



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2026 – 10:29 PM EDT

PDB ID : 5WIT / pdb_00005wit
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with pikromycin and bound to mRNA and A-, P- and E-site tRNAs at 2.6Å resolution
Authors : Almutairi, M.M.; Svetlov, M.S.; Hansen, D.A.; Khabibullina, N.F.; Klepacki, D.; Kang, H.Y.; Sherman, D.H.; Vazquez-Laslop, N.; Polikanov, Y.S.; Mankin, A.S.
Deposited on : 2017-07-20
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

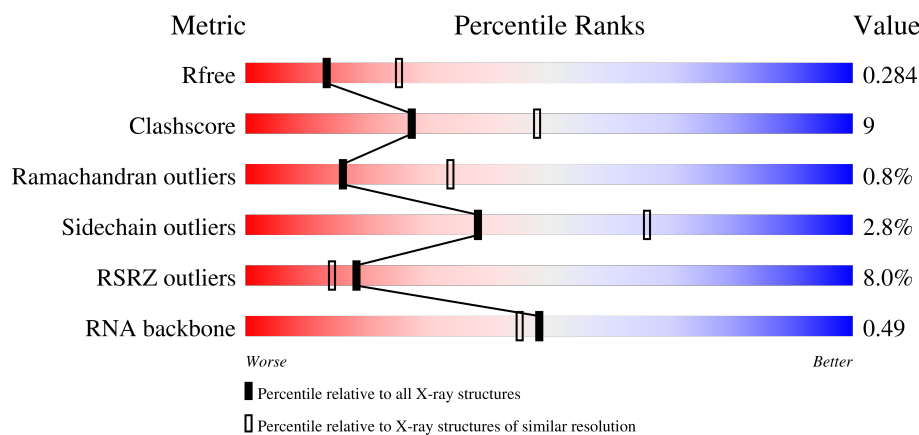
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

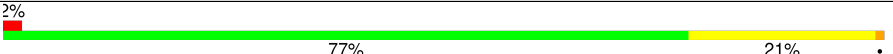
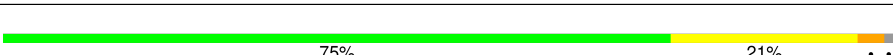
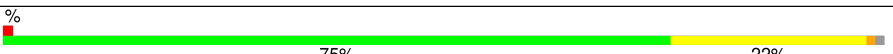
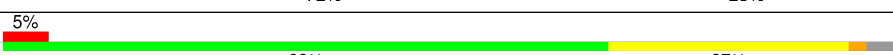
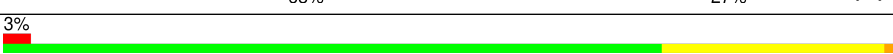
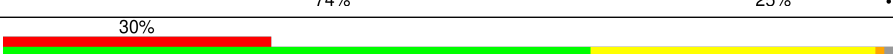
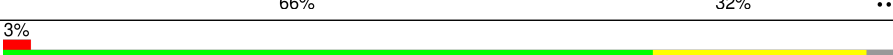
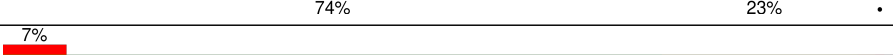
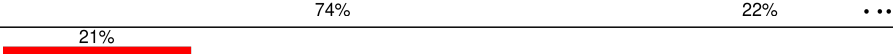
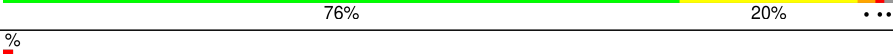
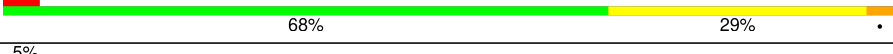
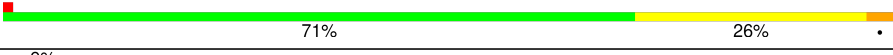
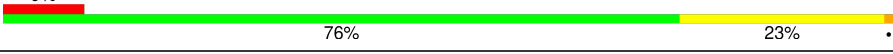
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	5% 64% 28% 6%
1	2A	2915	3% 55% 34% 7%

Continued on next page...

