1466	G
1	2A	1467	C
1	2A	1471	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1506	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1542	A
1	2A	1543	C
1	2A	1545	A
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	1640	C
1	2A	1647	G
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	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1853	A
1	2A	1861	G
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	1931	U
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	1975	G
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2016	U
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2098	U
1	2A	2104	G
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2129	C
1	2A	2130	U
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	2142	C
1	2A	2145	C
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2160	G
1	2A	2161	C
1	2A	2162	G
1	2A	2165	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2171	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2185	C
1	2A	2186	G
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	2219	G
1	2A	2225	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2297	C
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
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	2366	A
1	2A	2372	G
1	2A	2376	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2406	U
1	2A	2409	G
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2440	C
1	2A	2441	C
1	2A	2448	A
1	2A	2459	A
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2491	U
1	2A	2498	C
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2759	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2780	G
1	2A	2793	G
1	2A	2794	C
1	2A	2803	C
1	2A	2804	C
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	24	G
2	2B	32	C
2	2B	35	U
2	2B	41	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	51	G
2	2B	53	A
2	2B	56	G
2	2B	58	A
2	2B	63	G
2	2B	65	C
2	2B	66	A
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	89	G
2	2B	91	C
2	2B	94	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	44	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	56	U
32	2a	65	U
32	2a	66	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	115	G
32	2a	116	A
32	2a	117	G
32	2a	121	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	131	C
32	2a	137	C
32	2a	143	A
32	2a	144	G
32	2a	146	G
32	2a	159	G
32	2a	163	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	245	C
32	2a	247	G
32	2a	250	A
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	274	A
32	2a	279	A
32	2a	281	G
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	341	C
32	2a	344	A
32	2a	346	G
32	2a	350	G
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	404	U
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	422	C
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	451	A
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	477	A
32	2a	484	G
32	2a	485	G
32	2a	495	A
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C
32	2a	521	G
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	549	C
32	2a	559	A
32	2a	562	C
32	2a	564	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	587	G
32	2a	596	C
32	2a	597	G
32	2a	601	C
32	2a	618	C
32	2a	630	G
32	2a	641	U
32	2a	650	G
32	2a	652	U
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	666	G
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	746	A
32	2a	749	C
32	2a	755	G
32	2a	763	G
32	2a	773	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	835	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	840	C
32	2a	841	U
32	2a	855	G
32	2a	859	A
32	2a	872	A
32	2a	876	G
32	2a	880	C
32	2a	902	G
32	2a	914	A
32	2a	924	C
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	932	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	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	998	G
32	2a	1001	A
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1012	U
32	2a	1016	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1020	U
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	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1030(D)	A
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1053	G
32	2a	1054	C
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1084	G
32	2a	1085	U
32	2a	1086	U
32	2a	1088	G
32	2a	1091	U
32	2a	1092	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1105	A
32	2a	1108	G
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1130	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1155	G
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1177	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1187	G
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1208	C
32	2a	1211	U
32	2a	1213	A
32	2a	1214	C
32	2a	1227	A
32	2a	1233	G
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1246	C
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1262	C
32	2a	1264	C
32	2a	1270	C
32	2a	1272	G
32	2a	1275	A
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1283	G
32	2a	1285	A
32	2a	1287	A
32	2a	1299	A
32	2a	1301	U
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1319	A
32	2a	1320	C
32	2a	1322	C
32	2a	1323	G
32	2a	1336	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1354	C
32	2a	1358	U
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1368	G
32	2a	1370	G
32	2a	1381	U
32	2a	1397	C
32	2a	1400	5MC
32	2a	1404	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1487	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1506	U
32	2a	1517	G
32	2a	1519	MA6
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	15	A
53	2v	19	A
54	2w	3	G
54	2w	8	U
54	2w	10	G
54	2w	11	C
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	20	U
54	2w	22	G
54	2w	23	A
54	2w	24	G
54	2w	25	C
54	2w	28	U
54	2w	30	G
54	2w	31	A
54	2w	41	A
54	2w	42	A
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	49	G
54	2w	50	C
54	2w	52	G
54	2w	53	G
54	2w	54	5MU
54	2w	58	A
54	2w	60	U
54	2w	61	C
54	2w	62	C
54	2w	64	G
54	2w	65	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2w	66	A
54	2w	68	G
54	2w	69	A
54	2w	74	C
55	2x	8	4SU
55	2x	9	G
55	2x	16	C
55	2x	17	C
55	2x	18	G
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	28	C
55	2x	47	U
55	2x	53	G
55	2x	56	C
57	2y	3	G
57	2y	7	U
57	2y	8	U
57	2y	11	C
57	2y	13	C
57	2y	14	A
57	2y	15	G
57	2y	19	G
57	2y	20	U
57	2y	21	A
57	2y	24	G
57	2y	27	G
57	2y	29	U
57	2y	36	U
57	2y	40	C
57	2y	42	A
57	2y	44	U
57	2y	45	G
57	2y	46	G7M
57	2y	47	U
57	2y	48	C
57	2y	49	G
57	2y	50	C
57	2y	52	G
57	2y	53	G
57	2y	56	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	2y	57	G
57	2y	58	A
57	2y	59	A
57	2y	60	U
57	2y	61	C
57	2y	66	A
57	2y	68	G
57	2y	69	A
57	2y	70	C

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	974	G
1	1A	1174	A
1	1A	1176	G
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2126	A
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	229	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	310	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	528	A
1	2A	746	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	2156	G
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U

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

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	$\# Z > 2$
57	U8U	1y	34	57	17,21,25	1.56	4 (23%)	21,30,37	1.48	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.40	3 (16%)	21,30,33	2.01	4 (19%)
1	5MU	1A	1915	1	19,22,23	1.43	6 (31%)	27,32,35	2.12	7 (25%)
32	5MC	2a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.27	5 (19%)
1	5MC	1A	1942	1	19,22,23	1.64	3 (15%)	26,32,35	1.19	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	1A	2251	58,55,1	23,26,27	1.25	3 (13%)	32,38,41	2.04	6 (18%)
54	G7M	1w	46	54	23,26,27	1.50	3 (13%)	34,39,42	1.68	5 (14%)
55	8AN	2x	76	58,59,55	21,24,25	1.41	3 (14%)	26,35,38	2.31	10 (38%)
55	4SU	1x	8	55	18,21,22	2.29	5 (27%)	25,30,33	1.60	6 (24%)
54	5MU	1w	54	54	19,22,23	1.33	4 (21%)	27,32,35	2.68	6 (22%)
54	U8U	1w	34	53,54	20,24,25	1.42	2 (10%)	22,34,37	1.17	4 (18%)
57	T6A	2y	37	57	21,24,35	1.59	3 (14%)	30,35,52	2.03	8 (26%)
55	5MC	2x	32	55	19,22,23	1.69	3 (15%)	26,32,35	1.25	4 (15%)
54	A1B8A	2w	76	54	30,33,34	1.24	3 (10%)	36,46,49	1.88	9 (25%)
32	5MC	1a	1404	32	19,22,23	1.79	3 (15%)	26,32,35	1.25	4 (15%)
1	OMU	1A	2552	58,1	19,22,23	1.22	3 (15%)	25,31,34	1.85	5 (20%)
43	0TD	1l	92	43	8,9,10	4.54	1 (12%)	6,11,13	2.98	2 (33%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.90	6 (18%)
32	MA6	2a	1519	32	23,26,27	0.41	0	33,38,41	2.03	9 (27%)
57	U8U	2y	34	57	17,21,25	1.56	3 (17%)	21,30,37	1.49	3 (14%)
55	5MC	1x	32	55	19,22,23	1.58	3 (15%)	26,32,35	1.19	2 (7%)
57	5MU	1y	54	57	19,22,23	1.41	5 (26%)	27,32,35	2.15	8 (29%)
57	PSU	1y	39	57	18,21,22	1.39	2 (11%)	21,30,33	2.11	4 (19%)
32	UR3	2a	1498	32	19,22,23	1.03	2 (10%)	26,32,35	1.65	3 (11%)
55	PSU	1x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.12	4 (19%)
55	8AN	1x	76	58,55	21,24,25	1.44	3 (14%)	26,35,38	2.32	10 (38%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.03	4 (19%)
55	5MU	2x	54	55	19,22,23	1.38	6 (31%)	27,32,35	2.03	6 (22%)
57	G7M	1y	46	57	23,26,27	1.56	4 (17%)	34,39,42	1.83	4 (11%)
1	OMC	1A	1920	1	19,22,23	0.78	0	25,31,34	0.93	1 (4%)
32	5MC	2a	1407	32	19,22,23	1.57	3 (15%)	26,32,35	1.18	3 (11%)
1	5MC	2A	1962	58,1	19,22,23	1.64	3 (15%)	26,32,35	1.15	2 (7%)
1	2MA	1A	2503	58,1	22,25,26	1.49	5 (22%)	32,37,40	2.29	9 (28%)
57	T6A	1y	37	57	21,24,35	1.56	4 (19%)	30,35,52	2.01	7 (23%)
1	5MU	2A	1915	1	19,22,23	1.49	5 (26%)	27,32,35	2.04	5 (18%)
54	A1B8A	1w	76	54	30,33,34	1.26	3 (10%)	36,46,49	1.88	9 (25%)
56	FME	2z	1	56	8,9,10	1.00	0	8,9,11	1.57	2 (25%)
32	UR3	1a	1498	32	19,22,23	1.00	0	26,32,35	1.64	2 (7%)
54	PSU	2w	39	54	18,21,22	1.29	2 (11%)	21,30,33	2.09	3 (14%)
54	T6A	1w	37	54	31,34,35	1.41	5 (16%)	43,49,52	1.74	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1404	32	19,22,23	1.68	3 (15%)	26,32,35	1.19	3 (11%)
54	T6A	2w	37	53,54	31,34,35	1.39	4 (12%)	43,49,52	1.84	10 (23%)
1	2MA	2A	2503	58,1	22,25,26	1.51	4 (18%)	32,37,40	2.28	8 (25%)
32	PSU	2a	516	32	18,21,22	1.37	2 (11%)	21,30,33	2.03	5 (23%)
1	OMG	2A	2251	55,1	23,26,27	1.19	3 (13%)	32,38,41	1.99	6 (18%)
54	5MU	2w	54	54	19,22,23	1.54	6 (31%)	27,32,35	1.75	5 (18%)
55	5MU	1x	54	55	19,22,23	1.43	5 (26%)	27,32,35	1.94	5 (18%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.01	1 (4%)
54	G7M	2w	46	54	23,26,27	1.49	4 (17%)	34,39,42	1.71	6 (17%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	1.99	3 (14%)
32	4OC	2a	1402	32,58	20,23,24	0.77	0	25,32,35	1.09	2 (8%)
57	PSU	1y	55	57	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.91	6 (18%)
32	5MC	2a	967	32	19,22,23	1.77	3 (15%)	26,32,35	1.19	3 (11%)
1	5MC	1A	1962	58,1	19,22,23	1.80	3 (15%)	26,32,35	1.20	3 (11%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.14	3 (14%)
54	U8U	2w	34	32,53,54	20,24,25	1.48	3 (15%)	22,34,37	1.73	2 (9%)
32	2MG	2a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.25	7 (21%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.02	9 (27%)
54	PSU	2w	55	54	18,21,22	1.33	2 (11%)	21,30,33	1.96	4 (19%)
32	PSU	1a	516	32	18,21,22	1.36	3 (16%)	21,30,33	1.89	4 (19%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
57	G7M	2y	46	57	23,26,27	1.55	3 (13%)	34,39,42	1.69	4 (11%)
32	G7M	2a	527	32,58	23,26,27	1.51	3 (13%)	34,39,42	1.70	5 (14%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	2.04	9 (27%)
32	5MC	1a	1407	32	19,22,23	1.54	3 (15%)	26,32,35	1.14	3 (11%)
32	MA6	1a	1519	32	23,26,27	0.47	0	33,38,41	2.11	9 (27%)
1	5MC	2A	1942	1	19,22,23	1.58	3 (15%)	26,32,35	1.11	2 (7%)
32	5MC	1a	967	32	19,22,23	1.50	3 (15%)	26,32,35	1.07	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.40	2 (11%)	21,30,33	1.96	3 (14%)
54	PSU	1w	55	54	18,21,22	1.37	1 (5%)	21,30,33	2.00	4 (19%)
57	PSU	2y	55	57	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
32	5MC	1a	1400	32	19,22,23	1.61	3 (15%)	26,32,35	1.21	3 (11%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.08	3 (14%)
1	PSU	1A	2605	58,1	18,21,22	1.41	4 (22%)	21,30,33	2.20	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	4SU	2x	8	55	18,21,22	2.13	6 (33%)	25,30,33	1.32	4 (16%)
57	PSU	2y	39	57	18,21,22	1.42	2 (11%)	21,30,33	1.77	2 (9%)
1	OMU	2A	2552	58,1	19,22,23	1.12	2 (10%)	25,31,34	1.88	5 (20%)
1	5MU	1A	1939	58,1	19,22,23	1.50	4 (21%)	27,32,35	2.08	6 (22%)
32	2MG	1a	1207	32	23,26,27	1.24	2 (8%)	33,38,41	2.28	9 (27%)
57	5MU	2y	54	57	19,22,23	1.49	5 (26%)	27,32,35	1.61	7 (25%)
56	FME	1z	1	56	8,9,10	0.95	1 (12%)	8,9,11	2.12	2 (25%)
1	5MU	2A	1939	1	19,22,23	1.39	5 (26%)	27,32,35	2.25	6 (22%)
32	G7M	1a	527	32,58	23,26,27	1.51	3 (13%)	34,39,42	1.74	5 (14%)
43	0TD	2l	92	43	8,9,10	4.44	2 (25%)	6,11,13	6.78	1 (16%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.91	1 (4%)

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	U8U	1y	34	57	-	0/7/25/29	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	58,55,1	-	0/9/27/28	0/3/3/3
54	G7M	1w	46	54	-	0/7/25/26	0/3/3/3
55	8AN	2x	76	58,59,55	-	3/7/25/26	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	U8U	1w	34	53,54	-	2/10/28/29	0/2/2/2
57	T6A	2y	37	57	-	1/7/25/42	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	A1B8A	2w	76	54	-	3/20/38/39	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
57	U8U	2y	34	57	-	0/7/25/29	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
57	PSU	1y	39	57	-	4/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	58,55	-	3/7/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	0/7/25/26	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	58,1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	58,1	-	0/7/25/26	0/3/3/3
57	T6A	1y	37	57	-	1/7/25/42	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	A1B8A	1w	76	54	-	6/20/38/39	0/3/3/3
56	FME	2z	1	56	-	2/7/9/11	-
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	T6A	1w	37	54	-	6/23/41/42	0/3/3/3
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
54	T6A	2w	37	53,54	-	9/23/41/42	0/3/3/3
1	2MA	2A	2503	58,1	-	0/7/25/26	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
54	5MU	2w	54	54	-	3/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,58	-	2/9/29/30	0/2/2/2
57	PSU	1y	55	57	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	58,1	-	2/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	U8U	2w	34	32,53,54	-	6/10/28/29	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
54	PSU	2w	55	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
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
57	G7M	2y	46	57	-	0/7/25/26	0/3/3/3
32	G7M	2a	527	32,58	-	3/7/25/26	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
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	2/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	2/7/25/26	0/2/2/2
57	PSU	2y	55	57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	58,1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
57	PSU	2y	39	57	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
1	5MU	1A	1939	58,1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
57	5MU	2y	54	57	-	0/7/25/26	0/2/2/2
56	FME	1z	1	56	-	3/7/9/11	-
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,58	-	2/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	4/7/12/14	-
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2

All (241) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.29	1.69	1.82
43	2l	92	0TD	CB-SB	-12.04	1.70	1.82
1	1A	1962	5MC	C5-C4	6.74	1.49	1.44
32	2a	967	5MC	C5-C4	6.60	1.49	1.44
32	1a	1404	5MC	C5-C4	6.56	1.49	1.44
32	2a	1400	5MC	C5-C4	6.35	1.48	1.44
32	2a	1404	5MC	C5-C4	6.07	1.48	1.44
55	2x	32	5MC	C5-C4	6.05	1.48	1.44
1	1A	1942	5MC	C5-C4	5.94	1.48	1.44
1	2A	1962	5MC	C5-C4	5.79	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1400	5MC	C5-C4	5.77	1.48	1.44
1	2A	1942	5MC	C5-C4	5.57	1.48	1.44
32	1a	1407	5MC	C5-C4	5.54	1.48	1.44
32	2a	1407	5MC	C5-C4	5.54	1.48	1.44
55	1x	8	4SU	C4-N3	-5.53	1.31	1.37
55	1x	32	5MC	C5-C4	5.44	1.48	1.44
32	1a	967	5MC	C5-C4	5.27	1.48	1.44
57	2y	37	T6A	C5-C4	5.15	1.48	1.39
55	2x	8	4SU	C4-N3	-5.06	1.32	1.37
57	1y	37	T6A	C5-C4	5.05	1.48	1.39
54	2w	37	T6A	C5-C4	4.79	1.47	1.39
54	1w	37	T6A	C5-C4	4.73	1.47	1.39
32	2a	527	G7M	C5-N7	-4.71	1.33	1.39
54	1w	34	U8U	C2-S2	-4.71	1.60	1.67
55	1x	8	4SU	C4-S4	-4.67	1.60	1.68
55	2x	8	4SU	C4-S4	-4.64	1.60	1.68
57	2y	34	U8U	C2-S2	-4.55	1.60	1.67
32	1a	527	G7M	C5-N7	-4.54	1.34	1.39
1	2A	2503	2MA	C5-C4	4.52	1.47	1.39
54	2w	34	U8U	C2-S2	-4.49	1.60	1.67
54	2w	46	G7M	C5-N7	-4.49	1.34	1.39
57	2y	46	G7M	C5-N7	-4.46	1.34	1.39
57	1y	34	U8U	C2-S2	-4.44	1.60	1.67
1	1A	2503	2MA	C5-C4	4.41	1.47	1.39
54	1w	46	G7M	C5-N7	-4.38	1.34	1.39
57	1y	46	G7M	C5-N7	-4.19	1.34	1.39
54	1w	55	PSU	C6-C5	4.17	1.39	1.35
57	2y	39	PSU	C6-C5	4.05	1.39	1.35
57	1y	55	PSU	C6-C5	4.04	1.39	1.35
55	1x	8	4SU	C5-C4	-3.99	1.37	1.42
55	2x	76	8AN	C5-N7	-3.97	1.31	1.39
54	2w	55	PSU	C6-C5	3.95	1.39	1.35
57	2y	55	PSU	C6-C5	3.85	1.39	1.35
54	2w	76	A1B8A	C5-N7	-3.78	1.32	1.39
54	1w	76	A1B8A	C5-N7	-3.73	1.32	1.39
57	1y	39	PSU	C6-C5	3.69	1.39	1.35
1	2A	1917	PSU	C6-C5	3.67	1.39	1.35
54	1w	39	PSU	C6-C5	3.67	1.39	1.35
1	1A	1917	PSU	C6-C5	3.65	1.39	1.35
55	1x	55	PSU	C6-C5	3.62	1.39	1.35
57	1y	46	G7M	C5-C4	3.61	1.47	1.38
32	2a	516	PSU	C6-C5	3.60	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	76	8AN	C5-N7	-3.60	1.32	1.39
57	2y	46	G7M	C5-C4	3.57	1.47	1.38
55	1x	8	4SU	C2-N3	-3.57	1.31	1.38
55	1x	76	8AN	C5-C4	-3.51	1.32	1.39
54	2w	39	PSU	C6-C5	3.43	1.39	1.35
55	2x	55	PSU	C6-C5	3.41	1.39	1.35
32	1a	527	G7M	C5-C4	3.39	1.46	1.38
54	2w	34	U8U	C6-N1	-3.36	1.32	1.38
1	2A	2605	PSU	C6-C5	3.34	1.39	1.35
54	1w	46	G7M	C5-C4	3.32	1.46	1.38
1	2A	1911	PSU	C6-C5	3.31	1.39	1.35
54	2w	46	G7M	C5-C4	3.31	1.46	1.38
32	2a	1207	2MG	C5-C4	3.30	1.47	1.38
54	1w	76	A1B8A	C5-C4	-3.24	1.33	1.39
1	1A	1911	PSU	C6-C5	3.23	1.38	1.35
54	2w	54	5MU	C6-C5	3.23	1.39	1.34
1	1A	1939	5MU	C4-N3	-3.21	1.32	1.38
54	2w	76	A1B8A	C5-C4	-3.19	1.33	1.39
32	2a	966	M2G	C5-C4	3.18	1.47	1.38
55	2x	8	4SU	C5-C4	-3.18	1.38	1.42
32	1a	516	PSU	C6-C5	3.17	1.38	1.35
32	2a	527	G7M	C5-C4	3.15	1.46	1.38
32	1a	966	M2G	C5-C4	3.15	1.47	1.38
57	2y	37	T6A	C5-C6	3.07	1.49	1.41
1	2A	1915	5MU	C6-C5	2.99	1.39	1.34
1	1A	2251	OMG	C5-C4	2.98	1.46	1.38
1	2A	1942	5MC	C6-C5	2.97	1.39	1.34
55	1x	32	5MC	C6-C5	2.97	1.39	1.34
57	2y	54	5MU	C6-C5	2.97	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.96	1.33	1.38
32	1a	1207	2MG	C5-C4	2.94	1.46	1.38
1	2A	2251	OMG	C5-C4	2.91	1.46	1.38
32	2a	1404	5MC	C6-C5	2.90	1.39	1.34
55	2x	8	4SU	C2-N3	-2.89	1.32	1.38
1	2A	2605	PSU	C4-N3	-2.88	1.33	1.38
54	2w	37	T6A	C5-C6	2.85	1.48	1.41
54	2w	54	5MU	C2-N1	2.85	1.42	1.38
57	1y	37	T6A	C5-C6	2.85	1.48	1.41
1	1A	1939	5MU	C2-N3	-2.85	1.33	1.38
55	2x	76	8AN	C5-C4	-2.83	1.34	1.39
1	1A	1939	5MU	C6-C5	2.82	1.39	1.34
57	1y	54	5MU	C4-C5	2.82	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1915	5MU	C2-N1	2.80	1.42	1.38
32	1a	966	M2G	C2-N2	2.80	1.40	1.35
1	2A	1939	5MU	C4-N3	-2.78	1.33	1.38
55	2x	54	5MU	C6-C5	2.77	1.39	1.34
1	1A	1915	5MU	C6-C5	2.75	1.39	1.34
55	2x	32	5MC	C6-C5	2.74	1.39	1.34
55	1x	54	5MU	C6-C5	2.74	1.39	1.34
1	2A	1939	5MU	C6-C5	2.74	1.39	1.34
54	1w	34	U8U	C4-N3	-2.74	1.33	1.38
57	2y	54	5MU	C4-N3	-2.74	1.33	1.38
57	1y	54	5MU	C6-C5	2.73	1.39	1.34
55	1x	54	5MU	C4-N3	-2.71	1.33	1.38
32	2a	966	M2G	C2-N2	2.69	1.40	1.35
1	2A	1962	5MC	C6-C5	2.68	1.39	1.34
32	1a	1404	5MC	C6-N1	-2.68	1.33	1.38
1	2A	1911	PSU	C4-N3	-2.67	1.33	1.38
1	1A	2552	OMU	C4-N3	-2.67	1.34	1.38
1	2A	2503	2MA	C5-C6	2.67	1.48	1.41
32	2a	967	5MC	C6-C5	2.67	1.39	1.34
1	1A	1915	5MU	C4-C5	2.67	1.49	1.44
54	1w	37	T6A	C5-C6	2.67	1.48	1.41
1	2A	1915	5MU	C4-C5	2.66	1.49	1.44
1	2A	2251	OMG	C6-N1	-2.65	1.33	1.38
1	1A	2503	2MA	C5-C6	2.65	1.48	1.41
55	2x	76	8AN	C5-C6	-2.65	1.33	1.41
57	1y	34	U8U	C4-N3	-2.65	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.64	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.64	1.33	1.38
1	1A	2251	OMG	C6-N1	-2.63	1.33	1.38
32	1a	1404	5MC	C6-C5	2.62	1.38	1.34
57	2y	39	PSU	C4-N3	-2.62	1.33	1.38
32	1a	1400	5MC	C6-C5	2.62	1.38	1.34
57	2y	54	5MU	C2-N1	2.62	1.42	1.38
55	1x	76	8AN	C5-C6	-2.61	1.33	1.41
54	2w	54	5MU	C4-N3	-2.60	1.34	1.38
32	2a	1407	5MC	C6-C5	2.60	1.38	1.34
32	1a	1207	2MG	C6-N1	-2.59	1.34	1.38
54	1w	54	5MU	C2-N1	2.59	1.42	1.38
32	1a	966	M2G	C6-N1	-2.58	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.58	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.57	1.34	1.38
32	1a	516	PSU	C4-N3	-2.57	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1962	5MC	C6-N1	-2.56	1.33	1.38
54	1w	76	A1B8A	C5-C6	-2.55	1.33	1.41
54	1w	39	PSU	C4-N3	-2.55	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.54	1.33	1.38
57	2y	34	U8U	C5-C4	2.53	1.49	1.43
57	1y	34	U8U	C5-C4	2.52	1.49	1.43
54	2w	76	A1B8A	C5-C6	-2.52	1.34	1.41
1	1A	1942	5MC	C6-C5	2.51	1.38	1.34
57	1y	55	PSU	C4-N3	-2.50	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.50	1.33	1.38
32	2a	1400	5MC	C6-C5	2.50	1.38	1.34
55	2x	54	5MU	C4-N3	-2.49	1.34	1.38
55	2x	55	PSU	C4-N3	-2.49	1.34	1.38
57	2y	54	5MU	C4-C5	2.49	1.48	1.44
1	2A	1915	5MU	C4-N3	-2.48	1.34	1.38
1	2A	2503	2MA	C8-N7	2.48	1.36	1.31
57	2y	37	T6A	C8-N7	2.47	1.36	1.31
32	1a	967	5MC	C6-C5	2.47	1.38	1.34
57	1y	46	G7M	C6-N1	-2.45	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.45	1.33	1.38
1	1A	2251	OMG	C5-N7	-2.44	1.34	1.39
55	1x	32	5MC	C6-N1	-2.44	1.33	1.38
54	1w	37	T6A	C8-N7	2.43	1.36	1.31
55	2x	32	5MC	C6-N1	-2.43	1.33	1.38
54	1w	54	5MU	C6-C5	2.42	1.38	1.34
1	1A	1962	5MC	C6-C5	2.42	1.38	1.34
54	2w	54	5MU	O2-C2	2.42	1.27	1.23
54	1w	54	5MU	C4-C5	2.42	1.48	1.44
55	2x	54	5MU	C4-C5	2.41	1.48	1.44
54	2w	39	PSU	C4-N3	-2.41	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.40	1.34	1.38
54	2w	37	T6A	C8-N7	2.40	1.36	1.31
32	1a	1407	5MC	C6-C5	2.40	1.38	1.34
55	1x	54	5MU	C4-C5	2.39	1.48	1.44
57	1y	54	5MU	C2-N1	2.38	1.42	1.38
55	1x	54	5MU	C2-N1	2.38	1.42	1.38
1	1A	2605	PSU	C6-C5	2.37	1.37	1.35
1	1A	1915	5MU	C2-N1	2.37	1.42	1.38
1	2A	2503	2MA	C5-N7	-2.36	1.34	1.39
32	2a	966	M2G	C6-N1	-2.36	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.36	1.33	1.37
32	2a	1407	5MC	C6-N1	-2.35	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1400	5MC	C6-N1	-2.35	1.34	1.38
57	2y	34	U8U	C4-N3	-2.35	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.35	1.34	1.38
54	1w	54	5MU	C6-N1	-2.34	1.34	1.38
57	2y	46	G7M	C6-N1	-2.34	1.34	1.38
32	2a	516	PSU	C4-N3	-2.34	1.34	1.38
55	1x	8	4SU	O2-C2	2.33	1.27	1.23
32	1a	967	5MC	C6-N1	-2.33	1.34	1.38
1	1A	2503	2MA	C4-N9	-2.33	1.32	1.37
32	2a	1498	UR3	C2-N1	2.33	1.41	1.38
1	2A	2552	OMU	C4-N3	-2.32	1.34	1.38
55	2x	8	4SU	O2-C2	2.31	1.27	1.23
57	1y	39	PSU	C4-N3	-2.31	1.34	1.38
32	1a	527	G7M	C6-N1	-2.31	1.34	1.38
55	1x	55	PSU	C4-N3	-2.29	1.34	1.38
1	1A	2552	OMU	C2-N3	-2.29	1.34	1.38
1	1A	2503	2MA	C8-N7	2.28	1.36	1.31
57	1y	37	T6A	C8-N7	2.28	1.36	1.31
1	1A	2552	OMU	C5-C4	-2.28	1.38	1.43
54	2w	34	U8U	C4-N3	-2.28	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.26	1.34	1.38
54	1w	37	T6A	C5-N7	-2.26	1.35	1.39
54	2w	54	5MU	C4-C5	2.25	1.48	1.44
1	2A	1939	5MU	C2-N3	-2.22	1.34	1.38
57	1y	37	T6A	C5-N7	-2.19	1.35	1.39
32	2a	1404	5MC	C6-N1	-2.19	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.19	1.35	1.39
1	2A	2605	PSU	C2-N3	-2.19	1.33	1.37
32	2a	967	5MC	C6-N1	-2.19	1.34	1.38
32	2a	527	G7M	C6-N1	-2.18	1.34	1.38
54	1w	37	T6A	C4-N9	-2.17	1.33	1.37
32	1a	966	M2G	C5-N7	-2.17	1.34	1.39
1	2A	1939	5MU	C4-C5	2.16	1.48	1.44
32	2a	1207	2MG	C6-N1	-2.16	1.34	1.38
57	1y	54	5MU	C6-N1	-2.15	1.34	1.38
1	1A	2605	PSU	C2-N1	-2.14	1.33	1.36
55	1x	54	5MU	C2-N3	-2.14	1.34	1.38
57	2y	54	5MU	C2-N3	-2.14	1.34	1.38
54	2w	55	PSU	C4-N3	-2.13	1.34	1.38
54	1w	46	G7M	C5-C6	2.13	1.49	1.43
1	2A	1942	5MC	C6-N1	-2.13	1.34	1.38
57	1y	54	5MU	C4-N3	-2.12	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	C6-N1	-2.12	1.34	1.38
57	2y	55	PSU	C4-N3	-2.11	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.10	1.34	1.39
55	2x	54	5MU	C2-N3	-2.10	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.08	1.34	1.38
55	2x	8	4SU	C2-N1	2.07	1.41	1.38
54	2w	46	G7M	C4-N9	-2.06	1.32	1.38
57	1y	46	G7M	C5-C6	2.06	1.48	1.43
43	2l	92	0TD	CB-CA	2.06	1.55	1.54
55	2x	54	5MU	C6-N1	-2.06	1.34	1.38
57	1y	34	U8U	C6-C5	2.05	1.39	1.35
32	1a	516	PSU	C2-N3	-2.05	1.34	1.37
32	2a	966	M2G	C5-N7	-2.05	1.35	1.39
54	2w	37	T6A	C5-N7	-2.04	1.35	1.39
32	2a	1498	UR3	C6-C5	2.03	1.39	1.35
56	1z	1	FME	CN-N	2.03	1.39	1.33
54	2w	46	G7M	C5-C6	2.01	1.48	1.43
54	2w	54	5MU	C6-N1	-2.01	1.34	1.38
55	2x	54	5MU	C2-N1	2.01	1.41	1.38
1	1A	1915	5MU	C2-N3	-2.00	1.34	1.38
1	2A	2552	OMU	C6-C5	2.00	1.39	1.35

All (411) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	16.41	131.87	102.36
1	2A	2503	2MA	C5-C4-N3	-8.20	118.55	127.18
1	1A	2503	2MA	C5-C4-N3	-7.53	119.25	127.18
32	1a	1207	2MG	C2-N3-C4	7.19	120.99	112.00
32	2a	1207	2MG	C2-N3-C4	6.98	120.73	112.00
1	1A	2605	PSU	N1-C2-N3	6.81	122.35	115.17
54	1w	54	5MU	C4-N3-C2	-6.78	118.45	127.34
57	1y	39	PSU	N1-C2-N3	6.68	122.22	115.17
43	1l	92	0TD	CSB-SB-CB	-6.67	90.37	102.36
1	1A	1911	PSU	N1-C2-N3	6.65	122.18	115.17
54	1w	54	5MU	O4-C4-C5	-6.62	117.35	124.92
55	1x	55	PSU	N1-C2-N3	6.59	122.11	115.17
32	1a	1498	UR3	C4-N3-C2	-6.53	119.33	124.58
1	1A	1917	PSU	N1-C2-N3	6.52	122.04	115.17
32	1a	966	M2G	C5-C4-N3	-6.47	118.10	128.39
32	2a	1498	UR3	C4-N3-C2	-6.39	119.44	124.58
54	2w	39	PSU	N1-C2-N3	6.33	121.85	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1y	55	PSU	N1-C2-N3	6.31	121.82	115.17
32	2a	516	PSU	N1-C2-N3	6.27	121.78	115.17
55	2x	55	PSU	N1-C2-N3	6.25	121.76	115.17
1	2A	2503	2MA	N3-C4-N9	6.23	134.90	126.99
1	2A	1917	PSU	N1-C2-N3	6.22	121.73	115.17
54	1w	39	PSU	N1-C2-N3	6.20	121.71	115.17
57	2y	55	PSU	N1-C2-N3	6.18	121.68	115.17
1	2A	2605	PSU	N1-C2-N3	6.17	121.67	115.17
1	1A	2251	OMG	C5-C4-N3	-6.15	118.61	128.39
1	2A	1911	PSU	N1-C2-N3	6.10	121.61	115.17
32	2a	966	M2G	C5-C4-N3	-6.10	118.68	128.39
57	1y	46	G7M	N9-C4-N3	6.08	138.11	125.95
57	2y	37	T6A	C5-C4-N3	-6.06	118.37	126.72
54	2w	34	U8U	C1'-N1-C6	-6.04	111.20	121.15
1	1A	2503	2MA	N3-C4-N9	6.04	134.66	126.99
32	1a	1207	2MG	C5-C4-N3	-5.98	118.87	128.39
1	2A	2251	OMG	C5-C4-N3	-5.96	118.91	128.39
57	1y	37	T6A	C5-C4-N3	-5.83	118.69	126.72
32	2a	1207	2MG	C5-C4-N3	-5.80	119.15	128.39
32	1a	516	PSU	N1-C2-N3	5.78	121.26	115.17
54	2w	76	A1B8A	N3-C2-N1	-5.76	119.86	128.58
55	1x	76	8AN	N1-C2-N3	-5.75	119.88	128.58
55	2x	76	8AN	N1-C2-N3	-5.72	119.93	128.58
54	1w	76	A1B8A	N3-C2-N1	-5.69	119.97	128.58
54	1w	55	PSU	N1-C2-N3	5.69	121.17	115.17
54	1w	54	5MU	N3-C2-N1	5.69	122.29	114.89
57	1y	46	G7M	C5-C4-N3	-5.61	117.55	128.15
1	2A	1939	5MU	C4-N3-C2	-5.60	120.00	127.34
54	1w	54	5MU	C5-C4-N3	5.60	120.19	115.32
54	2w	37	T6A	C5-C4-N3	-5.55	119.08	126.72
54	2w	55	PSU	N1-C2-N3	5.53	121.00	115.17
32	1a	527	G7M	N9-C4-N3	5.50	136.95	125.95
57	2y	46	G7M	N9-C4-N3	5.39	136.73	125.95
32	1a	527	G7M	C5-C4-N3	-5.37	118.01	128.15
57	2y	39	PSU	N1-C2-N3	5.32	120.78	115.17
32	2a	527	G7M	N9-C4-N3	5.29	136.53	125.95
1	1A	1915	5MU	N3-C2-N1	5.29	121.77	114.89
57	1y	54	5MU	C4-N3-C2	-5.27	120.43	127.34
1	2A	1939	5MU	N3-C2-N1	5.26	121.74	114.89
32	2a	527	G7M	C5-C4-N3	-5.24	118.25	128.15
1	1A	2251	OMG	C2-N3-C4	5.20	121.25	112.30
54	1w	37	T6A	C5-C4-N3	-5.16	119.61	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	76	8AN	C5-C4-N3	-5.14	119.64	126.72
1	1A	1915	5MU	C4-N3-C2	-5.14	120.61	127.34
55	1x	76	8AN	C5-C4-N3	-5.13	119.65	126.72
54	1w	46	G7M	C5-C4-N3	-5.12	118.47	128.15
32	1a	1519	MA6	N1-C2-N3	-5.09	120.88	128.58
57	2y	46	G7M	C5-C4-N3	-5.09	118.54	128.15
1	2A	1915	5MU	N3-C2-N1	5.07	121.49	114.89
54	1w	76	A1B8A	C5-C4-N3	-5.05	119.76	126.72
54	2w	76	A1B8A	C5-C4-N3	-5.05	119.76	126.72
57	2y	34	U8U	C2-N3-C4	-5.04	121.13	127.33
57	1y	46	G7M	C2-N3-C4	5.03	120.96	112.30
55	2x	54	5MU	N3-C2-N1	5.03	121.44	114.89
1	1A	1939	5MU	C4-N3-C2	-5.02	120.76	127.34
54	1w	46	G7M	N9-C4-N3	5.02	135.98	125.95
57	1y	34	U8U	C2-N3-C4	-5.01	121.17	127.33
32	2a	1518	MA6	N1-C2-N3	-4.98	121.05	128.58
54	2w	46	G7M	C5-C4-N3	-4.97	118.75	128.15
32	1a	1518	MA6	N1-C2-N3	-4.94	121.11	128.58
1	1A	1939	5MU	N3-C2-N1	4.93	121.31	114.89
1	2A	1915	5MU	C4-N3-C2	-4.93	120.88	127.34
1	2A	2552	OMU	C4-N3-C2	-4.91	120.51	126.61
55	2x	54	5MU	C4-N3-C2	-4.90	120.92	127.34
1	2A	2251	OMG	C2-N3-C4	4.89	120.72	112.30
57	1y	54	5MU	N3-C2-N1	4.88	121.24	114.89
32	1a	966	M2G	N9-C4-N3	4.86	135.66	125.95
1	1A	2251	OMG	N9-C4-N3	4.84	135.64	125.95
1	1A	2552	OMU	C4-N3-C2	-4.82	120.63	126.61
57	1y	37	T6A	N3-C4-N9	4.81	135.35	127.17
1	2A	1939	5MU	C5-C4-N3	4.78	119.47	115.32
1	1A	1939	5MU	C5-C4-N3	4.75	119.45	115.32
32	1a	527	G7M	C2-N3-C4	4.74	120.47	112.30
32	2a	527	G7M	C2-N3-C4	4.74	120.46	112.30
54	1w	46	G7M	C2-N3-C4	4.72	120.44	112.30
56	1z	1	FME	CA-N-CN	4.70	130.06	122.82
55	1x	54	5MU	N3-C2-N1	4.69	120.99	114.89
57	2y	37	T6A	N3-C4-N9	4.67	135.11	127.17
54	2w	46	G7M	N9-C4-N3	4.67	135.28	125.95
32	1a	1519	MA6	C5-C4-N3	-4.66	120.30	126.72
1	1A	2552	OMU	N3-C2-N1	4.64	120.93	114.89
32	2a	1519	MA6	N1-C2-N3	-4.63	121.57	128.58
54	2w	46	G7M	C2-N3-C4	4.61	120.25	112.30
32	2a	966	M2G	N9-C4-N3	4.60	135.16	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	966	M2G	C2-N3-C4	4.60	121.01	112.51
54	2w	39	PSU	C4-N3-C2	-4.58	120.06	126.37
55	1x	54	5MU	C4-N3-C2	-4.57	121.34	127.34
57	2y	46	G7M	C2-N3-C4	4.55	120.14	112.30
1	1A	2605	PSU	C4-N3-C2	-4.53	120.14	126.37
57	1y	54	5MU	C5-C4-N3	4.52	119.25	115.32
1	2A	2552	OMU	N3-C2-N1	4.52	120.77	114.89
1	2A	2251	OMG	N9-C4-N3	4.43	134.80	125.95
54	2w	34	U8U	C-C5-C6	-4.41	114.59	121.21
57	2y	55	PSU	O2-C2-N1	-4.40	118.26	122.79
32	2a	966	M2G	C2-N3-C4	4.39	120.63	112.51
32	1a	1518	MA6	C5-C4-N3	-4.37	120.69	126.72
32	2a	1518	MA6	C5-C4-N3	-4.37	120.70	126.72
54	1w	55	PSU	O2-C2-N1	-4.37	118.28	122.79
57	1y	39	PSU	O2-C2-N1	-4.37	118.29	122.79
1	1A	1915	5MU	C5-C4-N3	4.36	119.11	115.32
1	2A	1939	5MU	O4-C4-C5	-4.35	119.94	124.92
55	2x	55	PSU	C4-N3-C2	-4.35	120.38	126.37
32	2a	1519	MA6	C5-C4-N3	-4.34	120.74	126.72
1	1A	1911	PSU	C4-N3-C2	-4.33	120.40	126.37
54	2w	37	T6A	N3-C4-N9	4.33	134.53	127.17
1	1A	1917	PSU	C4-N3-C2	-4.24	120.53	126.37
1	1A	1911	PSU	O2-C2-N1	-4.23	118.42	122.79
1	1A	1939	5MU	C5-C6-N1	-4.21	118.74	123.31
1	2A	1939	5MU	C5-C6-N1	-4.19	118.76	123.31
1	1A	2605	PSU	O2-C2-N1	-4.15	118.51	122.79
55	1x	55	PSU	C4-N3-C2	-4.14	120.67	126.37
1	2A	2605	PSU	C4-N3-C2	-4.14	120.67	126.37
32	2a	516	PSU	C4-N3-C2	-4.12	120.70	126.37
1	2A	1915	5MU	C5-C4-N3	4.09	118.88	115.32
54	1w	54	5MU	C5-C6-N1	-4.08	118.88	123.31
32	2a	1518	MA6	C2-N1-C6	4.08	121.79	111.83
55	1x	54	5MU	C5-C4-N3	4.07	118.86	115.32
54	2w	54	5MU	N3-C2-N1	4.06	120.18	114.89
55	2x	54	5MU	C5-C4-N3	4.05	118.84	115.32
54	1w	37	T6A	N3-C4-N9	4.03	134.02	127.17
57	1y	54	5MU	O4-C4-C5	-4.00	120.34	124.92
32	1a	1519	MA6	C2-N1-C6	4.00	121.59	111.83
55	1x	8	4SU	C6-C5-C4	-3.98	116.50	119.95
57	1y	55	PSU	C4-N3-C2	-3.97	120.90	126.37
54	1w	39	PSU	C4-N3-C2	-3.96	120.91	126.37
54	2w	55	PSU	C4-N3-C2	-3.96	120.92	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1519	MA6	C4-C5-N7	-3.95	106.06	110.58
1	2A	1911	PSU	C4-N3-C2	-3.95	120.94	126.37
32	1a	1518	MA6	C2-N1-C6	3.92	121.42	111.83
55	1x	55	PSU	O2-C2-N1	-3.92	118.75	122.79
57	1y	39	PSU	C4-N3-C2	-3.91	120.99	126.37
32	2a	1519	MA6	C5-N7-C8	3.91	109.59	103.45
32	1a	1518	MA6	C5-N7-C8	3.90	109.58	103.45
32	2a	1404	5MC	C5-C6-N1	-3.90	119.08	123.31
32	1a	1207	2MG	N9-C4-N3	3.89	133.72	125.95
32	2a	1207	2MG	C6-C5-N7	3.88	137.35	130.29
1	1A	1939	5MU	O4-C4-C5	-3.88	120.48	124.92
32	1a	1519	MA6	C5-N7-C8	3.87	109.54	103.45
55	2x	54	5MU	O4-C4-C5	-3.87	120.49	124.92
54	2w	54	5MU	C4-N3-C2	-3.85	122.29	127.34
32	2a	1519	MA6	C2-N1-C6	3.85	121.23	111.83
32	1a	1519	MA6	C4-C5-N7	-3.84	106.20	110.58
57	2y	37	T6A	C4-C5-N7	-3.83	106.20	110.58
1	2A	1917	PSU	C4-N3-C2	-3.82	121.10	126.37
1	1A	2503	2MA	N6-C6-N1	3.81	122.17	117.03
32	1a	1207	2MG	C6-C5-N7	3.80	137.21	130.29
55	1x	32	5MC	C5-C6-N1	-3.77	119.22	123.31
1	2A	1915	5MU	O4-C4-C5	-3.76	120.61	124.92
54	2w	39	PSU	O2-C2-N1	-3.72	118.96	122.79
32	2a	1518	MA6	C5-N7-C8	3.71	109.28	103.45
57	2y	54	5MU	N3-C2-N1	3.71	119.72	114.89
32	1a	516	PSU	C4-N3-C2	-3.71	121.26	126.37
54	2w	54	5MU	O4-C4-C5	-3.68	120.71	124.92
57	2y	55	PSU	C4-N3-C2	-3.67	121.32	126.37
32	1a	1518	MA6	C4-C5-N7	-3.66	106.39	110.58
57	2y	37	T6A	C2-N3-C4	3.66	120.78	111.83
1	1A	1915	5MU	O4-C4-C5	-3.66	120.73	124.92
54	2w	37	T6A	C6-C5-N7	3.65	136.41	132.43
54	2w	54	5MU	C5-C4-N3	3.64	118.49	115.32
54	1w	37	T6A	C6-C5-N7	3.63	136.38	132.43
55	1x	54	5MU	O4-C4-C5	-3.62	120.77	124.92
32	1a	1519	MA6	C2-N3-C4	3.62	120.68	111.83
1	1A	2552	OMU	C5-C4-N3	3.62	119.87	114.80
57	1y	37	T6A	C2-N3-C4	3.61	120.65	111.83
32	2a	1518	MA6	C4-C5-N7	-3.60	106.47	110.58
32	2a	1207	2MG	N9-C4-N3	3.59	133.13	125.95
1	2A	2503	2MA	C4-C5-N7	-3.58	106.49	110.58
32	1a	1518	MA6	N9-C8-N7	-3.58	108.86	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2552	OMU	O2-C2-N1	-3.57	118.15	122.80
54	2w	37	T6A	C2-N3-C4	3.56	120.52	111.83
1	2A	1911	PSU	O2-C2-N1	-3.55	119.13	122.79
54	2w	37	T6A	C4-C5-N7	-3.55	106.53	110.58
32	2a	1400	5MC	C5-C6-N1	-3.52	119.50	123.31
55	2x	76	8AN	N9-C8-N7	-3.49	108.98	113.94
32	2a	1207	2MG	N1-C2-N2	3.49	120.13	116.56
32	1a	1400	5MC	C5-C6-N1	-3.49	119.53	123.31
32	1a	1518	MA6	C2-N3-C4	3.47	120.31	111.83
32	2a	967	5MC	C5-C6-N1	-3.47	119.54	123.31
1	2A	2251	OMG	C6-C5-N7	3.46	136.58	130.29
55	2x	76	8AN	C2-N3-C4	3.46	120.28	111.83
1	1A	1917	PSU	O2-C2-N1	-3.44	119.24	122.79
1	2A	2552	OMU	C5-C4-N3	3.44	119.61	114.80
32	2a	1518	MA6	C2-N3-C4	3.43	120.21	111.83
32	1a	1519	MA6	N9-C8-N7	-3.43	109.07	113.94
54	1w	37	T6A	C2-N3-C4	3.43	120.20	111.83
1	1A	1962	5MC	C5-C6-N1	-3.41	119.61	123.31
56	2z	1	FME	CA-N-CN	3.41	128.06	122.82
55	2x	8	4SU	C5-C4-N3	3.40	117.92	114.75
55	1x	54	5MU	C5-C6-N1	-3.40	119.62	123.31
57	2y	54	5MU	C5-C4-N3	3.40	118.28	115.32
55	1x	76	8AN	N9-C8-N7	-3.39	109.12	113.94
32	2a	1407	5MC	C5-C6-N1	-3.39	119.63	123.31
1	1A	2503	2MA	C4-C5-N7	-3.38	106.72	110.58
1	2A	1917	PSU	O2-C2-N1	-3.38	119.30	122.79
54	1w	55	PSU	C4-N3-C2	-3.37	121.72	126.37
55	2x	54	5MU	C5-C6-N1	-3.37	119.65	123.31
54	2w	76	A1B8A	C2-N3-C4	3.37	120.07	111.83
54	1w	37	T6A	C4-C5-N7	-3.37	106.73	110.58
57	1y	54	5MU	C5-C6-N1	-3.36	119.66	123.31
32	2a	1519	MA6	N9-C8-N7	-3.36	109.17	113.94
54	2w	76	A1B8A	N9-C8-N7	-3.35	109.18	113.94
54	1w	76	A1B8A	C2-N3-C4	3.35	120.01	111.83
32	2a	1519	MA6	C2-N3-C4	3.34	119.99	111.83
55	1x	76	8AN	C2-N3-C4	3.34	119.98	111.83
1	2A	1962	5MC	C5-C6-N1	-3.34	119.69	123.31
32	2a	1518	MA6	N9-C8-N7	-3.32	109.22	113.94
54	1w	76	A1B8A	N9-C8-N7	-3.32	109.22	113.94
57	1y	37	T6A	C4-C5-N7	-3.31	106.79	110.58
57	1y	55	PSU	O2-C2-N1	-3.29	119.40	122.79
55	1x	8	4SU	O2-C2-N1	3.28	127.07	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	C4-N9-C8	3.28	109.18	105.74
57	2y	54	5MU	C4-N3-C2	-3.27	123.05	127.34
54	2w	37	T6A	N6-C10-N11	3.26	118.26	113.77
56	1z	1	FME	C-CA-N	3.26	115.79	109.50
57	2y	39	PSU	C4-N3-C2	-3.25	121.89	126.37
32	2a	516	PSU	O2-C2-N1	-3.25	119.44	122.79
54	2w	55	PSU	O2-C2-N1	-3.25	119.44	122.79
32	2a	966	M2G	C6-C5-N7	3.24	136.19	130.29
1	2A	1942	5MC	C5-C6-N1	-3.22	119.81	123.31
54	1w	37	T6A	N3-C2-N1	-3.21	123.73	128.58
32	1a	1404	5MC	C5-C6-N1	-3.20	119.83	123.31
32	1a	1207	2MG	N1-C2-N2	3.20	119.83	116.56
55	2x	76	8AN	C5-N7-C8	3.20	108.47	103.45
32	2a	1207	2MG	N2-C2-N3	-3.19	116.44	120.51
32	2a	1207	2MG	C4-C5-N7	-3.18	105.63	110.67
32	1a	967	5MC	C5-C6-N1	-3.14	119.90	123.31
1	2A	1915	5MU	C5-C6-N1	-3.14	119.91	123.31
54	1w	34	U8U	C5-C4-N3	3.13	119.99	115.21
55	1x	76	8AN	C4'-O4'-C1'	-3.12	102.57	109.47
54	1w	39	PSU	O2-C2-N1	-3.12	119.57	122.79
55	1x	8	4SU	C1'-N1-C2	3.12	123.19	117.59
32	1a	516	PSU	O2-C2-N1	-3.11	119.58	122.79
54	2w	37	T6A	N3-C2-N1	-3.11	123.88	128.58
57	1y	37	T6A	N3-C2-N1	-3.10	123.89	128.58
32	1a	1404	5MC	C5-C4-N3	-3.09	118.58	121.75
32	2a	1407	5MC	C5-C4-N3	-3.08	118.59	121.75
55	2x	32	5MC	C5-C6-N1	-3.07	119.98	123.31
32	1a	1207	2MG	C4-C5-N7	-3.07	105.81	110.67
1	1A	2251	OMG	C6-C5-N7	3.05	135.84	130.29
55	1x	76	8AN	C5-C4-N9	3.04	109.12	105.81
1	1A	1915	5MU	C5-C6-N1	-3.02	120.03	123.31
1	2A	2605	PSU	O2-C2-N1	-3.02	119.67	122.79
1	1A	2552	OMU	O2-C2-N1	-3.02	118.87	122.80
1	1A	1942	5MC	C5-C6-N1	-2.99	120.06	123.31
32	1a	1498	UR3	C5-C4-N3	2.99	118.98	115.04
32	2a	1498	UR3	C5-C4-N3	2.99	118.98	115.04
54	2w	76	A1B8A	C5-N7-C8	2.98	108.14	103.45
57	2y	34	U8U	C5-C4-N3	2.98	118.97	114.80
57	1y	34	U8U	C5-C4-N3	2.97	118.96	114.80
1	2A	1942	5MC	C5-C4-N3	-2.96	118.72	121.75
54	1w	76	A1B8A	C5-N7-C8	2.95	108.08	103.45
55	2x	8	4SU	C1'-N1-C2	2.94	122.87	117.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	O4-C4-C5	-2.92	120.13	125.16
54	2w	55	PSU	C6-C5-C4	-2.91	116.21	118.17
55	1x	76	8AN	C5-N7-C8	2.91	108.03	103.45
32	1a	966	M2G	C6-C5-N7	2.91	135.59	130.29
55	2x	32	5MC	C5-C4-N3	-2.91	118.78	121.75
57	2y	54	5MU	O4-C4-C5	-2.90	121.60	124.92
55	1x	32	5MC	C5-C4-N3	-2.89	118.79	121.75
55	1x	8	4SU	C5-C4-N3	2.89	117.44	114.75
57	2y	37	T6A	N3-C2-N1	-2.87	124.24	128.58
54	1w	76	A1B8A	C5-C4-N9	2.87	108.94	105.81
1	2A	1939	5MU	O2-C2-N1	-2.87	119.07	122.80
55	2x	55	PSU	O2-C2-N1	-2.86	119.84	122.79
32	1a	1519	MA6	N3-C4-N9	2.85	132.02	127.17
32	1a	1407	5MC	C5-C4-N3	-2.85	118.83	121.75
1	1A	1942	5MC	C5-C4-N3	-2.83	118.85	121.75
32	1a	1407	5MC	C5-C6-N1	-2.80	120.27	123.31
32	1a	1518	MA6	N3-C4-N9	2.80	131.93	127.17
1	2A	2251	OMG	C4-C5-N7	-2.76	106.30	110.67
32	2a	1518	MA6	N3-C4-N9	2.76	131.86	127.17
54	2w	76	A1B8A	C5-C4-N9	2.76	108.82	105.81
54	2w	46	G7M	O6-C6-C5	-2.76	121.86	128.01
1	1A	1962	5MC	CM5-C5-C6	-2.75	119.12	122.85
1	2A	2552	OMU	O4-C4-C5	-2.75	120.42	125.16
54	1w	54	5MU	O2-C2-N1	-2.73	119.25	122.80
54	1w	37	T6A	C4-N9-C8	2.72	108.59	105.74
1	1A	1962	5MC	C5-C4-N3	-2.72	118.97	121.75
54	2w	37	T6A	C4-N9-C8	2.71	108.58	105.74
1	1A	2503	2MA	C2-N1-C6	2.70	122.25	118.10
54	1w	34	U8U	O4-C4-C5	-2.70	120.17	124.71
32	1a	1207	2MG	N2-C2-N3	-2.70	117.07	120.51
55	1x	76	8AN	C6-C5-C4	2.67	120.83	117.18
57	2y	37	T6A	C5-N7-C8	2.67	107.65	103.45
55	2x	76	8AN	C5-C4-N9	2.67	108.72	105.81
54	2w	54	5MU	C5-C6-N1	-2.66	120.42	123.31
32	1a	1400	5MC	C5-C4-N3	-2.66	119.03	121.75
1	2A	2503	2MA	N6-C6-N1	2.66	120.61	117.03
55	2x	8	4SU	C6-C5-C4	-2.64	117.66	119.95
57	1y	54	5MU	C5M-C5-C4	2.64	121.60	118.78
55	2x	54	5MU	O2-C2-N1	-2.63	119.37	122.80
55	2x	76	8AN	N3-C4-N9	2.63	131.63	127.17
32	2a	966	M2G	C4-C5-N7	-2.62	106.53	110.67
57	1y	37	T6A	C4-N9-C8	2.61	108.48	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	55	PSU	C6-C5-C4	-2.61	116.42	118.17
57	2y	34	U8U	O4-C4-C5	-2.61	120.67	125.16
1	1A	2605	PSU	C5-C6-N1	-2.60	118.54	122.14
1	2A	1962	5MC	C5-C4-N3	-2.58	119.11	121.75
1	2A	2503	2MA	C5-N7-C8	2.58	107.51	103.45
57	2y	54	5MU	C5-C6-N1	-2.58	120.51	123.31
1	1A	1915	5MU	O2-C2-N1	-2.58	119.44	122.80
1	2A	2503	2MA	C2-N1-C6	2.55	122.02	118.10
54	2w	37	T6A	C5-N7-C8	2.54	107.44	103.45
1	1A	2251	OMG	O6-C6-C5	-2.53	119.84	126.53
57	1y	37	T6A	C5-N7-C8	2.53	107.42	103.45
32	2a	1519	MA6	N3-C4-N9	2.52	131.45	127.17
32	2a	967	5MC	C5-C4-N3	-2.52	119.17	121.75
32	2a	1400	5MC	O2-C2-N3	-2.51	118.37	122.33
55	2x	32	5MC	O2-C2-N3	-2.51	118.38	122.33
54	2w	76	A1B8A	N3-C4-N9	2.50	131.42	127.17
55	2x	76	8AN	C4'-O4'-C1'	-2.49	103.96	109.47
56	2z	1	FME	C-CA-N	2.49	114.30	109.50
1	1A	1915	5MU	C5M-C5-C4	2.49	121.44	118.78
1	2A	2503	2MA	C4-N9-C8	2.49	108.35	105.74
32	2a	1402	4OC	O2-C2-N3	-2.48	118.42	122.33
32	2a	1402	4OC	C6-C5-C4	2.47	119.98	117.00
32	2a	527	G7M	O6-C6-C5	-2.46	122.52	128.01
32	1a	1407	5MC	O2-C2-N3	-2.46	118.45	122.33
55	2x	55	PSU	C5-C6-N1	-2.46	118.73	122.14
32	1a	1404	5MC	CM5-C5-C6	-2.44	119.55	122.85
54	1w	76	A1B8A	N3-C4-N9	2.43	131.31	127.17
54	1w	37	T6A	N6-C10-N11	2.43	117.11	113.77
55	2x	76	8AN	C4-C5-N7	-2.43	107.81	110.58
32	1a	966	M2G	C4-C5-N7	-2.41	106.85	110.67
54	1w	76	A1B8A	C6-C5-C4	2.40	120.46	117.18
54	1w	46	G7M	O6-C6-C5	-2.39	122.67	128.01
57	1y	34	U8U	O4-C4-C5	-2.39	121.03	125.16
55	1x	76	8AN	N3-C4-N9	2.38	131.22	127.17
57	2y	37	T6A	C4-N9-C8	2.38	108.24	105.74
1	1A	1942	5MC	CM5-C5-C6	-2.38	119.62	122.85
32	2a	1400	5MC	C5-C4-N3	-2.37	119.33	121.75
54	2w	76	A1B8A	C6-C5-C4	2.36	120.40	117.18
32	1a	527	G7M	O6-C6-C5	-2.36	122.74	128.01
1	1A	2503	2MA	C5-N7-C8	2.36	107.16	103.45
32	1a	1404	5MC	O2-C2-N3	-2.35	118.63	122.33
1	1A	2251	OMG	C4-C5-N7	-2.34	106.95	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	T6A	C5-N7-C8	2.33	107.11	103.45
32	2a	1404	5MC	C5-C4-N3	-2.32	119.38	121.75
57	1y	54	5MU	O2-C2-N1	-2.32	119.78	122.80
32	1a	967	5MC	C5-C4-N3	-2.32	119.38	121.75
32	1a	1519	MA6	C4-C5-C6	2.31	118.30	115.91
32	1a	1402	4OC	C6-C5-C4	2.30	119.77	117.00
1	2A	2503	2MA	C6-C5-N7	2.30	136.52	132.09
32	2a	516	PSU	O4'-C1'-C2'	2.29	108.32	105.15
32	2a	1518	MA6	C4-C5-C6	2.28	118.27	115.91
32	1a	1207	2MG	CM2-N2-C2	-2.27	118.77	123.65
55	1x	76	8AN	C4-C5-N7	-2.26	108.00	110.58
1	1A	2503	2MA	C6-C5-N7	2.23	136.40	132.09
57	1y	39	PSU	O4'-C1'-C2'	2.23	108.23	105.15
54	2w	46	G7M	N2-C2-N3	-2.19	115.39	119.67
1	1A	1920	OMC	O2-C2-N3	-2.18	118.90	122.33
1	1A	2503	2MA	N9-C8-N7	-2.17	110.86	113.94
1	2A	2605	PSU	C5-C6-N1	-2.17	119.13	122.14
54	1w	76	A1B8A	C4-C5-N7	-2.16	108.11	110.58
32	1a	527	G7M	C5-C6-N1	2.15	116.29	111.84
32	2a	1519	MA6	C4-C5-C6	2.15	118.13	115.91
54	1w	39	PSU	C5-C6-N1	-2.14	119.17	122.14
54	2w	76	A1B8A	C4-C5-N7	-2.14	108.14	110.58
55	1x	8	4SU	C4-N3-C2	2.13	129.36	127.31
55	2x	8	4SU	O2-C2-N1	2.13	125.56	122.80
32	2a	1400	5MC	CM5-C5-C6	-2.13	119.97	122.85
57	2y	37	T6A	C6-C5-N7	2.13	136.19	132.09
32	2a	1498	UR3	C6-N1-C2	-2.13	120.06	121.80
32	2a	1404	5MC	O2-C2-N3	-2.12	118.99	122.33
32	2a	966	M2G	O6-C6-C5	-2.12	120.95	126.53
55	2x	32	5MC	C1'-N1-C6	-2.11	117.67	121.15
32	2a	967	5MC	O2-C2-N3	-2.10	119.01	122.33
32	1a	1400	5MC	O2-C2-N3	-2.10	119.01	122.33
54	1w	34	U8U	C5-C6-N1	-2.10	120.11	122.94
54	1w	46	G7M	C5-C6-N1	2.10	116.17	111.84
43	1l	92	0TD	OD2-CG-CB	2.09	117.68	113.15
54	1w	34	U8U	C1'-N1-C6	-2.09	117.70	121.15
32	2a	527	G7M	C5-C6-N1	2.09	116.17	111.84
32	2a	516	PSU	C5-C6-N1	-2.09	119.24	122.14
57	2y	46	G7M	O6-C6-C5	-2.08	123.37	128.01
57	1y	46	G7M	O6-C6-C5	-2.07	123.39	128.01
54	1w	37	T6A	C2-N1-C6	2.07	122.11	115.24
57	2y	54	5MU	C5M-C5-C4	2.07	120.99	118.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	76	8AN	C6-C5-C4	2.07	120.00	117.18
55	1x	55	PSU	C5-C6-N1	-2.06	119.27	122.14
57	2y	54	5MU	C1'-N1-C2	2.06	121.30	117.59
57	1y	54	5MU	C5M-C5-C6	-2.06	120.06	122.85
32	1a	1518	MA6	C4-C5-C6	2.06	118.04	115.91
1	2A	1920	OMC	O2-C2-N3	-2.05	119.09	122.33
55	1x	8	4SU	S4-C4-N3	-2.05	118.06	120.20
1	2A	2251	OMG	C8-N7-C5	2.04	107.89	104.26
32	2a	1407	5MC	O2-C2-N3	-2.03	119.13	122.33
54	2w	37	T6A	N9-C8-N7	-2.03	111.06	113.94
32	2a	1400	5MC	C1'-N1-C6	-2.03	117.81	121.15
1	1A	1939	5MU	O2-C2-N1	-2.02	120.16	122.80
32	1a	966	M2G	O6-C6-C5	-2.02	121.21	126.53
32	1a	1207	2MG	C8-N7-C5	2.01	107.84	104.26
54	2w	46	G7M	C5-C6-N1	2.01	115.99	111.84
32	1a	516	PSU	C6-C5-C4	-2.01	116.82	118.17

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
57	1y	39	PSU	C2'-C1'-C5-C4
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB
55	2x	76	8AN	O4'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
54	1w	34	U8U	C5-C-N-CA
54	2w	34	U8U	N-C-C5-C4
54	2w	34	U8U	C5-C-N-CA
54	1w	37	T6A	O10-C10-N6-C6
54	1w	37	T6A	N11-C10-N6-C6
54	1w	37	T6A	C14-C12-C13-ODA
54	1w	37	T6A	C14-C12-C13-ODB
54	2w	37	T6A	O10-C10-N6-C6
54	2w	37	T6A	N11-C10-N6-C6
54	2w	37	T6A	N6-C10-N11-C12
54	2w	37	T6A	C13-C12-C14-O14
54	2w	37	T6A	C13-C12-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	1w	76	A1B8A	O4'-C4'-C5'-O5'
54	2w	76	A1B8A	O4'-C4'-C5'-O5'
56	1z	1	FME	C-CA-CB-CG
56	2z	1	FME	O-C-CA-CB
54	2w	37	T6A	O10-C10-N11-C12
55	1x	76	8AN	C3'-C4'-C5'-O5'
54	2w	76	A1B8A	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
54	1w	76	A1B8A	C-CA-CB-CG
55	1x	76	8AN	O4'-C4'-C5'-O5'
56	1z	1	FME	CA-CB-CG-SD
56	1z	1	FME	N-CA-CB-CG
54	1w	76	A1B8A	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	37	T6A	N11-C12-C14-C15
54	1w	37	T6A	N11-C12-C13-ODA
54	1w	37	T6A	N11-C12-C13-ODB
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1404	5MC	O4'-C4'-C5'-O5'
54	2w	34	U8U	C3'-C4'-C5'-O5'
54	2w	34	U8U	O4'-C4'-C5'-O5'
54	2w	54	5MU	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
54	2w	54	5MU	C3'-C4'-C5'-O5'
54	2w	76	A1B8A	CA-CB-CG-CD
54	1w	76	A1B8A	CA-CB-CG-CD
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
57	1y	39	PSU	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
54	1w	76	A1B8A	N-CA-CB-CG
57	1y	39	PSU	C4'-C5'-O5'-P
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
55	1x	76	8AN	C4'-C5'-O5'-P
55	2x	76	8AN	C4'-C5'-O5'-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	1w	55	PSU	O4'-C1'-C5-C4
32	2a	1402	4OC	C3'-C4'-C5'-O5'
57	1y	37	T6A	C4'-C5'-O5'-P
54	1w	76	A1B8A	CE-CD-CG-CB
56	2z	1	FME	CA-CB-CG-SD
1	1A	1962	5MC	C2'-C1'-N1-C6
54	2w	46	G7M	C4'-C5'-O5'-P
54	2w	37	T6A	N11-C12-C14-O14
57	1y	39	PSU	O4'-C4'-C5'-O5'
1	2A	1917	PSU	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
32	2a	527	G7M	C4'-C5'-O5'-P
43	2l	92	0TD	SB-CB-CG-OD2
54	2w	54	5MU	C4'-C5'-O5'-P
54	1w	55	PSU	O4'-C1'-C5-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
54	1w	34	U8U	N-C-C5-C6
54	2w	34	U8U	N-C-C5-C6
57	2y	37	T6A	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
54	2w	37	T6A	N11-C12-C13-ODB
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
54	2w	34	U8U	C2'-C1'-N1-C2
32	2a	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

45 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1y	34	U8U	1	0
1	1A	1915	5MU	1	0
32	2a	1400	5MC	1	0
1	1A	2251	OMG	1	0
55	2x	76	8AN	2	0
55	1x	8	4SU	1	0
54	1w	54	5MU	1	0
54	1w	34	U8U	2	0
57	2y	37	T6A	1	0
54	2w	76	A1B8A	1	0
1	1A	2552	OMU	1	0
32	2a	1519	MA6	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	2y	34	U8U	1	0
57	1y	39	PSU	1	0
55	1x	76	8AN	1	0
55	2x	55	PSU	1	0
55	2x	54	5MU	1	0
1	2A	1962	5MC	1	0
57	1y	37	T6A	1	0
54	1w	76	A1B8A	1	0
54	2w	39	PSU	4	0
54	1w	37	T6A	1	0
32	2a	1404	5MC	1	0
32	2a	516	PSU	2	0
1	2A	2251	OMG	1	0
54	2w	54	5MU	4	0
1	2A	1911	PSU	1	0
32	2a	1402	4OC	1	0
57	1y	55	PSU	1	0
32	2a	967	5MC	1	0
54	2w	34	U8U	1	0
32	2a	1207	2MG	3	0
32	2a	1518	MA6	1	0
54	2w	55	PSU	3	0
57	2y	46	G7M	2	0
32	1a	1518	MA6	1	0
32	1a	1519	MA6	1	0
32	1a	1400	5MC	1	0
1	1A	2605	PSU	1	0
55	2x	8	4SU	2	0
1	1A	1939	5MU	1	0
57	2y	54	5MU	1	0
1	2A	1939	5MU	1	0
43	2l	92	0TD	1	0
1	2A	1920	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2540 ligands modelled in this entry, 2536 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	$\# Z > 2$
60	ERY	1A	4098	-	53,53,53	0.95	2 (3%)	82,82,82	1.49	12 (14%)
60	ERY	2A	3688	-	53,53,53	0.95	2 (3%)	82,82,82	1.36	9 (10%)
62	SF4	1d	303	35	0,12,12	-	-	-		
62	SF4	2d	303	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
60	ERY	1A	4098	-	-	1/72/107/107	0/3/3/3
60	ERY	2A	3688	-	-	5/72/107/107	0/3/3/3
62	SF4	1d	303	35	-	-	0/6/5/5
62	SF4	2d	303	35	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	2A	3688	ERY	O2-C1	4.85	1.45	1.34
60	1A	4098	ERY	O2-C1	4.77	1.45	1.34
60	1A	4098	ERY	O2-C13	-2.84	1.41	1.46
60	2A	3688	ERY	O2-C13	-2.41	1.42	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	2A	3688	ERY	C13-O2-C1	-5.08	109.32	118.20
60	1A	4098	ERY	O3-C3-C4	3.97	112.91	108.23
60	1A	4098	ERY	C6-C5-C4	-3.69	108.53	113.89
60	2A	3688	ERY	O5-C16-C15	-3.66	107.32	112.95
60	2A	3688	ERY	O5-C16-C17	3.58	109.05	103.86
60	2A	3688	ERY	O2-C1-C2	3.58	119.17	111.53
60	1A	4098	ERY	C13-O2-C1	-3.43	112.22	118.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	1A	4098	ERY	O2-C1-C2	3.10	118.15	111.53
60	1A	4098	ERY	C32-C6-C5	3.05	115.33	110.13
60	1A	4098	ERY	C15-C16-C17	2.99	112.76	107.64
60	1A	4098	ERY	O7-C5-C6	2.83	109.78	106.40
60	1A	4098	ERY	O4-C18-C17	2.82	114.90	110.04
60	1A	4098	ERY	O5-C16-C15	-2.71	108.78	112.95
60	1A	4098	ERY	C2-C3-C4	-2.55	105.57	112.91
60	1A	4098	ERY	O7-C5-C4	-2.50	107.97	111.58
60	2A	3688	ERY	C20-O5-C16	2.41	122.42	117.51
60	2A	3688	ERY	O2-C1-O1	-2.33	119.75	123.95
60	1A	4098	ERY	O2-C1-O1	-2.30	119.79	123.95
60	2A	3688	ERY	C6-C7-C8	-2.23	111.16	115.61
60	2A	3688	ERY	C2-C3-C4	-2.16	106.71	112.91
60	2A	3688	ERY	C31-C4-C3	-2.14	107.63	111.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	2A	3688	ERY	C15-C16-O5-C20
60	2A	3688	ERY	C17-C16-O5-C20
60	2A	3688	ERY	C19-C16-O5-C20
60	1A	4098	ERY	C32-C6-C7-C8
60	2A	3688	ERY	C32-C6-C7-C8
60	2A	3688	ERY	C30-C2-C3-C4

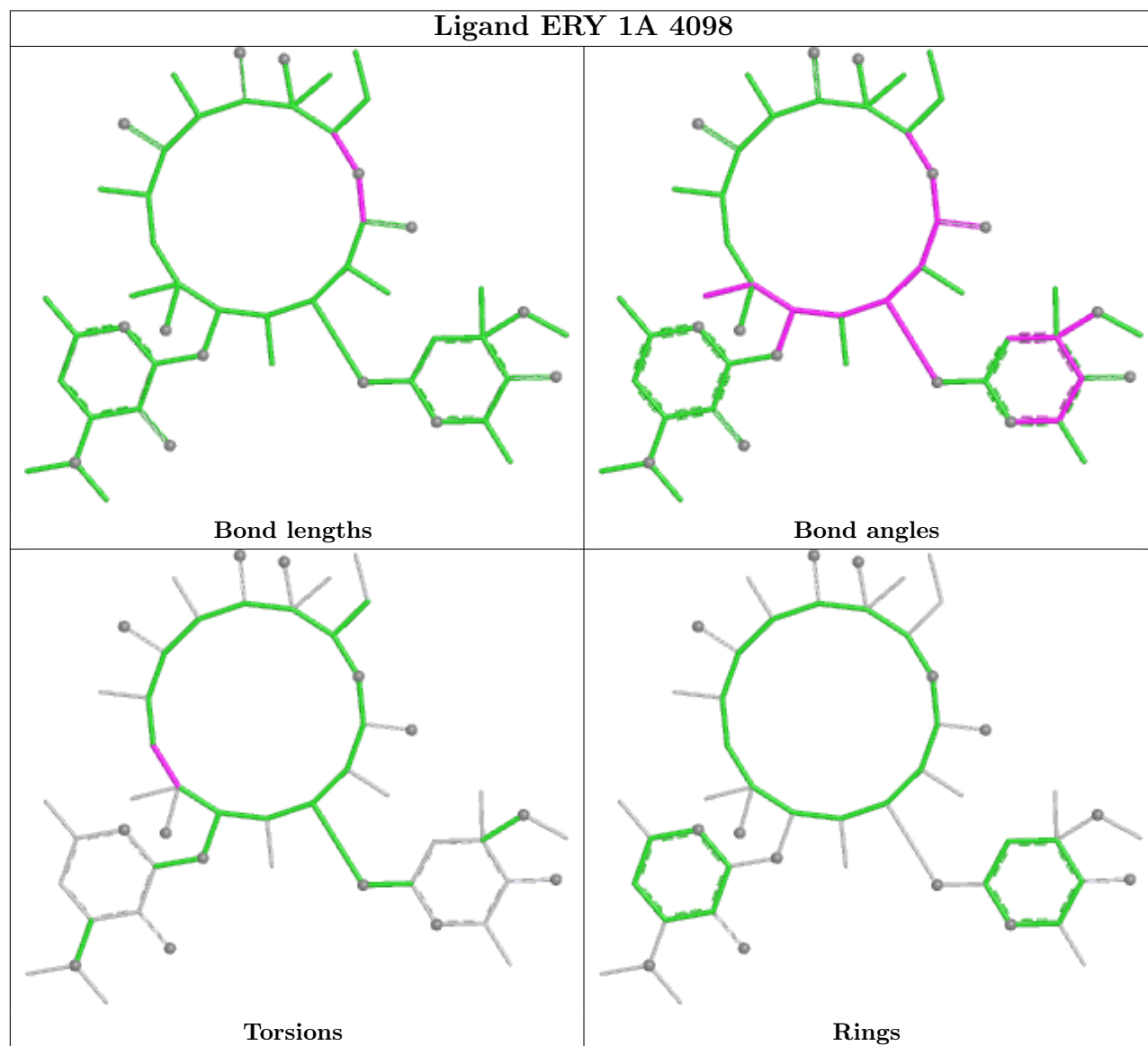
There are no ring outliers.