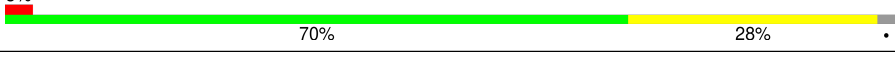
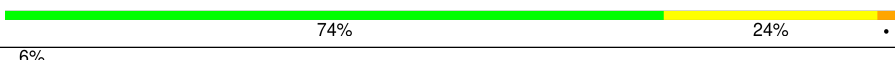
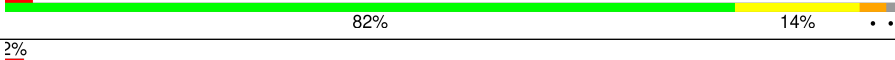
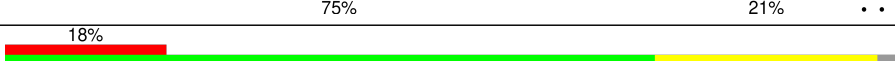
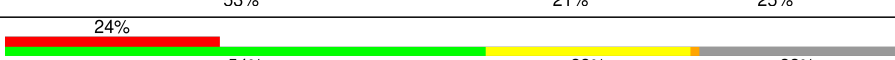
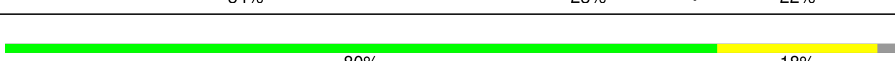
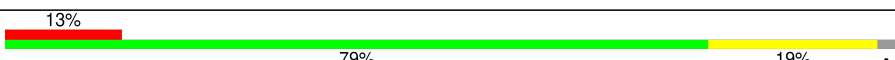
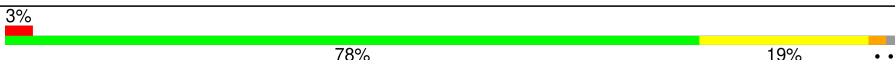
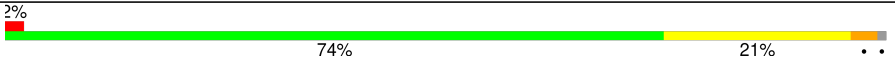
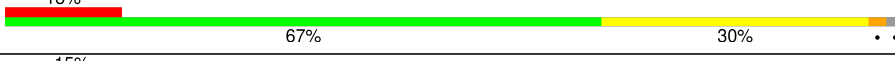
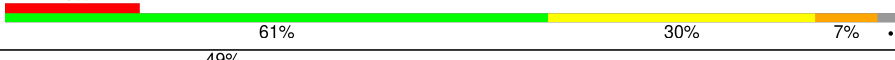
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	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
57	MG	2A	3305	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 298900 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
			1429	916	256	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 mRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0
			1603	722	287	518	74	2		
54	2w	72	Total	C	N	O	P	S	0	0
			1555	699	280	502	72	2		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
55	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
56	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1001	Total	Mg	0	0
			1001	1001		
57	1B	31	Total	Mg	0	0
			31	31		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	10	Total	Mg	0	0
			10	10		
57	1F	9	Total	Mg	0	0
			9	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	7	Total 7	Mg 7	0	0
57	1O	7	Total 7	Mg 7	0	0
57	1P	4	Total 4	Mg 4	0	0
57	1Q	6	Total 6	Mg 6	0	0
57	1R	3	Total 3	Mg 3	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	2	Total 2	Mg 2	0	0
57	1U	4	Total 4	Mg 4	0	0
57	1V	3	Total 3	Mg 3	0	0
57	1W	6	Total 6	Mg 6	0	0
57	1X	7	Total 7	Mg 7	0	0
57	1Y	4	Total 4	Mg 4	0	0
57	1Z	3	Total 3	Mg 3	0	0
57	10	5	Total 5	Mg 5	0	0
57	11	3	Total 3	Mg 3	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	1	Total 1	Mg 1	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	4	Total 4	Mg 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	1	Total 1	Mg 1	0	0
57	17	2	Total 2	Mg 2	0	0
57	18	4	Total 4	Mg 4	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	231	Total 231	Mg 231	0	0
57	1b	2	Total 2	Mg 2	0	0
57	1e	1	Total 1	Mg 1	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1n	2	Total 2	Mg 2	0	0
57	1q	1	Total 1	Mg 1	0	0
57	1r	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1w	4	Total 4	Mg 4	0	0
57	1x	11	Total 11	Mg 11	0	0
57	1y	2	Total 2	Mg 2	0	0
57	2A	687	Total 687	Mg 687	0	0
57	2B	21	Total 21	Mg 21	0	0
57	2D	8	Total 8	Mg 8	0	0
57	2E	6	Total 6	Mg 6	0	0
57	2F	6	Total 6	Mg 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2G	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2P	1	Total 1	Mg 1	0	0
57	2Q	3	Total 3	Mg 3	0	0
57	2R	2	Total 2	Mg 2	0	0
57	2U	2	Total 2	Mg 2	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	1	Total 1	Mg 1	0	0
57	2X	2	Total 2	Mg 2	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	3	Total 3	Mg 3	0	0
57	23	1	Total 1	Mg 1	0	0
57	25	3	Total 3	Mg 3	0	0
57	28	2	Total 2	Mg 2	0	0
57	2a	201	Total 201	Mg 201	0	0
57	2d	2	Total 2	Mg 2	0	0
57	2e	1	Total 1	Mg 1	0	0
57	2f	2	Total 2	Mg 2	0	0
57	2g	1	Total 1	Mg 1	0	0
57	2h	1	Total 1	Mg 1	0	0

Continued on next page...