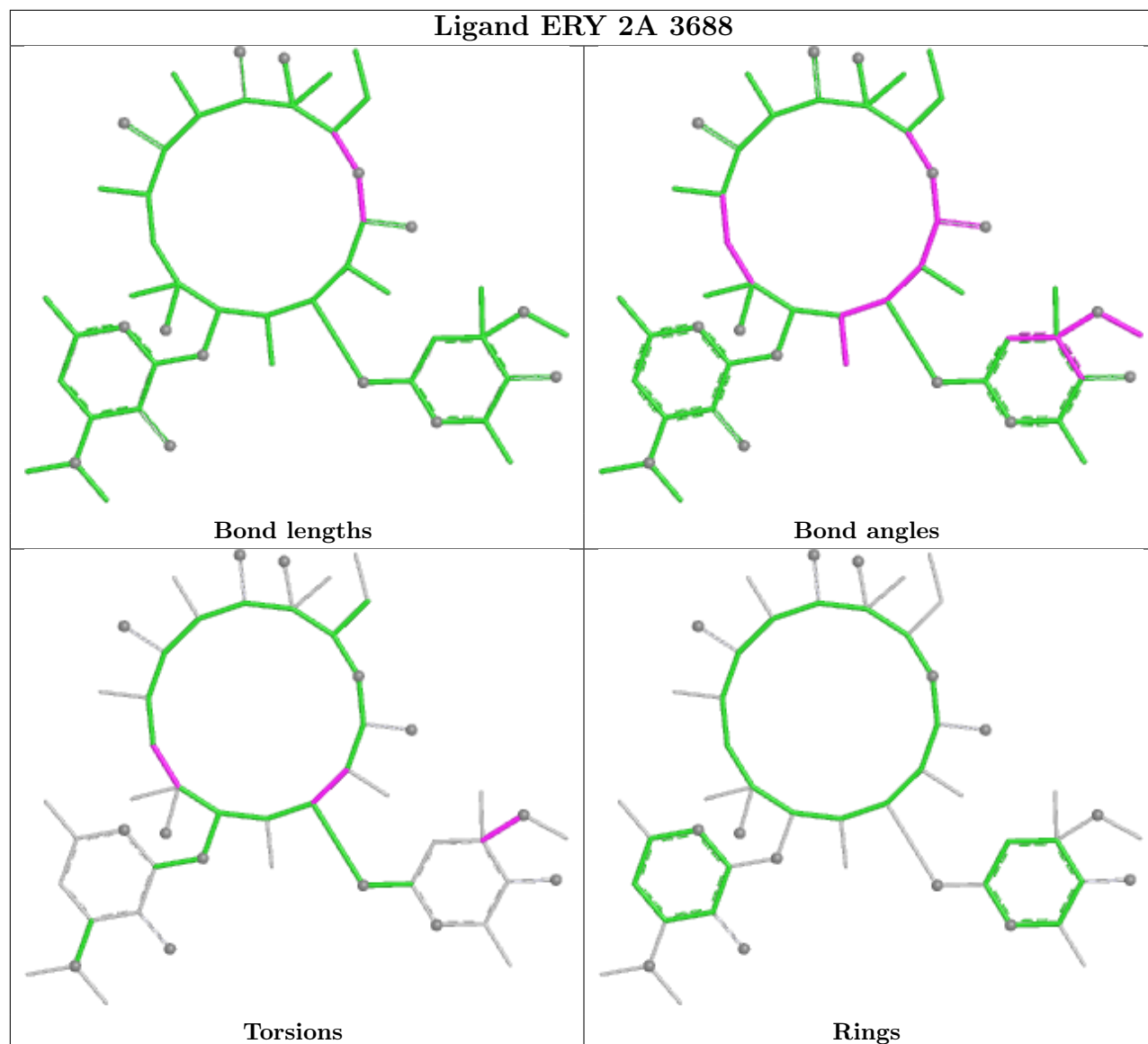
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1A	4098	ERY	1	0
60	2A	3688	ERY	4	0
62	2d	303	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%)	-0.42	123 (4%)	40	36	19, 38, 99, 111	0
1	2A	2789/2915 (95%)	0.01	103 (3%)	45	41	33, 59, 95, 113	0
2	1B	120/121 (99%)	-0.34	0	100	100	31, 52, 66, 91	0
2	2B	120/121 (99%)	1.04	10 (8%)	17	14	64, 82, 90, 97	0
3	1D	275/276 (99%)	-0.12	2 (0%)	84	83	21, 38, 52, 80	0
3	2D	275/276 (99%)	0.27	2 (0%)	84	83	32, 51, 65, 79	0
4	1E	204/206 (99%)	-0.07	0	100	100	20, 44, 63, 72	0
4	2E	204/206 (99%)	0.29	3 (1%)	72	70	36, 60, 74, 84	0
5	1F	203/210 (96%)	-0.03	0	100	100	19, 44, 67, 85	0
5	2F	203/210 (96%)	0.46	5 (2%)	58	55	36, 71, 83, 88	0
6	1G	181/182 (99%)	0.54	8 (4%)	39	35	41, 61, 77, 86	0
6	2G	181/182 (99%)	1.55	48 (26%)	1	1	70, 82, 89, 96	0
7	1H	174/180 (96%)	0.32	2 (1%)	78	76	41, 56, 68, 71	0
7	2H	174/180 (96%)	1.11	16 (9%)	14	12	70, 83, 90, 93	0
8	1I	146/148 (98%)	0.62	2 (1%)	73	72	44, 75, 84, 88	0
8	2I	146/148 (98%)	0.90	14 (9%)	13	11	60, 75, 87, 90	0
9	1N	140/140 (100%)	0.08	1 (0%)	84	83	28, 44, 62, 81	0
9	2N	140/140 (100%)	0.81	7 (5%)	34	30	45, 66, 78, 88	0
10	1O	122/122 (100%)	0.09	2 (1%)	70	68	29, 42, 58, 69	0
10	2O	122/122 (100%)	0.34	0	100	100	46, 59, 71, 79	0
11	1P	149/150 (99%)	0.00	0	100	100	21, 45, 68, 77	0
11	2P	149/150 (99%)	0.60	3 (2%)	65	62	36, 69, 83, 89	0
12	1Q	141/141 (100%)	-0.05	0	100	100	27, 43, 59, 73	0
12	2Q	141/141 (100%)	0.89	9 (6%)	25	22	50, 69, 79, 83	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%)	-0.08	1 (0%) 82 81	28, 39, 53, 64	0
13	2R	118/118 (100%)	0.22	2 (1%) 69 67	40, 54, 65, 73	0
14	1S	110/112 (98%)	0.18	1 (0%) 81 80	38, 51, 63, 71	0
14	2S	110/112 (98%)	1.40	18 (16%) 4 4	65, 75, 84, 87	0
15	1T	131/146 (89%)	0.28	5 (3%) 44 40	34, 46, 71, 78	0
15	2T	131/146 (89%)	0.47	2 (1%) 72 70	50, 62, 76, 80	0
16	1U	116/118 (98%)	-0.15	0 100 100	26, 36, 55, 67	0
16	2U	116/118 (98%)	0.62	1 (0%) 81 80	46, 63, 78, 83	0
17	1V	101/101 (100%)	0.09	1 (0%) 79 78	25, 48, 64, 72	0
17	2V	101/101 (100%)	0.71	4 (3%) 42 38	45, 73, 81, 86	0
18	1W	112/113 (99%)	-0.04	2 (1%) 67 65	26, 37, 55, 82	0
18	2W	112/113 (99%)	0.54	4 (3%) 46 42	40, 52, 70, 96	0
19	1X	95/96 (98%)	0.01	2 (2%) 63 61	26, 40, 62, 77	0
19	2X	95/96 (98%)	0.63	2 (2%) 63 61	44, 62, 77, 82	0
20	1Y	107/110 (97%)	0.44	3 (2%) 55 51	35, 52, 71, 80	0
20	2Y	107/110 (97%)	1.24	16 (14%) 5 4	62, 74, 85, 89	0
21	1Z	154/206 (74%)	0.79	13 (8%) 17 14	46, 68, 90, 100	0
21	2Z	160/206 (77%)	1.52	38 (23%) 2 1	68, 83, 94, 99	0
22	10	83/85 (97%)	0.14	6 (7%) 21 18	29, 40, 60, 70	0
22	20	83/85 (97%)	1.26	10 (12%) 9 7	45, 67, 76, 81	0
23	11	97/98 (98%)	0.26	2 (2%) 63 61	27, 47, 71, 78	0
23	21	97/98 (98%)	0.51	3 (3%) 51 48	41, 58, 79, 80	0
24	12	70/72 (97%)	0.22	1 (1%) 73 72	35, 51, 63, 71	0
24	22	70/72 (97%)	0.84	1 (1%) 73 72	59, 73, 81, 85	0
25	13	59/60 (98%)	0.02	1 (1%) 69 67	29, 43, 65, 75	0
25	23	59/60 (98%)	0.81	3 (5%) 33 29	56, 68, 79, 92	0
26	14	69/71 (97%)	0.93	10 (14%) 6 5	55, 77, 89, 94	0
26	24	69/71 (97%)	1.54	19 (27%) 1 1	81, 89, 97, 100	0
27	15	59/60 (98%)	0.10	2 (3%) 48 44	24, 39, 69, 78	0
27	25	59/60 (98%)	0.26	0 100 100	39, 53, 71, 86	0
28	16	53/54 (98%)	-0.05	1 (1%) 66 63	31, 42, 57, 60	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%)	0.85	3 (5%) 29 26	54, 64, 71, 75	0
29	17	48/49 (97%)	-0.18	3 (6%) 26 23	22, 28, 55, 63	0
29	27	48/49 (97%)	0.10	2 (4%) 40 37	32, 41, 64, 76	0
30	18	64/65 (98%)	-0.17	0 100 100	28, 35, 43, 55	0
30	28	64/65 (98%)	0.60	0 100 100	47, 58, 66, 74	0
31	19	37/37 (100%)	-0.15	1 (2%) 56 53	32, 43, 59, 67	0
31	29	37/37 (100%)	1.00	2 (5%) 31 27	64, 69, 80, 86	0
32	1a	1488/1521 (97%)	0.18	37 (2%) 58 55	36, 67, 94, 112	0
32	2a	1491/1521 (98%)	0.69	101 (6%) 23 20	52, 80, 98, 112	0
33	1b	231/256 (90%)	0.93	29 (12%) 8 7	66, 81, 89, 94	0
33	2b	231/256 (90%)	1.39	47 (20%) 3 2	75, 88, 93, 99	0
34	1c	206/239 (86%)	0.78	6 (2%) 53 50	61, 73, 82, 89	0
34	2c	206/239 (86%)	1.59	61 (29%) 1 1	75, 88, 93, 97	0
35	1d	208/209 (99%)	0.86	13 (6%) 26 23	58, 70, 81, 87	0
35	2d	208/209 (99%)	1.05	26 (12%) 8 7	62, 75, 85, 92	0
36	1e	148/162 (91%)	0.60	5 (3%) 48 44	51, 64, 75, 83	0
36	2e	148/162 (91%)	1.27	25 (16%) 4 3	69, 80, 87, 90	0
37	1f	100/101 (99%)	0.44	2 (2%) 65 62	58, 67, 77, 81	0
37	2f	100/101 (99%)	0.65	4 (4%) 42 38	64, 73, 80, 86	0
38	1g	155/156 (99%)	0.65	12 (7%) 19 17	61, 72, 89, 93	0
38	2g	155/156 (99%)	1.18	22 (14%) 6 5	74, 84, 91, 94	0
39	1h	137/138 (99%)	0.72	4 (2%) 53 50	58, 68, 76, 82	0
39	2h	137/138 (99%)	1.21	15 (10%) 10 9	71, 79, 85, 88	0
40	1i	127/128 (99%)	1.05	10 (7%) 18 16	56, 77, 85, 88	0
40	2i	127/128 (99%)	1.73	43 (33%) 1 1	76, 87, 93, 95	0
41	1j	97/105 (92%)	1.32	22 (22%) 2 2	59, 79, 87, 93	0
41	2j	96/105 (91%)	1.95	37 (38%) 1 0	75, 88, 94, 95	0
42	1k	114/129 (88%)	0.66	7 (6%) 27 24	45, 70, 81, 86	0
42	2k	114/129 (88%)	0.98	10 (8%) 15 13	60, 76, 85, 88	0
43	1l	121/132 (91%)	0.47	3 (2%) 58 55	41, 57, 68, 78	0
43	2l	121/132 (91%)	1.08	12 (9%) 13 10	57, 71, 80, 86	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%)	0.95	9 (7%) 21 18	57, 72, 82, 97	0
44	2m	122/126 (96%)	1.95	43 (35%) 1 1	73, 86, 92, 95	0
45	1n	60/61 (98%)	0.72	3 (5%) 34 30	60, 68, 76, 77	0
45	2n	60/61 (98%)	2.37	35 (58%) 0 0	78, 88, 92, 95	0
46	1o	88/89 (98%)	0.67	3 (3%) 48 44	52, 65, 75, 81	0
46	2o	88/89 (98%)	0.89	7 (7%) 18 15	63, 76, 84, 91	0
47	1p	82/88 (93%)	1.34	19 (23%) 2 2	59, 71, 79, 89	0
47	2p	82/88 (93%)	0.91	6 (7%) 21 18	59, 71, 82, 86	0
48	1q	99/105 (94%)	0.71	3 (3%) 52 49	57, 68, 78, 82	0
48	2q	99/105 (94%)	1.08	12 (12%) 8 7	65, 74, 83, 87	0
49	1r	68/88 (77%)	0.43	1 (1%) 72 70	56, 67, 78, 81	0
49	2r	68/88 (77%)	0.66	1 (1%) 72 70	66, 75, 84, 87	0
50	1s	83/93 (89%)	0.65	3 (3%) 46 42	65, 74, 83, 86	0
50	2s	83/93 (89%)	1.89	35 (42%) 0 0	81, 89, 94, 98	0
51	1t	96/106 (90%)	0.88	12 (12%) 8 7	60, 72, 82, 86	0
51	2t	96/106 (90%)	0.74	4 (4%) 40 37	60, 72, 81, 87	0
52	1u	23/27 (85%)	0.80	2 (8%) 16 13	60, 67, 73, 79	0
52	2u	23/27 (85%)	2.04	14 (60%) 0 0	78, 83, 87, 88	0
53	1v	13/24 (54%)	1.06	3 (23%) 2 2	46, 72, 98, 103	0
53	2v	11/24 (45%)	1.38	3 (27%) 1 1	69, 83, 94, 96	0
54	1w	67/76 (88%)	1.33	18 (26%) 1 1	49, 93, 103, 108	0
54	2w	67/76 (88%)	1.49	16 (23%) 2 1	66, 100, 108, 110	0
55	1x	72/77 (93%)	0.59	4 (5%) 30 26	31, 67, 84, 89	0
55	2x	72/77 (93%)	0.81	3 (4%) 40 37	47, 84, 93, 96	0
56	1z	2/3 (66%)	0.54	0 100 100	37, 37, 37, 38	0
56	2z	2/3 (66%)	1.10	0 100 100	52, 52, 52, 56	0
57	1y	68/76 (89%)	1.84	23 (33%) 1 1	59, 104, 108, 109	0
57	2y	68/76 (89%)	2.01	34 (50%) 0 0	69, 106, 110, 111	0
All	All	20882/21754 (95%)	0.42	1414 (6%) 23 20	19, 66, 93, 113	0

All (1414) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	13.3
44	2m	123	ALA	10.1
44	1m	124	PRO	9.3
44	2m	102	ARG	9.2
44	1m	122	LYS	8.3
1	1A	2113	U	8.2
44	2m	122	LYS	8.1
1	1A	2115	G	7.8
1	1A	2112	G	7.1
1	1A	2145	C	6.9
1	2A	2145	C	6.8
44	1m	123	ALA	6.4
45	2n	2	ALA	6.3
1	2A	2112	G	6.2
1	1A	2114	A	6.0
44	2m	121	LYS	6.0
32	2a	1032	G	5.9
1	2A	2146	C	5.7
45	1n	2	ALA	5.5
33	2b	165	VAL	5.4
7	1H	2	SER	5.3
44	1m	2	ALA	5.2
21	1Z	141	VAL	5.2
1	2A	2113	U	5.0
1	1A	2121	G	5.0
41	2j	47	PHE	4.9
32	2a	1031	G	4.9
45	2n	39	LEU	4.9
44	1m	121	LYS	4.9
1	2A	2111	C	4.9
32	2a	973	G	4.9
50	1s	84	GLY	4.8
40	2i	102	LEU	4.8
38	2g	84	ASN	4.8
38	2g	83	ALA	4.8
45	2n	34	TYR	4.8
32	2a	1030(B)	C	4.7
38	1g	81	GLY	4.7
1	1A	2117	A	4.7
45	2n	25	VAL	4.7
1	1A	2159	G	4.7
32	2a	1033	G	4.7
38	2g	82	GLY	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	24	51	ASP	4.7
40	2i	14	VAL	4.6
1	1A	2147	G	4.5
18	2W	112	GLY	4.5
53	1v	13	A	4.5
1	2A	2166	G	4.5
1	1A	2146	C	4.5
32	2a	1027	C	4.5
32	2a	1532	U	4.5
1	2A	2125	G	4.5
1	2A	2133	G	4.4
1	2A	2155	G	4.4
33	2b	237	ALA	4.4
23	11	2	SER	4.4
1	2A	2174	C	4.4
50	2s	9	VAL	4.4
40	1i	126	SER	4.4
22	20	7	LEU	4.4
43	2l	64	TYR	4.4
45	2n	33	VAL	4.4
50	2s	2	PRO	4.3
1	2A	2123	G	4.3
32	2a	1034	G	4.3
51	1t	13	LEU	4.3
1	1A	2136	C	4.3
1	1A	2178	C	4.3
32	1a	1257	U	4.3
32	2a	1116	C	4.3
1	2A	2167	U	4.3
32	2a	1149	C	4.3
33	2b	7	VAL	4.3
45	2n	21	TYR	4.3
35	1d	157	LEU	4.2
1	1A	2103	C	4.2
54	1w	49	G	4.2
27	15	60	VAL	4.2
1	2A	2175	C	4.2
15	1T	131	ALA	4.2
32	2a	972	C	4.2
1	2A	2165	G	4.2
20	2Y	1	MET	4.1
1	2A	2115	G	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2111	C	4.1
32	2a	1251	A	4.1
6	2G	50	ALA	4.1
1	1A	2141	G	4.0
1	2A	2168	G	4.0
32	2a	1030(A)	G	4.0
25	23	60	GLU	4.0
34	2c	189	ALA	4.0
31	29	37	GLY	4.0
23	21	2	SER	4.0
3	1D	276	LYS	4.0
38	1g	80	VAL	4.0
34	2c	188	LEU	4.0
51	1t	10	LEU	4.0
1	2A	2147	G	4.0
1	2A	2169	A	4.0
6	2G	52	ILE	3.9
33	1b	237	ALA	3.9
44	2m	90	LEU	3.9
1	1A	2143	C	3.9
6	2G	77	ILE	3.9
32	2a	1036	G	3.9
44	2m	6	GLY	3.9
1	1A	1096	A	3.9
26	14	56	VAL	3.9
34	2c	87	LEU	3.9
32	2a	1224	G	3.9
21	1Z	146	ILE	3.9
1	1A	2180	U	3.9
1	2A	2144	U	3.9
1	1A	2119	A	3.8
21	2Z	121	HIS	3.8
1	1A	2174	C	3.8
20	1Y	1	MET	3.8
8	2I	146	ALA	3.8
1	2A	2110	G	3.8
1	1A	1081	U	3.8
32	1a	1533	C	3.8
32	2a	1219	U	3.8
33	2b	21	ARG	3.8
40	2i	10	ARG	3.8
8	2I	1	MET	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	144	LEU	3.8
22	20	84	LEU	3.8
45	2n	13	THR	3.7
1	2A	2114	A	3.7
1	1A	2179	C	3.7
40	2i	11	LYS	3.7
1	1A	1057	A	3.7
38	2g	80	VAL	3.7
21	1Z	150	LEU	3.7
1	1A	2160	G	3.7
1	1A	2166	G	3.7
41	2j	40	LEU	3.7
1	1A	2142	C	3.7
41	2j	75	ILE	3.7
38	2g	85	TYR	3.7
41	2j	55	LYS	3.7
6	1G	146	TYR	3.6
46	2o	75	PRO	3.6
1	2A	2126	A	3.6
1	1A	2110	G	3.6
1	2A	1536	C	3.6
32	2a	1002	G	3.6
43	2l	32	PHE	3.6
21	2Z	146	ILE	3.6
1	1A	548	A	3.6
32	2a	1030(D)	A	3.6
12	2Q	121	ALA	3.6
52	2u	14	TRP	3.6
33	2b	236	TYR	3.6
38	1g	85	TYR	3.6
19	1X	95	LEU	3.6
1	1A	2104	G	3.6
32	2a	1202	G	3.6
57	2y	33	U	3.6
1	1A	2135	A	3.6
26	24	49	PHE	3.6
57	1y	5	C	3.5
22	20	69	PHE	3.5
1	1A	2122	U	3.5
1	1A	2130	U	3.5
1	1A	2144	U	3.5
1	1A	2167	U	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2169	A	3.5
21	1Z	171	ILE	3.5
40	2i	105	ASP	3.5
41	1j	32	ALA	3.5
57	2y	5	C	3.5
38	2g	16	LEU	3.5
32	2a	1358	U	3.5
45	2n	29	ARG	3.5
1	1A	2133	G	3.5
1	1A	1094	U	3.5
1	1A	2189	U	3.5
1	2A	2117	A	3.5
1	2A	2170	A	3.5
34	2c	2	GLY	3.5
45	2n	14	PRO	3.5
57	1y	75	C	3.4
38	2g	81	GLY	3.4
52	2u	2	GLY	3.4
32	2a	974	A	3.4
40	2i	126	SER	3.4
1	1A	2161	C	3.4
33	2b	86	GLU	3.4
1	1A	1078	U	3.4
34	2c	195	VAL	3.4
50	2s	58	VAL	3.4
1	2A	2127	G	3.4
32	1a	1030(A)	G	3.4
34	2c	124	ILE	3.4
1	1A	1095	A	3.4
1	1A	2170	A	3.4
53	1v	12	A	3.4
41	2j	79	ARG	3.4
1	2A	2143	C	3.4
44	2m	60	VAL	3.4
55	2x	47	U	3.4
44	2m	65	LYS	3.4
21	1Z	166	SER	3.4
40	2i	36	TYR	3.4
1	1A	2116	G	3.4
1	2A	2100	G	3.4
32	1a	1036	G	3.4
32	2a	1061	G	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	965	A	3.4
44	2m	104	ARG	3.4
44	2m	7	VAL	3.4
1	1A	886	C	3.3
1	2A	2164	C	3.3
57	1y	35	U	3.3
33	1b	134	GLU	3.3
33	2b	213	LEU	3.3
41	2j	8	LEU	3.3
41	2j	65	LEU	3.3
6	1G	50	ALA	3.3
22	10	3	HIS	3.3
34	2c	137	ALA	3.3
32	2a	1220	G	3.3
3	2D	276	LYS	3.3
6	2G	182	LYS	3.3
41	1j	4	ILE	3.3
1	1A	1026	U	3.3
2	2B	4	C	3.3
32	2a	1030	C	3.3
40	1i	2	GLU	3.3
45	2n	31	ARG	3.3
44	2m	101	GLN	3.3
1	2A	2116	G	3.3
32	2a	1117	G	3.3
33	2b	120	ALA	3.3
1	2A	2139	C	3.3
6	2G	15	VAL	3.3
7	2H	35	VAL	3.3
45	2n	40	CYS	3.3
32	2a	1035	A	3.3
1	1A	1059	G	3.3
32	2a	963	G	3.3
40	2i	96	LEU	3.3
38	2g	154	TYR	3.3
36	2e	21	ALA	3.3
34	2c	157	ILE	3.3
42	1k	14	VAL	3.3
6	2G	49	ASP	3.3
6	2G	53	LEU	3.2
1	1A	614(B)	G	3.2
1	1A	1058	G	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1068	G	3.2
1	2A	2162	G	3.2
32	2a	1353	G	3.2
45	2n	3	ARG	3.2
1	1A	889	C	3.2
34	2c	52	LEU	3.2
54	1w	50	C	3.2
38	1g	82	GLY	3.2
32	2a	978	A	3.2
6	1G	52	ILE	3.2
41	2j	38	ILE	3.2
1	1A	2165	G	3.2
39	2h	30	ARG	3.2
57	1y	15	G	3.2
1	2A	2189	U	3.2
34	2c	33	LEU	3.2
36	2e	12	LEU	3.2
39	1h	2	LEU	3.2
36	2e	74	GLY	3.2
44	2m	100	GLY	3.2
1	1A	2108	C	3.2
1	1A	2129	C	3.2
32	2a	1114	C	3.2
45	2n	20	ALA	3.2
40	1i	114	TYR	3.2
20	2Y	34	LYS	3.2
6	1G	48	GLU	3.2
22	10	7	LEU	3.2
1	1A	2120	G	3.2
32	2a	1026	G	3.2
45	2n	42	ILE	3.2
47	2p	38	TYR	3.2
35	2d	154	ASN	3.1
44	2m	69	GLU	3.1
47	2p	82	GLN	3.1
50	2s	79	THR	3.1
1	1A	1082	U	3.1
57	2y	20	U	3.1
1	1A	2181	G	3.1
1	2A	1533	G	3.1
1	2A	2148	G	3.1
20	2Y	55	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	1k	25	TYR	3.1
54	1w	19	G	3.1
57	2y	6	G	3.1
1	1A	2140	C	3.1
45	2n	6	LEU	3.1
22	20	68	GLU	3.1
34	2c	73	PRO	3.1
32	2a	1250	A	3.1
35	2d	2	GLY	3.1
33	2b	200	ILE	3.1
45	2n	30	ALA	3.1
34	2c	55	VAL	3.1
41	2j	63	PHE	3.1
40	2i	66	ARG	3.1
40	2i	95	LYS	3.1
45	2n	4	LYS	3.1
41	1j	76	ASN	3.1
6	2G	147	ASP	3.1
1	2A	2160	G	3.1
44	2m	58	GLU	3.1
33	2b	131	PRO	3.1
1	1A	2138	C	3.1
41	2j	48	THR	3.1
54	1w	56	C	3.1
15	1T	130	ALA	3.1
21	2Z	57	ILE	3.1
21	2Z	171	ILE	3.1
34	2c	160	ALA	3.1
53	2v	14	A	3.1
14	2S	92	TYR	3.1
57	2y	45	G	3.1
34	2c	4	LYS	3.1
1	1A	154(A)	C	3.1
1	1A	1064	C	3.1
21	2Z	174	VAL	3.1
45	2n	16	PHE	3.1
40	2i	99	LEU	3.0
8	2I	20	ASP	3.0
32	2a	1257	U	3.0
11	2P	28	GLY	3.0
22	10	6	GLY	3.0
42	2k	31	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	119	GLY	3.0
38	1g	79	ARG	3.0
41	1j	60	ARG	3.0
41	2j	32	ALA	3.0
14	2S	29	PHE	3.0
1	2A	1171	G	3.0
32	2a	1030(C)	G	3.0
1	2A	2128	C	3.0
26	14	57	GLU	3.0
32	1a	1027	C	3.0
38	1g	154	TYR	3.0
1	2A	2122	U	3.0
32	2a	950	U	3.0
57	1y	33	U	3.0
22	20	43	THR	3.0
6	2G	19	LEU	3.0
41	2j	76	ASN	3.0
1	1A	1087	G	3.0
1	2A	883	G	3.0
1	2A	2157	G	3.0
26	24	65	ASP	3.0
44	2m	120	LYS	3.0
57	1y	70	C	3.0
1	2A	2173	A	3.0
32	1a	1447	A	3.0
40	2i	7	THR	3.0
41	2j	74	ILE	3.0
46	2o	88	ARG	3.0
47	1p	19	ILE	3.0
33	1b	188	ALA	3.0
57	2y	36	U	3.0
6	2G	160	VAL	3.0
14	2S	46	VAL	3.0
34	2c	153	VAL	3.0
36	2e	20	GLN	3.0
41	2j	78	ASN	3.0
6	2G	161	THR	3.0
41	2j	93	GLY	3.0
1	2A	2182	G	3.0
44	2m	118	ALA	3.0
32	2a	1289	A	3.0
6	2G	175	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	2h	112	LEU	2.9
38	1g	84	ASN	2.9
33	1b	34	ALA	2.9
21	1Z	104	PHE	2.9
26	24	50	VAL	2.9
32	2a	980	C	2.9
32	2a	1223	C	2.9
1	2A	2119	A	2.9
32	1a	1030(D)	A	2.9
32	2a	1364	U	2.9
38	2g	32	ARG	2.9
20	2Y	107	ASP	2.9
40	2i	63	ILE	2.9
45	2n	38	GLY	2.9
50	2s	41	VAL	2.9
38	2g	12	LEU	2.9
20	2Y	54	LYS	2.9
48	1q	100	LYS	2.9
33	2b	234	PRO	2.9
6	2G	76	SER	2.9
6	1G	51	ARG	2.9
32	1a	1531	A	2.9
32	2a	532	A	2.9
1	2A	2104	G	2.9
34	2c	181	ASN	2.9
4	2E	10	GLY	2.9
26	24	54	GLY	2.9
40	2i	27	THR	2.9
21	2Z	172	ALA	2.9
26	24	5	ILE	2.9
34	2c	77	ILE	2.9
41	1j	74	ILE	2.9
1	1A	2164	C	2.9
40	2i	62	TYR	2.9
57	2y	13	C	2.9
1	2A	2154	G	2.9
1	2A	2156	G	2.9
21	2Z	139	VAL	2.9
34	2c	207	VAL	2.9
45	2n	18	VAL	2.9
49	1r	78	LEU	2.9
45	2n	36	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	11	26	ARG	2.8
41	1j	33	GLN	2.8
38	1g	156	TRP	2.8
38	2g	77	SER	2.8
36	2e	130	ASN	2.8
21	2Z	150	LEU	2.8
1	1A	2109	U	2.8
1	2A	2171	A	2.8
32	1a	149	A	2.8
32	1a	1532	U	2.8
33	2b	93	VAL	2.8
32	2a	1357	A	2.8
1	2A	2188	C	2.8
32	2a	1249	C	2.8
32	2a	1354	C	2.8
24	12	69	ARG	2.8
32	2a	630	G	2.8
48	2q	99	SER	2.8
6	2G	81	LYS	2.8
39	2h	130	GLY	2.8
40	2i	67	GLY	2.8
43	1l	64	TYR	2.8
47	1p	6	LEU	2.8
22	20	2	ALA	2.8
34	2c	24	ALA	2.8
9	2N	9	VAL	2.8
39	2h	9	MET	2.8
1	1A	1060	U	2.8
1	2A	2109	U	2.8
1	2A	2137	C	2.8
7	1H	175	LYS	2.8
12	2Q	22	LYS	2.8
14	2S	35	ILE	2.8
21	1Z	120	ILE	2.8
54	1w	18	G	2.8
33	2b	187	LEU	2.8
35	1d	2	GLY	2.8
45	2n	55	GLY	2.8
21	2Z	170	THR	2.8
39	1h	3	THR	2.8
33	2b	112	VAL	2.8
34	2c	128	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	184	TYR	2.8
34	2c	186	PHE	2.8
40	2i	28	VAL	2.8
41	2j	34	VAL	2.8
20	2Y	5	MET	2.8
21	2Z	95	PRO	2.8
52	1u	24	ARG	2.8
32	2a	1235	U	2.8
57	1y	4	U	2.8
34	2c	199	LYS	2.8
43	2l	13	LYS	2.8
1	1A	529	A	2.8
33	2b	208	ILE	2.8
53	2v	24	A	2.8
2	2B	6	C	2.8
33	2b	149	LEU	2.8
37	2f	21	LEU	2.8
45	2n	44	LEU	2.8
33	2b	48	MET	2.8
34	2c	129	ALA	2.8
38	1g	9	VAL	2.8
40	2i	13	ALA	2.8
33	2b	17	PHE	2.8
40	2i	17	VAL	2.8
1	1A	1056	G	2.8
1	1A	2123	G	2.8
1	2A	2101	G	2.8
32	1a	380	G	2.8
32	1a	1031	G	2.8
47	1p	81	ARG	2.8
33	1b	125	PRO	2.7
45	2n	7	ILE	2.7
57	2y	4	U	2.7
9	2N	45	ASN	2.7
21	2Z	155	LEU	2.7
51	1t	24	LEU	2.7
15	2T	69	GLY	2.7
32	2a	1248	A	2.7
1	1A	885	C	2.7
1	1A	2137	C	2.7
1	2A	2138	C	2.7
18	2W	92	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	14	58	ARG	2.7
32	2a	1039	C	2.7
33	2b	230	VAL	2.7
43	2l	39	VAL	2.7
54	1w	13	C	2.7
54	1w	67	C	2.7
57	2y	70	C	2.7
26	24	63	TYR	2.7
36	2e	133	TYR	2.7
50	2s	80	TYR	2.7
3	1D	275	LYS	2.7
6	2G	74	LYS	2.7
48	2q	100	LYS	2.7
1	1A	2125	G	2.7
1	1A	2162	G	2.7
2	2B	119	G	2.7
32	1a	1001(A)	G	2.7
33	2b	185	ILE	2.7
52	2u	13	ILE	2.7
47	2p	6	LEU	2.7
38	1g	153	HIS	2.7
41	1j	31	GLY	2.7
50	2s	35	SER	2.7
44	2m	73	GLU	2.7
6	2G	102	PHE	2.7
21	2Z	69	THR	2.7
33	2b	71	VAL	2.7
33	2b	197	VAL	2.7
34	2c	68	VAL	2.7
35	1d	111	ALA	2.7
36	2e	84	PHE	2.7
40	1i	28	VAL	2.7
47	1p	5	ARG	2.7
51	2t	97	ALA	2.7
1	1A	887	A	2.7
2	2B	120	A	2.7
57	1y	69	A	2.7
26	14	63	TYR	2.7
40	2i	92	TYR	2.7
40	2i	125	TYR	2.7
1	1A	2175	C	2.7
32	1a	1030(B)	C	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	1y	74	C	2.7
57	2y	74	C	2.7
34	2c	13	GLY	2.7
14	2S	3	ARG	2.7
38	2g	37	ASN	2.7
40	2i	128	ARG	2.7
7	2H	17	VAL	2.7
35	2d	92	VAL	2.7
41	2j	67	THR	2.7
1	2A	2132	U	2.7
32	1a	1025	U	2.7
54	1w	47	U	2.7
42	2k	25	TYR	2.7
54	2w	59	A	2.7
57	2y	69	A	2.7
34	1c	39	ILE	2.7
1	1A	888	C	2.7
32	1a	1028	C	2.7
32	2a	1038	C	2.7
57	1y	71	C	2.7
40	2i	50	LEU	2.7
18	1W	112	GLY	2.7
41	1j	79	ARG	2.7
39	2h	3	THR	2.7
50	2s	13	ASP	2.7
1	2A	2130	U	2.6
20	2Y	90	LEU	2.6
32	1a	1286	A	2.6
32	2a	1447	A	2.6
39	2h	107	LEU	2.6
52	2u	15	ARG	2.6
51	2t	103	GLY	2.6
1	1A	34	C	2.6
1	2A	2185	C	2.6
55	2x	1	C	2.6
7	2H	96	ALA	2.6
14	2S	12	PHE	2.6
33	1b	7	VAL	2.6
33	2b	97	TRP	2.6
50	2s	76	PRO	2.6
36	2e	101	ILE	2.6
41	1j	98	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1099	G	2.6
1	1A	2154	G	2.6
1	1A	2182	G	2.6
1	2A	882	G	2.6
2	2B	23	G	2.6
32	1a	1034	G	2.6
57	1y	12	U	2.6
57	2y	35	U	2.6
14	2S	45	GLY	2.6
19	1X	94	GLY	2.6
20	2Y	10	GLY	2.6
34	2c	155	GLY	2.6
9	1N	9	VAL	2.6
35	2d	164	ALA	2.6
38	1g	83	ALA	2.6
40	2i	101	PHE	2.6
47	1p	80	PHE	2.6
50	2s	11	VAL	2.6
9	2N	44	PRO	2.6
1	1A	2128	C	2.6
1	2A	2163	C	2.6
54	2w	50	C	2.6
50	2s	52	TYR	2.6
42	2k	126	ARG	2.6
17	1V	101	GLY	2.6
21	2Z	26	GLY	2.6
21	2Z	106	GLY	2.6
1	1A	2190	G	2.6
1	2A	530	G	2.6
1	2A	2318	G	2.6
8	1I	146	ALA	2.6
41	2j	77	PRO	2.6
51	1t	95	ALA	2.6
1	1A	1098	A	2.6
34	2c	14	ILE	2.6
34	2c	182	ILE	2.6
39	2h	2	LEU	2.6
35	2d	73	ARG	2.6
50	2s	78	ARG	2.6
14	2S	34	HIS	2.6
1	1A	2118	U	2.6
4	2E	204	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	108	ALA	2.6
50	2s	59	PRO	2.6
1	1A	2131	G	2.5
1	1A	2157	G	2.5
1	2A	2120	G	2.5
32	1a	1024	G	2.5
32	2a	1001(A)	G	2.5
32	2a	1356	G	2.5
35	2d	144	ASP	2.5
1	2A	229	A	2.5
32	2a	1286	A	2.5
32	2a	1287	A	2.5
57	2y	38	A	2.5
3	2D	38	LYS	2.5
12	2Q	10	ARG	2.5
19	2X	69	TYR	2.5
48	1q	78	GLU	2.5
32	2a	979	C	2.5
25	13	2	PRO	2.5
44	2m	113	PRO	2.5
5	2F	90	PHE	2.5
26	24	42	PHE	2.5
36	2e	94	ALA	2.5
41	2j	27	ALA	2.5
41	2j	54	PHE	2.5
44	2m	76	ALA	2.5
26	14	52	THR	2.5
32	1a	1000	U	2.5
57	2y	47	U	2.5
39	2h	4	ASP	2.5
33	2b	211	ILE	2.5
6	2G	172	LEU	2.5
11	2P	39	LYS	2.5
15	2T	111	ARG	2.5
29	27	47	ARG	2.5
33	2b	10	LEU	2.5
40	1i	56	LEU	2.5
48	2q	98	LEU	2.5
50	2s	32	LYS	2.5
1	1A	2101	G	2.5
1	1A	2156	G	2.5
54	1w	1	G	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	2y	3	G	2.5
57	2y	10	G	2.5
14	2S	7	TYR	2.5
32	1a	1035	A	2.5
32	2a	1001	A	2.5
22	20	76	GLY	2.5
34	2c	158	GLY	2.5
50	2s	68	GLY	2.5
46	1o	19	PRO	2.5
21	2Z	165	VAL	2.5
35	1d	110	PHE	2.5
50	2s	24	ALA	2.5
1	2A	885	C	2.5
1	2A	894	C	2.5
1	2A	2129	C	2.5
1	2A	2136	C	2.5
1	2A	2161	C	2.5
2	2B	12	C	2.5
57	1y	32	C	2.5
50	2s	53	ASN	2.5
50	2s	4	SER	2.5
40	1i	105	ASP	2.5
43	1l	28	LYS	2.5
1	1A	2132	U	2.5
2	2B	1	U	2.5
6	2G	128	ARG	2.5
9	2N	74	ARG	2.5
9	2N	112	LEU	2.5
18	2W	37	ARG	2.5
33	2b	11	LEU	2.5
44	2m	88	ARG	2.5
5	2F	16	GLY	2.5
34	2c	74	GLY	2.5
42	2k	90	GLY	2.5
51	1t	69	GLY	2.5
32	1a	630	G	2.5
32	2a	971	G	2.5
33	1b	165	VAL	2.5
34	1c	207	VAL	2.5
36	2e	100	VAL	2.5
40	1i	106	ALA	2.5
47	1p	7	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	33	THR	2.5
43	2l	126	LYS	2.5
21	2Z	41	LEU	2.5
40	1i	19	LEU	2.5
41	2j	23	ILE	2.5
44	2m	96	LEU	2.5
45	2n	53	LEU	2.5
50	2s	71	LEU	2.5
51	1t	8	ARG	2.5
1	1A	2794	C	2.5
1	2A	884	C	2.5
6	2G	4	ASP	2.5
32	1a	1029	C	2.5
40	2i	91	ASP	2.5
22	20	3	HIS	2.5
1	2A	2118	U	2.5
15	1T	109	GLU	2.5
20	2Y	29	GLU	2.5
57	1y	36	U	2.5
6	2G	146	TYR	2.5
52	2u	11	GLY	2.5
34	2c	75	VAL	2.5
41	1j	34	VAL	2.5
47	1p	21	VAL	2.5
21	2Z	173	ALA	2.5
45	2n	10	ALA	2.5
43	2l	28	LYS	2.4
32	2a	1531	A	2.4
36	2e	126	ARG	2.4
41	1j	78	ASN	2.4
6	2G	20	ILE	2.4
33	1b	127	ILE	2.4
33	2b	44	LEU	2.4
34	2c	84	ILE	2.4
44	2m	22	ILE	2.4
1	1A	1176	G	2.4
1	2A	2159	G	2.4
1	2A	2181	G	2.4
32	2a	1003	G	2.4
57	2y	57	G	2.4
40	2i	2	GLU	2.4
32	2a	1054	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2w	56	C	2.4
57	2y	25	C	2.4
32	1a	65	U	2.4
32	1a	202	U	2.4
32	1a	204	U	2.4
34	2c	25	GLY	2.4
42	2k	49	GLY	2.4
43	1l	63	GLY	2.4
57	2y	7	U	2.4
21	2Z	15	PRO	2.4
34	2c	48	TYR	2.4
6	2G	70	VAL	2.4
7	2H	107	VAL	2.4
33	1b	136	VAL	2.4
6	2G	57	ALA	2.4
21	2Z	88	PHE	2.4
48	2q	44	ALA	2.4
10	1O	49	ARG	2.4
41	2j	87	THR	2.4
52	2u	24	ARG	2.4
42	2k	117	ASN	2.4
51	1t	70	SER	2.4
6	2G	29	TRP	2.4
26	14	51	ASP	2.4
32	2a	1225	A	2.4
32	2a	1285	A	2.4
34	2c	62	ASP	2.4
54	1w	73	A	2.4
33	1b	9	GLU	2.4
33	2b	134	GLU	2.4
35	1d	179	GLU	2.4
1	1A	275	G	2.4
32	2a	1024	G	2.4
32	2a	1222	G	2.4
54	2w	1	G	2.4
55	1x	46	G	2.4
57	1y	68	G	2.4
6	2G	2	PRO	2.4
41	2j	53	PRO	2.4
29	17	48	LYS	2.4
29	27	48	LYS	2.4
1	1A	652(S)	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	34	C	2.4
17	2V	81	TYR	2.4
26	24	32	TYR	2.4
26	24	33	VAL	2.4
33	2b	136	VAL	2.4
34	2c	130	VAL	2.4
44	2m	53	VAL	2.4
35	2d	122	ARG	2.4
38	2g	5	ARG	2.4
41	2j	28	ARG	2.4
45	1n	3	ARG	2.4
21	1Z	170	THR	2.4
34	2c	192	THR	2.4
39	2h	86	ILE	2.4
44	2m	78	ILE	2.4
18	1W	60	ASN	2.4
34	2c	6	HIS	2.4
50	2s	14	HIS	2.4
6	2G	35	GLU	2.4
26	24	57	GLU	2.4
33	1b	128	GLU	2.4
47	1p	68	ASP	2.4
1	2A	896	A	2.4
1	2A	2158	A	2.4
22	10	5	LYS	2.4
36	1e	85	GLY	2.4
20	2Y	85	VAL	2.4
21	1Z	105	VAL	2.4
21	2Z	71	VAL	2.4
26	24	21	VAL	2.4
41	2j	49	VAL	2.4
1	1A	2127	G	2.4
32	1a	1023	G	2.4
38	2g	26	PHE	2.4
40	2i	52	ALA	2.4
43	2l	56	ALA	2.4
44	2m	5	ALA	2.4
52	2u	7	ARG	2.4
54	1w	68	G	2.4
57	2y	15	G	2.4
1	2A	2102	U	2.4
7	2H	89	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	2d	162	LEU	2.4
41	2j	88	LEU	2.4
48	2q	76	LEU	2.4
32	2a	1369	C	2.4
32	2a	1372	U	2.4
54	1w	61	C	2.4
54	2w	61	C	2.4
50	2s	83	HIS	2.4
34	2c	161	GLU	2.4
7	2H	36	PRO	2.4
33	1b	131	PRO	2.4
41	1j	77	PRO	2.4
36	2e	85	GLY	2.4
51	1t	103	GLY	2.4
20	2Y	57	GLN	2.4
47	2p	76	GLN	2.4
33	2b	175	ARG	2.4
35	2d	178	VAL	2.4
39	2h	53	VAL	2.4
41	2j	72	VAL	2.4
47	1p	20	VAL	2.4
48	2q	35	VAL	2.4
1	1A	2173	A	2.4
1	2A	2135	A	2.4
21	2Z	164	ALA	2.4
33	1b	17	PHE	2.4
57	2y	66	A	2.4
33	2b	123	ALA	2.4
44	2m	30	ALA	2.4
7	2H	83	TYR	2.3
14	2S	36	TYR	2.3
21	2Z	29	TYR	2.3
46	1o	57	LEU	2.3
36	2e	13	ILE	2.3
21	1Z	121	HIS	2.3
1	1A	1101	U	2.3
32	1a	1009	G	2.3
32	2a	631	G	2.3
32	2a	1370	G	2.3
54	1w	7	U	2.3
54	1w	60	U	2.3
54	2w	15	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2w	18	G	2.3
41	1j	64	GLU	2.3
41	2j	83	GLU	2.3
21	2Z	154	ASP	2.3
22	20	5	LYS	2.3
32	1a	1008	C	2.3
40	2i	71	SER	2.3
42	1k	51	LYS	2.3
34	2c	167	TRP	2.3
44	2m	64	TRP	2.3
7	2H	128	PRO	2.3
34	2c	197	GLY	2.3
40	2i	6	GLY	2.3
14	2S	20	ARG	2.3
34	1c	190	ARG	2.3
38	2g	4	ARG	2.3
7	2H	37	VAL	2.3
8	2I	15	VAL	2.3
21	2Z	74	VAL	2.3
41	1j	24	VAL	2.3
50	1s	9	VAL	2.3
25	23	26	LEU	2.3
34	2c	163	ALA	2.3
36	1e	94	ALA	2.3
51	1t	55	ILE	2.3
47	1p	17	TYR	2.3
32	2a	1363(A)	A	2.3
33	1b	19	HIS	2.3
41	1j	100	THR	2.3
45	2n	17	LYS	2.3
51	2t	74	LYS	2.3
1	1A	1065	U	2.3
32	2a	1205	U	2.3
32	2a	1232	U	2.3
50	2s	12	ASP	2.3
1	1A	880	G	2.3
1	2A	2106	G	2.3
16	2U	2	PRO	2.3
32	1a	1002	G	2.3
32	2a	947	G	2.3
41	2j	91	PRO	2.3
54	1w	57	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2188	C	2.3
1	2A	2794	C	2.3
21	2Z	131	ARG	2.3
32	1a	1038	C	2.3
33	1b	203	GLY	2.3
41	2j	5	ARG	2.3
52	2u	4	GLY	2.3
55	1x	1	C	2.3
57	1y	13	C	2.3
43	2l	104	VAL	2.3
35	2d	206	PHE	2.3
29	17	45	ALA	2.3
42	1k	15	ALA	2.3
20	2Y	44	ILE	2.3
35	2d	158	ILE	2.3
50	2s	31	ILE	2.3
18	2W	111	HIS	2.3
47	1p	16	HIS	2.3
17	2V	7	THR	2.3
34	2c	95	THR	2.3
44	2m	23	TYR	2.3
47	1p	38	TYR	2.3
12	2Q	103	MET	2.3
6	2G	48	GLU	2.3
20	2Y	63	LYS	2.3
27	15	59	GLU	2.3
1	1A	2134	A	2.3
53	2v	15	A	2.3
51	1t	11	SER	2.3
5	2F	62	ARG	2.3
6	2G	51	ARG	2.3
33	1b	97	TRP	2.3
41	1j	45	ARG	2.3
35	2d	87	GLY	2.3
46	2o	89	GLY	2.3
26	24	56	VAL	2.3
35	2d	88	VAL	2.3
37	1f	88	VAL	2.3
40	2i	41	VAL	2.3
40	2i	86	VAL	2.3
40	2i	108	VAL	2.3
6	2G	139	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	14	49	PHE	2.3
33	2b	121	LEU	2.3
33	1b	214	ILE	2.3
33	2b	13	ALA	2.3
34	2c	8	ILE	2.3
36	2e	86	ALA	2.3
1	1A	1075	C	2.3
1	2A	11	G	2.3
1	2A	645	C	2.3
1	2A	2131	G	2.3
2	2B	118	G	2.3
32	1a	136	C	2.3
32	2a	951	G	2.3
50	2s	49	ILE	2.3
32	2a	1192	C	2.3
40	2i	117	HIS	2.3
54	2w	32	C	2.3
57	1y	10	G	2.3
57	2y	1	G	2.3
9	2N	1	MET	2.3
45	2n	11	LYS	2.3
50	2s	77	THR	2.3
26	24	25	TYR	2.3
42	2k	75	TYR	2.3
28	16	4	GLU	2.3
6	2G	130	ASN	2.3
6	1G	76	SER	2.3
13	2R	68	ARG	2.3
13	2R	69	ASP	2.3