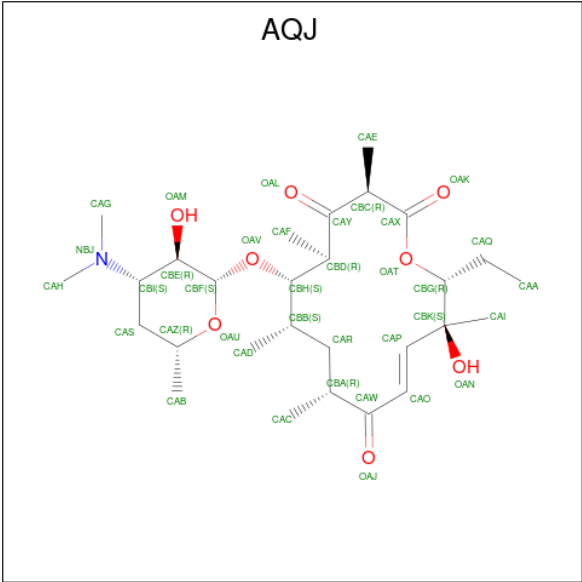
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2j	2	Total 2	Mg 2	0	0
57	2l	2	Total 2	Mg 2	0	0
57	2q	3	Total 3	Mg 3	0	0
57	2r	1	Total 1	Mg 1	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	2	Total 2	Mg 2	0	0
57	2w	4	Total 4	Mg 4	0	0
57	2x	5	Total 5	Mg 5	0	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1	Total 1	K 1	0	0
58	2A	1	Total 1	K 1	0	0

- Molecule 59 is (3R,5R,6S,7S,9R,11E,13S,14R)-14-ethyl-13-hydroxy-3,5,7,9,13-pentamethyl-2,4,10-trioxo-1-oxacyclotetradec-11-en-6-yl 3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-h exopyranoside (CCD ID: AQJ) (formula: C₂₈H₄₇NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1A	1	Total	C	N	O	0	0
			37	28	1	8		
59	2A	1	Total	C	N	O	0	0
			37	28	1	8		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

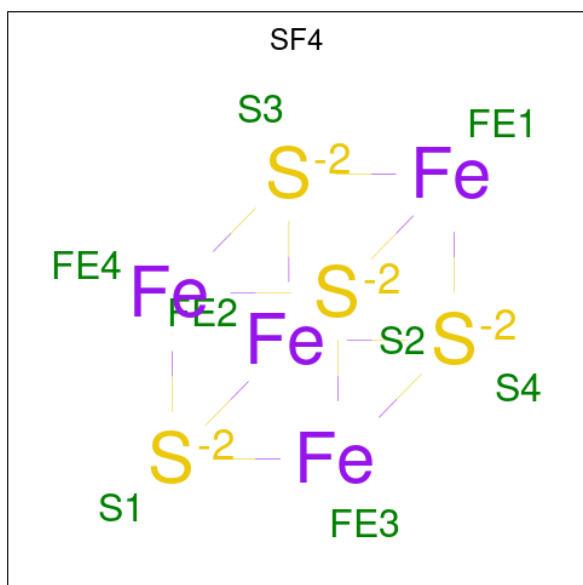
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	29	1	Total	Zn	0	0
			1	1		
60	2n	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1610	Total	O	0	0
			1610	1610		
62	1B	40	Total	O	0	0
			40	40		
62	1D	21	Total	O	0	0
			21	21		
62	1E	19	Total	O	0	0
			19	19		
62	1F	14	Total	O	0	0
			14	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1G	5	Total 5	O 5	0	0
62	1H	1	Total 1	O 1	0	0
62	1I	2	Total 2	O 2	0	0
62	1N	2	Total 2	O 2	0	0
62	1O	5	Total 5	O 5	0	0
62	1P	18	Total 18	O 18	0	0
62	1Q	3	Total 3	O 3	0	0
62	1R	6	Total 6	O 6	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	6	Total 6	O 6	0	0
62	1U	9	Total 9	O 9	0	0
62	1V	4	Total 4	O 4	0	0
62	1W	4	Total 4	O 4	0	0
62	1X	5	Total 5	O 5	0	0
62	1Y	3	Total 3	O 3	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	7	Total 7	O 7	0	0
62	11	2	Total 2	O 2	0	0
62	12	4	Total 4	O 4	0	0
62	13	3	Total 3	O 3	0	0
62	14	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	15	4	Total 4	O 4	0	0
62	17	4	Total 4	O 4	0	0
62	18	8	Total 8	O 8	0	0
62	19	1	Total 1	O 1	0	0
62	1a	276	Total 276	O 276	0	0
62	1b	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0
62	1j	1	Total 1	O 1	0	0
62	1k	1	Total 1	O 1	0	0
62	1l	3	Total 3	O 3	0	0
62	1q	1	Total 1	O 1	0	0
62	1v	3	Total 3	O 3	0	0
62	1w	6	Total 6	O 6	0	0
62	1x	9	Total 9	O 9	0	0
62	1y	1	Total 1	O 1	0	0
62	2A	926	Total 926	O 926	0	0
62	2B	10	Total 10	O 10	0	0
62	2D	16	Total 16	O 16	0	0
62	2E	10	Total 10	O 10	0	0
62	2F	5	Total 5	O 5	0	0
62	2I	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2N	1	Total O 1 1	0	0
62	2O	1	Total O 1 1	0	0
62	2P	10	Total O 10 10	0	0
62	2Q	1	Total O 1 1	0	0
62	2R	2	Total O 2 2	0	0
62	2T	2	Total O 2 2	0	0
62	2U	3	Total O 3 3	0	0
62	2V	1	Total O 1 1	0	0
62	2W	1	Total O 1 1	0	0
62	2X	3	Total O 3 3	0	0
62	2Z	2	Total O 2 2	0	0
62	20	3	Total O 3 3	0	0
62	21	3	Total O 3 3	0	0
62	22	1	Total O 1 1	0	0
62	25	3	Total O 3 3	0	0
62	27	4	Total O 4 4	0	0
62	28	4	Total O 4 4	0	0
62	29	1	Total O 1 1	0	0
62	2a	230	Total O 230 230	0	0
62	2d	2	Total O 2 2	0	0
62	2e	1	Total O 1 1	0	0

Continued on next page...

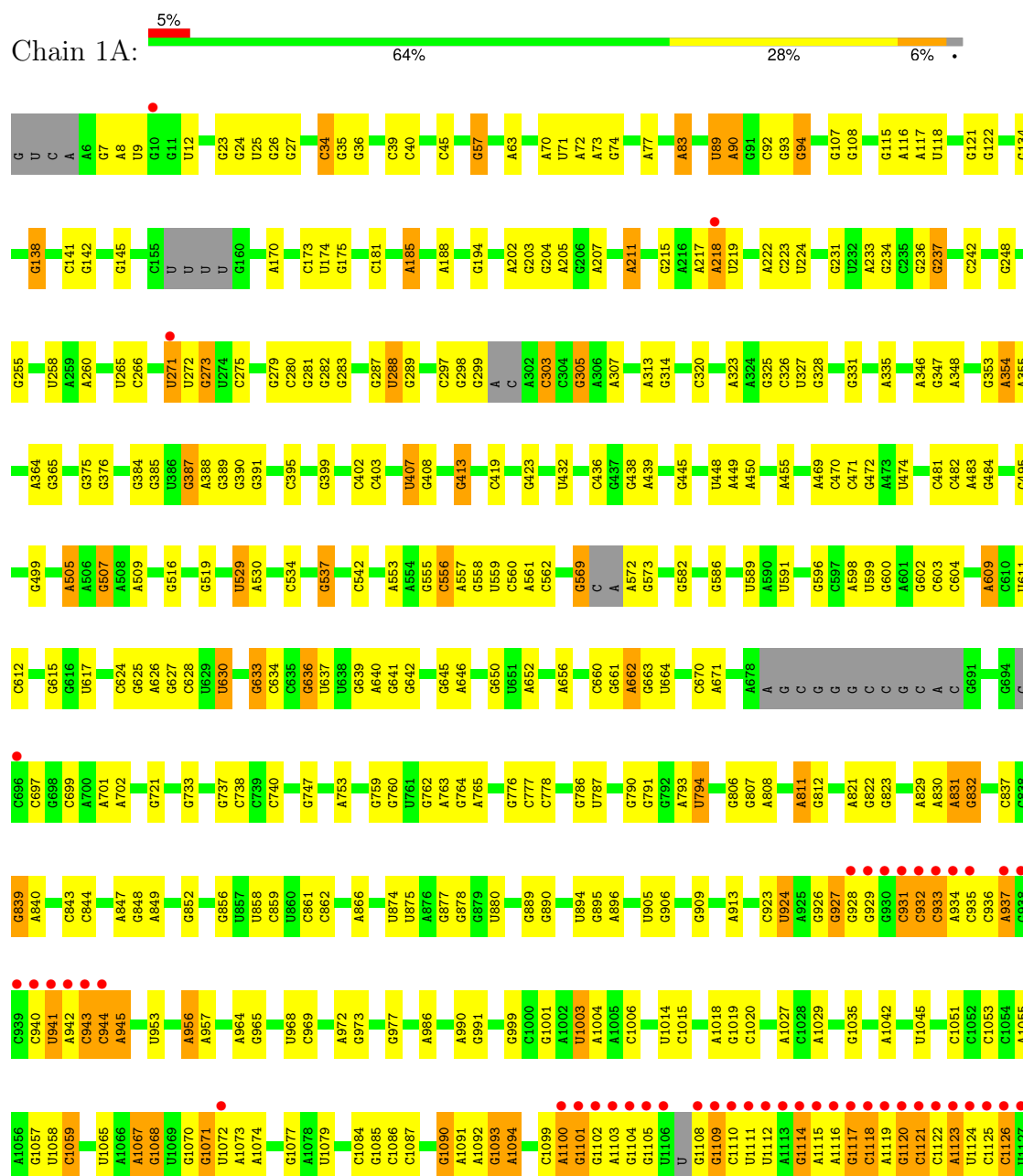
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2f	1	Total	O	0	0
			1	1		
62	2g	1	Total	O	0	0
			1	1		
62	2i	2	Total	O	0	0
			2	2		
62	2j	4	Total	O	0	0
			4	4		
62	2l	3	Total	O	0	0
			3	3		
62	2n	1	Total	O	0	0
			1	1		
62	2o	1	Total	O	0	0
			1	1		
62	2v	2	Total	O	0	0
			2	2		
62	2w	1	Total	O	0	0
			1	1		
62	2x	5	Total	O	0	0
			5	5		