14	2S	50	SER	2.3
33	1b	167	PRO	2.3
50	2s	38	SER	2.3
6	2G	41	GLN	2.3
41	1j	84	GLN	2.3
21	2Z	143	GLY	2.3
21	2Z	147	GLY	2.3
28	26	42	TRP	2.3
51	1t	47	GLY	2.3
5	2F	6	VAL	2.3
5	2F	24	LEU	2.3
7	2H	44	VAL	2.3
8	2I	68	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	229	VAL	2.3
35	1d	8	VAL	2.3
38	2g	38	LEU	2.3
39	1h	112	LEU	2.3
41	2j	44	VAL	2.3
47	1p	79	VAL	2.3
45	2n	37	PHE	2.3
22	10	2	ALA	2.2
26	24	22	ILE	2.2
32	2a	5	U	2.2
32	2a	1000	U	2.2
34	2c	5	ILE	2.2
36	2e	95	ALA	2.2
38	2g	49	ILE	2.2
40	2i	94	ALA	2.2
11	2P	35	HIS	2.2
9	2N	83	LYS	2.2
21	2Z	127	LYS	2.2
47	1p	35	LYS	2.2
45	2n	22	THR	2.2
24	22	66	GLU	2.2
33	2b	170	GLU	2.2
35	2d	20	TYR	2.2
35	2d	68	TYR	2.2
2	2B	5	C	2.2
1	1A	2148	G	2.2
1	2A	892	G	2.2
1	2A	2149	G	2.2
6	2G	123	ASN	2.2
32	1a	1003	G	2.2
32	2a	953	G	2.2
54	2w	57	G	2.2
57	2y	2	G	2.2
57	2y	22	G	2.2
57	2y	68	G	2.2
19	2X	68	ARG	2.2
34	2c	79	ARG	2.2
50	1s	29	ARG	2.2
52	2u	6	ARG	2.2
26	24	7	PRO	2.2
6	2G	126	ASP	2.2
35	1d	83	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	59	SER	2.2
34	2c	78	GLY	2.2
8	2I	3	VAL	2.2
33	1b	15	VAL	2.2
33	2b	145	LEU	2.2
34	2c	151	VAL	2.2
42	1k	98	LEU	2.2
44	2m	19	LEU	2.2
44	2m	54	VAL	2.2
44	2m	81	LEU	2.2
49	2r	86	VAL	2.2
1	1A	1077	A	2.2
1	2A	2134	A	2.2
6	1G	46	ALA	2.2
32	2a	983	A	2.2
33	2b	70	PHE	2.2
33	2b	122	PHE	2.2
35	2d	166	LYS	2.2
41	1j	55	LYS	2.2
57	2y	73	A	2.2
1	1A	2102	U	2.2
1	2A	12	U	2.2
6	2G	64	THR	2.2
32	2a	1125	U	2.2
32	2a	1150	U	2.2
48	2q	86	GLU	2.2
52	2u	8	THR	2.2
31	29	24	TYR	2.2
46	2o	68	ARG	2.2
48	2q	68	ARG	2.2
17	2V	50	PRO	2.2
1	1A	1079	C	2.2
1	2A	2105	C	2.2
1	2A	2186	G	2.2
1	2A	2319	G	2.2
15	1T	37	GLY	2.2
12	2Q	17	LEU	2.2
20	2Y	31	LEU	2.2
32	1a	148	G	2.2
32	2a	1221	G	2.2
35	2d	183	GLY	2.2
50	2s	46	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	118	LEU	2.2
57	1y	27	G	2.2
6	2G	92	VAL	2.2
33	2b	81	VAL	2.2
34	2c	138	VAL	2.2
36	2e	115	VAL	2.2
48	2q	87	LYS	2.2
6	2G	141	PHE	2.2
40	2i	18	PHE	2.2
6	2G	46	ALA	2.2
8	2I	55	ALA	2.2
33	1b	13	ALA	2.2
34	2c	168	ALA	2.2
34	2c	180	ALA	2.2
44	1m	30	ALA	2.2
35	1d	163	GLU	2.2
43	2l	16	GLU	2.2
32	2a	1110	A	2.2
54	1w	66	A	2.2
32	1a	841	U	2.2
32	2a	1065	U	2.2
44	2m	94	ARG	2.2
40	2i	4	TYR	2.2
48	2q	95	TYR	2.2
54	2w	33	U	2.2
54	2w	47	U	2.2
33	1b	202	PRO	2.2
38	2g	112	PRO	2.2
47	1p	82	GLN	2.2
6	2G	129	GLY	2.2
21	2Z	87	ASP	2.2
22	10	8	GLY	2.2
22	20	62	LEU	2.2
26	14	64	GLY	2.2
34	1c	47	LEU	2.2
34	1c	135	LYS	2.2
38	2g	34	GLY	2.2
39	2h	133	LEU	2.2
41	1j	59	SER	2.2
44	2m	66	LEU	2.2
7	2H	24	VAL	2.2
25	23	6	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	26	VAL	2.2
44	2m	117	VAL	2.2
47	1p	62	VAL	2.2
50	2s	51	VAL	2.2
1	1A	1080	C	2.2
1	2A	886	C	2.2
1	2A	2107	C	2.2
20	2Y	89	PHE	2.2
33	1b	122	PHE	2.2
33	2b	214	ILE	2.2
39	2h	80	ILE	2.2
41	1j	75	ILE	2.2
57	1y	25	C	2.2
40	2i	119	ALA	2.2
44	1m	118	ALA	2.2
1	1A	2151	G	2.2
1	2A	2751	G	2.2
32	2a	1190	G	2.2
47	2p	45	THR	2.2
1	1A	890	A	2.2
8	2I	137	PRO	2.2
26	24	67	TYR	2.2
32	2a	1252	A	2.2
34	2c	7	PRO	2.2
34	2c	29	TYR	2.2
44	2m	41	PRO	2.2
51	2t	98	PRO	2.2
55	1x	72	A	2.2
57	2y	14	A	2.2
8	2I	17	GLN	2.2
32	2a	961	U	2.2
7	2H	88	LEU	2.2
35	1d	87	GLY	2.2
44	2m	56	LEU	2.2
44	2m	112	GLY	2.2
6	2G	159	VAL	2.2
12	2Q	106	VAL	2.2
21	2Z	16	SER	2.2
28	26	48	VAL	2.2
35	2d	105	VAL	2.2
36	2e	33	VAL	2.2
40	1i	108	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	96	ILE	2.2
48	1q	45	HIS	2.2
12	2Q	104	PHE	2.2
36	2e	30	ALA	2.1
6	2G	54	GLU	2.1
21	1Z	119	GLU	2.1
35	1d	192	GLU	2.1
1	2A	2108	C	2.1
14	2S	5	THR	2.1
34	2c	127	ARG	2.1
35	2d	209	ARG	2.1
54	2w	71	C	2.1
1	2A	2321	G	2.1
40	2i	49	PRO	2.1
48	2q	2	PRO	2.1
57	1y	1	G	2.1
57	1y	24	G	2.1
57	1y	49	G	2.1
6	2G	47	LYS	2.1
33	1b	22	LYS	2.1
33	2b	199	TYR	2.1
38	2g	151	TYR	2.1
47	1p	39	TYR	2.1
14	2S	56	LEU	2.1
34	2c	175	LEU	2.1
41	1j	86	MET	2.1
1	1A	1067	A	2.1
1	1A	1086	A	2.1
6	1G	44	GLY	2.1
13	1R	7	GLY	2.1
14	2S	22	GLY	2.1
32	2a	969	A	2.1
32	2a	1004	A	2.1
53	1v	15	A	2.1
2	2B	22	U	2.1
32	2a	982	U	2.1
37	2f	88	VAL	2.1
39	2h	134	ILE	2.1
41	2j	82	ILE	2.1
47	2p	16	HIS	2.1
54	2w	60	U	2.1
6	2G	180	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	14	59	PHE	2.1
35	2d	117	ALA	2.1
35	2d	156	GLU	2.1
26	24	68	ARG	2.1
38	2g	76	ARG	2.1
44	2m	99	ARG	2.1
45	2n	41	ARG	2.1
46	2o	54	ARG	2.1
47	1p	75	ARG	2.1
7	2H	29	PRO	2.1
14	2S	59	LYS	2.1
55	1x	16	C	2.1
21	2Z	76	LEU	2.1
34	1c	87	LEU	2.1
35	2d	174	LEU	2.1
37	2f	89	MET	2.1
33	1b	33	TYR	2.1
23	21	28	GLY	2.1
33	1b	228	GLY	2.1
50	2s	82	GLY	2.1
1	2A	2141	G	2.1
7	2H	9	ILE	2.1
7	2H	15	VAL	2.1
32	2a	587	G	2.1
36	2e	90	VAL	2.1
41	1j	50	ILE	2.1
42	2k	29	ILE	2.1
45	1n	33	VAL	2.1
54	2w	49	G	2.1
57	1y	19	G	2.1
57	2y	49	G	2.1
33	2b	163	PHE	2.1
35	2d	110	PHE	2.1
42	1k	79	SER	2.1
1	1A	1045	A	2.1
32	2a	949	A	2.1
32	2a	1503	A	2.1
36	1e	95	ALA	2.1
54	1w	69	A	2.1
42	1k	92	GLU	2.1
6	2G	100	TRP	2.1
34	2c	190	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	156	TRP	2.1
46	2o	17	ARG	2.1
8	2I	121	LYS	2.1
20	1Y	63	LYS	2.1
33	2b	169	LYS	2.1
40	1i	25	LYS	2.1
42	2k	13	GLN	2.1
8	2I	75	LEU	2.1
21	2Z	70	LEU	2.1
33	1b	10	LEU	2.1
39	1h	107	LEU	2.1
40	2i	19	LEU	2.1
50	2s	15	LEU	2.1
39	2h	135	CYS	2.1
17	2V	63	GLY	2.1
41	2j	31	GLY	2.1
44	1m	87	TYR	2.1
46	1o	78	TYR	2.1
52	1u	21	TYR	2.1
1	1A	1509	C	2.1
1	1A	2107	C	2.1
1	2A	893	C	2.1
28	26	54	ILE	2.1
32	2a	962	C	2.1
32	2a	999	C	2.1
33	2b	80	ILE	2.1
37	1f	90	VAL	2.1
6	2G	178	PHE	2.1
15	1T	107	ASP	2.1
31	19	12	ASP	2.1
36	1e	6	PHE	2.1
36	2e	45	PHE	2.1
52	2u	5	ASP	2.1
8	2I	49	ALA	2.1
35	1d	208	SER	2.1
14	2S	13	ARG	2.1
35	1d	191	ARG	2.1
36	1e	21	ALA	2.1
1	1A	545	G	2.1
1	1A	2149	G	2.1
1	2A	2151	G	2.1
1	1A	1088	A	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2158	A	2.1
1	2A	2320	A	2.1
32	1a	1503	A	2.1
33	2b	22	LYS	2.1
35	1d	84	LYS	2.1
54	2w	68	G	2.1
57	2y	26	A	2.1
45	2n	54	PRO	2.1
46	2o	2	PRO	2.1
52	2u	23	PRO	2.1
21	1Z	1	MET	2.1
33	2b	215	LEU	2.1
34	2c	196	LEU	2.1
39	2h	59	LEU	2.1
12	2Q	19	GLY	2.1
50	2s	26	GLY	2.1
52	2u	16	GLY	2.1
26	14	67	TYR	2.1
34	2c	193	TYR	2.1
36	2e	118	ILE	2.1
48	2q	32	TYR	2.1
8	2I	145	VAL	2.1
14	2S	98	VAL	2.1
37	2f	40	VAL	2.1
44	2m	98	VAL	2.1
50	2s	45	VAL	2.1
21	1Z	136	PHE	2.1
12	2Q	16	ARG	2.0
29	17	23	ARG	2.0
40	2i	9	ARG	2.0
45	2n	12	ARG	2.0
51	1t	17	ARG	2.0
35	2d	48	ALA	2.0
40	2i	106	ALA	2.0
1	1A	1092	C	2.0
1	2A	888	C	2.0
43	2l	111	LYS	2.0
43	2l	114	LYS	2.0
55	2x	71	C	2.0
57	2y	11	C	2.0
44	2m	103	THR	2.0
40	2i	21	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1097	U	2.0
1	1A	2150	U	2.0
1	2A	895	U	2.0
43	2l	9	GLN	2.0
54	1w	20	U	2.0
1	1A	892	G	2.0
1	1A	1103	A	2.0
1	2A	2121	G	2.0
32	2a	1058	G	2.0
57	1y	6	G	2.0
57	2y	19	G	2.0
23	2l	79	GLY	2.0
26	24	15	ILE	2.0
36	2e	80	ILE	2.0
41	2j	10	GLY	2.0
47	1p	78	GLY	2.0
6	2G	28	VAL	2.0
6	2G	37	VAL	2.0
21	2Z	141	VAL	2.0
35	2d	8	VAL	2.0
42	2k	50	TYR	2.0
14	1S	3	ARG	2.0
10	1O	108	GLU	2.0
21	2Z	104	PHE	2.0
33	2b	57	PHE	2.0
38	1g	4	ARG	2.0
41	2j	43	ARG	2.0
45	2n	19	ARG	2.0
50	2s	10	PHE	2.0
52	2u	22	ARG	2.0
6	2G	163	ALA	2.0
8	2l	59	ALA	2.0
21	2Z	21	ALA	2.0
33	1b	29	ALA	2.0
34	2c	149	ALA	2.0
7	2H	41	MET	2.0
20	2Y	12	THR	2.0
45	2n	61	TRP	2.0
50	2s	66	MET	2.0
1	1A	2177	C	2.0
32	2a	91	C	2.0
32	2a	948	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2w	67	C	2.0
57	2y	67	C	2.0
57	2y	71	C	2.0
32	2a	4	U	2.0
32	2a	1148	U	2.0
57	2y	12	U	2.0
6	2G	44	GLY	2.0
20	1Y	59	GLY	2.0
33	1b	172	ILE	2.0
34	2c	185	GLY	2.0
1	1A	1073	A	2.0
1	1A	2171	A	2.0
1	2A	652(B)	A	2.0
1	2A	899	A	2.0
1	2A	1847	A	2.0
4	2E	150	VAL	2.0
8	1I	3	VAL	2.0
21	2Z	86	VAL	2.0
32	1a	160	A	2.0
32	2a	1005	A	2.0
32	2a	1288	A	2.0
35	2d	47	ARG	2.0
36	2e	67	VAL	2.0
36	2e	105	VAL	2.0
44	1m	3	ARG	2.0
44	2m	17	VAL	2.0
21	2Z	9	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
57	G7M	1y	46	24/25	0.35	0.17	95,104,109,118	0
57	G7M	2y	46	24/25	0.36	0.18	96,105,116,132	0
57	T6A	2y	37	22/33	0.41	0.18	89,102,113,126	0
57	U8U	1y	34	20/24	0.41	0.20	88,105,112,125	0
57	U8U	2y	34	20/24	0.42	0.23	97,108,116,129	0
57	T6A	1y	37	22/33	0.48	0.17	95,98,103,113	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	G7M	2w	46	24/25	0.52	0.14	91,102,116,128	0
54	PSU	2w	55	20/21	0.54	0.16	90,102,108,109	0
57	PSU	2y	55	20/21	0.55	0.15	97,107,113,117	0
54	G7M	1w	46	24/25	0.55	0.15	87,96,107,118	0
57	PSU	2y	39	20/21	0.57	0.16	93,101,106,120	0
54	PSU	1w	55	20/21	0.58	0.18	84,100,107,112	0
57	5MU	2y	54	21/22	0.58	0.14	97,105,113,122	0
57	PSU	1y	39	20/21	0.63	0.14	94,102,109,116	0
57	PSU	1y	55	20/21	0.65	0.11	99,102,112,123	0
54	5MU	2w	54	21/22	0.65	0.14	82,93,101,104	0
57	5MU	1y	54	21/22	0.66	0.12	95,101,104,119	0
54	5MU	1w	54	21/22	0.79	0.12	74,86,94,97	0
1	5MU	2A	1915	21/22	0.80	0.15	79,84,87,90	0
54	U8U	2w	34	23/24	0.80	0.20	78,89,97,100	0
32	2MG	2a	1207	24/25	0.81	0.15	81,90,101,106	0
54	PSU	2w	39	20/21	0.82	0.13	84,89,96,96	0
32	PSU	2a	516	20/21	0.83	0.14	73,85,91,92	0
54	T6A	2w	37	32/33	0.84	0.15	77,89,96,98	0
55	PSU	2x	55	20/21	0.84	0.13	79,84,89,90	0
55	4SU	2x	8	20/21	0.85	0.12	80,85,93,96	0
54	U8U	1w	34	23/24	0.86	0.14	69,76,84,87	0
55	5MU	2x	54	21/22	0.87	0.12	78,86,92,107	0
54	T6A	1w	37	32/33	0.88	0.14	60,72,81,85	0
56	FME	2z	1	10/11	0.88	0.24	51,59,66,70	0
55	PSU	1x	55	20/21	0.89	0.10	58,65,76,77	0
56	FME	1z	1	10/11	0.89	0.23	44,54,62,77	0
32	M2G	2a	966	25/26	0.89	0.16	62,72,88,91	0
32	5MC	2a	967	21/22	0.90	0.14	70,76,83,89	0
1	PSU	2A	1917	20/21	0.90	0.10	65,75,80,84	0
55	4SU	1x	8	20/21	0.91	0.12	59,65,71,77	0
55	5MU	1x	54	21/22	0.92	0.10	65,71,77,79	0
54	A1B8A	2w	76	31/32	0.92	0.12	41,56,64,65	0
43	0TD	2l	92	10/11	0.92	0.13	69,71,78,87	0
32	G7M	2a	527	24/25	0.92	0.11	59,68,74,83	0
32	5MC	2a	1404	21/22	0.93	0.11	55,62,71,74	0
1	PSU	2A	1911	20/21	0.93	0.10	57,70,78,80	0
1	5MU	1A	1915	21/22	0.93	0.10	52,59,63,68	0
54	PSU	1w	39	20/21	0.93	0.10	77,80,86,87	0
32	PSU	1a	516	20/21	0.93	0.09	62,67,70,70	0
43	0TD	1l	92	10/11	0.93	0.09	49,52,54,61	0
32	4OC	2a	1402	22/23	0.93	0.11	55,69,74,76	0
55	5MC	2x	32	21/22	0.94	0.12	71,75,82,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	2a	1407	21/22	0.94	0.11	54,60,67,69	0
54	A1B8A	1w	76	31/32	0.94	0.11	34,42,47,50	0
1	OMC	2A	1920	21/22	0.94	0.10	58,69,73,76	0
55	8AN	2x	76	22/23	0.94	0.11	42,50,56,58	0
32	5MC	2a	1400	21/22	0.94	0.14	72,77,81,84	0
1	5MC	2A	1962	21/22	0.95	0.09	39,51,58,70	0
32	MA6	1a	1519	24/25	0.95	0.10	35,45,48,51	0
32	G7M	1a	527	24/25	0.95	0.09	36,44,57,57	0
32	2MG	1a	1207	24/25	0.95	0.10	57,66,72,74	0
1	5MC	2A	1942	21/22	0.95	0.10	51,63,71,75	0
32	UR3	2a	1498	21/22	0.95	0.10	52,60,65,71	0
32	MA6	2a	1518	24/25	0.95	0.11	55,66,74,76	0
32	M2G	1a	966	25/26	0.96	0.09	51,54,62,63	0
1	OMG	2A	2251	24/25	0.96	0.09	37,43,45,48	0
1	PSU	2A	2605	20/21	0.96	0.07	31,41,44,45	0
55	5MC	1x	32	21/22	0.96	0.10	46,54,59,63	0
32	MA6	2a	1519	24/25	0.96	0.11	56,66,74,76	0
32	5MC	1a	967	21/22	0.96	0.10	50,57,64,67	0
1	5MC	1A	1942	21/22	0.96	0.10	38,42,48,59	0
55	8AN	1x	76	22/23	0.96	0.09	30,36,40,44	0
32	5MC	1a	1400	21/22	0.96	0.10	44,50,53,53	0
1	PSU	1A	1911	20/21	0.96	0.09	42,51,56,58	0
1	PSU	1A	1917	20/21	0.96	0.07	47,52,57,61	0
1	5MU	1A	1939	21/22	0.97	0.07	23,28,35,36	0
1	OMC	1A	1920	21/22	0.97	0.08	35,45,49,50	0
1	2MA	2A	2503	23/24	0.97	0.08	33,37,39,41	0
1	OMU	2A	2552	21/22	0.97	0.08	34,43,48,49	0
32	4OC	1a	1402	22/23	0.97	0.09	40,47,51,53	0
32	5MC	1a	1404	21/22	0.97	0.09	33,42,47,48	0
32	5MC	1a	1407	21/22	0.97	0.08	35,40,43,48	0
1	5MU	2A	1939	21/22	0.97	0.07	37,42,46,46	0
32	UR3	1a	1498	21/22	0.97	0.08	36,41,46,48	0
32	MA6	1a	1518	24/25	0.98	0.09	27,43,47,56	0
1	OMU	1A	2552	21/22	0.98	0.07	25,30,34,37	0
1	PSU	1A	2605	20/21	0.98	0.07	24,28,34,35	0
1	5MC	1A	1962	21/22	0.98	0.07	30,36,43,48	0
1	2MA	1A	2503	23/24	0.98	0.06	18,22,26,28	0
1	OMG	1A	2251	24/25	0.99	0.06	21,26,29,31	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(Å ²)	Q<0.9
58	MG	2a	1753	1/1	0.40	0.16	93,93,93,93	0
58	MG	2a	1789	1/1	0.58	0.24	88,88,88,88	0
58	MG	2A	3538	1/1	0.59	0.31	77,77,77,77	0
58	MG	1A	3813	1/1	0.60	0.23	60,60,60,60	0
58	MG	2A	3668	1/1	0.60	0.15	73,73,73,73	0
58	MG	1A	3569	1/1	0.61	0.19	64,64,64,64	0
58	MG	2a	1606	1/1	0.62	0.31	81,81,81,81	0
58	MG	1a	1680	1/1	0.63	0.33	80,80,80,80	0
58	MG	2a	1741	1/1	0.63	0.29	84,84,84,84	0
58	MG	1v	101	1/1	0.64	0.27	88,88,88,88	0
58	MG	2A	3107	1/1	0.64	0.26	63,63,63,63	0
58	MG	2a	1802	1/1	0.64	0.14	82,82,82,82	0
58	MG	1A	3960	1/1	0.65	0.14	64,64,64,64	0
58	MG	2a	1727	1/1	0.66	0.20	70,70,70,70	0
58	MG	2a	1762	1/1	0.66	0.15	81,81,81,81	0
58	MG	1a	1788	1/1	0.67	0.17	82,82,82,82	0
58	MG	1B	233	1/1	0.67	0.21	76,76,76,76	0
58	MG	1A	3998	1/1	0.68	0.30	83,83,83,83	0
58	MG	2A	3595	1/1	0.68	0.21	70,70,70,70	0
58	MG	1A	4094	1/1	0.68	0.21	79,79,79,79	0
58	MG	1a	1747	1/1	0.68	0.28	75,75,75,75	0
58	MG	2A	3535	1/1	0.68	0.20	79,79,79,79	0
58	MG	2A	3576	1/1	0.69	0.21	51,51,51,51	0
58	MG	2a	1708	1/1	0.69	0.15	88,88,88,88	0
58	MG	1A	4087	1/1	0.69	0.26	72,72,72,72	0
58	MG	2A	3243	1/1	0.69	0.28	83,83,83,83	0
58	MG	1a	1777	1/1	0.70	0.18	75,75,75,75	0
58	MG	1a	1812	1/1	0.70	0.20	79,79,79,79	0
58	MG	1U	212	1/1	0.71	0.44	60,60,60,60	0
58	MG	1a	1796	1/1	0.71	0.13	80,80,80,80	0
58	MG	2A	3610	1/1	0.71	0.21	89,89,89,89	0
58	MG	1A	3326	1/1	0.72	0.32	70,70,70,70	0
58	MG	2a	1644	1/1	0.72	0.12	79,79,79,79	0
58	MG	2a	1649	1/1	0.72	0.18	86,86,86,86	0
58	MG	2A	3341	1/1	0.72	0.22	73,73,73,73	0
58	MG	2A	3534	1/1	0.72	0.18	73,73,73,73	0
58	MG	1A	3512	1/1	0.73	0.17	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
58	MG	1A	3719	1/1	0.73	0.25	70,70,70,70	0
58	MG	2A	3025	1/1	0.74	0.25	61,61,61,61	0
58	MG	1B	229	1/1	0.74	0.21	71,71,71,71	0
58	MG	1a	1604	1/1	0.74	0.20	65,65,65,65	0
58	MG	2A	3553	1/1	0.74	0.18	50,50,50,50	0
58	MG	2a	1766	1/1	0.74	0.28	75,75,75,75	0
58	MG	1A	3796	1/1	0.74	0.18	80,80,80,80	0
58	MG	2A	3434	1/1	0.74	0.14	49,49,49,49	0
58	MG	2a	1808	1/1	0.74	0.28	63,63,63,63	0
58	MG	2v	101	1/1	0.74	0.18	69,69,69,69	0
58	MG	1A	3843	1/1	0.75	0.19	63,63,63,63	0
58	MG	1A	3883	1/1	0.75	0.36	76,76,76,76	0
58	MG	18	107	1/1	0.75	0.22	76,76,76,76	0
58	MG	1A	3926	1/1	0.75	0.13	44,44,44,44	0
58	MG	1a	1808	1/1	0.75	0.23	88,88,88,88	0
58	MG	1A	3266	1/1	0.75	0.20	68,68,68,68	0
58	MG	2l	201	1/1	0.75	0.18	69,69,69,69	0
58	MG	2l	206	1/1	0.75	0.14	77,77,77,77	0
58	MG	2A	3526	1/1	0.75	0.15	82,82,82,82	0
58	MG	2B	212	1/1	0.76	0.17	73,73,73,73	0
58	MG	2A	3342	1/1	0.76	0.13	59,59,59,59	0
58	MG	2a	1625	1/1	0.76	0.37	76,76,76,76	0
58	MG	2a	1643	1/1	0.76	0.19	66,66,66,66	0
58	MG	2A	3356	1/1	0.76	0.11	51,51,51,51	0
58	MG	1A	4021	1/1	0.76	0.20	54,54,54,54	0
58	MG	1A	3369	1/1	0.76	0.24	65,65,65,65	0
58	MG	1a	1607	1/1	0.76	0.35	71,71,71,71	0
58	MG	1a	1665	1/1	0.76	0.29	68,68,68,68	0
58	MG	2a	1783	1/1	0.77	0.17	73,73,73,73	0
58	MG	1l	201	1/1	0.77	0.20	79,79,79,79	0
58	MG	2a	1613	1/1	0.77	0.41	77,77,77,77	0
58	MG	1A	3463	1/1	0.77	0.13	53,53,53,53	0
58	MG	2A	3371	1/1	0.77	0.29	65,65,65,65	0
58	MG	2A	3406	1/1	0.77	0.16	61,61,61,61	0
58	MG	1A	4078	1/1	0.77	0.15	67,67,67,67	0
58	MG	1A	3754	1/1	0.78	0.10	33,33,33,33	0
58	MG	2A	3318	1/1	0.78	0.25	71,71,71,71	0
58	MG	2a	1745	1/1	0.78	0.22	76,76,76,76	0
58	MG	1a	1809	1/1	0.78	0.21	73,73,73,73	0
58	MG	2a	1607	1/1	0.78	0.25	75,75,75,75	0
58	MG	1a	1741	1/1	0.78	0.24	68,68,68,68	0
58	MG	2A	3544	1/1	0.78	0.30	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
58	MG	2a	1785	1/1	0.78	0.17	83,83,83,83	0
58	MG	1A	3961	1/1	0.78	0.10	24,24,24,24	0
58	MG	1A	3523	1/1	0.78	0.23	71,71,71,71	0
58	MG	2a	1804	1/1	0.78	0.21	73,73,73,73	0
58	MG	1A	3942	1/1	0.78	0.11	22,22,22,22	0
58	MG	2a	1675	1/1	0.78	0.29	78,78,78,78	0
58	MG	2a	1691	1/1	0.78	0.35	85,85,85,85	0
58	MG	1A	4069	1/1	0.78	0.22	45,45,45,45	0
58	MG	1a	1707	1/1	0.79	0.25	68,68,68,68	0
58	MG	1a	1720	1/1	0.79	0.24	75,75,75,75	0
58	MG	2A	3614	1/1	0.79	0.14	50,50,50,50	0
58	MG	1a	1722	1/1	0.79	0.13	75,75,75,75	0
58	MG	2a	1748	1/1	0.79	0.14	79,79,79,79	0
58	MG	1A	3632	1/1	0.79	0.17	61,61,61,61	0
58	MG	1B	230	1/1	0.79	0.19	70,70,70,70	0
58	MG	2A	3057	1/1	0.79	0.11	56,56,56,56	0
58	MG	1A	3691	1/1	0.79	0.21	65,65,65,65	0
58	MG	1I	201	1/1	0.79	0.12	72,72,72,72	0
58	MG	2a	1788	1/1	0.79	0.18	70,70,70,70	0
58	MG	2a	1634	1/1	0.79	0.22	66,66,66,66	0
58	MG	2a	1799	1/1	0.79	0.25	79,79,79,79	0
58	MG	2a	1642	1/1	0.79	0.17	78,78,78,78	0
58	MG	2A	3260	1/1	0.79	0.29	59,59,59,59	0
58	MG	2a	1807	1/1	0.79	0.25	79,79,79,79	0
58	MG	2A	3306	1/1	0.79	0.15	50,50,50,50	0
58	MG	2d	301	1/1	0.79	0.17	75,75,75,75	0
58	MG	1a	1671	1/1	0.79	0.34	74,74,74,74	0
58	MG	2A	3572	1/1	0.79	0.16	72,72,72,72	0
58	MG	1A	3588	1/1	0.79	0.13	69,69,69,69	0
58	MG	2a	1703	1/1	0.80	0.20	70,70,70,70	0
58	MG	2A	3232	1/1	0.80	0.26	63,63,63,63	0
58	MG	2a	1723	1/1	0.80	0.23	81,81,81,81	0
58	MG	1A	3840	1/1	0.80	0.14	60,60,60,60	0
58	MG	1B	202	1/1	0.80	0.30	68,68,68,68	0
58	MG	1a	1781	1/1	0.80	0.15	64,64,64,64	0
58	MG	1a	1639	1/1	0.80	0.18	76,76,76,76	0
58	MG	1A	3656	1/1	0.80	0.20	55,55,55,55	0
58	MG	1A	4015	1/1	0.80	0.20	62,62,62,62	0
58	MG	1A	3264	1/1	0.80	0.27	72,72,72,72	0
58	MG	2a	1603	1/1	0.80	0.19	71,71,71,71	0
58	MG	2A	3361	1/1	0.80	0.25	80,80,80,80	0
58	MG	2A	3366	1/1	0.80	0.17	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
58	MG	1A	3381	1/1	0.80	0.28	66,66,66,66	0
58	MG	2a	1620	1/1	0.80	0.29	87,87,87,87	0
58	MG	2a	1800	1/1	0.80	0.30	65,65,65,65	0
58	MG	1O	202	1/1	0.80	0.25	69,69,69,69	0
58	MG	1A	3815	1/1	0.80	0.12	42,42,42,42	0
58	MG	2A	3444	1/1	0.80	0.21	39,39,39,39	0
58	MG	1a	1735	1/1	0.80	0.21	67,67,67,67	0
58	MG	1a	1737	1/1	0.80	0.15	80,80,80,80	0
58	MG	2A	3070	1/1	0.80	0.17	79,79,79,79	0
58	MG	1A	3824	1/1	0.80	0.14	60,60,60,60	0
58	MG	2A	3230	1/1	0.80	0.24	77,77,77,77	0
58	MG	2A	3247	1/1	0.81	0.15	73,73,73,73	0
58	MG	1A	3753	1/1	0.81	0.20	66,66,66,66	0
58	MG	2A	3541	1/1	0.81	0.17	60,60,60,60	0
58	MG	2a	1660	1/1	0.81	0.14	77,77,77,77	0
58	MG	1A	3972	1/1	0.81	0.12	66,66,66,66	0
58	MG	2A	3547	1/1	0.81	0.29	71,71,71,71	0
58	MG	1e	201	1/1	0.81	0.18	76,76,76,76	0
58	MG	1B	226	1/1	0.81	0.14	67,67,67,67	0
58	MG	2a	1709	1/1	0.81	0.26	65,65,65,65	0
58	MG	1A	3616	1/1	0.81	0.11	57,57,57,57	0
58	MG	1A	3462	1/1	0.81	0.15	75,75,75,75	0
58	MG	1A	3913	1/1	0.81	0.22	38,38,38,38	0
58	MG	2a	1743	1/1	0.81	0.40	86,86,86,86	0
58	MG	1a	1779	1/1	0.81	0.14	56,56,56,56	0
58	MG	2A	3666	1/1	0.81	0.22	73,73,73,73	0
58	MG	1A	3529	1/1	0.81	0.34	59,59,59,59	0
58	MG	2A	3682	1/1	0.81	0.18	56,56,56,56	0
58	MG	2B	201	1/1	0.81	0.29	76,76,76,76	0
58	MG	2B	208	1/1	0.81	0.27	79,79,79,79	0
58	MG	2A	3376	1/1	0.81	0.15	51,51,51,51	0
58	MG	2E	305	1/1	0.81	0.23	82,82,82,82	0
58	MG	2A	3404	1/1	0.81	0.26	71,71,71,71	0
58	MG	2A	3179	1/1	0.81	0.11	65,65,65,65	0
58	MG	2A	3198	1/1	0.81	0.30	71,71,71,71	0
58	MG	2a	1609	1/1	0.81	0.44	71,71,71,71	0
58	MG	2a	1612	1/1	0.81	0.50	80,80,80,80	0
58	MG	1a	1700	1/1	0.81	0.35	75,75,75,75	0
58	MG	2A	3466	1/1	0.81	0.10	52,52,52,52	0
58	MG	2a	1622	1/1	0.81	0.34	68,68,68,68	0
58	MG	2j	201	1/1	0.81	0.15	77,77,77,77	0
58	MG	2A	3495	1/1	0.81	0.20	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
58	MG	1A	3351	1/1	0.81	0.20	60,60,60,60	0
58	MG	1A	3401	1/1	0.81	0.24	63,63,63,63	0
58	MG	2A	3436	1/1	0.82	0.26	58,58,58,58	0
58	MG	2B	209	1/1	0.82	0.24	80,80,80,80	0
58	MG	2a	1722	1/1	0.82	0.24	81,81,81,81	0
58	MG	1A	3477	1/1	0.82	0.13	67,67,67,67	0
58	MG	2E	303	1/1	0.82	0.12	66,66,66,66	0
58	MG	2a	1737	1/1	0.82	0.46	78,78,78,78	0
58	MG	1b	301	1/1	0.82	0.14	79,79,79,79	0
58	MG	1A	3102	1/1	0.82	0.28	66,66,66,66	0
58	MG	2a	1604	1/1	0.82	0.25	80,80,80,80	0
58	MG	1A	3513	1/1	0.82	0.17	81,81,81,81	0
58	MG	1a	1669	1/1	0.82	0.34	77,77,77,77	0
58	MG	2A	3328	1/1	0.82	0.17	66,66,66,66	0
58	MG	2A	3335	1/1	0.82	0.25	68,68,68,68	0
58	MG	1a	1762	1/1	0.82	0.16	65,65,65,65	0
58	MG	2a	1618	1/1	0.82	0.20	76,76,76,76	0
58	MG	1A	3806	1/1	0.82	0.10	52,52,52,52	0
58	MG	2A	3343	1/1	0.82	0.20	57,57,57,57	0
58	MG	2A	3353	1/1	0.82	0.18	67,67,67,67	0
58	MG	1A	3648	1/1	0.82	0.24	58,58,58,58	0
58	MG	2A	3360	1/1	0.82	0.19	55,55,55,55	0
58	MG	2A	3090	1/1	0.82	0.26	66,66,66,66	0
58	MG	1A	3412	1/1	0.82	0.27	74,74,74,74	0
58	MG	2A	3176	1/1	0.82	0.23	69,69,69,69	0
58	MG	2a	1812	1/1	0.82	0.32	73,73,73,73	0
58	MG	1A	4092	1/1	0.82	0.12	49,49,49,49	0
58	MG	1A	3185	1/1	0.82	0.15	68,68,68,68	0
58	MG	1A	3205	1/1	0.82	0.10	56,56,56,56	0
58	MG	2a	1701	1/1	0.82	0.29	71,71,71,71	0
58	MG	1a	1734	1/1	0.82	0.13	61,61,61,61	0
58	MG	2x	3303	1/1	0.82	0.24	79,79,79,79	0
58	MG	1a	1742	1/1	0.83	0.18	75,75,75,75	0
58	MG	1A	3362	1/1	0.83	0.36	51,51,51,51	0
58	MG	2A	3188	1/1	0.83	0.15	69,69,69,69	0
58	MG	2a	1652	1/1	0.83	0.28	71,71,71,71	0
58	MG	2a	1657	1/1	0.83	0.18	75,75,75,75	0
58	MG	1a	1758	1/1	0.83	0.18	64,64,64,64	0
58	MG	2A	3205	1/1	0.83	0.35	71,71,71,71	0
58	MG	2A	3222	1/1	0.83	0.30	80,80,80,80	0
58	MG	2A	3225	1/1	0.83	0.31	76,76,76,76	0
58	MG	1A	3767	1/1	0.83	0.11	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1765	1/1	0.83	0.14	65,65,65,65	0
58	MG	1a	1772	1/1	0.83	0.19	78,78,78,78	0
58	MG	2a	1714	1/1	0.83	0.19	73,73,73,73	0
58	MG	1A	3422	1/1	0.83	0.23	71,71,71,71	0
58	MG	1a	1623	1/1	0.83	0.39	65,65,65,65	0
58	MG	2a	1726	1/1	0.83	0.21	73,73,73,73	0
58	MG	1A	3028	1/1	0.83	0.29	77,77,77,77	0
58	MG	1a	1652	1/1	0.83	0.20	68,68,68,68	0
58	MG	2a	1739	1/1	0.83	0.36	74,74,74,74	0
58	MG	2A	3319	1/1	0.83	0.12	68,68,68,68	0
58	MG	1A	3341	1/1	0.83	0.12	54,54,54,54	0
58	MG	1B	225	1/1	0.83	0.17	55,55,55,55	0
58	MG	2B	204	1/1	0.83	0.21	79,79,79,79	0
58	MG	1A	3473	1/1	0.83	0.10	62,62,62,62	0
58	MG	1A	3821	1/1	0.83	0.16	54,54,54,54	0
58	MG	2B	210	1/1	0.83	0.28	69,69,69,69	0
58	MG	1A	3705	1/1	0.83	0.10	55,55,55,55	0
58	MG	1A	3309	1/1	0.83	0.22	63,63,63,63	0
58	MG	1a	1709	1/1	0.83	0.30	62,62,62,62	0
58	MG	20	103	1/1	0.83	0.26	58,58,58,58	0
58	MG	1n	101	1/1	0.83	0.12	51,51,51,51	0
58	MG	1t	201	1/1	0.83	0.19	65,65,65,65	0
58	MG	1A	3597	1/1	0.83	0.35	42,42,42,42	0
58	MG	1w	101	1/1	0.83	0.09	66,66,66,66	0
58	MG	1N	201	1/1	0.83	0.20	52,52,52,52	0
58	MG	2A	3028	1/1	0.83	0.22	65,65,65,65	0
58	MG	1A	3871	1/1	0.83	0.17	39,39,39,39	0
58	MG	1T	202	1/1	0.83	0.21	52,52,52,52	0
58	MG	1A	4070	1/1	0.83	0.14	61,61,61,61	0
58	MG	2A	3102	1/1	0.83	0.32	79,79,79,79	0
58	MG	2A	3458	1/1	0.83	0.15	53,53,53,53	0
58	MG	2t	201	1/1	0.83	0.17	54,54,54,54	0
58	MG	1W	201	1/1	0.83	0.22	52,52,52,52	0
58	MG	2A	3119	1/1	0.83	0.18	72,72,72,72	0
58	MG	1A	3979	1/1	0.84	0.15	65,65,65,65	0
58	MG	2a	1640	1/1	0.84	0.16	59,59,59,59	0
58	MG	1a	1663	1/1	0.84	0.12	58,58,58,58	0
58	MG	2A	3531	1/1	0.84	0.16	76,76,76,76	0
58	MG	2A	3237	1/1	0.84	0.33	56,56,56,56	0
58	MG	1a	1759	1/1	0.84	0.13	60,60,60,60	0
58	MG	2A	3246	1/1	0.84	0.15	61,61,61,61	0
58	MG	2a	1654	1/1	0.84	0.13	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3539	1/1	0.84	0.26	70,70,70,70	0
58	MG	1w	106	1/1	0.84	0.12	76,76,76,76	0
58	MG	1x	104	1/1	0.84	0.22	62,62,62,62	0
58	MG	2A	3267	1/1	0.84	0.35	66,66,66,66	0
58	MG	2A	3268	1/1	0.84	0.26	72,72,72,72	0
58	MG	2A	3557	1/1	0.84	0.20	66,66,66,66	0
58	MG	2A	3566	1/1	0.84	0.14	58,58,58,58	0
58	MG	2A	3273	1/1	0.84	0.24	62,62,62,62	0
58	MG	2A	3278	1/1	0.84	0.17	72,72,72,72	0
58	MG	2A	3582	1/1	0.84	0.18	63,63,63,63	0
58	MG	1x	109	1/1	0.84	0.32	67,67,67,67	0
58	MG	2A	3606	1/1	0.84	0.11	72,72,72,72	0
58	MG	2A	3307	1/1	0.84	0.28	70,70,70,70	0
58	MG	2A	3612	1/1	0.84	0.13	70,70,70,70	0
58	MG	1A	3270	1/1	0.84	0.14	54,54,54,54	0
58	MG	1P	202	1/1	0.84	0.20	46,46,46,46	0
58	MG	2A	3056	1/1	0.84	0.13	63,63,63,63	0
58	MG	2A	3330	1/1	0.84	0.35	70,70,70,70	0
58	MG	2A	3333	1/1	0.84	0.23	62,62,62,62	0
58	MG	1A	3251	1/1	0.84	0.15	56,56,56,56	0
58	MG	2a	1756	1/1	0.84	0.30	66,66,66,66	0
58	MG	2B	205	1/1	0.84	0.24	73,73,73,73	0
58	MG	1A	3578	1/1	0.84	0.10	32,32,32,32	0
58	MG	2A	3089	1/1	0.84	0.24	69,69,69,69	0
58	MG	1a	1696	1/1	0.84	0.27	62,62,62,62	0
58	MG	1A	4042	1/1	0.84	0.17	57,57,57,57	0
58	MG	1Y	203	1/1	0.84	0.13	71,71,71,71	0
58	MG	2a	1795	1/1	0.84	0.22	64,64,64,64	0
58	MG	1A	3263	1/1	0.84	0.27	70,70,70,70	0
58	MG	2A	3127	1/1	0.84	0.10	71,71,71,71	0
58	MG	2A	3128	1/1	0.84	0.24	61,61,61,61	0
58	MG	1A	3870	1/1	0.84	0.20	46,46,46,46	0
58	MG	2a	1806	1/1	0.84	0.22	73,73,73,73	0
58	MG	1A	3593	1/1	0.84	0.29	60,60,60,60	0
58	MG	2A	3378	1/1	0.84	0.34	64,64,64,64	0
58	MG	2A	3180	1/1	0.84	0.22	59,59,59,59	0
58	MG	2a	1817	1/1	0.84	0.28	67,67,67,67	0
58	MG	2a	1820	1/1	0.84	0.33	75,75,75,75	0
58	MG	2a	1610	1/1	0.84	0.26	72,72,72,72	0
58	MG	1G	203	1/1	0.84	0.13	61,61,61,61	0
58	MG	1a	1630	1/1	0.84	0.34	59,59,59,59	0
58	MG	2l	204	1/1	0.84	0.28	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
58	MG	2A	3203	1/1	0.84	0.33	65,65,65,65	0
58	MG	1A	3878	1/1	0.84	0.27	63,63,63,63	0
58	MG	1a	1641	1/1	0.84	0.18	73,73,73,73	0
58	MG	1a	1647	1/1	0.84	0.25	70,70,70,70	0
58	MG	2A	3139	1/1	0.85	0.14	68,68,68,68	0
58	MG	1A	3603	1/1	0.85	0.30	71,71,71,71	0
58	MG	1A	3349	1/1	0.85	0.15	65,65,65,65	0
58	MG	1A	3896	1/1	0.85	0.28	81,81,81,81	0
58	MG	2A	3355	1/1	0.85	0.20	67,67,67,67	0
58	MG	1A	3033	1/1	0.85	0.18	38,38,38,38	0