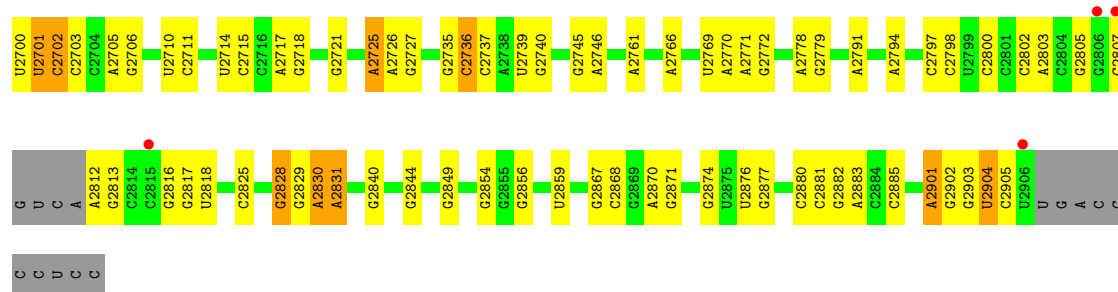
3 Residue-property plots

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.

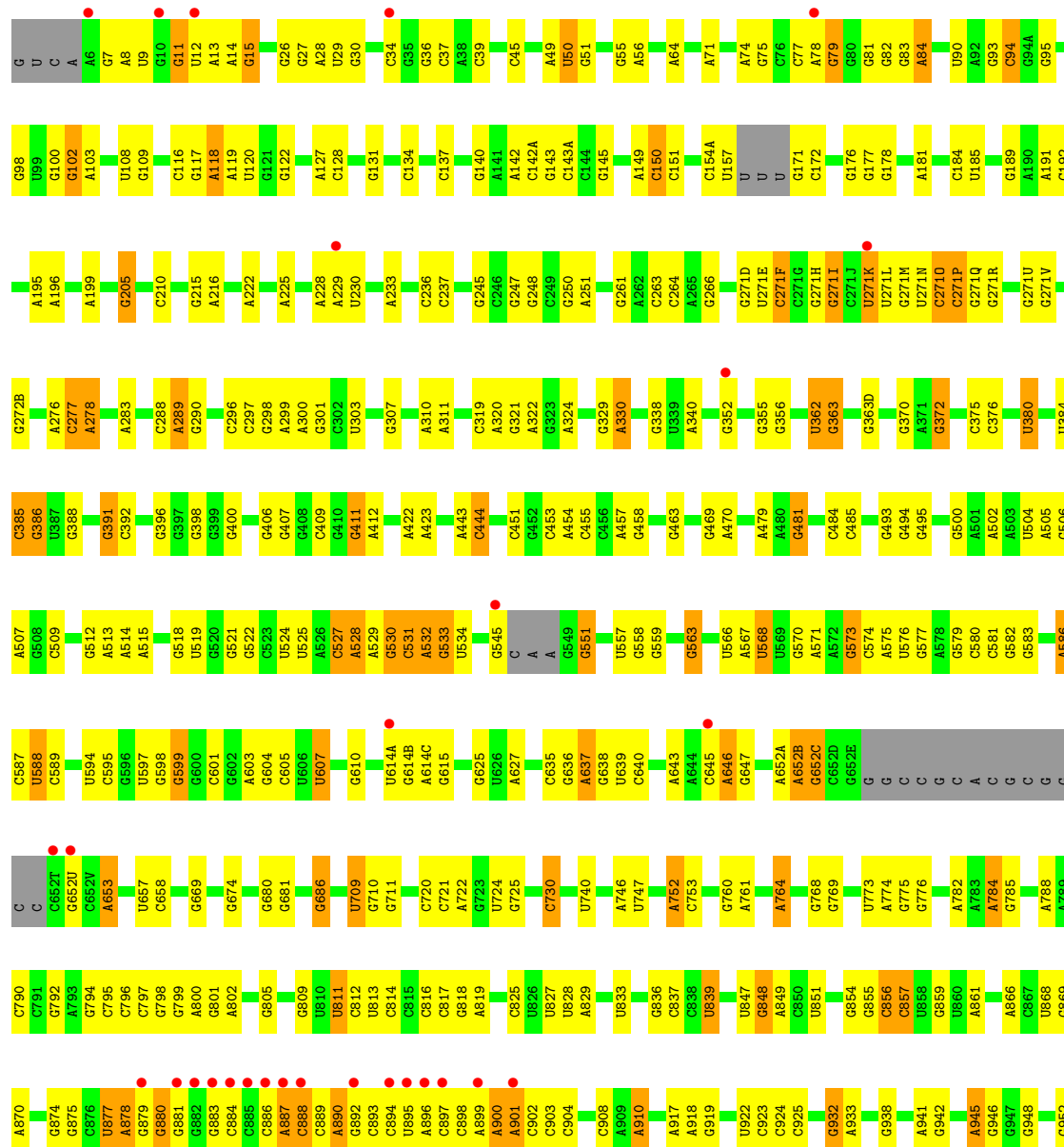
• Molecule 1: 23S Ribosomal RNA



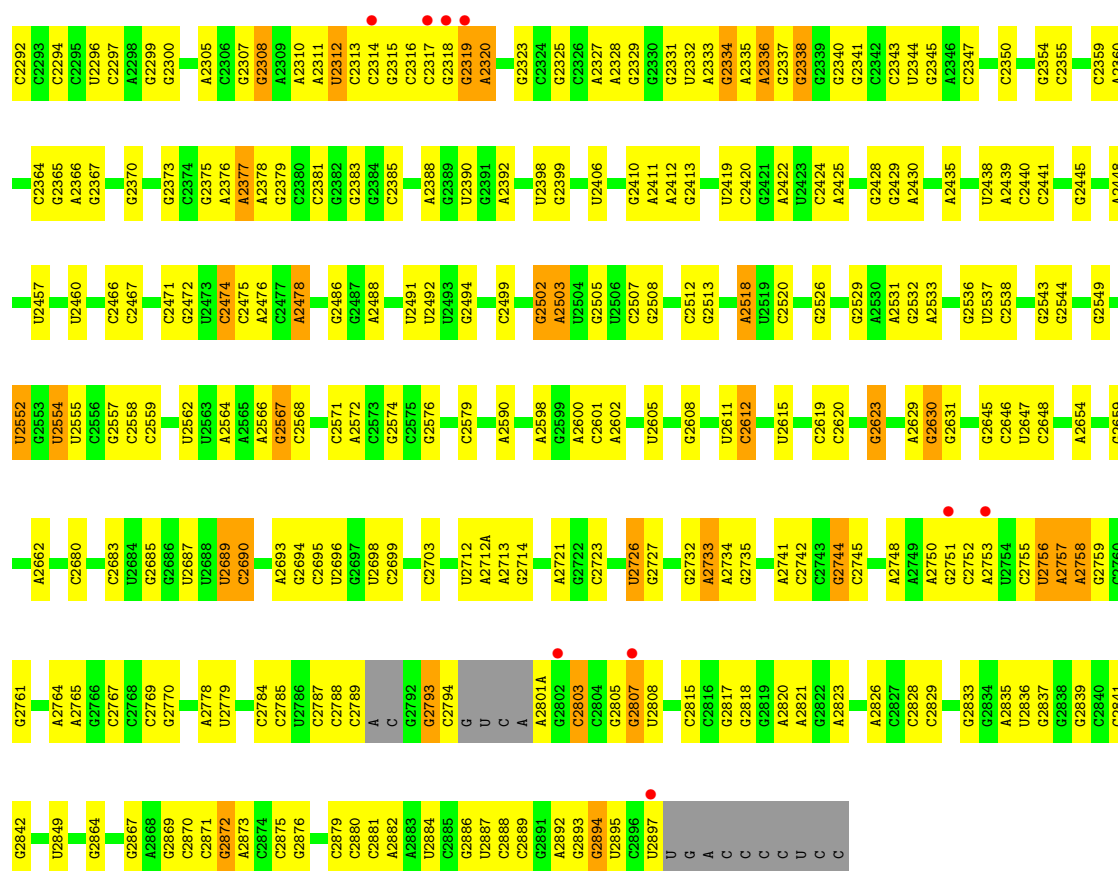
G2569	U2450	A2347	C2326	C2160	G1951	U1829	A1712	G1576	U1466	U1346	G1218	U1128
C2570	A2451	A2348	G2227	C2161	G1952	G1830	A1715	C1577	G1467	A1347	A1219	U1129
C2452	C2453	G2353	G2228	C2162	A1959	C1831	A1716	C1578	G1472	U1359	U1220	A1130
A2357	A2460	G2357	A2237	C2164	A1960	A1833	G1719	C1579	G1473	C1361	G1221	A1131
A2358	U2461	C2358	G2247	U2166	U1961	A1834	U1720	G	C1474	C1364	C1222	A1132
C2359	G2466	C2360	C2248	C2167	C1964	G1845	G1721	U	G1475	G1365	C1223	A1133
C2360	G2361	G2250	C2249	G2168	G1971	A1846	G1729	A	C1476	C1366	C1224	A1134
C2362	C2362	G2251	G2251	G2169	G1972	G1847	G1733	C	U1477	U1376	U1232	U1135
G2365	G2482	U2255	U2255	G2170	U1973	G1848	G1734	G1584	U1478	C1376	C1246	U1136
G2366	G2365	U2256	U2256	G2171	A1974	G1857	G1734	G1586	U1479	U1377	C1247	U1137
C2367	G2484	U2257	U2257	G2172	A1975	C1858	G1734	G1587	C1483	A1377	U1376	U1138
G2368	U2485	G2257	G2257	G2173	U1976	G1859	U1740	G1588	A1491	G1378	U1255	U1139
U2486	G2486	G2258	G2258	G2174	U1977	A1860	U1740	C1589	U1492	U1379	A1255	A1141
A2372	A2372	G2259	G2259	G2175	U1977	C1861	A1747	C1590	C1493	G1380	U1256	A1142
A2373	A2373	G2260	G2260	G2176	C1980	C1861	A1747	A1601	C1493	U1380	A1265	A1144
G2379	A2279	G2261	G2261	G2177	U1981	U1864	G1750	A1605	G1497	G1384	U1269	U1145
A2380	A2280	G2262	G2262	G2178	A1982	C1868	G1750	A1605	G1502	C1391	A1272	U1147
G2383	G2282	G2282	G2282	A2180	C1983	C1869	U1765	A1613	G1506	G1394	A1272	C1150
A2389	C2283	G2283	G2283	G2181	C1984	G1870	A1767	A1614	G1507	U1398	G1277	U1151
C2391	C2283	G2283	G2283	G2182	U1985	A1878	U1768	G1615	A1507	A1406	A1283	G1152
C2392	C2283	G2283	G2283	G2183	G1986	C1878	U1768	G1615	A1507	A1406	A1283	C1155
C2393	C2283	G2283	G2283	G2184	C1987	A1878	U1768	G1615	A1507	A1406	A1283	G1156
C2394	C2283	G2283	G2283	G2185	A1988	A1890	U1770	A1619	A1518	A1406	G1285	G1157
C2395	C2283	G2283	G2283	G2186	C1989	A1890	U1770	A1619	A1518	A1406	G1285	G1158
C2396	C2283	G2283	G2283	G2187	G1990	G1896	G1776	U1625	G1525	G1410	A1299	C1170
C2397	C2283	G2283	G2283	G2188	A1991	C1897	G1776	A1633	G1526	G1410	A1300	G1171
C2398	C2283	G2283	G2283	G2189	A1992	A1897	G1776	A1633	G1526	A1411	U1301	U1176
C2399	C2283	G2283	G2283	G2190	A1993	A1898	G1776	A1634	G1527	C1416	G1302	U1176
C2400	C2283	G2283	G2283	G2191	A1994	A1899	G1776	C1634	U1528	C1416	U1302	U1176
C2401	C2283	G2283	G2283	G2192	A1995	A1900	G1776	G1639	U1529	C1416	U1302	U1176
C2402	C2283	G2283	G2283	G2193	A1996	C1901	G1776	G1640	U1530	C1416	U1302	U1176
C2403	C2283	G2283	G2283	G2194	U1997	G1904	G1776	G1640	U1530	C1416	U1302	U1176
C2404	C2283	G2283	G2283	G2195	U1998	C1905	G1776	G1640	U1530	C1416	U1302	U1176
C2405	C2283	G2283	G2283	G2196	G2014	G1905	G1776	G1640	U1530	C1416	U1302	U1176
C2406	C2283	G2283	G2283	G2197	U2015	A1911	G1793	G1640	U1530	C1416	U1302	U1176
C2407	C2283	G2283	G2283	G2198	U2016	A1912	G1793	G1640	U1530	C1416	U1302	U1176
C2408	C2283	G2283	G2283	G2199	C2018	A1913	G1793	G1640	U1530	C1416	U1302	U1176
C2409	C2283	G2283	G2283	G2200	G2019	A1914	G1793	G1640	U1530	C1416	U1302	U1176
C2410	C2283	G2283	G2283	G2201	G2020	A1915	G1793	G1640	U1530	C1416	U1302	U1176
C2411	C2283	G2283	G2283	G2202	G2021	A1916	G1793	G1640	U1530	C1416	U1302	U1176
C2412	C2283	G2283	G2283	G2203	G2022	A1917	G1793	G1640	U1530	C1416	U1302	U1176
C2413	C2283	G2283	G2283	G2204	A2023	A1918	G1793	G1640	U1530	C1416	U1302	U1176
C2414	C2283	G2283	G2283	G2205	G2024	A1919	G1793	G1640	U1530	C1416	U1302	U1176
C2415	C2283	G2283	G2283	G2206	G2025	A1920	G1793	G1640	U1530	C1416	U1302	U1176
C2416	C2283	G2283	G2283	G2207	G2026	A1921	G1793	G1640	U1530	C1416	U1302	U1176