58	MG	2A	3623	1/1	0.85	0.13	58,58,58,58	0
58	MG	2A	3628	1/1	0.85	0.11	35,35,35,35	0
58	MG	1d	301	1/1	0.85	0.39	61,61,61,61	0
58	MG	1a	1708	1/1	0.85	0.21	61,61,61,61	0
58	MG	2A	3671	1/1	0.85	0.17	67,67,67,67	0
58	MG	2A	3674	1/1	0.85	0.11	58,58,58,58	0
58	MG	2A	3678	1/1	0.85	0.13	60,60,60,60	0
58	MG	2A	3680	1/1	0.85	0.21	65,65,65,65	0
58	MG	2a	1729	1/1	0.85	0.23	57,57,57,57	0
58	MG	1A	3920	1/1	0.85	0.14	47,47,47,47	0
58	MG	2A	3221	1/1	0.85	0.14	73,73,73,73	0
58	MG	2A	3373	1/1	0.85	0.19	64,64,64,64	0
58	MG	15	104	1/1	0.85	0.11	59,59,59,59	0
58	MG	1A	3441	1/1	0.85	0.12	52,52,52,52	0
58	MG	2A	3379	1/1	0.85	0.18	64,64,64,64	0
58	MG	2A	3400	1/1	0.85	0.22	64,64,64,64	0
58	MG	1A	3538	1/1	0.85	0.14	62,62,62,62	0
58	MG	1A	3954	1/1	0.85	0.16	65,65,65,65	0
58	MG	1w	104	1/1	0.85	0.09	83,83,83,83	0
58	MG	2V	201	1/1	0.85	0.16	62,62,62,62	0
58	MG	1a	1614	1/1	0.85	0.12	66,66,66,66	0
58	MG	28	101	1/1	0.85	0.19	64,64,64,64	0
58	MG	2A	3244	1/1	0.85	0.15	67,67,67,67	0
58	MG	1a	1619	1/1	0.85	0.18	61,61,61,61	0
58	MG	1A	3816	1/1	0.85	0.13	39,39,39,39	0
58	MG	2A	3005	1/1	0.85	0.20	66,66,66,66	0
58	MG	2A	3263	1/1	0.85	0.20	58,58,58,58	0
58	MG	2A	3528	1/1	0.85	0.15	62,62,62,62	0
58	MG	1A	3189	1/1	0.85	0.25	61,61,61,61	0
58	MG	1A	3193	1/1	0.85	0.14	54,54,54,54	0
58	MG	1A	3149	1/1	0.85	0.14	40,40,40,40	0
58	MG	1a	1644	1/1	0.85	0.18	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
58	MG	2a	1813	1/1	0.85	0.19	61,61,61,61	0
58	MG	1A	3346	1/1	0.85	0.12	52,52,52,52	0
58	MG	1a	1767	1/1	0.85	0.12	63,63,63,63	0
58	MG	1E	311	1/1	0.85	0.21	57,57,57,57	0
58	MG	2g	201	1/1	0.85	0.15	78,78,78,78	0
58	MG	1A	3404	1/1	0.85	0.10	55,55,55,55	0
58	MG	2A	3324	1/1	0.85	0.34	63,63,63,63	0
58	MG	1A	3758	1/1	0.85	0.17	56,56,56,56	0
58	MG	1A	4028	1/1	0.85	0.14	56,56,56,56	0
58	MG	2q	202	1/1	0.85	0.15	83,83,83,83	0
58	MG	2a	1645	1/1	0.85	0.19	77,77,77,77	0
58	MG	1A	4036	1/1	0.85	0.11	25,25,25,25	0
58	MG	1a	1678	1/1	0.85	0.19	68,68,68,68	0
58	MG	2A	3096	1/1	0.86	0.20	54,54,54,54	0
58	MG	1A	3514	1/1	0.86	0.16	75,75,75,75	0
58	MG	1A	3405	1/1	0.86	0.11	68,68,68,68	0
58	MG	2a	1674	1/1	0.86	0.28	69,69,69,69	0
58	MG	1A	4072	1/1	0.86	0.25	58,58,58,58	0
58	MG	2a	1689	1/1	0.86	0.22	71,71,71,71	0
58	MG	2A	3122	1/1	0.86	0.19	70,70,70,70	0
58	MG	2a	1700	1/1	0.86	0.16	72,72,72,72	0
58	MG	1A	3526	1/1	0.86	0.28	58,58,58,58	0
58	MG	2A	3638	1/1	0.86	0.11	45,45,45,45	0
58	MG	1A	3880	1/1	0.86	0.14	59,59,59,59	0
58	MG	1A	3350	1/1	0.86	0.13	53,53,53,53	0
58	MG	2A	3175	1/1	0.86	0.26	63,63,63,63	0
58	MG	1A	3166	1/1	0.86	0.37	63,63,63,63	0
58	MG	1A	3548	1/1	0.86	0.41	41,41,41,41	0
58	MG	1a	1648	1/1	0.86	0.26	60,60,60,60	0
58	MG	2A	3181	1/1	0.86	0.26	56,56,56,56	0
58	MG	1a	1802	1/1	0.86	0.10	60,60,60,60	0
58	MG	2a	1732	1/1	0.86	0.42	84,84,84,84	0
58	MG	1B	216	1/1	0.86	0.13	70,70,70,70	0
58	MG	1A	3756	1/1	0.86	0.11	64,64,64,64	0
58	MG	1A	3325	1/1	0.86	0.20	54,54,54,54	0
58	MG	1A	3937	1/1	0.86	0.12	61,61,61,61	0
58	MG	1A	3455	1/1	0.86	0.17	39,39,39,39	0
58	MG	1A	3584	1/1	0.86	0.19	71,71,71,71	0
58	MG	2a	1751	1/1	0.86	0.23	72,72,72,72	0
58	MG	1A	3025	1/1	0.86	0.18	52,52,52,52	0
58	MG	1A	3104	1/1	0.86	0.11	63,63,63,63	0
58	MG	1A	3967	1/1	0.86	0.15	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
58	MG	20	102	1/1	0.86	0.09	62,62,62,62	0
58	MG	1A	3814	1/1	0.86	0.15	38,38,38,38	0
58	MG	2A	3482	1/1	0.86	0.19	68,68,68,68	0
58	MG	2a	1787	1/1	0.86	0.24	68,68,68,68	0
58	MG	1A	3390	1/1	0.86	0.13	55,55,55,55	0
58	MG	1A	3994	1/1	0.86	0.11	34,34,34,34	0
58	MG	2a	1792	1/1	0.86	0.16	71,71,71,71	0
58	MG	1R	206	1/1	0.86	0.12	41,41,41,41	0
58	MG	1A	3997	1/1	0.86	0.20	83,83,83,83	0
58	MG	1A	3393	1/1	0.86	0.35	39,39,39,39	0
58	MG	2A	3264	1/1	0.86	0.19	54,54,54,54	0
58	MG	1x	111	1/1	0.86	0.33	69,69,69,69	0
58	MG	1A	3604	1/1	0.86	0.24	75,75,75,75	0
58	MG	2a	1617	1/1	0.86	0.17	70,70,70,70	0
58	MG	2A	3271	1/1	0.86	0.34	70,70,70,70	0
58	MG	2A	3023	1/1	0.86	0.21	54,54,54,54	0
58	MG	1A	3502	1/1	0.86	0.16	56,56,56,56	0
58	MG	10	104	1/1	0.86	0.24	51,51,51,51	0
58	MG	2a	1628	1/1	0.86	0.23	78,78,78,78	0
58	MG	1A	3107	1/1	0.86	0.15	52,52,52,52	0
58	MG	2a	1639	1/1	0.86	0.14	79,79,79,79	0
58	MG	2A	3560	1/1	0.86	0.18	47,47,47,47	0
58	MG	1a	1746	1/1	0.86	0.14	56,56,56,56	0
58	MG	2l	203	1/1	0.86	0.17	70,70,70,70	0
58	MG	1A	3090	1/1	0.86	0.12	53,53,53,53	0
58	MG	2A	3083	1/1	0.86	0.17	66,66,66,66	0
58	MG	1A	4040	1/1	0.86	0.16	56,56,56,56	0
58	MG	2r	101	1/1	0.86	0.24	74,74,74,74	0
58	MG	2A	3587	1/1	0.86	0.11	62,62,62,62	0
58	MG	1A	3856	1/1	0.86	0.14	48,48,48,48	0
58	MG	2a	1653	1/1	0.86	0.34	74,74,74,74	0
58	MG	2A	3655	1/1	0.87	0.12	60,60,60,60	0
58	MG	2a	1694	1/1	0.87	0.20	57,57,57,57	0
58	MG	2a	1699	1/1	0.87	0.13	78,78,78,78	0
58	MG	2A	3217	1/1	0.87	0.23	59,59,59,59	0
58	MG	1A	3912	1/1	0.87	0.21	44,44,44,44	0
58	MG	1a	1716	1/1	0.87	0.19	63,63,63,63	0
58	MG	1A	3027	1/1	0.87	0.19	69,69,69,69	0
58	MG	1A	3728	1/1	0.87	0.14	65,65,65,65	0
58	MG	1Z	301	1/1	0.87	0.07	55,55,55,55	0
58	MG	2a	1719	1/1	0.87	0.16	69,69,69,69	0
58	MG	1A	3924	1/1	0.87	0.14	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
58	MG	2A	3419	1/1	0.87	0.16	33,33,33,33	0
58	MG	2a	1725	1/1	0.87	0.38	52,52,52,52	0
58	MG	2A	3242	1/1	0.87	0.29	60,60,60,60	0
58	MG	1A	3491	1/1	0.87	0.20	72,72,72,72	0
58	MG	1A	4074	1/1	0.87	0.16	65,65,65,65	0
58	MG	2A	3006	1/1	0.87	0.26	56,56,56,56	0
58	MG	2a	1733	1/1	0.87	0.22	74,74,74,74	0
58	MG	1A	3831	1/1	0.87	0.12	56,56,56,56	0
58	MG	2A	3470	1/1	0.87	0.13	53,53,53,53	0
58	MG	2D	306	1/1	0.87	0.18	67,67,67,67	0
58	MG	1A	3605	1/1	0.87	0.14	49,49,49,49	0
58	MG	2A	3483	1/1	0.87	0.16	66,66,66,66	0
58	MG	2a	1747	1/1	0.87	0.34	79,79,79,79	0
58	MG	2A	3487	1/1	0.87	0.13	32,32,32,32	0
58	MG	1A	3943	1/1	0.87	0.14	38,38,38,38	0
58	MG	2A	3499	1/1	0.87	0.17	61,61,61,61	0
58	MG	2a	1754	1/1	0.87	0.22	70,70,70,70	0
58	MG	1A	3842	1/1	0.87	0.12	58,58,58,58	0
58	MG	1A	3501	1/1	0.87	0.38	53,53,53,53	0
58	MG	1a	1627	1/1	0.87	0.12	49,49,49,49	0
58	MG	2a	1776	1/1	0.87	0.22	61,61,61,61	0
58	MG	1A	3854	1/1	0.87	0.13	47,47,47,47	0
58	MG	1A	3580	1/1	0.87	0.12	48,48,48,48	0
58	MG	2A	3277	1/1	0.87	0.21	55,55,55,55	0
58	MG	1A	3644	1/1	0.87	0.12	52,52,52,52	0
58	MG	1A	3343	1/1	0.87	0.20	55,55,55,55	0
58	MG	2A	3542	1/1	0.87	0.10	64,64,64,64	0
58	MG	1a	1778	1/1	0.87	0.14	36,36,36,36	0
58	MG	1A	3505	1/1	0.87	0.23	46,46,46,46	0
58	MG	1A	3530	1/1	0.87	0.27	71,71,71,71	0
58	MG	2a	1621	1/1	0.87	0.19	67,67,67,67	0
58	MG	1A	3881	1/1	0.87	0.10	29,29,29,29	0
58	MG	1A	4012	1/1	0.87	0.14	74,74,74,74	0
58	MG	2A	3562	1/1	0.87	0.12	51,51,51,51	0
58	MG	1a	1797	1/1	0.87	0.21	62,62,62,62	0
58	MG	1G	204	1/1	0.87	0.14	64,64,64,64	0
58	MG	2A	3573	1/1	0.87	0.14	53,53,53,53	0
58	MG	1A	3320	1/1	0.87	0.14	45,45,45,45	0
58	MG	1A	4017	1/1	0.87	0.21	63,63,63,63	0
58	MG	1N	204	1/1	0.87	0.13	57,57,57,57	0
58	MG	2d	302	1/1	0.87	0.24	53,53,53,53	0
58	MG	2f	202	1/1	0.87	0.15	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
58	MG	2A	3590	1/1	0.87	0.12	55,55,55,55	0
58	MG	2a	1647	1/1	0.87	0.23	63,63,63,63	0
58	MG	1A	3884	1/1	0.87	0.13	30,30,30,30	0
58	MG	2A	3602	1/1	0.87	0.25	75,75,75,75	0
58	MG	1A	3888	1/1	0.87	0.16	51,51,51,51	0
58	MG	2A	3186	1/1	0.87	0.15	63,63,63,63	0
58	MG	1A	4033	1/1	0.87	0.17	55,55,55,55	0
58	MG	1a	1705	1/1	0.87	0.26	73,73,73,73	0
58	MG	1A	3714	1/1	0.87	0.13	45,45,45,45	0
58	MG	1U	203	1/1	0.87	0.21	68,68,68,68	0
58	MG	2A	3215	1/1	0.87	0.12	66,66,66,66	0
58	MG	1A	3002	1/1	0.88	0.23	57,57,57,57	0
58	MG	2A	3386	1/1	0.88	0.23	65,65,65,65	0
58	MG	2A	3395	1/1	0.88	0.23	67,67,67,67	0
58	MG	1A	3704	1/1	0.88	0.11	32,32,32,32	0
58	MG	2A	3402	1/1	0.88	0.25	63,63,63,63	0
58	MG	1a	1712	1/1	0.88	0.11	62,62,62,62	0
58	MG	1A	3154	1/1	0.88	0.13	36,36,36,36	0
58	MG	1A	3370	1/1	0.88	0.20	45,45,45,45	0
58	MG	2a	1614	1/1	0.88	0.20	60,60,60,60	0
58	MG	1A	3718	1/1	0.88	0.10	52,52,52,52	0
58	MG	1E	308	1/1	0.88	0.12	30,30,30,30	0
58	MG	1A	3097	1/1	0.88	0.10	59,59,59,59	0
58	MG	2A	3447	1/1	0.88	0.17	47,47,47,47	0
58	MG	2A	3151	1/1	0.88	0.27	71,71,71,71	0
58	MG	2A	3459	1/1	0.88	0.11	48,48,48,48	0
58	MG	1A	3271	1/1	0.88	0.10	45,45,45,45	0
58	MG	2a	1633	1/1	0.88	0.26	76,76,76,76	0
58	MG	1A	3730	1/1	0.88	0.20	55,55,55,55	0
58	MG	2a	1635	1/1	0.88	0.26	75,75,75,75	0
58	MG	2a	1637	1/1	0.88	0.14	55,55,55,55	0
58	MG	2A	3472	1/1	0.88	0.27	62,62,62,62	0
58	MG	2A	3474	1/1	0.88	0.20	46,46,46,46	0
58	MG	2A	3481	1/1	0.88	0.18	57,57,57,57	0
58	MG	1A	3731	1/1	0.88	0.16	62,62,62,62	0
58	MG	1A	3739	1/1	0.88	0.15	51,51,51,51	0
58	MG	1A	3747	1/1	0.88	0.10	19,19,19,19	0
58	MG	2a	1646	1/1	0.88	0.09	65,65,65,65	0
58	MG	1A	3949	1/1	0.88	0.19	72,72,72,72	0
58	MG	1A	3041	1/1	0.88	0.14	52,52,52,52	0
58	MG	2A	3503	1/1	0.88	0.11	65,65,65,65	0
58	MG	2A	3509	1/1	0.88	0.29	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3513	1/1	0.88	0.16	40,40,40,40	0
58	MG	2a	1655	1/1	0.88	0.30	81,81,81,81	0
58	MG	2A	3522	1/1	0.88	0.19	52,52,52,52	0
58	MG	1A	3054	1/1	0.88	0.11	52,52,52,52	0
58	MG	2A	3200	1/1	0.88	0.28	63,63,63,63	0
58	MG	1a	1764	1/1	0.88	0.11	70,70,70,70	0
58	MG	2a	1678	1/1	0.88	0.14	70,70,70,70	0
58	MG	1A	3190	1/1	0.88	0.20	42,42,42,42	0
58	MG	2a	1690	1/1	0.88	0.15	80,80,80,80	0
58	MG	1A	3063	1/1	0.88	0.17	61,61,61,61	0
58	MG	1A	3334	1/1	0.88	0.20	52,52,52,52	0
58	MG	1A	3773	1/1	0.88	0.14	44,44,44,44	0
58	MG	1A	3980	1/1	0.88	0.13	64,64,64,64	0
58	MG	1A	3336	1/1	0.88	0.09	50,50,50,50	0
58	MG	1A	3803	1/1	0.88	0.10	21,21,21,21	0
58	MG	2A	3546	1/1	0.88	0.15	49,49,49,49	0
58	MG	1A	3435	1/1	0.88	0.34	54,54,54,54	0
58	MG	2a	1710	1/1	0.88	0.28	77,77,77,77	0
58	MG	1A	3338	1/1	0.88	0.16	62,62,62,62	0
58	MG	1A	3453	1/1	0.88	0.10	61,61,61,61	0
58	MG	1A	3340	1/1	0.88	0.17	39,39,39,39	0
58	MG	1A	3118	1/1	0.88	0.28	52,52,52,52	0
58	MG	1A	3594	1/1	0.88	0.10	59,59,59,59	0
58	MG	2A	3567	1/1	0.88	0.13	64,64,64,64	0
58	MG	2A	3569	1/1	0.88	0.14	54,54,54,54	0
58	MG	1A	4032	1/1	0.88	0.12	55,55,55,55	0
58	MG	2A	3257	1/1	0.88	0.23	41,41,41,41	0
58	MG	2A	3574	1/1	0.88	0.11	78,78,78,78	0
58	MG	2a	1734	1/1	0.88	0.28	65,65,65,65	0
58	MG	2a	1735	1/1	0.88	0.20	65,65,65,65	0
58	MG	1A	3130	1/1	0.88	0.18	62,62,62,62	0
58	MG	2A	3577	1/1	0.88	0.15	61,61,61,61	0
58	MG	1A	3471	1/1	0.88	0.17	49,49,49,49	0
58	MG	1a	1631	1/1	0.88	0.16	61,61,61,61	0
58	MG	1A	3253	1/1	0.88	0.15	76,76,76,76	0
58	MG	1A	3258	1/1	0.88	0.15	64,64,64,64	0
58	MG	1p	101	1/1	0.88	0.23	64,64,64,64	0
58	MG	2A	3605	1/1	0.88	0.12	54,54,54,54	0
58	MG	1a	1643	1/1	0.88	0.20	59,59,59,59	0
58	MG	1A	4046	1/1	0.88	0.14	59,59,59,59	0
58	MG	2A	3611	1/1	0.88	0.10	62,62,62,62	0
58	MG	2a	1761	1/1	0.88	0.15	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
58	MG	1A	3486	1/1	0.88	0.12	61,61,61,61	0
58	MG	2A	3302	1/1	0.88	0.37	78,78,78,78	0
58	MG	2A	3615	1/1	0.88	0.11	62,62,62,62	0
58	MG	1A	3617	1/1	0.88	0.10	26,26,26,26	0
58	MG	1w	105	1/1	0.88	0.23	79,79,79,79	0
58	MG	2A	3633	1/1	0.88	0.11	54,54,54,54	0
58	MG	2A	3315	1/1	0.88	0.16	63,63,63,63	0
58	MG	2A	3645	1/1	0.88	0.11	71,71,71,71	0
58	MG	1A	3260	1/1	0.88	0.12	51,51,51,51	0
58	MG	2A	3664	1/1	0.88	0.17	77,77,77,77	0
58	MG	2a	1798	1/1	0.88	0.22	67,67,67,67	0
58	MG	2A	3665	1/1	0.88	0.10	63,63,63,63	0
58	MG	1A	3493	1/1	0.88	0.12	51,51,51,51	0
58	MG	2a	1801	1/1	0.88	0.17	55,55,55,55	0
58	MG	1x	107	1/1	0.88	0.29	71,71,71,71	0
58	MG	1A	3139	1/1	0.88	0.36	36,36,36,36	0
58	MG	1x	110	1/1	0.88	0.30	65,65,65,65	0
58	MG	2A	3675	1/1	0.88	0.18	74,74,74,74	0
58	MG	2A	3332	1/1	0.88	0.28	58,58,58,58	0
58	MG	1A	4081	1/1	0.88	0.12	47,47,47,47	0
58	MG	1A	4084	1/1	0.88	0.12	54,54,54,54	0
58	MG	1a	1672	1/1	0.88	0.15	62,62,62,62	0
58	MG	1A	3875	1/1	0.88	0.25	44,44,44,44	0
58	MG	1A	4088	1/1	0.88	0.22	63,63,63,63	0
58	MG	1a	1681	1/1	0.88	0.17	76,76,76,76	0
58	MG	2A	3041	1/1	0.88	0.14	68,68,68,68	0
58	MG	1a	1691	1/1	0.88	0.23	61,61,61,61	0
58	MG	1A	3361	1/1	0.88	0.18	43,43,43,43	0
58	MG	2A	3063	1/1	0.88	0.13	54,54,54,54	0
58	MG	1A	3663	1/1	0.88	0.16	52,52,52,52	0
58	MG	2A	3367	1/1	0.88	0.08	62,62,62,62	0
58	MG	2F	303	1/1	0.88	0.20	52,52,52,52	0
58	MG	2A	3075	1/1	0.88	0.10	70,70,70,70	0
58	MG	1a	1704	1/1	0.88	0.16	64,64,64,64	0
58	MG	1A	3685	1/1	0.88	0.13	46,46,46,46	0
58	MG	1A	3689	1/1	0.88	0.10	47,47,47,47	0
58	MG	2a	1602	1/1	0.88	0.14	74,74,74,74	0
58	MG	2x	3304	1/1	0.88	0.16	67,67,67,67	0
58	MG	1B	212	1/1	0.89	0.17	62,62,62,62	0
58	MG	1a	1684	1/1	0.89	0.14	55,55,55,55	0
58	MG	1a	1689	1/1	0.89	0.32	64,64,64,64	0
58	MG	1A	3269	1/1	0.89	0.19	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
58	MG	2a	1608	1/1	0.89	0.53	72,72,72,72	0
58	MG	2A	3078	1/1	0.89	0.19	66,66,66,66	0
58	MG	1a	1692	1/1	0.89	0.31	55,55,55,55	0
58	MG	1A	3928	1/1	0.89	0.11	47,47,47,47	0
58	MG	2A	3407	1/1	0.89	0.17	43,43,43,43	0
58	MG	1A	3113	1/1	0.89	0.19	42,42,42,42	0
58	MG	2a	1616	1/1	0.89	0.10	72,72,72,72	0
58	MG	2A	3433	1/1	0.89	0.13	48,48,48,48	0
58	MG	1A	3776	1/1	0.89	0.12	27,27,27,27	0
58	MG	2A	3435	1/1	0.89	0.16	44,44,44,44	0
58	MG	2A	3099	1/1	0.89	0.12	58,58,58,58	0
58	MG	1A	3608	1/1	0.89	0.12	46,46,46,46	0
58	MG	2A	3106	1/1	0.89	0.10	52,52,52,52	0
58	MG	1B	231	1/1	0.89	0.13	54,54,54,54	0
58	MG	2A	3112	1/1	0.89	0.22	50,50,50,50	0
58	MG	1A	3945	1/1	0.89	0.15	65,65,65,65	0
58	MG	1A	3798	1/1	0.89	0.12	45,45,45,45	0
58	MG	2A	3471	1/1	0.89	0.14	54,54,54,54	0
58	MG	1A	3133	1/1	0.89	0.21	56,56,56,56	0
58	MG	1A	3291	1/1	0.89	0.15	59,59,59,59	0
58	MG	2A	3134	1/1	0.89	0.10	67,67,67,67	0
58	MG	1a	1718	1/1	0.89	0.27	69,69,69,69	0
58	MG	2A	3150	1/1	0.89	0.15	49,49,49,49	0
58	MG	1a	1719	1/1	0.89	0.27	59,59,59,59	0
58	MG	1A	3807	1/1	0.89	0.12	54,54,54,54	0
58	MG	1A	3304	1/1	0.89	0.36	62,62,62,62	0
58	MG	2A	3501	1/1	0.89	0.23	51,51,51,51	0
58	MG	2A	3177	1/1	0.89	0.43	71,71,71,71	0
58	MG	1a	1729	1/1	0.89	0.14	66,66,66,66	0
58	MG	1A	3348	1/1	0.89	0.44	44,44,44,44	0
58	MG	2A	3520	1/1	0.89	0.22	57,57,57,57	0
58	MG	1A	3974	1/1	0.89	0.16	70,70,70,70	0
58	MG	1O	201	1/1	0.89	0.09	65,65,65,65	0
58	MG	2a	1664	1/1	0.89	0.14	65,65,65,65	0
58	MG	2a	1668	1/1	0.89	0.30	59,59,59,59	0
58	MG	2a	1669	1/1	0.89	0.24	70,70,70,70	0
58	MG	1A	3416	1/1	0.89	0.08	58,58,58,58	0
58	MG	1O	205	1/1	0.89	0.18	56,56,56,56	0
58	MG	2a	1676	1/1	0.89	0.24	69,69,69,69	0
58	MG	1A	3420	1/1	0.89	0.14	52,52,52,52	0
58	MG	2a	1686	1/1	0.89	0.21	71,71,71,71	0
58	MG	2A	3201	1/1	0.89	0.20	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
58	MG	1P	206	1/1	0.89	0.24	57,57,57,57	0
58	MG	2A	3204	1/1	0.89	0.21	55,55,55,55	0
58	MG	1R	201	1/1	0.89	0.18	58,58,58,58	0
58	MG	2a	1696	1/1	0.89	0.13	76,76,76,76	0
58	MG	1A	3515	1/1	0.89	0.07	67,67,67,67	0
58	MG	1A	3995	1/1	0.89	0.12	24,24,24,24	0
58	MG	1A	3666	1/1	0.89	0.09	33,33,33,33	0
58	MG	1U	207	1/1	0.89	0.25	48,48,48,48	0
58	MG	1A	3164	1/1	0.89	0.43	35,35,35,35	0
58	MG	1a	1769	1/1	0.89	0.10	62,62,62,62	0
58	MG	1A	3053	1/1	0.89	0.24	46,46,46,46	0
58	MG	1A	4014	1/1	0.89	0.11	63,63,63,63	0
58	MG	2A	3239	1/1	0.89	0.12	61,61,61,61	0
58	MG	1A	3324	1/1	0.89	0.10	45,45,45,45	0
58	MG	1A	3695	1/1	0.89	0.12	25,25,25,25	0
58	MG	14	101	1/1	0.89	0.23	78,78,78,78	0
58	MG	1A	4018	1/1	0.89	0.12	58,58,58,58	0
58	MG	1A	3851	1/1	0.89	0.14	60,60,60,60	0
58	MG	2a	1728	1/1	0.89	0.33	80,80,80,80	0
58	MG	1a	1602	1/1	0.89	0.45	74,74,74,74	0
58	MG	1A	3442	1/1	0.89	0.09	43,43,43,43	0
58	MG	2A	3578	1/1	0.89	0.19	55,55,55,55	0
58	MG	1A	3452	1/1	0.89	0.15	64,64,64,64	0
58	MG	1a	1611	1/1	0.89	0.12	71,71,71,71	0
58	MG	1a	1811	1/1	0.89	0.10	65,65,65,65	0
58	MG	2A	3593	1/1	0.89	0.14	68,68,68,68	0
58	MG	1A	3167	1/1	0.89	0.09	33,33,33,33	0
58	MG	2A	3269	1/1	0.89	0.30	56,56,56,56	0
58	MG	2A	3270	1/1	0.89	0.27	61,61,61,61	0
58	MG	1A	3566	1/1	0.89	0.14	45,45,45,45	0
58	MG	1A	3874	1/1	0.89	0.18	33,33,33,33	0
58	MG	1a	1626	1/1	0.89	0.40	64,64,64,64	0
58	MG	1A	3221	1/1	0.89	0.23	44,44,44,44	0
58	MG	2A	3281	1/1	0.89	0.30	53,53,53,53	0
58	MG	2A	3285	1/1	0.89	0.23	63,63,63,63	0
58	MG	2A	3619	1/1	0.89	0.13	53,53,53,53	0
58	MG	1A	3329	1/1	0.89	0.16	44,44,44,44	0
58	MG	2A	3304	1/1	0.89	0.30	60,60,60,60	0
58	MG	1A	4064	1/1	0.89	0.11	53,53,53,53	0
58	MG	2a	1778	1/1	0.89	0.18	55,55,55,55	0
58	MG	1a	1638	1/1	0.89	0.16	59,59,59,59	0
58	MG	1A	3265	1/1	0.89	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
58	MG	2A	3648	1/1	0.89	0.10	60,60,60,60	0
58	MG	2A	3654	1/1	0.89	0.11	36,36,36,36	0
58	MG	1A	3468	1/1	0.89	0.13	50,50,50,50	0
58	MG	1w	102	1/1	0.89	0.24	73,73,73,73	0
58	MG	2A	3321	1/1	0.89	0.18	63,63,63,63	0
58	MG	2A	3323	1/1	0.89	0.17	62,62,62,62	0
58	MG	1a	1642	1/1	0.89	0.25	78,78,78,78	0
58	MG	1A	3587	1/1	0.89	0.16	64,64,64,64	0
58	MG	1A	3740	1/1	0.89	0.17	62,62,62,62	0
58	MG	1A	4077	1/1	0.89	0.14	54,54,54,54	0
58	MG	1x	106	1/1	0.89	0.20	73,73,73,73	0
58	MG	1A	3371	1/1	0.89	0.10	46,46,46,46	0
58	MG	1A	3378	1/1	0.89	0.10	68,68,68,68	0
58	MG	1a	1659	1/1	0.89	0.24	72,72,72,72	0
58	MG	1A	3897	1/1	0.89	0.08	46,46,46,46	0
58	MG	2A	3345	1/1	0.89	0.14	46,46,46,46	0
58	MG	2a	1816	1/1	0.89	0.17	64,64,64,64	0
58	MG	2A	3348	1/1	0.89	0.17	64,64,64,64	0
58	MG	1a	1664	1/1	0.89	0.15	64,64,64,64	0
58	MG	1A	3908	1/1	0.89	0.10	52,52,52,52	0
58	MG	2A	3019	1/1	0.89	0.27	65,65,65,65	0
58	MG	2f	201	1/1	0.89	0.18	61,61,61,61	0
58	MG	2B	215	1/1	0.89	0.22	75,75,75,75	0
58	MG	1A	3379	1/1	0.89	0.12	63,63,63,63	0
58	MG	1A	4090	1/1	0.89	0.17	60,60,60,60	0
58	MG	2E	304	1/1	0.89	0.09	34,34,34,34	0
58	MG	2A	3363	1/1	0.89	0.23	54,54,54,54	0
58	MG	1A	3233	1/1	0.89	0.10	48,48,48,48	0
58	MG	2P	201	1/1	0.89	0.13	50,50,50,50	0
58	MG	2A	3031	1/1	0.89	0.24	63,63,63,63	0
58	MG	2Z	301	1/1	0.89	0.23	71,71,71,71	0
58	MG	2A	3033	1/1	0.89	0.22	56,56,56,56	0
58	MG	1A	3489	1/1	0.89	0.12	61,61,61,61	0
58	MG	2w	101	1/1	0.89	0.27	68,68,68,68	0
58	MG	2A	3043	1/1	0.89	0.12	69,69,69,69	0
58	MG	1A	3764	1/1	0.89	0.13	16,16,16,16	0
58	MG	2x	3305	1/1	0.89	0.28	66,66,66,66	0
58	MG	2A	3013	1/1	0.90	0.27	49,49,49,49	0
58	MG	2B	202	1/1	0.90	0.33	71,71,71,71	0
58	MG	2A	3018	1/1	0.90	0.31	43,43,43,43	0
58	MG	1A	3018	1/1	0.90	0.19	32,32,32,32	0
58	MG	1A	3804	1/1	0.90	0.10	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1673	1/1	0.90	0.12	58,58,58,58	0
58	MG	1a	1674	1/1	0.90	0.28	68,68,68,68	0
58	MG	2A	3339	1/1	0.90	0.28	49,49,49,49	0
58	MG	1A	3311	1/1	0.90	0.26	57,57,57,57	0
58	MG	1A	3408	1/1	0.90	0.20	61,61,61,61	0
58	MG	2E	301	1/1	0.90	0.16	70,70,70,70	0
58	MG	2A	3034	1/1	0.90	0.09	62,62,62,62	0
58	MG	2A	3036	1/1	0.90	0.13	56,56,56,56	0
58	MG	2A	3040	1/1	0.90	0.20	67,67,67,67	0
58	MG	2A	3352	1/1	0.90	0.13	45,45,45,45	0
58	MG	1A	3618	1/1	0.90	0.15	52,52,52,52	0
58	MG	1A	3411	1/1	0.90	0.09	55,55,55,55	0
58	MG	2X	101	1/1	0.90	0.09	71,71,71,71	0
58	MG	2A	3045	1/1	0.90	0.23	71,71,71,71	0
58	MG	2A	3048	1/1	0.90	0.15	56,56,56,56	0
58	MG	1A	3503	1/1	0.90	0.16	70,70,70,70	0
58	MG	2A	3362	1/1	0.90	0.20	62,62,62,62	0
58	MG	2a	1601	1/1	0.90	0.16	67,67,67,67	0
58	MG	1A	3315	1/1	0.90	0.08	34,34,34,34	0
58	MG	2A	3364	1/1	0.90	0.26	63,63,63,63	0
58	MG	1A	3817	1/1	0.90	0.11	52,52,52,52	0
58	MG	2a	1605	1/1	0.90	0.32	71,71,71,71	0
58	MG	2A	3064	1/1	0.90	0.35	65,65,65,65	0
58	MG	1a	1695	1/1	0.90	0.28	72,72,72,72	0
58	MG	1A	3983	1/1	0.90	0.10	34,34,34,34	0
58	MG	1A	3655	1/1	0.90	0.11	58,58,58,58	0
58	MG	1a	1701	1/1	0.90	0.19	49,49,49,49	0
58	MG	2A	3088	1/1	0.90	0.13	59,59,59,59	0
58	MG	2A	3383	1/1	0.90	0.17	50,50,50,50	0
58	MG	1A	3211	1/1	0.90	0.14	68,68,68,68	0
58	MG	2A	3390	1/1	0.90	0.31	73,73,73,73	0
58	MG	1A	3220	1/1	0.90	0.13	54,54,54,54	0
58	MG	2A	3399	1/1	0.90	0.36	66,66,66,66	0
58	MG	2a	1619	1/1	0.90	0.10	74,74,74,74	0
58	MG	2A	3092	1/1	0.90	0.14	50,50,50,50	0
58	MG	1A	3837	1/1	0.90	0.13	63,63,63,63	0
58	MG	1A	4004	1/1	0.90	0.10	37,37,37,37	0
58	MG	1A	4007	1/1	0.90	0.07	43,43,43,43	0
58	MG	1A	3354	1/1	0.90	0.13	62,62,62,62	0
58	MG	2A	3416	1/1	0.90	0.12	47,47,47,47	0
58	MG	1a	1715	1/1	0.90	0.23	55,55,55,55	0
58	MG	2A	3426	1/1	0.90	0.17	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
58	MG	2A	3429	1/1	0.90	0.13	56,56,56,56	0
58	MG	2a	1638	1/1	0.90	0.22	64,64,64,64	0
58	MG	1A	3683	1/1	0.90	0.09	26,26,26,26	0
58	MG	1A	3424	1/1	0.90	0.12	55,55,55,55	0
58	MG	2A	3121	1/1	0.90	0.28	63,63,63,63	0
58	MG	1T	201	1/1	0.90	0.14	57,57,57,57	0
58	MG	2A	3442	1/1	0.90	0.20	41,41,41,41	0
58	MG	1A	4016	1/1	0.90	0.11	62,62,62,62	0
58	MG	1a	1721	1/1	0.90	0.29	71,71,71,71	0
58	MG	2A	3131	1/1	0.90	0.36	63,63,63,63	0
58	MG	2a	1648	1/1	0.90	0.11	81,81,81,81	0
58	MG	1A	3844	1/1	0.90	0.12	51,51,51,51	0
58	MG	2A	3135	1/1	0.90	0.20	73,73,73,73	0
58	MG	2A	3469	1/1	0.90	0.23	39,39,39,39	0
58	MG	2A	3136	1/1	0.90	0.10	50,50,50,50	0
58	MG	2A	3138	1/1	0.90	0.12	51,51,51,51	0
58	MG	2a	1656	1/1	0.90	0.14	59,59,59,59	0
58	MG	1U	205	1/1	0.90	0.13	43,43,43,43	0
58	MG	2a	1658	1/1	0.90	0.30	76,76,76,76	0
58	MG	2A	3147	1/1	0.90	0.24	64,64,64,64	0
58	MG	2A	3477	1/1	0.90	0.27	64,64,64,64	0
58	MG	2a	1666	1/1	0.90	0.29	61,61,61,61	0
58	MG	2A	3479	1/1	0.90	0.17	45,45,45,45	0
58	MG	1A	3432	1/1	0.90	0.08	61,61,61,61	0
58	MG	1A	3852	1/1	0.90	0.23	44,44,44,44	0
58	MG	2A	3158	1/1	0.90	0.16	58,58,58,58	0
58	MG	2A	3486	1/1	0.90	0.14	35,35,35,35	0
58	MG	2A	3159	1/1	0.90	0.16	61,61,61,61	0
58	MG	2a	1680	1/1	0.90	0.22	64,64,64,64	0
58	MG	2a	1682	1/1	0.90	0.19	77,77,77,77	0
58	MG	2a	1684	1/1	0.90	0.28	68,68,68,68	0
58	MG	1A	4027	1/1	0.90	0.12	46,46,46,46	0
58	MG	1A	3433	1/1	0.90	0.13	49,49,49,49	0
58	MG	1A	3355	1/1	0.90	0.10	45,45,45,45	0
58	MG	10	101	1/1	0.90	0.10	42,42,42,42	0
58	MG	2A	3508	1/1	0.90	0.16	40,40,40,40	0
58	MG	1A	3075	1/1	0.90	0.20	57,57,57,57	0
58	MG	2a	1697	1/1	0.90	0.23	63,63,63,63	0
58	MG	1a	1757	1/1	0.90	0.20	68,68,68,68	0
58	MG	2A	3517	1/1	0.90	0.17	53,53,53,53	0
58	MG	10	107	1/1	0.90	0.15	61,61,61,61	0
58	MG	13	103	1/1	0.90	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
58	MG	2a	1706	1/1	0.90	0.18	75,75,75,75	0
58	MG	2A	3524	1/1	0.90	0.19	66,66,66,66	0
58	MG	2A	3525	1/1	0.90	0.26	63,63,63,63	0
58	MG	2A	3195	1/1	0.90	0.11	46,46,46,46	0
58	MG	2A	3527	1/1	0.90	0.19	64,64,64,64	0
58	MG	2a	1718	1/1	0.90	0.19	70,70,70,70	0
58	MG	1A	3534	1/1	0.90	0.30	61,61,61,61	0
58	MG	15	102	1/1	0.90	0.37	34,34,34,34	0
58	MG	2A	3533	1/1	0.90	0.09	69,69,69,69	0
58	MG	2a	1724	1/1	0.90	0.17	64,64,64,64	0
58	MG	1A	3713	1/1	0.90	0.15	42,42,42,42	0
58	MG	2A	3202	1/1	0.90	0.28	61,61,61,61	0
58	MG	1A	3056	1/1	0.90	0.13	60,60,60,60	0
58	MG	1A	4043	1/1	0.90	0.11	56,56,56,56	0
58	MG	1a	1770	1/1	0.90	0.11	57,57,57,57	0
58	MG	2A	3208	1/1	0.90	0.34	47,47,47,47	0
58	MG	2A	3543	1/1	0.90	0.17	72,72,72,72	0
58	MG	2A	3211	1/1	0.90	0.13	63,63,63,63	0
58	MG	1A	3234	1/1	0.90	0.09	55,55,55,55	0
58	MG	1a	1605	1/1	0.90	0.13	51,51,51,51	0
58	MG	2A	3548	1/1	0.90	0.13	64,64,64,64	0
58	MG	2A	3551	1/1	0.90	0.28	61,61,61,61	0
58	MG	1A	3551	1/1	0.90	0.19	36,36,36,36	0
58	MG	1A	3564	1/1	0.90	0.42	39,39,39,39	0
58	MG	1A	3245	1/1	0.90	0.11	60,60,60,60	0
58	MG	2A	3229	1/1	0.90	0.21	46,46,46,46	0
58	MG	1a	1617	1/1	0.90	0.10	51,51,51,51	0
58	MG	2a	1752	1/1	0.90	0.17	76,76,76,76	0
58	MG	1A	3335	1/1	0.90	0.19	53,53,53,53	0
58	MG	1a	1622	1/1	0.90	0.16	59,59,59,59	0
58	MG	2A	3238	1/1	0.90	0.36	78,78,78,78	0
58	MG	1A	3373	1/1	0.90	0.09	47,47,47,47	0
58	MG	1a	1806	1/1	0.90	0.38	73,73,73,73	0
58	MG	2a	1763	1/1	0.90	0.12	66,66,66,66	0
58	MG	2a	1764	1/1	0.90	0.20	70,70,70,70	0
58	MG	2a	1765	1/1	0.90	0.19	50,50,50,50	0
58	MG	1a	1624	1/1	0.90	0.18	60,60,60,60	0
58	MG	2a	1768	1/1	0.90	0.18	77,77,77,77	0
58	MG	2a	1771	1/1	0.90	0.18	73,73,73,73	0
58	MG	1A	4076	1/1	0.90	0.14	65,65,65,65	0
58	MG	1A	3249	1/1	0.90	0.34	67,67,67,67	0
58	MG	2a	1779	1/1	0.90	0.24	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
58	MG	2A	3579	1/1	0.90	0.15	40,40,40,40	0
58	MG	1A	3583	1/1	0.90	0.33	40,40,40,40	0
58	MG	1A	3465	1/1	0.90	0.30	54,54,54,54	0
58	MG	2A	3258	1/1	0.90	0.20	54,54,54,54	0
58	MG	2A	3591	1/1	0.90	0.16	52,52,52,52	0
58	MG	2a	1790	1/1	0.90	0.14	72,72,72,72	0
58	MG	1A	3586	1/1	0.90	0.14	44,44,44,44	0
58	MG	1A	4086	1/1	0.90	0.13	50,50,50,50	0
58	MG	2A	3597	1/1	0.90	0.12	61,61,61,61	0
58	MG	2A	3600	1/1	0.90	0.23	81,81,81,81	0
58	MG	1A	3122	1/1	0.90	0.17	40,40,40,40	0
58	MG	1A	3339	1/1	0.90	0.09	65,65,65,65	0
58	MG	1A	3760	1/1	0.90	0.08	32,32,32,32	0
58	MG	1A	3472	1/1	0.90	0.10	42,42,42,42	0
58	MG	1a	1645	1/1	0.90	0.18	49,49,49,49	0
58	MG	1A	3194	1/1	0.90	0.35	45,45,45,45	0
58	MG	1A	4095	1/1	0.90	0.13	55,55,55,55	0
58	MG	2a	1811	1/1	0.90	0.23	65,65,65,65	0
58	MG	1A	3295	1/1	0.90	0.14	59,59,59,59	0
58	MG	1B	210	1/1	0.90	0.15	53,53,53,53	0
58	MG	2A	3620	1/1	0.90	0.12	76,76,76,76	0
58	MG	1a	1660	1/1	0.90	0.13	65,65,65,65	0
58	MG	2a	1818	1/1	0.90	0.14	74,74,74,74	0
58	MG	2a	1819	1/1	0.90	0.20	60,60,60,60	0
58	MG	1w	107	1/1	0.90	0.15	71,71,71,71	0
58	MG	2a	1821	1/1	0.90	0.27	70,70,70,70	0
58	MG	2A	3287	1/1	0.90	0.15	58,58,58,58	0
58	MG	2A	3296	1/1	0.90	0.20	54,54,54,54	0
58	MG	2A	3299	1/1	0.90	0.13	59,59,59,59	0
58	MG	1a	1661	1/1	0.90	0.20	66,66,66,66	0