C2417	C2283	G2283	G2283	G2208	G2027	A1922	G1793	G1640	U1530	C1416	U1302	U1176
C2418	C2283	G2283	G2283	G2209	G2028	A1923	G1793	G1640	U1530	C1416	U1302	U1176
C2419	C2283	G2283	G2283	G2210	G2029	A1924	G1793	G1640	U1530	C1416	U1302	U1176
C2420	C2283	G2283	G2283	G2211	G2030	A1925	G1793	G1640	U1530	C1416	U1302	U1176
C2421	C2283	G2283	G2283	G2212	G2031	A1926	G1793	G1640	U1530	C1416	U1302	U1176
C2422	C2283	G2283	G2283	G2213	G2032	A1927	G1793	G1640	U1530	C1416	U1302	U1176
C2423	C2283	G2283	G2283	G2214	G2033	A1928	G1793	G1640	U1530	C1416	U1302	U1176
C2424	C2283	G2283	G2283	G2215	G2034	A1929	G1793	G1640	U1530	C1416	U1302	U1176
C2425	C2283	G2283	G2283	G2216	G2035	A1930	G1793	G1640	U1530	C1416	U1302	U1176
C2426	C2283	G2283	G2283	G2217	G2036	A1931	G1793	G1640	U1530	C1416	U1302	U1176
C2427	C2283	G2283	G2283	G2218	G2037	A1932	G1793	G1640	U1530	C1416	U1302	U1176
C2428	C2283	G2283	G2283	G2219	G2038	A1933	G1793	G1640	U1530	C1416	U1302	U1176
C2429	C2283	G2283	G2283	G2220	G2039	A1934	G1793	G1640	U1530	C1416	U1302	U1176
C2430	C2283	G2283	G2283	G2221	G2040	A1935	G1793	G1640	U1530	C1416	U1302	U1176
C2431	C2283	G2283	G2283	G2222	G2041	A1936	G1793	G1640	U1530	C1416	U1302	U1176
C2432	C2283	G2283	G2283	G2223	G2042	A1937	G1793	G1640	U1530	C1416	U1302	U1176
C2433	C2283	G2283	G2283	G2224	G2043	A1938	G1793	G1640	U1530	C1416	U1302	U1176
C2434	C2283	G2283	G2283	G2225	G2044	A1939	G1793	G1640	U1530	C1416	U1302	U1176
C2435	C2283	G2283	G2283	G2226	G2045	A1940	G1793	G1640	U1530	C1416	U1302	U1176
C2436	C2283	G2283	G2283	G2227	G2046	A1941	G1793	G1640	U1530	C1416	U1302	U1176
C2437	C2283	G2283	G2283	G2228	G2047	A1942	G1793	G1640	U1530	C1416	U1302	U1176
C2438	C2283	G2283	G2283	G2229	G2048	A1943	G1793	G1640	U1530	C1416	U1302	U1176
C2439	C2283	G2283	G2283	G2230	G2049	A1944	G1793	G1640	U1530	C1416	U1302	U1176
C2440	C2283	G2283	G2283	G2231	G2050	A1945	G1793	G1640	U1530	C1416	U1302	U1176