58	MG	2A	3652	1/1	0.90	0.16	50,50,50,50	0
58	MG	1x	105	1/1	0.90	0.28	67,67,67,67	0
58	MG	2A	3305	1/1	0.90	0.11	55,55,55,55	0
58	MG	1a	1662	1/1	0.90	0.12	64,64,64,64	0
58	MG	1A	3479	1/1	0.90	0.16	61,61,61,61	0
58	MG	2A	3309	1/1	0.90	0.17	69,69,69,69	0
58	MG	2A	3311	1/1	0.90	0.07	52,52,52,52	0
58	MG	2A	3313	1/1	0.90	0.37	55,55,55,55	0
58	MG	1B	215	1/1	0.90	0.17	60,60,60,60	0
58	MG	1A	3394	1/1	0.90	0.16	46,46,46,46	0
58	MG	1a	1666	1/1	0.90	0.26	64,64,64,64	0
58	MG	2x	3302	1/1	0.90	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
58	MG	1a	1667	1/1	0.90	0.22	63,63,63,63	0
58	MG	1A	3255	1/1	0.90	0.21	61,61,61,61	0
58	MG	2A	3685	1/1	0.90	0.12	65,65,65,65	0
58	MG	1A	3459	1/1	0.91	0.09	54,54,54,54	0
58	MG	2A	3493	1/1	0.91	0.14	77,77,77,77	0
58	MG	1x	102	1/1	0.91	0.16	68,68,68,68	0
58	MG	2A	3234	1/1	0.91	0.16	58,58,58,58	0
58	MG	2a	1624	1/1	0.91	0.12	66,66,66,66	0
58	MG	1A	3552	1/1	0.91	0.07	49,49,49,49	0
58	MG	2a	1626	1/1	0.91	0.25	63,63,63,63	0
58	MG	1A	3999	1/1	0.91	0.18	60,60,60,60	0
58	MG	1A	3183	1/1	0.91	0.21	49,49,49,49	0
58	MG	1A	4006	1/1	0.91	0.12	39,39,39,39	0
58	MG	1A	3845	1/1	0.91	0.23	65,65,65,65	0
58	MG	2A	3514	1/1	0.91	0.23	52,52,52,52	0
58	MG	1A	4008	1/1	0.91	0.08	42,42,42,42	0
58	MG	2A	3518	1/1	0.91	0.25	66,66,66,66	0
58	MG	1O	204	1/1	0.91	0.11	60,60,60,60	0
58	MG	2a	1641	1/1	0.91	0.09	61,61,61,61	0
58	MG	1A	3847	1/1	0.91	0.08	65,65,65,65	0
58	MG	2A	3523	1/1	0.91	0.15	66,66,66,66	0
58	MG	2A	3248	1/1	0.91	0.16	67,67,67,67	0
58	MG	1a	1682	1/1	0.91	0.21	64,64,64,64	0
58	MG	1A	3386	1/1	0.91	0.27	43,43,43,43	0
58	MG	2A	3259	1/1	0.91	0.29	53,53,53,53	0
58	MG	1a	1688	1/1	0.91	0.31	46,46,46,46	0
58	MG	1A	3388	1/1	0.91	0.14	52,52,52,52	0
58	MG	2A	3022	1/1	0.91	0.18	51,51,51,51	0
58	MG	1A	3274	1/1	0.91	0.11	51,51,51,51	0
58	MG	1A	3579	1/1	0.91	0.15	37,37,37,37	0
58	MG	1S	202	1/1	0.91	0.10	73,73,73,73	0
58	MG	1A	3862	1/1	0.91	0.15	59,59,59,59	0
58	MG	2A	3540	1/1	0.91	0.19	66,66,66,66	0
58	MG	2A	3032	1/1	0.91	0.13	57,57,57,57	0
58	MG	1a	1698	1/1	0.91	0.12	60,60,60,60	0
58	MG	1A	3280	1/1	0.91	0.31	48,48,48,48	0
58	MG	1A	3083	1/1	0.91	0.13	40,40,40,40	0
58	MG	1A	3293	1/1	0.91	0.07	38,38,38,38	0
58	MG	2A	3284	1/1	0.91	0.23	55,55,55,55	0
58	MG	1A	3402	1/1	0.91	0.15	49,49,49,49	0
58	MG	2A	3549	1/1	0.91	0.16	64,64,64,64	0
58	MG	1A	3067	1/1	0.91	0.22	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
58	MG	2a	1677	1/1	0.91	0.21	64,64,64,64	0
58	MG	2A	3552	1/1	0.91	0.11	54,54,54,54	0
58	MG	2a	1679	1/1	0.91	0.25	62,62,62,62	0
58	MG	2A	3294	1/1	0.91	0.15	62,62,62,62	0
58	MG	1A	4035	1/1	0.91	0.16	29,29,29,29	0
58	MG	2A	3559	1/1	0.91	0.11	61,61,61,61	0
58	MG	1W	202	1/1	0.91	0.14	49,49,49,49	0
58	MG	2A	3054	1/1	0.91	0.08	43,43,43,43	0
58	MG	1A	3745	1/1	0.91	0.10	59,59,59,59	0
58	MG	1A	3480	1/1	0.91	0.18	52,52,52,52	0
58	MG	2a	1692	1/1	0.91	0.19	57,57,57,57	0
58	MG	1A	3297	1/1	0.91	0.12	49,49,49,49	0
58	MG	1A	3300	1/1	0.91	0.18	44,44,44,44	0
58	MG	10	105	1/1	0.91	0.27	73,73,73,73	0
58	MG	2a	1698	1/1	0.91	0.12	78,78,78,78	0
58	MG	2A	3073	1/1	0.91	0.28	50,50,50,50	0
58	MG	1A	3093	1/1	0.91	0.28	53,53,53,53	0
58	MG	10	108	1/1	0.91	0.17	62,62,62,62	0
58	MG	2A	3079	1/1	0.91	0.22	64,64,64,64	0
58	MG	2A	3081	1/1	0.91	0.19	56,56,56,56	0
58	MG	11	101	1/1	0.91	0.42	44,44,44,44	0
58	MG	2A	3086	1/1	0.91	0.24	53,53,53,53	0
58	MG	11	103	1/1	0.91	0.10	71,71,71,71	0
58	MG	13	102	1/1	0.91	0.15	59,59,59,59	0
58	MG	2a	1716	1/1	0.91	0.40	75,75,75,75	0
58	MG	1A	4047	1/1	0.91	0.19	46,46,46,46	0
58	MG	2A	3091	1/1	0.91	0.14	48,48,48,48	0
58	MG	1A	4050	1/1	0.91	0.10	47,47,47,47	0
58	MG	1A	3146	1/1	0.91	0.12	56,56,56,56	0
58	MG	2A	3601	1/1	0.91	0.15	59,59,59,59	0
58	MG	1A	3494	1/1	0.91	0.13	57,57,57,57	0
58	MG	2A	3340	1/1	0.91	0.16	58,58,58,58	0
58	MG	1A	3415	1/1	0.91	0.13	49,49,49,49	0
58	MG	2A	3105	1/1	0.91	0.13	50,50,50,50	0
58	MG	1a	1601	1/1	0.91	0.19	59,59,59,59	0
58	MG	1a	1751	1/1	0.91	0.12	53,53,53,53	0
58	MG	2A	3613	1/1	0.91	0.12	78,78,78,78	0
58	MG	1A	3116	1/1	0.91	0.07	50,50,50,50	0
58	MG	2A	3115	1/1	0.91	0.26	66,66,66,66	0
58	MG	1A	3198	1/1	0.91	0.31	52,52,52,52	0
58	MG	1A	3152	1/1	0.91	0.27	44,44,44,44	0
58	MG	1A	3921	1/1	0.91	0.09	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
58	MG	2A	3627	1/1	0.91	0.12	34,34,34,34	0
58	MG	2A	3358	1/1	0.91	0.12	70,70,70,70	0
58	MG	2a	1746	1/1	0.91	0.12	58,58,58,58	0
58	MG	1A	3507	1/1	0.91	0.14	56,56,56,56	0
58	MG	1A	4079	1/1	0.91	0.10	55,55,55,55	0
58	MG	1a	1615	1/1	0.91	0.14	55,55,55,55	0
58	MG	1A	3925	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	3423	1/1	0.91	0.23	75,75,75,75	0
58	MG	1A	3322	1/1	0.91	0.11	51,51,51,51	0
58	MG	1a	1773	1/1	0.91	0.23	62,62,62,62	0
58	MG	2A	3657	1/1	0.91	0.15	59,59,59,59	0
58	MG	2A	3661	1/1	0.91	0.09	55,55,55,55	0
58	MG	2A	3370	1/1	0.91	0.16	58,58,58,58	0
58	MG	1A	3117	1/1	0.91	0.18	38,38,38,38	0
58	MG	1A	3805	1/1	0.91	0.10	47,47,47,47	0
58	MG	1A	4089	1/1	0.91	0.12	54,54,54,54	0
58	MG	1a	1780	1/1	0.91	0.17	62,62,62,62	0
58	MG	2a	1770	1/1	0.91	0.16	76,76,76,76	0
58	MG	2A	3152	1/1	0.91	0.14	58,58,58,58	0
58	MG	2a	1775	1/1	0.91	0.16	60,60,60,60	0
58	MG	2A	3381	1/1	0.91	0.25	48,48,48,48	0
58	MG	2a	1777	1/1	0.91	0.15	51,51,51,51	0
58	MG	2A	3153	1/1	0.91	0.22	63,63,63,63	0
58	MG	2A	3157	1/1	0.91	0.13	62,62,62,62	0
58	MG	2a	1780	1/1	0.91	0.11	62,62,62,62	0
58	MG	2A	3387	1/1	0.91	0.26	66,66,66,66	0
58	MG	2A	3389	1/1	0.91	0.29	63,63,63,63	0
58	MG	1A	3649	1/1	0.91	0.13	60,60,60,60	0
58	MG	1A	3650	1/1	0.91	0.18	34,34,34,34	0
58	MG	2A	3161	1/1	0.91	0.19	55,55,55,55	0
58	MG	2A	3168	1/1	0.91	0.15	45,45,45,45	0
58	MG	2B	206	1/1	0.91	0.15	57,57,57,57	0
58	MG	2B	207	1/1	0.91	0.15	72,72,72,72	0
58	MG	2a	1796	1/1	0.91	0.16	60,60,60,60	0
58	MG	1A	3948	1/1	0.91	0.26	66,66,66,66	0
58	MG	1a	1634	1/1	0.91	0.28	70,70,70,70	0
58	MG	1a	1636	1/1	0.91	0.15	61,61,61,61	0
58	MG	1a	1803	1/1	0.91	0.10	67,67,67,67	0
58	MG	1A	3812	1/1	0.91	0.45	36,36,36,36	0
58	MG	1A	3952	1/1	0.91	0.10	61,61,61,61	0
58	MG	2A	3185	1/1	0.91	0.18	68,68,68,68	0
58	MG	1A	3363	1/1	0.91	0.15	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
58	MG	1B	211	1/1	0.91	0.17	63,63,63,63	0
58	MG	2A	3191	1/1	0.91	0.20	68,68,68,68	0
58	MG	2F	301	1/1	0.91	0.09	54,54,54,54	0
58	MG	2F	302	1/1	0.91	0.11	63,63,63,63	0
58	MG	2a	1815	1/1	0.91	0.27	65,65,65,65	0
58	MG	1A	3006	1/1	0.91	0.15	64,64,64,64	0
58	MG	1a	1813	1/1	0.91	0.31	77,77,77,77	0
58	MG	2A	3199	1/1	0.91	0.17	63,63,63,63	0
58	MG	1B	213	1/1	0.91	0.12	44,44,44,44	0
58	MG	1A	3121	1/1	0.91	0.13	37,37,37,37	0
58	MG	2A	3449	1/1	0.91	0.29	58,58,58,58	0
58	MG	2A	3454	1/1	0.91	0.14	44,44,44,44	0
58	MG	23	101	1/1	0.91	0.31	70,70,70,70	0
58	MG	1A	3231	1/1	0.91	0.14	24,24,24,24	0
58	MG	1B	222	1/1	0.91	0.09	58,58,58,58	0
58	MG	2A	3462	1/1	0.91	0.11	37,37,37,37	0
58	MG	2A	3464	1/1	0.91	0.21	57,57,57,57	0
58	MG	1A	3669	1/1	0.91	0.12	58,58,58,58	0
58	MG	1A	3681	1/1	0.91	0.11	22,22,22,22	0
58	MG	1A	3977	1/1	0.91	0.11	65,65,65,65	0
58	MG	1A	3445	1/1	0.91	0.20	53,53,53,53	0
58	MG	2A	3214	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	3331	1/1	0.91	0.24	62,62,62,62	0
58	MG	1A	3832	1/1	0.91	0.14	47,47,47,47	0
58	MG	1w	103	1/1	0.91	0.10	65,65,65,65	0
58	MG	2v	102	1/1	0.91	0.17	74,74,74,74	0
58	MG	1A	3232	1/1	0.91	0.23	34,34,34,34	0
58	MG	1A	3081	1/1	0.91	0.12	65,65,65,65	0
58	MG	2A	3228	1/1	0.91	0.18	66,66,66,66	0
58	MG	2A	3484	1/1	0.91	0.17	54,54,54,54	0
58	MG	1F	310	1/1	0.91	0.09	58,58,58,58	0
58	MG	2A	3155	1/1	0.92	0.06	51,51,51,51	0
58	MG	1A	3464	1/1	0.92	0.08	51,51,51,51	0
58	MG	1W	206	1/1	0.92	0.11	44,44,44,44	0
58	MG	1X	101	1/1	0.92	0.47	41,41,41,41	0
58	MG	2A	3160	1/1	0.92	0.15	48,48,48,48	0
58	MG	1A	3134	1/1	0.92	0.15	31,31,31,31	0
58	MG	1Y	204	1/1	0.92	0.20	51,51,51,51	0
58	MG	2A	3171	1/1	0.92	0.15	63,63,63,63	0
58	MG	2A	3172	1/1	0.92	0.14	40,40,40,40	0
58	MG	1A	3103	1/1	0.92	0.17	38,38,38,38	0
58	MG	2A	3453	1/1	0.92	0.17	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3591	1/1	0.92	0.14	54,54,54,54	0
58	MG	2A	3455	1/1	0.92	0.16	45,45,45,45	0
58	MG	2A	3456	1/1	0.92	0.12	45,45,45,45	0
58	MG	1A	3169	1/1	0.92	0.08	31,31,31,31	0
58	MG	2A	3178	1/1	0.92	0.20	73,73,73,73	0
58	MG	1A	3170	1/1	0.92	0.14	40,40,40,40	0
58	MG	2A	3463	1/1	0.92	0.14	47,47,47,47	0
58	MG	1A	3144	1/1	0.92	0.15	53,53,53,53	0
58	MG	1a	1774	1/1	0.92	0.15	77,77,77,77	0
58	MG	1A	3406	1/1	0.92	0.12	56,56,56,56	0
58	MG	2a	1623	1/1	0.92	0.18	65,65,65,65	0
58	MG	1A	3819	1/1	0.92	0.15	70,70,70,70	0
58	MG	1A	3319	1/1	0.92	0.35	36,36,36,36	0
58	MG	2A	3189	1/1	0.92	0.17	66,66,66,66	0
58	MG	1A	3225	1/1	0.92	0.19	44,44,44,44	0
58	MG	2A	3475	1/1	0.92	0.23	65,65,65,65	0
58	MG	1A	4025	1/1	0.92	0.10	54,54,54,54	0
58	MG	1a	1784	1/1	0.92	0.18	71,71,71,71	0
58	MG	1A	3827	1/1	0.92	0.17	30,30,30,30	0
58	MG	1a	1790	1/1	0.92	0.09	73,73,73,73	0
58	MG	1A	3830	1/1	0.92	0.09	41,41,41,41	0
58	MG	1A	3483	1/1	0.92	0.09	55,55,55,55	0
58	MG	1A	3609	1/1	0.92	0.08	41,41,41,41	0
58	MG	19	101	1/1	0.92	0.16	53,53,53,53	0
58	MG	1a	1804	1/1	0.92	0.15	60,60,60,60	0
58	MG	2A	3207	1/1	0.92	0.11	57,57,57,57	0
58	MG	2A	3496	1/1	0.92	0.15	41,41,41,41	0
58	MG	1A	3834	1/1	0.92	0.23	62,62,62,62	0
58	MG	2A	3209	1/1	0.92	0.09	54,54,54,54	0
58	MG	1A	3227	1/1	0.92	0.14	58,58,58,58	0
58	MG	2A	3506	1/1	0.92	0.13	43,43,43,43	0
58	MG	1a	1603	1/1	0.92	0.20	71,71,71,71	0
58	MG	1A	3323	1/1	0.92	0.13	47,47,47,47	0
58	MG	1A	3490	1/1	0.92	0.17	45,45,45,45	0
58	MG	2A	3219	1/1	0.92	0.08	45,45,45,45	0
58	MG	1A	3619	1/1	0.92	0.21	38,38,38,38	0
58	MG	1A	3626	1/1	0.92	0.12	35,35,35,35	0
58	MG	1a	1613	1/1	0.92	0.21	47,47,47,47	0
58	MG	2A	3521	1/1	0.92	0.22	70,70,70,70	0
58	MG	2a	1662	1/1	0.92	0.28	63,63,63,63	0
58	MG	1A	3357	1/1	0.92	0.16	57,57,57,57	0
58	MG	1f	202	1/1	0.92	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
58	MG	1A	4048	1/1	0.92	0.13	49,49,49,49	0
58	MG	1A	3492	1/1	0.92	0.08	44,44,44,44	0
58	MG	2a	1671	1/1	0.92	0.23	59,59,59,59	0
58	MG	1A	4053	1/1	0.92	0.11	53,53,53,53	0
58	MG	2A	3236	1/1	0.92	0.20	48,48,48,48	0
58	MG	1A	4061	1/1	0.92	0.09	43,43,43,43	0
58	MG	1A	4063	1/1	0.92	0.09	54,54,54,54	0
58	MG	1A	3645	1/1	0.92	0.18	60,60,60,60	0
58	MG	1A	3417	1/1	0.92	0.26	47,47,47,47	0
58	MG	1A	3045	1/1	0.92	0.13	38,38,38,38	0
58	MG	1a	1629	1/1	0.92	0.28	61,61,61,61	0
58	MG	1A	3421	1/1	0.92	0.20	50,50,50,50	0
58	MG	1A	3858	1/1	0.92	0.09	52,52,52,52	0
58	MG	1A	4075	1/1	0.92	0.23	73,73,73,73	0
58	MG	1x	101	1/1	0.92	0.35	70,70,70,70	0
58	MG	1A	3096	1/1	0.92	0.21	53,53,53,53	0
58	MG	1A	3088	1/1	0.92	0.19	33,33,33,33	0
58	MG	2A	3545	1/1	0.92	0.20	61,61,61,61	0
58	MG	1A	3659	1/1	0.92	0.11	40,40,40,40	0
58	MG	1A	3504	1/1	0.92	0.38	33,33,33,33	0
58	MG	1A	3327	1/1	0.92	0.23	59,59,59,59	0
58	MG	2A	3266	1/1	0.92	0.28	64,64,64,64	0
58	MG	1A	3426	1/1	0.92	0.13	58,58,58,58	0
58	MG	1A	3672	1/1	0.92	0.11	27,27,27,27	0
58	MG	1A	3510	1/1	0.92	0.11	47,47,47,47	0
58	MG	1A	3430	1/1	0.92	0.30	56,56,56,56	0
58	MG	1A	3431	1/1	0.92	0.11	53,53,53,53	0
58	MG	1A	3328	1/1	0.92	0.14	55,55,55,55	0
58	MG	1a	1656	1/1	0.92	0.15	63,63,63,63	0
58	MG	2a	1711	1/1	0.92	0.15	71,71,71,71	0
58	MG	2a	1713	1/1	0.92	0.22	63,63,63,63	0
58	MG	1a	1658	1/1	0.92	0.12	59,59,59,59	0
58	MG	1A	3191	1/1	0.92	0.18	34,34,34,34	0
58	MG	1A	4093	1/1	0.92	0.11	74,74,74,74	0
58	MG	2A	3571	1/1	0.92	0.21	53,53,53,53	0
58	MG	1A	3517	1/1	0.92	0.10	52,52,52,52	0
58	MG	1A	3905	1/1	0.92	0.14	46,46,46,46	0
58	MG	2A	3288	1/1	0.92	0.25	43,43,43,43	0
58	MG	2A	3289	1/1	0.92	0.23	53,53,53,53	0
58	MG	1B	201	1/1	0.92	0.19	62,62,62,62	0
58	MG	2A	3295	1/1	0.92	0.21	70,70,70,70	0
58	MG	1A	3907	1/1	0.92	0.11	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
58	MG	2A	3581	1/1	0.92	0.08	52,52,52,52	0
58	MG	1B	204	1/1	0.92	0.28	67,67,67,67	0
58	MG	1B	207	1/1	0.92	0.15	69,69,69,69	0
58	MG	1A	3519	1/1	0.92	0.35	56,56,56,56	0
58	MG	1A	3521	1/1	0.92	0.48	49,49,49,49	0
58	MG	2A	3592	1/1	0.92	0.14	61,61,61,61	0
58	MG	1A	3114	1/1	0.92	0.16	34,34,34,34	0
58	MG	1A	3917	1/1	0.92	0.09	42,42,42,42	0
58	MG	2A	3308	1/1	0.92	0.09	51,51,51,51	0
58	MG	1A	3437	1/1	0.92	0.28	38,38,38,38	0
58	MG	2A	3046	1/1	0.92	0.18	61,61,61,61	0
58	MG	1A	3715	1/1	0.92	0.08	53,53,53,53	0
58	MG	2A	3050	1/1	0.92	0.17	52,52,52,52	0
58	MG	2A	3316	1/1	0.92	0.17	60,60,60,60	0
58	MG	1A	3527	1/1	0.92	0.18	41,41,41,41	0
58	MG	1B	223	1/1	0.92	0.20	63,63,63,63	0
58	MG	1A	3439	1/1	0.92	0.24	39,39,39,39	0
58	MG	2A	3062	1/1	0.92	0.15	34,34,34,34	0
58	MG	2a	1758	1/1	0.92	0.07	50,50,50,50	0
58	MG	1A	3374	1/1	0.92	0.14	56,56,56,56	0
58	MG	1A	3333	1/1	0.92	0.26	52,52,52,52	0
58	MG	2A	3065	1/1	0.92	0.12	58,58,58,58	0
58	MG	2A	3067	1/1	0.92	0.12	52,52,52,52	0
58	MG	1a	1687	1/1	0.92	0.21	47,47,47,47	0
58	MG	1A	3929	1/1	0.92	0.09	47,47,47,47	0
58	MG	2A	3338	1/1	0.92	0.27	65,65,65,65	0
58	MG	2a	1769	1/1	0.92	0.10	76,76,76,76	0
58	MG	1A	3281	1/1	0.92	0.28	32,32,32,32	0
58	MG	1A	3738	1/1	0.92	0.14	65,65,65,65	0
58	MG	2A	3644	1/1	0.92	0.10	69,69,69,69	0
58	MG	1E	302	1/1	0.92	0.23	35,35,35,35	0
58	MG	1A	3543	1/1	0.92	0.23	38,38,38,38	0
58	MG	1A	3446	1/1	0.92	0.13	51,51,51,51	0
58	MG	1F	307	1/1	0.92	0.10	52,52,52,52	0
58	MG	2A	3347	1/1	0.92	0.11	53,53,53,53	0
58	MG	1a	1699	1/1	0.92	0.22	52,52,52,52	0
58	MG	2A	3659	1/1	0.92	0.10	56,56,56,56	0
58	MG	1A	3550	1/1	0.92	0.29	44,44,44,44	0
58	MG	1A	3285	1/1	0.92	0.15	45,45,45,45	0
58	MG	1A	3750	1/1	0.92	0.08	22,22,22,22	0
58	MG	1A	3247	1/1	0.92	0.17	54,54,54,54	0
58	MG	1A	3555	1/1	0.92	0.10	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
58	MG	2a	1793	1/1	0.92	0.14	76,76,76,76	0
58	MG	2A	3670	1/1	0.92	0.14	54,54,54,54	0
58	MG	1A	3556	1/1	0.92	0.10	52,52,52,52	0
58	MG	1A	3966	1/1	0.92	0.11	41,41,41,41	0
58	MG	1A	3454	1/1	0.92	0.21	59,59,59,59	0
58	MG	2A	3676	1/1	0.92	0.13	66,66,66,66	0
58	MG	1A	3971	1/1	0.92	0.08	65,65,65,65	0
58	MG	1A	3387	1/1	0.92	0.12	65,65,65,65	0
58	MG	1A	3761	1/1	0.92	0.10	53,53,53,53	0
58	MG	2a	1805	1/1	0.92	0.10	62,62,62,62	0
58	MG	2A	3114	1/1	0.92	0.15	49,49,49,49	0
58	MG	2A	3686	1/1	0.92	0.20	58,58,58,58	0
58	MG	1A	3976	1/1	0.92	0.11	76,76,76,76	0
58	MG	2a	1810	1/1	0.92	0.18	57,57,57,57	0
58	MG	1A	3567	1/1	0.92	0.20	46,46,46,46	0
58	MG	2B	203	1/1	0.92	0.17	59,59,59,59	0
58	MG	2A	3120	1/1	0.92	0.15	46,46,46,46	0
58	MG	2a	1814	1/1	0.92	0.13	68,68,68,68	0
58	MG	1R	205	1/1	0.92	0.11	32,32,32,32	0
58	MG	1A	3456	1/1	0.92	0.07	60,60,60,60	0
58	MG	1a	1724	1/1	0.92	0.18	59,59,59,59	0
58	MG	1A	3571	1/1	0.92	0.16	61,61,61,61	0
58	MG	2A	3129	1/1	0.92	0.12	58,58,58,58	0
58	MG	2A	3384	1/1	0.92	0.14	68,68,68,68	0
58	MG	1a	1733	1/1	0.92	0.14	59,59,59,59	0
58	MG	2A	3132	1/1	0.92	0.20	53,53,53,53	0
58	MG	2D	305	1/1	0.92	0.16	45,45,45,45	0
58	MG	1A	3982	1/1	0.92	0.10	29,29,29,29	0
58	MG	1A	3572	1/1	0.92	0.14	51,51,51,51	0
58	MG	1U	201	1/1	0.92	0.29	40,40,40,40	0
58	MG	2A	3397	1/1	0.92	0.21	45,45,45,45	0
58	MG	1A	3057	1/1	0.92	0.09	35,35,35,35	0
58	MG	1A	3460	1/1	0.92	0.17	63,63,63,63	0
58	MG	2A	3140	1/1	0.92	0.19	65,65,65,65	0
58	MG	2A	3403	1/1	0.92	0.16	60,60,60,60	0
58	MG	2O	201	1/1	0.92	0.12	61,61,61,61	0
58	MG	1a	1743	1/1	0.92	0.19	59,59,59,59	0
58	MG	1A	3461	1/1	0.92	0.25	54,54,54,54	0
58	MG	1A	3195	1/1	0.92	0.28	36,36,36,36	0
58	MG	2A	3408	1/1	0.92	0.10	52,52,52,52	0
58	MG	2A	3410	1/1	0.92	0.17	55,55,55,55	0
58	MG	1V	204	1/1	0.92	0.26	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
58	MG	1A	3197	1/1	0.92	0.36	34,34,34,34	0
58	MG	25	102	1/1	0.92	0.17	61,61,61,61	0
58	MG	27	102	1/1	0.92	0.08	49,49,49,49	0
58	MG	2A	3385	1/1	0.93	0.26	51,51,51,51	0
58	MG	1A	3962	1/1	0.93	0.09	44,44,44,44	0
58	MG	1A	3795	1/1	0.93	0.06	24,24,24,24	0
58	MG	1A	3089	1/1	0.93	0.26	41,41,41,41	0
58	MG	1A	3969	1/1	0.93	0.09	63,63,63,63	0
58	MG	1O	203	1/1	0.93	0.27	69,69,69,69	0
58	MG	2A	3396	1/1	0.93	0.19	55,55,55,55	0
58	MG	1A	3970	1/1	0.93	0.13	59,59,59,59	0
58	MG	2A	3398	1/1	0.93	0.26	63,63,63,63	0
58	MG	1A	3052	1/1	0.93	0.13	26,26,26,26	0
58	MG	2N	201	1/1	0.93	0.06	59,59,59,59	0
58	MG	1A	3802	1/1	0.93	0.11	24,24,24,24	0
58	MG	2A	3401	1/1	0.93	0.17	49,49,49,49	0
58	MG	1a	1725	1/1	0.93	0.13	55,55,55,55	0
58	MG	1A	3625	1/1	0.93	0.20	39,39,39,39	0
58	MG	2X	102	1/1	0.93	0.21	54,54,54,54	0
58	MG	2A	3146	1/1	0.93	0.10	59,59,59,59	0
58	MG	1A	3236	1/1	0.93	0.20	44,44,44,44	0
58	MG	1A	3389	1/1	0.93	0.39	71,71,71,71	0
58	MG	1A	3640	1/1	0.93	0.10	57,57,57,57	0
58	MG	1S	201	1/1	0.93	0.10	56,56,56,56	0
58	MG	25	104	1/1	0.93	0.15	59,59,59,59	0
58	MG	1A	3643	1/1	0.93	0.08	47,47,47,47	0
58	MG	2A	3418	1/1	0.93	0.15	59,59,59,59	0
58	MG	1A	3287	1/1	0.93	0.07	51,51,51,51	0
58	MG	2A	3423	1/1	0.93	0.21	58,58,58,58	0
58	MG	1A	3055	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	3990	1/1	0.93	0.10	59,59,59,59	0
58	MG	1A	3992	1/1	0.93	0.07	46,46,46,46	0
58	MG	1a	1749	1/1	0.93	0.19	44,44,44,44	0
58	MG	1a	1750	1/1	0.93	0.17	55,55,55,55	0
58	MG	1A	3246	1/1	0.93	0.10	48,48,48,48	0
58	MG	1a	1756	1/1	0.93	0.15	54,54,54,54	0
58	MG	1U	206	1/1	0.93	0.28	42,42,42,42	0
58	MG	1A	3400	1/1	0.93	0.12	56,56,56,56	0
58	MG	2A	3448	1/1	0.93	0.16	57,57,57,57	0
58	MG	1A	3125	1/1	0.93	0.16	47,47,47,47	0
58	MG	2a	1615	1/1	0.93	0.16	63,63,63,63	0
58	MG	2A	3450	1/1	0.93	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
58	MG	1a	1760	1/1	0.93	0.07	56,56,56,56	0
58	MG	1a	1761	1/1	0.93	0.13	66,66,66,66	0
58	MG	1A	3533	1/1	0.93	0.16	58,58,58,58	0
58	MG	1A	3818	1/1	0.93	0.10	50,50,50,50	0
58	MG	1A	4003	1/1	0.93	0.07	31,31,31,31	0
58	MG	2A	3183	1/1	0.93	0.10	57,57,57,57	0
58	MG	2A	3461	1/1	0.93	0.23	40,40,40,40	0
58	MG	1W	205	1/1	0.93	0.17	31,31,31,31	0
58	MG	1A	3153	1/1	0.93	0.35	30,30,30,30	0
58	MG	1A	3403	1/1	0.93	0.16	56,56,56,56	0
58	MG	1Y	201	1/1	0.93	0.10	54,54,54,54	0
58	MG	2a	1629	1/1	0.93	0.28	69,69,69,69	0
58	MG	2A	3190	1/1	0.93	0.07	63,63,63,63	0
58	MG	1A	3540	1/1	0.93	0.07	53,53,53,53	0
58	MG	2A	3192	1/1	0.93	0.14	59,59,59,59	0
58	MG	2a	1636	1/1	0.93	0.32	71,71,71,71	0
58	MG	2A	3193	1/1	0.93	0.13	62,62,62,62	0
58	MG	1A	3299	1/1	0.93	0.38	62,62,62,62	0
58	MG	1A	4011	1/1	0.93	0.12	57,57,57,57	0
58	MG	1A	3829	1/1	0.93	0.09	33,33,33,33	0
58	MG	1A	3196	1/1	0.93	0.17	32,32,32,32	0
58	MG	1A	3670	1/1	0.93	0.07	37,37,37,37	0
58	MG	10	106	1/1	0.93	0.10	48,48,48,48	0
58	MG	1A	3302	1/1	0.93	0.18	35,35,35,35	0
58	MG	1a	1787	1/1	0.93	0.11	58,58,58,58	0
58	MG	1A	3676	1/1	0.93	0.08	37,37,37,37	0
58	MG	1A	3467	1/1	0.93	0.23	56,56,56,56	0
58	MG	2A	3488	1/1	0.93	0.13	54,54,54,54	0
58	MG	2A	3489	1/1	0.93	0.15	54,54,54,54	0
58	MG	2a	1651	1/1	0.93	0.18	76,76,76,76	0
58	MG	2A	3490	1/1	0.93	0.20	44,44,44,44	0
58	MG	2A	3492	1/1	0.93	0.17	41,41,41,41	0
58	MG	11	102	1/1	0.93	0.20	51,51,51,51	0
58	MG	1A	3838	1/1	0.93	0.19	45,45,45,45	0
58	MG	1A	3303	1/1	0.93	0.17	40,40,40,40	0
58	MG	2A	3497	1/1	0.93	0.10	44,44,44,44	0
58	MG	1A	4026	1/1	0.93	0.07	43,43,43,43	0
58	MG	1A	3553	1/1	0.93	0.17	53,53,53,53	0
58	MG	1A	3470	1/1	0.93	0.18	41,41,41,41	0
58	MG	1A	4031	1/1	0.93	0.09	34,34,34,34	0
58	MG	2a	1665	1/1	0.93	0.13	62,62,62,62	0
58	MG	2A	3220	1/1	0.93	0.25	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
58	MG	1A	3410	1/1	0.93	0.13	51,51,51,51	0
58	MG	1A	3128	1/1	0.93	0.18	37,37,37,37	0
58	MG	2a	1670	1/1	0.93	0.13	60,60,60,60	0
58	MG	1A	3696	1/1	0.93	0.13	21,21,21,21	0
58	MG	2a	1672	1/1	0.93	0.08	75,75,75,75	0
58	MG	2A	3515	1/1	0.93	0.11	56,56,56,56	0
58	MG	2A	3227	1/1	0.93	0.23	61,61,61,61	0
58	MG	1A	3849	1/1	0.93	0.16	45,45,45,45	0
58	MG	1A	4037	1/1	0.93	0.17	39,39,39,39	0
58	MG	1A	4039	1/1	0.93	0.12	43,43,43,43	0
58	MG	2A	3231	1/1	0.93	0.23	54,54,54,54	0
58	MG	1A	3699	1/1	0.93	0.10	26,26,26,26	0
58	MG	2a	1681	1/1	0.93	0.29	63,63,63,63	0
58	MG	1a	1606	1/1	0.93	0.06	69,69,69,69	0
58	MG	1A	3701	1/1	0.93	0.09	32,32,32,32	0
58	MG	1A	3307	1/1	0.93	0.22	56,56,56,56	0
58	MG	2a	1687	1/1	0.93	0.21	42,42,42,42	0
58	MG	1n	102	1/1	0.93	0.21	54,54,54,54	0
58	MG	1A	3476	1/1	0.93	0.08	42,42,42,42	0
58	MG	2A	3240	1/1	0.93	0.14	60,60,60,60	0
58	MG	1A	3857	1/1	0.93	0.13	63,63,63,63	0
58	MG	1A	3712	1/1	0.93	0.10	49,49,49,49	0
58	MG	1a	1616	1/1	0.93	0.08	57,57,57,57	0
58	MG	1A	3859	1/1	0.93	0.08	32,32,32,32	0
58	MG	1A	3051	1/1	0.93	0.09	42,42,42,42	0
58	MG	1a	1620	1/1	0.93	0.06	45,45,45,45	0
58	MG	2A	3252	1/1	0.93	0.23	41,41,41,41	0
58	MG	2A	3253	1/1	0.93	0.20	45,45,45,45	0
58	MG	2A	3254	1/1	0.93	0.24	52,52,52,52	0
58	MG	2a	1704	1/1	0.93	0.22	63,63,63,63	0
58	MG	2A	3255	1/1	0.93	0.21	52,52,52,52	0
58	MG	2a	1707	1/1	0.93	0.11	75,75,75,75	0
58	MG	1A	3863	1/1	0.93	0.08	48,48,48,48	0
58	MG	1A	4062	1/1	0.93	0.16	70,70,70,70	0
58	MG	1A	3867	1/1	0.93	0.08	25,25,25,25	0
58	MG	1A	3570	1/1	0.93	0.14	43,43,43,43	0
58	MG	1A	3131	1/1	0.93	0.15	39,39,39,39	0
58	MG	1A	3259	1/1	0.93	0.23	40,40,40,40	0
58	MG	2a	1715	1/1	0.93	0.18	62,62,62,62	0
58	MG	1A	3482	1/1	0.93	0.13	52,52,52,52	0
58	MG	2a	1717	1/1	0.93	0.42	60,60,60,60	0
58	MG	1A	3721	1/1	0.93	0.10	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
58	MG	2A	3554	1/1	0.93	0.13	27,27,27,27	0
58	MG	2a	1720	1/1	0.93	0.24	51,51,51,51	0
58	MG	2a	1721	1/1	0.93	0.28	63,63,63,63	0
58	MG	2A	3556	1/1	0.93	0.12	38,38,38,38	0
58	MG	1A	3879	1/1	0.93	0.15	36,36,36,36	0
58	MG	1A	3132	1/1	0.93	0.09	64,64,64,64	0
58	MG	1A	3215	1/1	0.93	0.18	53,53,53,53	0
58	MG	1A	3218	1/1	0.93	0.24	49,49,49,49	0
58	MG	2A	3564	1/1	0.93	0.08	32,32,32,32	0
58	MG	1A	3732	1/1	0.93	0.18	58,58,58,58	0
58	MG	2A	3275	1/1	0.93	0.22	59,59,59,59	0
58	MG	2A	3568	1/1	0.93	0.10	63,63,63,63	0
58	MG	2A	3276	1/1	0.93	0.28	50,50,50,50	0
58	MG	1A	3733	1/1	0.93	0.16	64,64,64,64	0
58	MG	2A	3007	1/1	0.93	0.17	53,53,53,53	0
58	MG	2A	3279	1/1	0.93	0.20	54,54,54,54	0
58	MG	1A	3894	1/1	0.93	0.07	33,33,33,33	0
58	MG	2A	3282	1/1	0.93	0.21	58,58,58,58	0
58	MG	2A	3283	1/1	0.93	0.16	50,50,50,50	0
58	MG	2A	3014	1/1	0.93	0.15	48,48,48,48	0
58	MG	1A	3895	1/1	0.93	0.11	26,26,26,26	0
58	MG	1A	3364	1/1	0.93	0.24	47,47,47,47	0
58	MG	1A	3585	1/1	0.93	0.20	59,59,59,59	0
58	MG	2A	3585	1/1	0.93	0.17	41,41,41,41	0
58	MG	1A	3898	1/1	0.93	0.17	41,41,41,41	0
58	MG	2A	3589	1/1	0.93	0.17	47,47,47,47	0
58	MG	1a	1650	1/1	0.93	0.19	46,46,46,46	0
58	MG	1A	3902	1/1	0.93	0.15	63,63,63,63	0
58	MG	1a	1653	1/1	0.93	0.11	51,51,51,51	0
58	MG	1a	1655	1/1	0.93	0.22	59,59,59,59	0
58	MG	1A	4091	1/1	0.93	0.24	57,57,57,57	0
58	MG	1a	1657	1/1	0.93	0.09	63,63,63,63	0
58	MG	2A	3599	1/1	0.93	0.16	57,57,57,57	0
58	MG	1A	3903	1/1	0.93	0.12	53,53,53,53	0
58	MG	1A	3365	1/1	0.93	0.14	49,49,49,49	0
58	MG	1A	3906	1/1	0.93	0.35	31,31,31,31	0
58	MG	1A	3741	1/1	0.93	0.07	53,53,53,53	0
58	MG	1A	3742	1/1	0.93	0.08	43,43,43,43	0
58	MG	2A	3607	1/1	0.93	0.07	58,58,58,58	0
58	MG	2A	3609	1/1	0.93	0.12	79,79,79,79	0
58	MG	1A	3910	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3911	1/1	0.93	0.13	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
58	MG	2A	3314	1/1	0.93	0.27	58,58,58,58	0
58	MG	1A	3743	1/1	0.93	0.09	43,43,43,43	0
58	MG	1B	209	1/1	0.93	0.09	56,56,56,56	0
58	MG	2a	1782	1/1	0.93	0.14	67,67,67,67	0
58	MG	2A	3317	1/1	0.93	0.42	75,75,75,75	0
58	MG	2a	1784	1/1	0.93	0.14	73,73,73,73	0
58	MG	2A	3055	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	3425	1/1	0.93	0.12	59,59,59,59	0
58	MG	2A	3621	1/1	0.93	0.12	52,52,52,52	0
58	MG	1a	1668	1/1	0.93	0.15	62,62,62,62	0
58	MG	2A	3058	1/1	0.93	0.16	61,61,61,61	0
58	MG	2A	3059	1/1	0.93	0.10	46,46,46,46	0
58	MG	1A	3746	1/1	0.93	0.10	52,52,52,52	0
58	MG	1a	1670	1/1	0.93	0.17	64,64,64,64	0
58	MG	2A	3640	1/1	0.93	0.13	46,46,46,46	0
58	MG	1A	3087	1/1	0.93	0.18	32,32,32,32	0
58	MG	1A	3429	1/1	0.93	0.29	55,55,55,55	0
58	MG	2A	3646	1/1	0.93	0.08	62,62,62,62	0
58	MG	2A	3334	1/1	0.93	0.23	72,72,72,72	0
58	MG	2A	3650	1/1	0.93	0.07	74,74,74,74	0
58	MG	2A	3651	1/1	0.93	0.10	51,51,51,51	0
58	MG	1A	3099	1/1	0.93	0.08	39,39,39,39	0
58	MG	1A	3181	1/1	0.93	0.19	35,35,35,35	0
58	MG	1a	1675	1/1	0.93	0.18	46,46,46,46	0
58	MG	1B	219	1/1	0.93	0.06	43,43,43,43	0
58	MG	2a	1809	1/1	0.93	0.28	64,64,64,64	0
58	MG	1B	220	1/1	0.93	0.09	37,37,37,37	0
58	MG	1A	3136	1/1	0.93	0.14	38,38,38,38	0
58	MG	2A	3080	1/1	0.93	0.10	34,34,34,34	0
58	MG	1A	3137	1/1	0.93	0.09	39,39,39,39	0
58	MG	1a	1683	1/1	0.93	0.23	68,68,68,68	0
58	MG	1A	3272	1/1	0.93	0.13	54,54,54,54	0
58	MG	1A	3273	1/1	0.93	0.15	37,37,37,37	0
58	MG	1B	227	1/1	0.93	0.15	59,59,59,59	0
58	MG	1A	3380	1/1	0.93	0.10	48,48,48,48	0
58	MG	1a	1690	1/1	0.93	0.33	50,50,50,50	0
58	MG	1A	3440	1/1	0.93	0.09	40,40,40,40	0
58	MG	2A	3093	1/1	0.93	0.17	56,56,56,56	0
58	MG	1A	3944	1/1	0.93	0.07	53,53,53,53	0
58	MG	2A	3097	1/1	0.93	0.12	66,66,66,66	0
58	MG	2A	3683	1/1	0.93	0.12	67,67,67,67	0
58	MG	1A	3772	1/1	0.93	0.11	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
58	MG	1D	306	1/1	0.93	0.15	43,43,43,43	0
58	MG	2A	3687	1/1	0.93	0.13	62,62,62,62	0
58	MG	1D	309	1/1	0.93	0.13	51,51,51,51	0
58	MG	2I	202	1/1	0.93	0.12	67,67,67,67	0
58	MG	1A	3070	1/1	0.93	0.10	57,57,57,57	0
58	MG	1A	3385	1/1	0.93	0.11	63,63,63,63	0
58	MG	1A	3785	1/1	0.93	0.10	33,33,33,33	0
58	MG	2q	201	1/1	0.93	0.10	75,75,75,75	0
58	MG	1A	3791	1/1	0.93	0.06	30,30,30,30	0
58	MG	1A	3958	1/1	0.93	0.09	37,37,37,37	0
58	MG	1a	1706	1/1	0.93	0.15	45,45,45,45	0
58	MG	1F	312	1/1	0.93	0.07	49,49,49,49	0
58	MG	1A	3959	1/1	0.93	0.10	55,55,55,55	0
58	MG	1A	3792	1/1	0.93	0.06	50,50,50,50	0
58	MG	2B	211	1/1	0.93	0.18	66,66,66,66	0
58	MG	1A	3794	1/1	0.93	0.07	45,45,45,45	0
58	MG	2B	213	1/1	0.93	0.21	59,59,59,59	0
58	MG	2B	214	1/1	0.93	0.12	60,60,60,60	0
58	MG	2x	3306	1/1	0.93	0.17	71,71,71,71	0
58	MG	1A	3040	1/1	0.94	0.19	31,31,31,31	0
58	MG	1A	4044	1/1	0.94	0.08	18,18,18,18	0
58	MG	1A	4045	1/1	0.94	0.15	50,50,50,50	0
58	MG	1A	3565	1/1	0.94	0.10	41,41,41,41	0
58	MG	23	102	1/1	0.94	0.08	63,63,63,63	0
58	MG	1a	1771	1/1	0.94	0.18	65,65,65,65	0
58	MG	2A	3445	1/1	0.94	0.19	43,43,43,43	0
58	MG	1A	3727	1/1	0.94	0.09	22,22,22,22	0
58	MG	1A	3174	1/1	0.94	0.16	43,43,43,43	0
58	MG	2A	3182	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3073	1/1	0.94	0.23	32,32,32,32	0
58	MG	17	104	1/1	0.94	0.15	31,31,31,31	0
58	MG	18	101	1/1	0.94	0.25	52,52,52,52	0
58	MG	2A	3187	1/1	0.94	0.09	50,50,50,50	0
58	MG	18	102	1/1	0.94	0.25	38,38,38,38	0
58	MG	18	105	1/1	0.94	0.14	45,45,45,45	0
58	MG	1A	4051	1/1	0.94	0.15	53,53,53,53	0
58	MG	1A	3138	1/1	0.94	0.21	26,26,26,26	0
58	MG	1A	4057	1/1	0.94	0.06	25,25,25,25	0
58	MG	2a	1611	1/1	0.94	0.28	72,72,72,72	0
58	MG	1A	3885	1/1	0.94	0.07	28,28,28,28	0
58	MG	2A	3194	1/1	0.94	0.21	59,59,59,59	0
58	MG	1A	3886	1/1	0.94	0.09	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3196	1/1	0.94	0.09	49,49,49,49	0
58	MG	1a	1795	1/1	0.94	0.07	77,77,77,77	0
58	MG	1A	3887	1/1	0.94	0.12	28,28,28,28	0
58	MG	1A	3474	1/1	0.94	0.22	55,55,55,55	0
58	MG	1A	4068	1/1	0.94	0.10	43,43,43,43	0
58	MG	1A	3475	1/1	0.94	0.07	49,49,49,49	0
58	MG	1a	1609	1/1	0.94	0.13	59,59,59,59	0
58	MG	1A	3094	1/1	0.94	0.09	46,46,46,46	0
58	MG	1A	3574	1/1	0.94	0.07	53,53,53,53	0
58	MG	2A	3206	1/1	0.94	0.18	58,58,58,58	0
58	MG	1A	3576	1/1	0.94	0.08	41,41,41,41	0
58	MG	1A	3241	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3901	1/1	0.94	0.08	59,59,59,59	0
58	MG	2A	3210	1/1	0.94	0.09	71,71,71,71	0
58	MG	1A	3478	1/1	0.94	0.17	62,62,62,62	0
58	MG	2A	3212	1/1	0.94	0.07	52,52,52,52	0
58	MG	1A	3187	1/1	0.94	0.07	45,45,45,45	0
58	MG	1A	3744	1/1	0.94	0.08	46,46,46,46	0
58	MG	1A	4080	1/1	0.94	0.19	46,46,46,46	0
58	MG	2A	3218	1/1	0.94	0.22	52,52,52,52	0
58	MG	1e	202	1/1	0.94	0.19	60,60,60,60	0
58	MG	1f	201	1/1	0.94	0.13	51,51,51,51	0
58	MG	1A	3582	1/1	0.94	0.18	53,53,53,53	0
58	MG	2A	3500	1/1	0.94	0.09	36,36,36,36	0
58	MG	1k	201	1/1	0.94	0.19	58,58,58,58	0
58	MG	2A	3223	1/1	0.94	0.11	61,61,61,61	0
58	MG	2A	3224	1/1	0.94	0.17	58,58,58,58	0
58	MG	1A	3140	1/1	0.94	0.10	48,48,48,48	0
58	MG	2A	3226	1/1	0.94	0.09	44,44,44,44	0
58	MG	1a	1625	1/1	0.94	0.20	56,56,56,56	0
58	MG	1A	3481	1/1	0.94	0.15	47,47,47,47	0
58	MG	2a	1650	1/1	0.94	0.07	83,83,83,83	0
58	MG	1A	3748	1/1	0.94	0.12	31,31,31,31	0
58	MG	1A	3749	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	3353	1/1	0.94	0.17	36,36,36,36	0
58	MG	1A	3141	1/1	0.94	0.18	37,37,37,37	0
58	MG	1a	1633	1/1	0.94	0.23	57,57,57,57	0
58	MG	1A	3916	1/1	0.94	0.09	26,26,26,26	0
58	MG	1A	3026	1/1	0.94	0.13	40,40,40,40	0
58	MG	1a	1637	1/1	0.94	0.21	51,51,51,51	0
58	MG	2a	1659	1/1	0.94	0.13	47,47,47,47	0
58	MG	1A	3918	1/1	0.94	0.14	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1661	1/1	0.94	0.09	62,62,62,62	0
58	MG	1A	3755	1/1	0.94	0.10	45,45,45,45	0
58	MG	1A	3356	1/1	0.94	0.09	49,49,49,49	0
58	MG	1A	3590	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3145	1/1	0.94	0.14	62,62,62,62	0
58	MG	2A	3532	1/1	0.94	0.18	57,57,57,57	0
58	MG	2A	3245	1/1	0.94	0.15	64,64,64,64	0
58	MG	1A	3308	1/1	0.94	0.29	45,45,45,45	0
58	MG	1A	3252	1/1	0.94	0.25	36,36,36,36	0
58	MG	2A	3537	1/1	0.94	0.12	55,55,55,55	0
58	MG	2a	1673	1/1	0.94	0.13	67,67,67,67	0
58	MG	1A	3765	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3080	1/1	0.94	0.10	38,38,38,38	0
58	MG	1A	3313	1/1	0.94	0.14	52,52,52,52	0
58	MG	1A	3497	1/1	0.94	0.10	49,49,49,49	0
58	MG	2A	3002	1/1	0.94	0.15	59,59,59,59	0
58	MG	2A	3003	1/1	0.94	0.23	53,53,53,53	0
58	MG	1A	3498	1/1	0.94	0.06	39,39,39,39	0
58	MG	1B	214	1/1	0.94	0.15	57,57,57,57	0
58	MG	1A	3428	1/1	0.94	0.08	47,47,47,47	0
58	MG	2A	3009	1/1	0.94	0.08	48,48,48,48	0
58	MG	2a	1685	1/1	0.94	0.24	74,74,74,74	0
58	MG	1A	3788	1/1	0.94	0.08	19,19,19,19	0
58	MG	1A	3314	1/1	0.94	0.16	47,47,47,47	0
58	MG	2a	1688	1/1	0.94	0.33	57,57,57,57	0
58	MG	1A	3613	1/1	0.94	0.10	24,24,24,24	0
58	MG	1A	3004	1/1	0.94	0.04	24,24,24,24	0
58	MG	1A	3957	1/1	0.94	0.12	54,54,54,54	0
58	MG	1A	3318	1/1	0.94	0.10	44,44,44,44	0
58	MG	1A	3257	1/1	0.94	0.07	56,56,56,56	0
58	MG	2A	3272	1/1	0.94	0.35	55,55,55,55	0
58	MG	1A	3150	1/1	0.94	0.11	42,42,42,42	0
58	MG	2A	3030	1/1	0.94	0.09	31,31,31,31	0
58	MG	1A	3624	1/1	0.94	0.13	15,15,15,15	0
58	MG	1A	3321	1/1	0.94	0.22	35,35,35,35	0
58	MG	1A	3963	1/1	0.94	0.08	62,62,62,62	0
58	MG	1B	232	1/1	0.94	0.09	53,53,53,53	0
58	MG	2A	3280	1/1	0.94	0.15	50,50,50,50	0
58	MG	2a	1705	1/1	0.94	0.09	81,81,81,81	0
58	MG	1A	3964	1/1	0.94	0.12	47,47,47,47	0
58	MG	2A	3038	1/1	0.94	0.13	45,45,45,45	0
58	MG	2A	3039	1/1	0.94	0.25	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
58	MG	1D	301	1/1	0.94	0.31	34,34,34,34	0
58	MG	1A	3377	1/1	0.94	0.34	46,46,46,46	0
58	MG	1A	3630	1/1	0.94	0.11	42,42,42,42	0
58	MG	2A	3044	1/1	0.94	0.13	53,53,53,53	0
58	MG	1D	310	1/1	0.94	0.07	40,40,40,40	0
58	MG	2A	3290	1/1	0.94	0.16	47,47,47,47	0
58	MG	2A	3580	1/1	0.94	0.12	59,59,59,59	0
58	MG	2A	3291	1/1	0.94	0.11	50,50,50,50	0
58	MG	1A	3631	1/1	0.94	0.11	49,49,49,49	0
58	MG	2A	3047	1/1	0.94	0.17	58,58,58,58	0
58	MG	1E	307	1/1	0.94	0.08	54,54,54,54	0
58	MG	1a	1676	1/1	0.94	0.20	65,65,65,65	0
58	MG	2A	3301	1/1	0.94	0.08	46,46,46,46	0
58	MG	1a	1677	1/1	0.94	0.19	54,54,54,54	0
58	MG	1A	3438	1/1	0.94	0.12	42,42,42,42	0
58	MG	1A	3635	1/1	0.94	0.05	26,26,26,26	0
58	MG	1F	301	1/1	0.94	0.10	33,33,33,33	0
58	MG	1F	305	1/1	0.94	0.17	34,34,34,34	0
58	MG	2A	3598	1/1	0.94	0.14	73,73,73,73	0
58	MG	1A	3020	1/1	0.94	0.09	39,39,39,39	0
58	MG	2a	1730	1/1	0.94	0.30	68,68,68,68	0
58	MG	2a	1731	1/1	0.94	0.26	69,69,69,69	0
58	MG	1A	3642	1/1	0.94	0.06	26,26,26,26	0
58	MG	1a	1685	1/1	0.94	0.05	62,62,62,62	0
58	MG	1A	3084	1/1	0.94	0.27	38,38,38,38	0
58	MG	2A	3604	1/1	0.94	0.08	49,49,49,49	0
58	MG	1A	3030	1/1	0.94	0.07	41,41,41,41	0
58	MG	1A	3518	1/1	0.94	0.11	43,43,43,43	0
58	MG	1A	3208	1/1	0.94	0.14	55,55,55,55	0
58	MG	2A	3608	1/1	0.94	0.12	59,59,59,59	0
58	MG	1A	3444	1/1	0.94	0.14	65,65,65,65	0
58	MG	1A	3382	1/1	0.94	0.21	56,56,56,56	0
58	MG	2A	3077	1/1	0.94	0.07	51,51,51,51	0
58	MG	1A	3987	1/1	0.94	0.11	36,36,36,36	0
58	MG	1A	3989	1/1	0.94	0.09	55,55,55,55	0
58	MG	1A	3524	1/1	0.94	0.23	40,40,40,40	0
58	MG	1A	3826	1/1	0.94	0.06	29,29,29,29	0
58	MG	2A	3617	1/1	0.94	0.06	48,48,48,48	0
58	MG	2a	1755	1/1	0.94	0.15	66,66,66,66	0
58	MG	2A	3082	1/1	0.94	0.14	64,64,64,64	0
58	MG	2a	1757	1/1	0.94	0.18	67,67,67,67	0
58	MG	1A	3158	1/1	0.94	0.23	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3084	1/1	0.94	0.17	55,55,55,55	0
58	MG	1A	3213	1/1	0.94	0.15	45,45,45,45	0
58	MG	1A	3160	1/1	0.94	0.13	55,55,55,55	0
58	MG	1Q	202	1/1	0.94	0.19	38,38,38,38	0
58	MG	1Q	206	1/1	0.94	0.07	45,45,45,45	0
58	MG	2A	3635	1/1	0.94	0.10	52,52,52,52	0
58	MG	2A	3637	1/1	0.94	0.09	57,57,57,57	0
58	MG	1Q	207	1/1	0.94	0.09	36,36,36,36	0
58	MG	1A	3105	1/1	0.94	0.17	38,38,38,38	0
58	MG	2A	3642	1/1	0.94	0.11	43,43,43,43	0
58	MG	2a	1773	1/1	0.94	0.12	60,60,60,60	0
58	MG	2a	1774	1/1	0.94	0.10	60,60,60,60	0
58	MG	1A	3668	1/1	0.94	0.07	28,28,28,28	0
58	MG	1a	1710	1/1	0.94	0.16	47,47,47,47	0
58	MG	1a	1711	1/1	0.94	0.37	66,66,66,66	0
58	MG	1A	3532	1/1	0.94	0.21	45,45,45,45	0
58	MG	2A	3100	1/1	0.94	0.09	69,69,69,69	0
58	MG	2A	3349	1/1	0.94	0.10	41,41,41,41	0
58	MG	2A	3101	1/1	0.94	0.19	49,49,49,49	0
58	MG	1a	1713	1/1	0.94	0.06	47,47,47,47	0
58	MG	2A	3354	1/1	0.94	0.17	62,62,62,62	0
58	MG	2A	3103	1/1	0.94	0.11	61,61,61,61	0
58	MG	2a	1786	1/1	0.94	0.24	60,60,60,60	0
58	MG	1A	3165	1/1	0.94	0.19	49,49,49,49	0
58	MG	1A	4005	1/1	0.94	0.08	19,19,19,19	0
58	MG	2A	3662	1/1	0.94	0.12	57,57,57,57	0
58	MG	1A	3064	1/1	0.94	0.10	42,42,42,42	0
58	MG	2a	1791	1/1	0.94	0.15	60,60,60,60	0
58	MG	1A	3536	1/1	0.94	0.19	58,58,58,58	0
58	MG	1A	3457	1/1	0.94	0.20	47,47,47,47	0
58	MG	2a	1794	1/1	0.94	0.10	58,58,58,58	0
58	MG	1A	3391	1/1	0.94	0.19	43,43,43,43	0
58	MG	2A	3117	1/1	0.94	0.23	47,47,47,47	0
58	MG	1A	3541	1/1	0.94	0.26	54,54,54,54	0
58	MG	1A	3542	1/1	0.94	0.28	36,36,36,36	0
58	MG	1A	3223	1/1	0.94	0.13	51,51,51,51	0
58	MG	1a	1728	1/1	0.94	0.07	58,58,58,58	0
58	MG	2A	3677	1/1	0.94	0.13	69,69,69,69	0
58	MG	2A	3372	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3224	1/1	0.94	0.09	53,53,53,53	0
58	MG	2A	3681	1/1	0.94	0.13	53,53,53,53	0
58	MG	1V	201	1/1	0.94	0.41	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3549	1/1	0.94	0.16	35,35,35,35	0
58	MG	2A	3684	1/1	0.94	0.18	50,50,50,50	0
58	MG	1A	3397	1/1	0.94	0.09	53,53,53,53	0
58	MG	1a	1736	1/1	0.94	0.09	46,46,46,46	0
58	MG	2A	3133	1/1	0.94	0.19	38,38,38,38	0
58	MG	1A	3398	1/1	0.94	0.06	48,48,48,48	0
58	MG	1a	1738	1/1	0.94	0.15	54,54,54,54	0
58	MG	1A	4024	1/1	0.94	0.10	48,48,48,48	0
58	MG	1A	3703	1/1	0.94	0.14	35,35,35,35	0
58	MG	1W	207	1/1	0.94	0.12	55,55,55,55	0
58	MG	1a	1744	1/1	0.94	0.10	54,54,54,54	0
58	MG	2A	3142	1/1	0.94	0.16	55,55,55,55	0
58	MG	2A	3145	1/1	0.94	0.17	61,61,61,61	0
58	MG	1a	1745	1/1	0.94	0.17	59,59,59,59	0
58	MG	1A	3108	1/1	0.94	0.13	33,33,33,33	0
58	MG	1X	102	1/1	0.94	0.11	35,35,35,35	0
58	MG	2e	201	1/1	0.94	0.06	74,74,74,74	0
58	MG	1A	3337	1/1	0.94	0.08	49,49,49,49	0
58	MG	1A	3709	1/1	0.94	0.08	44,44,44,44	0
58	MG	1A	3711	1/1	0.94	0.13	40,40,40,40	0
58	MG	1a	1752	1/1	0.94	0.28	66,66,66,66	0
58	MG	1A	3001	1/1	0.94	0.08	37,37,37,37	0
58	MG	1A	3229	1/1	0.94	0.09	52,52,52,52	0
58	MG	1A	3868	1/1	0.94	0.20	54,54,54,54	0
58	MG	1A	3560	1/1	0.94	0.08	53,53,53,53	0
58	MG	1A	3562	1/1	0.94	0.10	45,45,45,45	0
58	MG	2A	3411	1/1	0.94	0.13	24,24,24,24	0
58	MG	2A	3412	1/1	0.94	0.27	56,56,56,56	0
58	MG	2A	3163	1/1	0.94	0.20	42,42,42,42	0
58	MG	2A	3164	1/1	0.94	0.09	50,50,50,50	0
58	MG	1A	3872	1/1	0.94	0.18	37,37,37,37	0
58	MG	2A	3170	1/1	0.94	0.13	55,55,55,55	0
58	MG	1A	3717	1/1	0.94	0.12	51,51,51,51	0
58	MG	2Q	202	1/1	0.94	0.11	49,49,49,49	0
58	MG	2R	201	1/1	0.94	0.17	32,32,32,32	0
58	MG	1A	3563	1/1	0.94	0.21	43,43,43,43	0
58	MG	2A	3431	1/1	0.94	0.16	56,56,56,56	0
58	MG	2A	3173	1/1	0.94	0.10	60,60,60,60	0
59	K	2x	3301	1/1	0.94	0.08	59,59,59,59	0
61	ZN	14	102	1/1	0.94	0.11	121,121,121,121	0
61	ZN	24	501	1/1	0.94	0.12	136,136,136,136	0
58	MG	1a	1608	1/1	0.95	0.09	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
58	MG	1A	3932	1/1	0.95	0.06	53,53,53,53	0
58	MG	2F	304	1/1	0.95	0.11	55,55,55,55	0
58	MG	2A	3420	1/1	0.95	0.07	45,45,45,45	0
58	MG	2A	3421	1/1	0.95	0.10	36,36,36,36	0
58	MG	2A	3422	1/1	0.95	0.12	63,63,63,63	0
58	MG	2Q	201	1/1	0.95	0.10	64,64,64,64	0
58	MG	1a	1798	1/1	0.95	0.09	59,59,59,59	0
58	MG	2A	3425	1/1	0.95	0.11	46,46,46,46	0
58	MG	2T	201	1/1	0.95	0.11	60,60,60,60	0
58	MG	2T	202	1/1	0.95	0.13	60,60,60,60	0
58	MG	1A	3936	1/1	0.95	0.06	39,39,39,39	0
58	MG	1A	3161	1/1	0.95	0.09	32,32,32,32	0
58	MG	2A	3430	1/1	0.95	0.09	34,34,34,34	0
58	MG	1A	3939	1/1	0.95	0.12	40,40,40,40	0
58	MG	1A	3162	1/1	0.95	0.23	38,38,38,38	0
58	MG	1a	1807	1/1	0.95	0.23	64,64,64,64	0
58	MG	1A	3100	1/1	0.95	0.12	25,25,25,25	0
58	MG	1A	3043	1/1	0.95	0.21	34,34,34,34	0
58	MG	25	101	1/1	0.95	0.38	49,49,49,49	0
58	MG	2A	3437	1/1	0.95	0.13	38,38,38,38	0
58	MG	1a	1618	1/1	0.95	0.06	52,52,52,52	0
58	MG	27	101	1/1	0.95	0.16	49,49,49,49	0
58	MG	2A	3443	1/1	0.95	0.13	47,47,47,47	0
58	MG	1A	3495	1/1	0.95	0.06	51,51,51,51	0
58	MG	1A	3496	1/1	0.95	0.19	47,47,47,47	0
58	MG	1A	3678	1/1	0.95	0.10	24,24,24,24	0
58	MG	1A	4096	1/1	0.95	0.14	46,46,46,46	0
58	MG	1d	302	1/1	0.95	0.18	50,50,50,50	0
58	MG	1A	3680	1/1	0.95	0.10	23,23,23,23	0
58	MG	2A	3451	1/1	0.95	0.25	58,58,58,58	0
58	MG	1A	3124	1/1	0.95	0.17	43,43,43,43	0
58	MG	1B	203	1/1	0.95	0.13	49,49,49,49	0
58	MG	1A	3202	1/1	0.95	0.14	26,26,26,26	0
58	MG	1a	1628	1/1	0.95	0.20	56,56,56,56	0
58	MG	2A	3197	1/1	0.95	0.24	58,58,58,58	0
58	MG	1B	205	1/1	0.95	0.06	51,51,51,51	0
58	MG	1B	206	1/1	0.95	0.17	46,46,46,46	0
58	MG	1A	3500	1/1	0.95	0.07	48,48,48,48	0
58	MG	1A	3687	1/1	0.95	0.05	32,32,32,32	0
58	MG	1A	3143	1/1	0.95	0.17	16,16,16,16	0
58	MG	1a	1635	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3690	1/1	0.95	0.06	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3575	1/1	0.95	0.07	52,52,52,52	0
58	MG	1A	3694	1/1	0.95	0.06	33,33,33,33	0
58	MG	1A	3206	1/1	0.95	0.13	27,27,27,27	0
58	MG	1A	3344	1/1	0.95	0.30	46,46,46,46	0
58	MG	1A	3447	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	3345	1/1	0.95	0.20	40,40,40,40	0
58	MG	2A	3478	1/1	0.95	0.13	60,60,60,60	0
58	MG	1A	3702	1/1	0.95	0.06	29,29,29,29	0
58	MG	2A	3480	1/1	0.95	0.12	50,50,50,50	0
58	MG	1B	221	1/1	0.95	0.07	39,39,39,39	0
58	MG	2a	1630	1/1	0.95	0.20	49,49,49,49	0
58	MG	2a	1631	1/1	0.95	0.30	54,54,54,54	0
58	MG	2a	1632	1/1	0.95	0.31	55,55,55,55	0
58	MG	2A	3213	1/1	0.95	0.08	41,41,41,41	0
58	MG	1x	103	1/1	0.95	0.23	63,63,63,63	0
58	MG	1a	1646	1/1	0.95	0.13	49,49,49,49	0
58	MG	1A	3581	1/1	0.95	0.20	28,28,28,28	0
58	MG	1A	3015	1/1	0.95	0.09	40,40,40,40	0
58	MG	1B	224	1/1	0.95	0.09	47,47,47,47	0
58	MG	1x	108	1/1	0.95	0.10	27,27,27,27	0
58	MG	1A	3209	1/1	0.95	0.14	43,43,43,43	0
58	MG	1A	3210	1/1	0.95	0.08	56,56,56,56	0
58	MG	1a	1654	1/1	0.95	0.17	47,47,47,47	0
58	MG	2A	3001	1/1	0.95	0.17	51,51,51,51	0
58	MG	1A	3841	1/1	0.95	0.24	66,66,66,66	0
58	MG	1A	3254	1/1	0.95	0.07	48,48,48,48	0
58	MG	2A	3498	1/1	0.95	0.07	39,39,39,39	0
58	MG	2A	3004	1/1	0.95	0.29	57,57,57,57	0
58	MG	1A	3068	1/1	0.95	0.10	38,38,38,38	0
58	MG	1A	3981	1/1	0.95	0.05	54,54,54,54	0
58	MG	1A	3171	1/1	0.95	0.18	58,58,58,58	0
58	MG	1A	3516	1/1	0.95	0.09	74,74,74,74	0
58	MG	2A	3011	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3233	1/1	0.95	0.16	40,40,40,40	0
58	MG	2A	3510	1/1	0.95	0.09	37,37,37,37	0
58	MG	2A	3511	1/1	0.95	0.10	61,61,61,61	0
58	MG	1A	3986	1/1	0.95	0.10	34,34,34,34	0
58	MG	1D	304	1/1	0.95	0.17	33,33,33,33	0
58	MG	1A	3173	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3988	1/1	0.95	0.08	47,47,47,47	0
58	MG	2A	3020	1/1	0.95	0.22	44,44,44,44	0
58	MG	2A	3519	1/1	0.95	0.26	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
58	MG	1A	3848	1/1	0.95	0.12	51,51,51,51	0
58	MG	1A	3407	1/1	0.95	0.17	49,49,49,49	0
58	MG	2A	3024	1/1	0.95	0.08	51,51,51,51	0
58	MG	1A	3991	1/1	0.95	0.16	38,38,38,38	0
58	MG	1A	3850	1/1	0.95	0.10	50,50,50,50	0
58	MG	1A	3312	1/1	0.95	0.13	41,41,41,41	0
58	MG	1E	313	1/1	0.95	0.15	44,44,44,44	0
58	MG	1A	3409	1/1	0.95	0.08	48,48,48,48	0
58	MG	2A	3251	1/1	0.95	0.19	68,68,68,68	0
58	MG	2A	3529	1/1	0.95	0.07	37,37,37,37	0
58	MG	2A	3530	1/1	0.95	0.09	54,54,54,54	0
58	MG	1F	304	1/1	0.95	0.05	42,42,42,42	0
58	MG	1A	3853	1/1	0.95	0.09	52,52,52,52	0
58	MG	2A	3035	1/1	0.95	0.16	54,54,54,54	0
58	MG	1A	3216	1/1	0.95	0.06	47,47,47,47	0
58	MG	1F	309	1/1	0.95	0.09	47,47,47,47	0
58	MG	2A	3536	1/1	0.95	0.10	49,49,49,49	0
58	MG	1A	3855	1/1	0.95	0.07	17,17,17,17	0
58	MG	1F	311	1/1	0.95	0.13	28,28,28,28	0
58	MG	2a	1683	1/1	0.95	0.17	60,60,60,60	0
58	MG	1A	4002	1/1	0.95	0.06	32,32,32,32	0
58	MG	2A	3262	1/1	0.95	0.09	40,40,40,40	0
58	MG	2A	3042	1/1	0.95	0.16	69,69,69,69	0
58	MG	1a	1679	1/1	0.95	0.18	69,69,69,69	0
58	MG	1G	201	1/1	0.95	0.12	42,42,42,42	0
58	MG	1A	3722	1/1	0.95	0.09	44,44,44,44	0
58	MG	1A	3598	1/1	0.95	0.12	39,39,39,39	0
58	MG	1A	3019	1/1	0.95	0.17	42,42,42,42	0
58	MG	1A	3525	1/1	0.95	0.16	40,40,40,40	0
58	MG	2A	3049	1/1	0.95	0.06	44,44,44,44	0
58	MG	1A	3466	1/1	0.95	0.11	60,60,60,60	0
58	MG	2A	3051	1/1	0.95	0.18	55,55,55,55	0
58	MG	2A	3274	1/1	0.95	0.19	55,55,55,55	0
58	MG	2A	3052	1/1	0.95	0.16	50,50,50,50	0
58	MG	1A	3606	1/1	0.95	0.13	28,28,28,28	0
58	MG	1A	4010	1/1	0.95	0.12	40,40,40,40	0
58	MG	2a	1702	1/1	0.95	0.16	55,55,55,55	0
58	MG	1A	3607	1/1	0.95	0.17	48,48,48,48	0
58	MG	1A	3358	1/1	0.95	0.16	49,49,49,49	0
58	MG	1A	4013	1/1	0.95	0.08	46,46,46,46	0
58	MG	2A	3561	1/1	0.95	0.13	61,61,61,61	0
58	MG	1P	201	1/1	0.95	0.21	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
58	MG	1A	3262	1/1	0.95	0.18	60,60,60,60	0
58	MG	1P	203	1/1	0.95	0.15	35,35,35,35	0
58	MG	1P	204	1/1	0.95	0.24	35,35,35,35	0
58	MG	1A	3612	1/1	0.95	0.08	48,48,48,48	0
58	MG	2a	1712	1/1	0.95	0.16	58,58,58,58	0
58	MG	2A	3286	1/1	0.95	0.17	48,48,48,48	0
58	MG	2A	3066	1/1	0.95	0.10	46,46,46,46	0
58	MG	1A	3219	1/1	0.95	0.29	43,43,43,43	0
58	MG	1Q	205	1/1	0.95	0.10	53,53,53,53	0
58	MG	2A	3072	1/1	0.95	0.07	43,43,43,43	0
58	MG	2A	3575	1/1	0.95	0.11	56,56,56,56	0
58	MG	1a	1702	1/1	0.95	0.07	51,51,51,51	0
58	MG	1A	3873	1/1	0.95	0.10	36,36,36,36	0
58	MG	2A	3076	1/1	0.95	0.12	50,50,50,50	0
58	MG	1A	3615	1/1	0.95	0.10	24,24,24,24	0
58	MG	2A	3297	1/1	0.95	0.13	51,51,51,51	0
58	MG	1A	4019	1/1	0.95	0.16	45,45,45,45	0
58	MG	1A	4020	1/1	0.95	0.08	41,41,41,41	0
58	MG	2A	3583	1/1	0.95	0.19	51,51,51,51	0
58	MG	1A	3531	1/1	0.95	0.12	34,34,34,34	0
58	MG	1A	4023	1/1	0.95	0.16	24,24,24,24	0
58	MG	2A	3588	1/1	0.95	0.18	60,60,60,60	0
58	MG	1A	3017	1/1	0.95	0.12	65,65,65,65	0
58	MG	1A	3182	1/1	0.95	0.24	54,54,54,54	0
58	MG	1A	3222	1/1	0.95	0.09	47,47,47,47	0
58	MG	1A	3620	1/1	0.95	0.14	47,47,47,47	0
58	MG	2A	3087	1/1	0.95	0.15	49,49,49,49	0
58	MG	2A	3594	1/1	0.95	0.07	66,66,66,66	0
58	MG	2a	1736	1/1	0.95	0.24	54,54,54,54	0
58	MG	2A	3310	1/1	0.95	0.20	54,54,54,54	0
58	MG	2a	1738	1/1	0.95	0.16	60,60,60,60	0
58	MG	1A	3882	1/1	0.95	0.09	58,58,58,58	0
58	MG	1A	3267	1/1	0.95	0.17	44,44,44,44	0
58	MG	1A	3268	1/1	0.95	0.15	45,45,45,45	0
58	MG	1A	3091	1/1	0.95	0.12	38,38,38,38	0
58	MG	1U	209	1/1	0.95	0.42	42,42,42,42	0
58	MG	1U	211	1/1	0.95	0.27	40,40,40,40	0
58	MG	2A	3094	1/1	0.95	0.11	43,43,43,43	0
58	MG	1A	3752	1/1	0.95	0.06	47,47,47,47	0
58	MG	1A	3060	1/1	0.95	0.11	41,41,41,41	0
58	MG	2A	3098	1/1	0.95	0.14	58,58,58,58	0
58	MG	1A	3078	1/1	0.95	0.23	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1V	206	1/1	0.95	0.14	63,63,63,63	0
58	MG	2A	3329	1/1	0.95	0.25	57,57,57,57	0
58	MG	1A	3891	1/1	0.95	0.11	25,25,25,25	0
58	MG	1A	3893	1/1	0.95	0.09	23,23,23,23	0
58	MG	1A	4041	1/1	0.95	0.09	25,25,25,25	0
58	MG	2A	3104	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3226	1/1	0.95	0.12	40,40,40,40	0
58	MG	2A	3616	1/1	0.95	0.09	49,49,49,49	0
58	MG	1A	3544	1/1	0.95	0.28	50,50,50,50	0
58	MG	2A	3618	1/1	0.95	0.12	54,54,54,54	0
58	MG	1A	3636	1/1	0.95	0.11	29,29,29,29	0
58	MG	2A	3110	1/1	0.95	0.17	36,36,36,36	0
58	MG	1A	3759	1/1	0.95	0.15	30,30,30,30	0
58	MG	1X	105	1/1	0.95	0.09	47,47,47,47	0
58	MG	2a	1772	1/1	0.95	0.22	64,64,64,64	0
58	MG	2A	3625	1/1	0.95	0.06	39,39,39,39	0
58	MG	1A	3061	1/1	0.95	0.15	51,51,51,51	0
58	MG	2A	3344	1/1	0.95	0.27	61,61,61,61	0
58	MG	2A	3629	1/1	0.95	0.13	50,50,50,50	0
58	MG	2A	3631	1/1	0.95	0.11	49,49,49,49	0
58	MG	1A	3062	1/1	0.95	0.06	42,42,42,42	0
58	MG	2A	3346	1/1	0.95	0.08	45,45,45,45	0
58	MG	2A	3636	1/1	0.95	0.05	50,50,50,50	0
58	MG	2A	3118	1/1	0.95	0.06	36,36,36,36	0
58	MG	1A	3762	1/1	0.95	0.12	47,47,47,47	0
58	MG	1A	3279	1/1	0.95	0.28	37,37,37,37	0
58	MG	2A	3641	1/1	0.95	0.12	61,61,61,61	0
58	MG	1A	3332	1/1	0.95	0.15	51,51,51,51	0
58	MG	10	103	1/1	0.95	0.07	40,40,40,40	0
58	MG	2A	3123	1/1	0.95	0.13	52,52,52,52	0
58	MG	2A	3124	1/1	0.95	0.06	57,57,57,57	0
58	MG	2A	3125	1/1	0.95	0.11	45,45,45,45	0
58	MG	1a	1748	1/1	0.95	0.20	48,48,48,48	0
58	MG	1A	3484	1/1	0.95	0.08	47,47,47,47	0
58	MG	1A	4054	1/1	0.95	0.13	14,14,14,14	0
58	MG	2A	3653	1/1	0.95	0.08	37,37,37,37	0
58	MG	2A	3130	1/1	0.95	0.08	46,46,46,46	0
58	MG	1A	4056	1/1	0.95	0.13	51,51,51,51	0
58	MG	2a	1797	1/1	0.95	0.24	56,56,56,56	0
58	MG	1A	3768	1/1	0.95	0.10	40,40,40,40	0
58	MG	2A	3365	1/1	0.95	0.14	63,63,63,63	0
58	MG	1A	3646	1/1	0.95	0.07	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3647	1/1	0.95	0.08	19,19,19,19	0
58	MG	2A	3368	1/1	0.95	0.17	51,51,51,51	0
58	MG	1A	3774	1/1	0.95	0.09	31,31,31,31	0
58	MG	1A	3485	1/1	0.95	0.26	68,68,68,68	0
58	MG	2A	3667	1/1	0.95	0.09	67,67,67,67	0
58	MG	12	101	1/1	0.95	0.14	48,48,48,48	0
58	MG	1A	4065	1/1	0.95	0.12	37,37,37,37	0
58	MG	2A	3374	1/1	0.95	0.27	65,65,65,65	0
58	MG	2A	3672	1/1	0.95	0.07	54,54,54,54	0
58	MG	2A	3375	1/1	0.95	0.17	46,46,46,46	0
58	MG	1A	4066	1/1	0.95	0.10	53,53,53,53	0
58	MG	2A	3141	1/1	0.95	0.09	54,54,54,54	0
58	MG	1a	1763	1/1	0.95	0.09	53,53,53,53	0
58	MG	2A	3380	1/1	0.95	0.07	36,36,36,36	0
58	MG	2A	3143	1/1	0.95	0.10	54,54,54,54	0
58	MG	1A	3778	1/1	0.95	0.12	34,34,34,34	0
58	MG	15	101	1/1	0.95	0.20	42,42,42,42	0
58	MG	1a	1766	1/1	0.95	0.06	52,52,52,52	0
58	MG	1A	3782	1/1	0.95	0.09	39,39,39,39	0
58	MG	1A	3159	1/1	0.95	0.10	39,39,39,39	0
58	MG	2a	1822	1/1	0.95	0.09	56,56,56,56	0
58	MG	2A	3388	1/1	0.95	0.13	56,56,56,56	0
58	MG	1A	3487	1/1	0.95	0.31	42,42,42,42	0
58	MG	1A	3652	1/1	0.95	0.09	37,37,37,37	0
58	MG	2A	3393	1/1	0.95	0.28	51,51,51,51	0
58	MG	2A	3394	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3654	1/1	0.95	0.07	37,37,37,37	0
58	MG	2A	3156	1/1	0.95	0.10	49,49,49,49	0
58	MG	18	104	1/1	0.95	0.10	61,61,61,61	0
58	MG	1A	3923	1/1	0.95	0.08	44,44,44,44	0
58	MG	18	106	1/1	0.95	0.11	49,49,49,49	0
58	MG	1A	3558	1/1	0.95	0.15	33,33,33,33	0
58	MG	1A	3434	1/1	0.95	0.31	36,36,36,36	0
58	MG	2A	3162	1/1	0.95	0.23	59,59,59,59	0
58	MG	1A	3561	1/1	0.95	0.33	35,35,35,35	0
58	MG	1A	3927	1/1	0.95	0.09	34,34,34,34	0
58	MG	2A	3405	1/1	0.95	0.12	47,47,47,47	0
58	MG	2A	3166	1/1	0.95	0.12	43,43,43,43	0
58	MG	2D	302	1/1	0.95	0.17	43,43,43,43	0
58	MG	2D	304	1/1	0.95	0.22	41,41,41,41	0
58	MG	2A	3167	1/1	0.95	0.31	64,64,64,64	0
58	MG	1A	3661	1/1	0.95	0.07	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
58	MG	1A	4082	1/1	0.95	0.13	58,58,58,58	0
58	MG	1A	4083	1/1	0.95	0.12	61,61,61,61	0
58	MG	1A	3022	1/1	0.95	0.06	37,37,37,37	0
59	K	1A	3554	1/1	0.95	0.08	55,55,55,55	0
58	MG	2A	3415	1/1	0.95	0.14	51,51,51,51	0
58	MG	2E	306	1/1	0.95	0.13	52,52,52,52	0
58	MG	1A	4085	1/1	0.95	0.21	54,54,54,54	0
61	ZN	2n	501	1/1	0.95	0.07	103,103,103,103	0
58	MG	1V	207	1/1	0.96	0.09	66,66,66,66	0
58	MG	1A	3781	1/1	0.96	0.11	63,63,63,63	0
58	MG	1A	3660	1/1	0.96	0.07	34,34,34,34	0
58	MG	1a	1717	1/1	0.96	0.14	44,44,44,44	0
58	MG	2A	3069	1/1	0.96	0.07	49,49,49,49	0
58	MG	2A	3512	1/1	0.96	0.07	54,54,54,54	0
58	MG	1A	3568	1/1	0.96	0.14	45,45,45,45	0
58	MG	2A	3071	1/1	0.96	0.10	48,48,48,48	0
58	MG	1A	3787	1/1	0.96	0.14	55,55,55,55	0
58	MG	1A	3919	1/1	0.96	0.19	61,61,61,61	0
58	MG	1A	3276	1/1	0.96	0.07	45,45,45,45	0
58	MG	1A	3790	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3922	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3664	1/1	0.96	0.09	35,35,35,35	0
58	MG	1a	1726	1/1	0.96	0.14	57,57,57,57	0
58	MG	1Y	202	1/1	0.96	0.16	46,46,46,46	0
58	MG	2a	1627	1/1	0.96	0.06	71,71,71,71	0
58	MG	1A	3277	1/1	0.96	0.09	37,37,37,37	0
58	MG	1a	1730	1/1	0.96	0.07	40,40,40,40	0
58	MG	1a	1731	1/1	0.96	0.10	30,30,30,30	0
58	MG	1A	3793	1/1	0.96	0.10	43,43,43,43	0
58	MG	1A	3278	1/1	0.96	0.21	23,23,23,23	0
58	MG	1Z	302	1/1	0.96	0.13	54,54,54,54	0
58	MG	1A	3032	1/1	0.96	0.29	28,28,28,28	0
58	MG	1A	3443	1/1	0.96	0.10	39,39,39,39	0
58	MG	1A	3238	1/1	0.96	0.34	35,35,35,35	0
58	MG	1A	3799	1/1	0.96	0.15	53,53,53,53	0
58	MG	1A	3800	1/1	0.96	0.10	25,25,25,25	0
58	MG	1A	3673	1/1	0.96	0.05	23,23,23,23	0
58	MG	1A	3675	1/1	0.96	0.12	27,27,27,27	0
58	MG	2A	3095	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3298	1/1	0.96	0.27	44,44,44,44	0
58	MG	10	109	1/1	0.96	0.04	49,49,49,49	0
58	MG	2A	3300	1/1	0.96	0.12	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
58	MG	1A	3239	1/1	0.96	0.17	30,30,30,30	0
58	MG	1A	3577	1/1	0.96	0.12	46,46,46,46	0
58	MG	2A	3303	1/1	0.96	0.17	55,55,55,55	0
58	MG	1A	3098	1/1	0.96	0.19	37,37,37,37	0
58	MG	11	104	1/1	0.96	0.07	47,47,47,47	0
58	MG	1A	3392	1/1	0.96	0.12	36,36,36,36	0
58	MG	13	101	1/1	0.96	0.08	38,38,38,38	0
58	MG	1A	3946	1/1	0.96	0.10	57,57,57,57	0
58	MG	1a	1755	1/1	0.96	0.08	44,44,44,44	0
58	MG	1A	3509	1/1	0.96	0.09	47,47,47,47	0
58	MG	1A	3684	1/1	0.96	0.06	29,29,29,29	0
58	MG	1A	3950	1/1	0.96	0.11	61,61,61,61	0
58	MG	2A	3109	1/1	0.96	0.14	62,62,62,62	0
58	MG	2A	3555	1/1	0.96	0.10	46,46,46,46	0
58	MG	1A	3448	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3111	1/1	0.96	0.12	54,54,54,54	0
58	MG	2A	3558	1/1	0.96	0.17	59,59,59,59	0
58	MG	1A	3953	1/1	0.96	0.12	58,58,58,58	0
58	MG	2a	1663	1/1	0.96	0.17	58,58,58,58	0
58	MG	1A	3511	1/1	0.96	0.09	48,48,48,48	0
58	MG	17	105	1/1	0.96	0.06	44,44,44,44	0
58	MG	1A	3955	1/1	0.96	0.07	50,50,50,50	0
58	MG	2a	1667	1/1	0.96	0.13	54,54,54,54	0
58	MG	1A	3688	1/1	0.96	0.12	25,25,25,25	0
58	MG	2A	3565	1/1	0.96	0.10	33,33,33,33	0
58	MG	18	103	1/1	0.96	0.19	46,46,46,46	0
58	MG	2A	3326	1/1	0.96	0.20	49,49,49,49	0
58	MG	2A	3327	1/1	0.96	0.30	63,63,63,63	0
58	MG	1A	3451	1/1	0.96	0.19	48,48,48,48	0
58	MG	1A	3244	1/1	0.96	0.15	41,41,41,41	0
58	MG	1a	1768	1/1	0.96	0.12	57,57,57,57	0
58	MG	1A	4097	1/1	0.96	0.16	45,45,45,45	0
58	MG	1A	3288	1/1	0.96	0.17	52,52,52,52	0
58	MG	1A	3692	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3396	1/1	0.96	0.05	47,47,47,47	0
58	MG	2A	3336	1/1	0.96	0.08	44,44,44,44	0
58	MG	2A	3337	1/1	0.96	0.22	58,58,58,58	0
58	MG	1A	3289	1/1	0.96	0.09	50,50,50,50	0
58	MG	1A	3290	1/1	0.96	0.11	47,47,47,47	0
58	MG	1a	1776	1/1	0.96	0.08	71,71,71,71	0
58	MG	1A	3697	1/1	0.96	0.06	28,28,28,28	0
58	MG	1A	3698	1/1	0.96	0.09	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
58	MG	1A	3968	1/1	0.96	0.09	54,54,54,54	0
58	MG	1A	3399	1/1	0.96	0.10	54,54,54,54	0
58	MG	1A	3342	1/1	0.96	0.05	55,55,55,55	0
58	MG	1a	1782	1/1	0.96	0.15	55,55,55,55	0
58	MG	1a	1783	1/1	0.96	0.08	56,56,56,56	0
58	MG	1A	3833	1/1	0.96	0.16	43,43,43,43	0
58	MG	1a	1610	1/1	0.96	0.12	27,27,27,27	0
58	MG	1A	3050	1/1	0.96	0.06	25,25,25,25	0
58	MG	1a	1789	1/1	0.96	0.10	55,55,55,55	0
58	MG	1a	1612	1/1	0.96	0.08	70,70,70,70	0
58	MG	2A	3144	1/1	0.96	0.10	43,43,43,43	0
58	MG	1a	1791	1/1	0.96	0.14	48,48,48,48	0
58	MG	2A	3357	1/1	0.96	0.12	53,53,53,53	0
58	MG	1A	3835	1/1	0.96	0.09	45,45,45,45	0
58	MG	2A	3359	1/1	0.96	0.12	34,34,34,34	0
58	MG	1A	3204	1/1	0.96	0.14	37,37,37,37	0
58	MG	2A	3149	1/1	0.96	0.17	59,59,59,59	0
58	MG	1A	3142	1/1	0.96	0.14	38,38,38,38	0
58	MG	1B	218	1/1	0.96	0.09	46,46,46,46	0
58	MG	1a	1799	1/1	0.96	0.11	61,61,61,61	0
58	MG	1a	1801	1/1	0.96	0.07	58,58,58,58	0
58	MG	1A	3839	1/1	0.96	0.07	36,36,36,36	0
58	MG	1A	3086	1/1	0.96	0.17	33,33,33,33	0
58	MG	1A	3706	1/1	0.96	0.09	28,28,28,28	0
58	MG	1A	3707	1/1	0.96	0.06	19,19,19,19	0
58	MG	1a	1621	1/1	0.96	0.18	51,51,51,51	0
58	MG	1A	3599	1/1	0.96	0.17	56,56,56,56	0
58	MG	1A	3985	1/1	0.96	0.08	23,23,23,23	0
58	MG	1a	1810	1/1	0.96	0.10	64,64,64,64	0
58	MG	1A	3600	1/1	0.96	0.11	43,43,43,43	0
58	MG	1A	3347	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3377	1/1	0.96	0.22	50,50,50,50	0
58	MG	2A	3165	1/1	0.96	0.07	62,62,62,62	0
58	MG	1A	3846	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3250	1/1	0.96	0.24	41,41,41,41	0
58	MG	1A	3528	1/1	0.96	0.19	39,39,39,39	0
58	MG	2A	3626	1/1	0.96	0.11	59,59,59,59	0
58	MG	2A	3382	1/1	0.96	0.14	45,45,45,45	0
58	MG	1A	3101	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3123	1/1	0.96	0.28	37,37,37,37	0
58	MG	2A	3630	1/1	0.96	0.06	47,47,47,47	0
58	MG	1A	3172	1/1	0.96	0.09	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1B	234	1/1	0.96	0.09	50,50,50,50	0
58	MG	2A	3174	1/1	0.96	0.14	46,46,46,46	0
58	MG	1A	3469	1/1	0.96	0.12	43,43,43,43	0
58	MG	1D	302	1/1	0.96	0.06	34,34,34,34	0
58	MG	1D	303	1/1	0.96	0.16	40,40,40,40	0
58	MG	2A	3391	1/1	0.96	0.32	52,52,52,52	0
58	MG	1l	202	1/1	0.96	0.13	61,61,61,61	0
58	MG	1A	3720	1/1	0.96	0.04	17,17,17,17	0
58	MG	2A	3643	1/1	0.96	0.10	32,32,32,32	0
58	MG	2a	1740	1/1	0.96	0.30	62,62,62,62	0
58	MG	1A	3610	1/1	0.96	0.06	22,22,22,22	0
58	MG	2a	1742	1/1	0.96	0.21	63,63,63,63	0
58	MG	1A	3611	1/1	0.96	0.08	42,42,42,42	0
58	MG	2a	1744	1/1	0.96	0.06	65,65,65,65	0
58	MG	1A	4000	1/1	0.96	0.19	44,44,44,44	0
58	MG	1A	4001	1/1	0.96	0.08	29,29,29,29	0
58	MG	2A	3649	1/1	0.96	0.08	26,26,26,26	0
58	MG	2A	3184	1/1	0.96	0.24	52,52,52,52	0
58	MG	2a	1749	1/1	0.96	0.09	64,64,64,64	0
58	MG	1E	304	1/1	0.96	0.16	34,34,34,34	0
58	MG	1E	305	1/1	0.96	0.09	47,47,47,47	0
58	MG	1A	3723	1/1	0.96	0.07	59,59,59,59	0
58	MG	1A	3726	1/1	0.96	0.12	34,34,34,34	0
58	MG	1E	309	1/1	0.96	0.12	23,23,23,23	0
58	MG	2A	3656	1/1	0.96	0.07	48,48,48,48	0
58	MG	1A	3352	1/1	0.96	0.11	63,63,63,63	0
58	MG	1A	3014	1/1	0.96	0.10	28,28,28,28	0
58	MG	1a	1651	1/1	0.96	0.12	54,54,54,54	0
58	MG	1A	3861	1/1	0.96	0.11	51,51,51,51	0
58	MG	1A	3535	1/1	0.96	0.09	58,58,58,58	0
58	MG	1A	3016	1/1	0.96	0.27	56,56,56,56	0
58	MG	1A	4009	1/1	0.96	0.07	31,31,31,31	0
58	MG	2A	3414	1/1	0.96	0.13	74,74,74,74	0
58	MG	1F	308	1/1	0.96	0.07	47,47,47,47	0
58	MG	2A	3669	1/1	0.96	0.11	49,49,49,49	0
58	MG	1A	3413	1/1	0.96	0.20	48,48,48,48	0
58	MG	2A	3417	1/1	0.96	0.11	32,32,32,32	0
58	MG	1A	3539	1/1	0.96	0.05	56,56,56,56	0
58	MG	1A	3735	1/1	0.96	0.07	38,38,38,38	0
58	MG	1A	3414	1/1	0.96	0.10	51,51,51,51	0
58	MG	1A	3256	1/1	0.96	0.07	57,57,57,57	0
58	MG	1A	3621	1/1	0.96	0.09	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
58	MG	1A	3177	1/1	0.96	0.09	34,34,34,34	0
58	MG	2A	3424	1/1	0.96	0.14	52,52,52,52	0
58	MG	1H	201	1/1	0.96	0.17	44,44,44,44	0
58	MG	1A	3180	1/1	0.96	0.05	33,33,33,33	0
58	MG	2a	1781	1/1	0.96	0.17	58,58,58,58	0
58	MG	1A	3419	1/1	0.96	0.07	45,45,45,45	0
58	MG	1N	202	1/1	0.96	0.05	44,44,44,44	0
58	MG	1N	203	1/1	0.96	0.06	51,51,51,51	0
58	MG	2A	3008	1/1	0.96	0.05	45,45,45,45	0
58	MG	1A	3627	1/1	0.96	0.06	59,59,59,59	0
58	MG	2A	3010	1/1	0.96	0.12	48,48,48,48	0
58	MG	1A	3628	1/1	0.96	0.06	27,27,27,27	0
58	MG	1A	3545	1/1	0.96	0.14	39,39,39,39	0
58	MG	2A	3441	1/1	0.96	0.21	39,39,39,39	0
58	MG	1A	4022	1/1	0.96	0.08	43,43,43,43	0
58	MG	2A	3015	1/1	0.96	0.11	56,56,56,56	0
58	MG	1A	3546	1/1	0.96	0.18	37,37,37,37	0
58	MG	1A	3021	1/1	0.96	0.07	24,24,24,24	0
58	MG	1A	3151	1/1	0.96	0.22	28,28,28,28	0
58	MG	1A	3077	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3751	1/1	0.96	0.25	61,61,61,61	0
58	MG	1A	3637	1/1	0.96	0.05	20,20,20,20	0
58	MG	1A	4029	1/1	0.96	0.08	44,44,44,44	0
58	MG	2A	3452	1/1	0.96	0.09	35,35,35,35	0
58	MG	1P	208	1/1	0.96	0.09	64,64,64,64	0
58	MG	2D	301	1/1	0.96	0.07	41,41,41,41	0
58	MG	2a	1803	1/1	0.96	0.20	61,61,61,61	0
58	MG	1Q	201	1/1	0.96	0.13	42,42,42,42	0
58	MG	1A	3184	1/1	0.96	0.04	49,49,49,49	0
58	MG	1Q	204	1/1	0.96	0.11	60,60,60,60	0
58	MG	2A	3457	1/1	0.96	0.18	53,53,53,53	0
58	MG	1A	3890	1/1	0.96	0.07	43,43,43,43	0
58	MG	1A	3641	1/1	0.96	0.10	28,28,28,28	0
58	MG	1A	3042	1/1	0.96	0.06	31,31,31,31	0
58	MG	1A	3031	1/1	0.96	0.33	36,36,36,36	0
58	MG	2A	3037	1/1	0.96	0.14	39,39,39,39	0
58	MG	2E	307	1/1	0.96	0.10	49,49,49,49	0
58	MG	1R	204	1/1	0.96	0.29	43,43,43,43	0
58	MG	2A	3465	1/1	0.96	0.07	27,27,27,27	0
58	MG	2A	3235	1/1	0.96	0.07	51,51,51,51	0
58	MG	1A	3188	1/1	0.96	0.15	37,37,37,37	0
58	MG	1A	3157	1/1	0.96	0.14	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3557	1/1	0.96	0.20	33,33,33,33	0
58	MG	1a	1693	1/1	0.96	0.27	50,50,50,50	0
58	MG	2A	3473	1/1	0.96	0.11	40,40,40,40	0
58	MG	1a	1694	1/1	0.96	0.30	57,57,57,57	0
58	MG	2A	3241	1/1	0.96	0.14	56,56,56,56	0
58	MG	2R	202	1/1	0.96	0.20	60,60,60,60	0
58	MG	1A	3109	1/1	0.96	0.05	31,31,31,31	0
58	MG	1A	3900	1/1	0.96	0.13	42,42,42,42	0
58	MG	1a	1697	1/1	0.96	0.30	62,62,62,62	0
58	MG	1A	3112	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3192	1/1	0.96	0.29	32,32,32,32	0
58	MG	1A	3065	1/1	0.96	0.35	50,50,50,50	0
58	MG	1U	204	1/1	0.96	0.18	40,40,40,40	0
58	MG	1A	3904	1/1	0.96	0.08	37,37,37,37	0
58	MG	1A	3651	1/1	0.96	0.07	29,29,29,29	0
58	MG	2A	3053	1/1	0.96	0.08	51,51,51,51	0
58	MG	23	103	1/1	0.96	0.25	54,54,54,54	0
58	MG	1A	3082	1/1	0.96	0.15	42,42,42,42	0
58	MG	1A	4049	1/1	0.96	0.05	30,30,30,30	0
58	MG	2A	3256	1/1	0.96	0.22	50,50,50,50	0
58	MG	1U	210	1/1	0.96	0.17	39,39,39,39	0
58	MG	1A	3115	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	3163	1/1	0.96	0.07	30,30,30,30	0
58	MG	1A	3275	1/1	0.96	0.18	47,47,47,47	0
58	MG	2A	3261	1/1	0.96	0.33	58,58,58,58	0
58	MG	2A	3060	1/1	0.96	0.14	45,45,45,45	0
58	MG	2A	3061	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	3658	1/1	0.96	0.06	45,45,45,45	0
58	MG	2A	3265	1/1	0.96	0.32	54,54,54,54	0
58	MG	2A	3502	1/1	0.96	0.16	45,45,45,45	0
60	ERY	1A	4098	51/51	0.96	0.09	19,32,41,45	0
60	ERY	2A	3688	51/51	0.96	0.10	35,47,57,68	0
58	MG	1A	3330	1/1	0.96	0.18	49,49,49,49	0
61	ZN	2Y	501	1/1	0.96	0.06	104,104,104,104	0
58	MG	2A	3504	1/1	0.96	0.12	55,55,55,55	0
58	MG	2A	3505	1/1	0.96	0.09	34,34,34,34	0
58	MG	2A	3126	1/1	0.97	0.17	53,53,53,53	0
58	MG	1A	3499	1/1	0.97	0.07	37,37,37,37	0
58	MG	1A	3126	1/1	0.97	0.13	33,33,33,33	0
58	MG	1m	3001	1/1	0.97	0.09	53,53,53,53	0
58	MG	1A	3186	1/1	0.97	0.04	36,36,36,36	0
58	MG	1U	208	1/1	0.97	0.15	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
58	MG	1A	3127	1/1	0.97	0.36	32,32,32,32	0
58	MG	1A	3036	1/1	0.97	0.06	34,34,34,34	0
58	MG	1A	3066	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3384	1/1	0.97	0.28	32,32,32,32	0
58	MG	2A	3639	1/1	0.97	0.11	43,43,43,43	0
58	MG	1A	3573	1/1	0.97	0.05	52,52,52,52	0
58	MG	1V	202	1/1	0.97	0.16	35,35,35,35	0
58	MG	1A	3506	1/1	0.97	0.33	39,39,39,39	0
58	MG	2A	3292	1/1	0.97	0.06	50,50,50,50	0
58	MG	1V	205	1/1	0.97	0.08	43,43,43,43	0
58	MG	1A	3653	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3973	1/1	0.97	0.05	48,48,48,48	0
58	MG	2A	3647	1/1	0.97	0.11	70,70,70,70	0
58	MG	1A	3039	1/1	0.97	0.15	33,33,33,33	0
58	MG	2A	3467	1/1	0.97	0.18	55,55,55,55	0
58	MG	2A	3468	1/1	0.97	0.09	44,44,44,44	0
58	MG	1a	1686	1/1	0.97	0.13	46,46,46,46	0
58	MG	1A	3975	1/1	0.97	0.12	31,31,31,31	0
58	MG	1W	203	1/1	0.97	0.11	39,39,39,39	0
58	MG	2a	1693	1/1	0.97	0.20	64,64,64,64	0
58	MG	1W	204	1/1	0.97	0.15	43,43,43,43	0
58	MG	2a	1695	1/1	0.97	0.10	74,74,74,74	0
58	MG	2A	3148	1/1	0.97	0.18	54,54,54,54	0
58	MG	1A	3228	1/1	0.97	0.10	45,45,45,45	0
58	MG	1A	3005	1/1	0.97	0.06	40,40,40,40	0
58	MG	2A	3658	1/1	0.97	0.18	55,55,55,55	0
58	MG	1A	3230	1/1	0.97	0.12	31,31,31,31	0
58	MG	2A	3660	1/1	0.97	0.10	60,60,60,60	0
58	MG	1A	3860	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3024	1/1	0.97	0.17	40,40,40,40	0
58	MG	2A	3663	1/1	0.97	0.07	46,46,46,46	0
58	MG	2A	3154	1/1	0.97	0.14	61,61,61,61	0
58	MG	1X	103	1/1	0.97	0.10	42,42,42,42	0
58	MG	1A	3072	1/1	0.97	0.09	19,19,19,19	0
58	MG	1A	3135	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3984	1/1	0.97	0.15	30,30,30,30	0
58	MG	2A	3485	1/1	0.97	0.11	56,56,56,56	0
58	MG	1A	3864	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3865	1/1	0.97	0.06	50,50,50,50	0
58	MG	1A	3662	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3111	1/1	0.97	0.23	37,37,37,37	0
58	MG	1A	3007	1/1	0.97	0.06	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
58	MG	2A	3491	1/1	0.97	0.10	35,35,35,35	0
58	MG	1A	3665	1/1	0.97	0.05	27,27,27,27	0
58	MG	1A	3237	1/1	0.97	0.06	70,70,70,70	0
58	MG	2A	3494	1/1	0.97	0.07	40,40,40,40	0
58	MG	2A	3322	1/1	0.97	0.18	46,46,46,46	0
58	MG	1A	3667	1/1	0.97	0.04	19,19,19,19	0
58	MG	1A	3993	1/1	0.97	0.06	44,44,44,44	0
58	MG	2A	3325	1/1	0.97	0.11	30,30,30,30	0
58	MG	1A	3092	1/1	0.97	0.08	53,53,53,53	0
58	MG	1A	3282	1/1	0.97	0.27	35,35,35,35	0
58	MG	2A	3016	1/1	0.97	0.04	40,40,40,40	0
58	MG	1A	3996	1/1	0.97	0.09	44,44,44,44	0
58	MG	1A	3876	1/1	0.97	0.25	38,38,38,38	0
58	MG	2A	3331	1/1	0.97	0.22	66,66,66,66	0
58	MG	1A	3877	1/1	0.97	0.24	32,32,32,32	0
58	MG	1a	1714	1/1	0.97	0.14	37,37,37,37	0
58	MG	1A	3763	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3520	1/1	0.97	0.11	39,39,39,39	0
58	MG	1A	3458	1/1	0.97	0.13	32,32,32,32	0
58	MG	2A	3026	1/1	0.97	0.05	44,44,44,44	0
58	MG	12	102	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3589	1/1	0.97	0.10	41,41,41,41	0
58	MG	1A	3674	1/1	0.97	0.04	19,19,19,19	0
58	MG	1A	3769	1/1	0.97	0.08	34,34,34,34	0
58	MG	2A	3516	1/1	0.97	0.12	40,40,40,40	0
58	MG	1A	3771	1/1	0.97	0.05	26,26,26,26	0
58	MG	1B	228	1/1	0.97	0.07	42,42,42,42	0
58	MG	1A	3522	1/1	0.97	0.24	44,44,44,44	0
58	MG	2D	303	1/1	0.97	0.04	30,30,30,30	0
58	MG	15	103	1/1	0.97	0.11	33,33,33,33	0
58	MG	1A	3074	1/1	0.97	0.04	13,13,13,13	0
58	MG	16	101	1/1	0.97	0.07	60,60,60,60	0
58	MG	17	103	1/1	0.97	0.08	28,28,28,28	0
58	MG	1A	3677	1/1	0.97	0.08	32,32,32,32	0
58	MG	2a	1750	1/1	0.97	0.11	71,71,71,71	0
58	MG	2A	3350	1/1	0.97	0.24	42,42,42,42	0
58	MG	1A	3592	1/1	0.97	0.09	34,34,34,34	0
58	MG	1A	3240	1/1	0.97	0.19	32,32,32,32	0
58	MG	1A	3200	1/1	0.97	0.19	37,37,37,37	0
58	MG	1A	3595	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	3201	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3168	1/1	0.97	0.08	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
58	MG	1A	3686	1/1	0.97	0.07	54,54,54,54	0
58	MG	2a	1760	1/1	0.97	0.08	53,53,53,53	0
58	MG	1A	3009	1/1	0.97	0.04	34,34,34,34	0
58	MG	1D	308	1/1	0.97	0.15	41,41,41,41	0
58	MG	1A	3292	1/1	0.97	0.20	28,28,28,28	0
58	MG	1A	3095	1/1	0.97	0.07	19,19,19,19	0
58	MG	1D	311	1/1	0.97	0.14	36,36,36,36	0
58	MG	1A	3294	1/1	0.97	0.10	51,51,51,51	0
58	MG	2a	1767	1/1	0.97	0.04	82,82,82,82	0
58	MG	1A	3248	1/1	0.97	0.07	53,53,53,53	0
58	MG	2R	203	1/1	0.97	0.06	48,48,48,48	0
58	MG	1A	3296	1/1	0.97	0.07	48,48,48,48	0
58	MG	1E	306	1/1	0.97	0.07	52,52,52,52	0
58	MG	1A	3059	1/1	0.97	0.04	29,29,29,29	0
58	MG	2A	3369	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3797	1/1	0.97	0.09	54,54,54,54	0
58	MG	1a	1753	1/1	0.97	0.08	62,62,62,62	0
58	MG	1A	3207	1/1	0.97	0.07	31,31,31,31	0
58	MG	1E	310	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3044	1/1	0.97	0.28	32,32,32,32	0
58	MG	1E	312	1/1	0.97	0.10	46,46,46,46	0
58	MG	2A	3550	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	3301	1/1	0.97	0.10	29,29,29,29	0
58	MG	1A	3119	1/1	0.97	0.13	29,29,29,29	0
58	MG	25	103	1/1	0.97	0.07	52,52,52,52	0
58	MG	1F	302	1/1	0.97	0.21	28,28,28,28	0
58	MG	1F	303	1/1	0.97	0.11	44,44,44,44	0
58	MG	2A	3068	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3120	1/1	0.97	0.08	35,35,35,35	0
58	MG	1A	3700	1/1	0.97	0.11	38,38,38,38	0
58	MG	1A	4030	1/1	0.97	0.10	38,38,38,38	0
58	MG	1A	3175	1/1	0.97	0.42	37,37,37,37	0
58	MG	1A	3614	1/1	0.97	0.13	48,48,48,48	0
58	MG	2A	3074	1/1	0.97	0.07	39,39,39,39	0
58	MG	1A	3306	1/1	0.97	0.06	35,35,35,35	0
58	MG	2A	3563	1/1	0.97	0.15	36,36,36,36	0
58	MG	1A	3212	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3418	1/1	0.97	0.07	44,44,44,44	0
58	MG	1A	3079	1/1	0.97	0.14	38,38,38,38	0
58	MG	1G	202	1/1	0.97	0.19	51,51,51,51	0
58	MG	1A	4038	1/1	0.97	0.11	36,36,36,36	0
58	MG	1A	3359	1/1	0.97	0.13	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3570	1/1	0.97	0.14	58,58,58,58	0
58	MG	1A	3214	1/1	0.97	0.31	37,37,37,37	0
58	MG	1A	3179	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	3147	1/1	0.97	0.26	32,32,32,32	0
58	MG	2A	3085	1/1	0.97	0.18	50,50,50,50	0
58	MG	1A	3217	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	3820	1/1	0.97	0.05	24,24,24,24	0
58	MG	1A	3261	1/1	0.97	0.24	44,44,44,44	0
58	MG	1N	205	1/1	0.97	0.12	45,45,45,45	0
58	MG	1A	3822	1/1	0.97	0.27	25,25,25,25	0
58	MG	1A	3823	1/1	0.97	0.06	33,33,33,33	0
58	MG	1a	1785	1/1	0.97	0.12	62,62,62,62	0
58	MG	1A	3366	1/1	0.97	0.17	33,33,33,33	0
58	MG	1A	3933	1/1	0.97	0.06	50,50,50,50	0
58	MG	2A	3584	1/1	0.97	0.15	54,54,54,54	0
58	MG	1A	3825	1/1	0.97	0.07	23,23,23,23	0
58	MG	2A	3586	1/1	0.97	0.12	38,38,38,38	0
58	MG	2A	3409	1/1	0.97	0.13	32,32,32,32	0
58	MG	1A	3716	1/1	0.97	0.04	47,47,47,47	0
58	MG	2A	3249	1/1	0.97	0.10	55,55,55,55	0
58	MG	1A	3367	1/1	0.97	0.08	60,60,60,60	0
58	MG	1A	3940	1/1	0.97	0.08	55,55,55,55	0
58	MG	1A	3629	1/1	0.97	0.10	24,24,24,24	0
58	MG	1P	205	1/1	0.97	0.29	32,32,32,32	0
58	MG	1a	1649	1/1	0.97	0.07	51,51,51,51	0
58	MG	1A	3368	1/1	0.97	0.09	53,53,53,53	0
58	MG	1A	3010	1/1	0.97	0.08	40,40,40,40	0
58	MG	1A	3316	1/1	0.97	0.10	48,48,48,48	0
58	MG	1A	3633	1/1	0.97	0.06	20,20,20,20	0
58	MG	1A	3559	1/1	0.97	0.18	37,37,37,37	0
58	MG	1A	3724	1/1	0.97	0.15	40,40,40,40	0
58	MG	2A	3108	1/1	0.97	0.08	44,44,44,44	0
58	MG	1A	3836	1/1	0.97	0.17	61,61,61,61	0
58	MG	2I	205	1/1	0.97	0.06	67,67,67,67	0
58	MG	1A	3951	1/1	0.97	0.11	46,46,46,46	0
58	MG	2A	3427	1/1	0.97	0.09	60,60,60,60	0
58	MG	1A	3725	1/1	0.97	0.14	50,50,50,50	0
58	MG	1R	202	1/1	0.97	0.10	38,38,38,38	0
58	MG	2A	3113	1/1	0.97	0.11	41,41,41,41	0
58	MG	2A	3432	1/1	0.97	0.09	41,41,41,41	0
58	MG	1R	203	1/1	0.97	0.10	50,50,50,50	0
58	MG	1A	3317	1/1	0.97	0.11	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
58	MG	1A	4071	1/1	0.97	0.13	42,42,42,42	0
58	MG	1A	3047	1/1	0.97	0.06	35,35,35,35	0
58	MG	1A	3639	1/1	0.97	0.04	21,21,21,21	0
58	MG	2A	3438	1/1	0.97	0.09	44,44,44,44	0
58	MG	2A	3440	1/1	0.97	0.14	41,41,41,41	0
58	MG	1A	3956	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3729	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3034	1/1	0.97	0.31	27,27,27,27	0
58	MG	1A	3375	1/1	0.97	0.07	42,42,42,42	0
58	MG	2A	3622	1/1	0.97	0.10	39,39,39,39	0
58	MG	1A	3436	1/1	0.97	0.16	36,36,36,36	0
58	MG	2A	3446	1/1	0.97	0.09	27,27,27,27	0
58	MG	1A	3035	1/1	0.97	0.27	35,35,35,35	0
58	MG	2A	3507	1/1	0.98	0.12	51,51,51,51	0
58	MG	1A	3243	1/1	0.98	0.11	28,28,28,28	0
58	MG	1A	3203	1/1	0.98	0.06	33,33,33,33	0
58	MG	1a	1800	1/1	0.98	0.08	48,48,48,48	0
58	MG	1A	4034	1/1	0.98	0.13	39,39,39,39	0
58	MG	2A	3634	1/1	0.98	0.08	45,45,45,45	0
58	MG	2A	3392	1/1	0.98	0.25	42,42,42,42	0
58	MG	1A	3376	1/1	0.98	0.06	26,26,26,26	0
58	MG	2A	3169	1/1	0.98	0.14	39,39,39,39	0
58	MG	1A	3708	1/1	0.98	0.11	20,20,20,20	0
58	MG	1A	3058	1/1	0.98	0.17	39,39,39,39	0
58	MG	1a	1805	1/1	0.98	0.04	57,57,57,57	0
58	MG	1A	3085	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3889	1/1	0.98	0.07	50,50,50,50	0
58	MG	1A	3965	1/1	0.98	0.10	20,20,20,20	0
58	MG	1A	3508	1/1	0.98	0.14	33,33,33,33	0
58	MG	1U	202	1/1	0.98	0.13	36,36,36,36	0
58	MG	1A	3828	1/1	0.98	0.03	34,34,34,34	0
58	MG	1A	3892	1/1	0.98	0.06	26,26,26,26	0
58	MG	1A	3011	1/1	0.98	0.07	33,33,33,33	0
58	MG	1A	3110	1/1	0.98	0.25	38,38,38,38	0
58	MG	1A	3622	1/1	0.98	0.10	19,19,19,19	0
58	MG	1A	3623	1/1	0.98	0.09	43,43,43,43	0
58	MG	1A	3076	1/1	0.98	0.05	32,32,32,32	0
58	MG	1B	235	1/1	0.98	0.07	30,30,30,30	0
58	MG	1A	3770	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3899	1/1	0.98	0.07	48,48,48,48	0
58	MG	1A	3547	1/1	0.98	0.14	35,35,35,35	0
58	MG	2a	1759	1/1	0.98	0.21	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
58	MG	1A	4052	1/1	0.98	0.08	42,42,42,42	0
58	MG	1V	203	1/1	0.98	0.24	34,34,34,34	0
58	MG	1A	3012	1/1	0.98	0.04	26,26,26,26	0
58	MG	1D	307	1/1	0.98	0.07	35,35,35,35	0
58	MG	1a	1723	1/1	0.98	0.12	54,54,54,54	0
58	MG	1a	1632	1/1	0.98	0.10	28,28,28,28	0
58	MG	1A	3383	1/1	0.98	0.20	32,32,32,32	0
58	MG	1A	3155	1/1	0.98	0.10	30,30,30,30	0
58	MG	1a	1727	1/1	0.98	0.08	49,49,49,49	0
58	MG	1A	3775	1/1	0.98	0.06	24,24,24,24	0
58	MG	1A	3156	1/1	0.98	0.07	43,43,43,43	0
58	MG	1E	301	1/1	0.98	0.19	36,36,36,36	0
58	MG	2A	3312	1/1	0.98	0.06	53,53,53,53	0
58	MG	1A	3777	1/1	0.98	0.05	63,63,63,63	0
58	MG	1A	3013	1/1	0.98	0.16	23,23,23,23	0
58	MG	1a	1640	1/1	0.98	0.23	53,53,53,53	0
58	MG	2A	3673	1/1	0.98	0.06	28,28,28,28	0
58	MG	1A	3780	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3909	1/1	0.98	0.10	42,42,42,42	0
58	MG	1A	3449	1/1	0.98	0.10	44,44,44,44	0
58	MG	1A	3450	1/1	0.98	0.06	39,39,39,39	0
58	MG	2A	3320	1/1	0.98	0.14	46,46,46,46	0
58	MG	2A	3679	1/1	0.98	0.07	34,34,34,34	0
58	MG	1a	1739	1/1	0.98	0.05	39,39,39,39	0
58	MG	1a	1740	1/1	0.98	0.10	33,33,33,33	0
58	MG	2A	3439	1/1	0.98	0.11	38,38,38,38	0
58	MG	1A	3069	1/1	0.98	0.04	29,29,29,29	0
58	MG	1X	104	1/1	0.98	0.05	38,38,38,38	0
58	MG	1A	3786	1/1	0.98	0.05	49,49,49,49	0
58	MG	1A	3679	1/1	0.98	0.08	31,31,31,31	0
58	MG	1A	3048	1/1	0.98	0.10	35,35,35,35	0
58	MG	1A	4073	1/1	0.98	0.10	41,41,41,41	0
58	MG	2A	3216	1/1	0.98	0.07	48,48,48,48	0
58	MG	1A	3789	1/1	0.98	0.04	61,61,61,61	0
58	MG	1A	3129	1/1	0.98	0.23	39,39,39,39	0
58	MG	1A	3682	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	3305	1/1	0.98	0.05	35,35,35,35	0
58	MG	10	102	1/1	0.98	0.09	42,42,42,42	0
58	MG	1A	3638	1/1	0.98	0.05	38,38,38,38	0
58	MG	1A	3596	1/1	0.98	0.12	28,28,28,28	0
58	MG	1a	1754	1/1	0.98	0.07	54,54,54,54	0
58	MG	2A	3116	1/1	0.98	0.25	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
58	MG	1A	3734	1/1	0.98	0.04	31,31,31,31	0
58	MG	1A	3235	1/1	0.98	0.06	47,47,47,47	0
58	MG	2A	3012	1/1	0.98	0.06	43,43,43,43	0
58	MG	1A	3737	1/1	0.98	0.04	29,29,29,29	0
58	MG	2A	3460	1/1	0.98	0.12	42,42,42,42	0
58	MG	1A	3071	1/1	0.98	0.09	33,33,33,33	0
58	MG	1A	3037	1/1	0.98	0.06	36,36,36,36	0
58	MG	1A	3199	1/1	0.98	0.05	43,43,43,43	0
58	MG	2A	3017	1/1	0.98	0.05	37,37,37,37	0
58	MG	1A	3930	1/1	0.98	0.07	45,45,45,45	0
58	MG	1A	3931	1/1	0.98	0.03	20,20,20,20	0
58	MG	2E	302	1/1	0.98	0.06	45,45,45,45	0
58	MG	1A	3601	1/1	0.98	0.12	26,26,26,26	0
58	MG	2A	3021	1/1	0.98	0.04	45,45,45,45	0
58	MG	2A	3351	1/1	0.98	0.08	52,52,52,52	0
58	MG	1A	3602	1/1	0.98	0.03	22,22,22,22	0
58	MG	1A	3935	1/1	0.98	0.04	29,29,29,29	0
58	MG	1A	3310	1/1	0.98	0.05	50,50,50,50	0
58	MG	1A	3693	1/1	0.98	0.05	22,22,22,22	0
58	MG	1A	3938	1/1	0.98	0.09	38,38,38,38	0
58	MG	1A	3866	1/1	0.98	0.06	49,49,49,49	0
58	MG	2A	3476	1/1	0.98	0.05	42,42,42,42	0
58	MG	2A	3029	1/1	0.98	0.14	44,44,44,44	0
58	MG	2A	3596	1/1	0.98	0.04	37,37,37,37	0
58	MG	1A	3427	1/1	0.98	0.08	43,43,43,43	0
58	MG	2A	3137	1/1	0.98	0.14	37,37,37,37	0
58	MG	1A	3941	1/1	0.98	0.06	46,46,46,46	0
58	MG	1A	3283	1/1	0.98	0.27	28,28,28,28	0
58	MG	1A	3869	1/1	0.98	0.04	32,32,32,32	0
58	MG	2A	3250	1/1	0.98	0.13	35,35,35,35	0
58	MG	1A	3808	1/1	0.98	0.11	28,28,28,28	0
58	MG	1a	1775	1/1	0.98	0.05	40,40,40,40	0
58	MG	17	101	1/1	0.98	0.04	33,33,33,33	0
58	MG	17	102	1/1	0.98	0.17	33,33,33,33	0
58	MG	1A	3809	1/1	0.98	0.06	25,25,25,25	0
58	MG	20	101	1/1	0.98	0.09	53,53,53,53	0
58	MG	1A	3810	1/1	0.98	0.06	40,40,40,40	0
58	MG	1A	3947	1/1	0.98	0.10	44,44,44,44	0
58	MG	1A	3811	1/1	0.98	0.07	24,24,24,24	0
58	MG	1A	3284	1/1	0.98	0.12	43,43,43,43	0
58	MG	1B	208	1/1	0.98	0.07	52,52,52,52	0
58	MG	1A	3038	1/1	0.98	0.07	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3286	1/1	0.98	0.10	38,38,38,38	0
58	MG	1a	1786	1/1	0.98	0.06	53,53,53,53	0
58	MG	1A	3106	1/1	0.98	0.12	29,29,29,29	0
58	MG	1A	3148	1/1	0.98	0.19	31,31,31,31	0
58	MG	1Q	203	1/1	0.98	0.06	44,44,44,44	0
58	MG	1A	3372	1/1	0.98	0.07	42,42,42,42	0
58	MG	1A	3242	1/1	0.98	0.17	34,34,34,34	0
58	MG	1a	1792	1/1	0.98	0.04	46,46,46,46	0
58	MG	1a	1793	1/1	0.98	0.06	61,61,61,61	0
58	MG	1A	3537	1/1	0.98	0.08	58,58,58,58	0
58	MG	1A	3657	1/1	0.98	0.06	41,41,41,41	0
58	MG	1B	217	1/1	0.98	0.05	50,50,50,50	0
62	SF4	2d	303	8/8	0.98	0.05	71,78,88,104	0
58	MG	1A	3671	1/1	0.99	0.04	34,34,34,34	0
58	MG	1A	3978	1/1	0.99	0.06	53,53,53,53	0
58	MG	1A	3008	1/1	0.99	0.06	27,27,27,27	0
58	MG	1D	305	1/1	0.99	0.03	24,24,24,24	0
58	MG	1A	3298	1/1	0.99	0.04	31,31,31,31	0
58	MG	1A	3934	1/1	0.99	0.04	23,23,23,23	0
58	MG	1A	3757	1/1	0.99	0.04	41,41,41,41	0
58	MG	2A	3293	1/1	0.99	0.16	27,27,27,27	0
58	MG	1A	3029	1/1	0.99	0.15	30,30,30,30	0
58	MG	1A	3914	1/1	0.99	0.03	22,22,22,22	0
58	MG	1A	4058	1/1	0.99	0.04	44,44,44,44	0
58	MG	2A	3603	1/1	0.99	0.13	42,42,42,42	0
58	MG	1A	4059	1/1	0.99	0.07	52,52,52,52	0
58	MG	1A	4060	1/1	0.99	0.05	25,25,25,25	0
58	MG	1E	303	1/1	0.99	0.12	33,33,33,33	0
58	MG	1A	3915	1/1	0.99	0.02	22,22,22,22	0
58	MG	1A	3046	1/1	0.99	0.03	34,34,34,34	0
58	MG	2A	3413	1/1	0.99	0.08	36,36,36,36	0
58	MG	1A	3023	1/1	0.99	0.03	18,18,18,18	0
58	MG	1A	3003	1/1	0.99	0.07	25,25,25,25	0
58	MG	1A	3395	1/1	0.99	0.21	39,39,39,39	0
58	MG	1A	3779	1/1	0.99	0.04	17,17,17,17	0
58	MG	1a	1794	1/1	0.99	0.04	57,57,57,57	0
58	MG	1A	4067	1/1	0.99	0.13	39,39,39,39	0
58	MG	1A	3049	1/1	0.99	0.17	32,32,32,32	0
58	MG	1A	3360	1/1	0.99	0.04	51,51,51,51	0
58	MG	1A	3801	1/1	0.99	0.07	24,24,24,24	0
58	MG	1A	3488	1/1	0.99	0.18	34,34,34,34	0
58	MG	1A	3783	1/1	0.99	0.04	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1732	1/1	0.99	0.12	40,40,40,40	0
58	MG	1A	3784	1/1	0.99	0.03	24,24,24,24	0
58	MG	1P	207	1/1	0.99	0.04	32,32,32,32	0
58	MG	2A	3624	1/1	0.99	0.10	42,42,42,42	0
58	MG	2A	3428	1/1	0.99	0.05	40,40,40,40	0
58	MG	2A	3027	1/1	0.99	0.16	40,40,40,40	0
58	MG	1A	3766	1/1	0.99	0.09	40,40,40,40	0
61	ZN	1Y	205	1/1	0.99	0.02	66,66,66,66	0
58	MG	1A	3176	1/1	0.99	0.16	32,32,32,32	0
61	ZN	15	105	1/1	0.99	0.04	67,67,67,67	0
61	ZN	19	102	1/1	0.99	0.04	44,44,44,44	0
61	ZN	1n	103	1/1	0.99	0.03	67,67,67,67	0
58	MG	1a	1703	1/1	0.99	0.05	49,49,49,49	0
58	MG	1F	306	1/1	0.99	0.20	31,31,31,31	0
61	ZN	25	105	1/1	0.99	0.05	91,91,91,91	0
61	ZN	26	501	1/1	0.99	0.06	71,71,71,71	0
61	ZN	29	501	1/1	0.99	0.03	70,70,70,70	0
58	MG	1A	3634	1/1	0.99	0.04	52,52,52,52	0
62	SF4	1d	303	8/8	0.99	0.06	59,66,69,71	0
58	MG	1A	3710	1/1	0.99	0.05	31,31,31,31	0
58	MG	1A	4055	1/1	1.00	0.03	17,17,17,17	0
58	MG	1A	3178	1/1	1.00	0.06	19,19,19,19	0
58	MG	1A	3736	1/1	1.00	0.02	27,27,27,27	0
58	MG	2A	3632	1/1	1.00	0.06	28,28,28,28	0
61	ZN	16	102	1/1	1.00	0.05	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.