C2441	C2283	G2283	G2283	G2232	G2051	A1946	G1793	G1640	U1530	C1416	U1302	U1176
C2442	C2283	G2283	G2283	G2233	G2052	A1947	G1793	G1640	U1530	C1416	U1302	U1176
C2443	C2283	G2283	G2283	G2234	G2053	A1948	G1793	G1640	U1530	C1416	U1302	U1176
C2444	C2283	G2283	G2283	G2235	G2054	A1949	G1793	G1640	U1530	C1416	U1302	U1176
C2445	C2283	G2283	G2283	G2236	G2055	A1950	G1793	G1640	U1530	C1416	U1302	U1176
C2446	C2283	G2283	G2283	G2237	G2056	A1951	G1793	G1640	U1530	C1416	U1302	U1176
C2447	C2283	G2283	G2283	G2238	G2057	A1952	G1793	G1640	U1530	C1416	U1302	U1176
C2448	C2283	G2283	G2283	G2239	G2058	A1953	G1793	G1640	U1530	C1416	U1302	U1176
C2449	C2283	G2283	G2283	G2240	G2059	A1954	G1793	G1640	U1530	C1416	U1302	U1176
C2450	C2283	G2283	G2283	G2241	G2060	A1955	G1793	G1640	U1530	C1416	U1302	U1176
C2451	C2283	G2283	G2283	G2242	G2061	A1956	G1793	G1640	U1530	C1416	U1302	U1176
C2452	C2283	G2283	G2283	G2243	G2062	A1957	G1793	G1640	U1530	C1416	U1302	U1176
C2453	C2283	G2283	G2283	G2244	G2063	A1958	G1793	G1640	U1530	C1416	U1302	U1176
C2454	C2283	G2283	G2283	G2245	G2064	A1959	G1793	G1640	U1530	C1416	U1302	U1176
C2455	C2283	G2283	G2283	G2246	G2065	A1960	G1793	G1640	U1530	C1416	U1302	U1176
C2456	C2283	G2283	G2283	G2247	G2066	A1961	G1793	G1640	U1530	C1416	U1302	U1176
C2457	C2283	G2283	G2283	G2248	G2067	A1962	G1793	G1640	U1530	C1416	U1302	U1176
C2458	C2283	G2283	G2283	G2249	G2068	A1963	G1793	G1640	U1530	C1416	U1302	U1176
C2459	C2283	G2283	G2283	G2250	G2069	A1964	G1793	G1640	U1530	C1416	U1302	U1176
C2460	C2283	G2283	G2283	G2251	G2070	A1965	G1793	G1640	U1530	C1416	U1302	U1176
C2461	C2283	G2283	G2283	G2252	G2071	A1966	G1793	G1640	U1530	C1416	U1302	U1176
C2462	C2283	G2283	G2283	G2253	G2072	A1967	G1793	G1640	U1530	C1416	U1302	U1176
C2463	C2283	G2283	G2283	G2254	G2073	A1968	G1793	G1640	U1530	C1416	U1302	U1176
C2464	C2283	G2283	G2283	G2255	G2074	A1969	G1793	G1640	U1530	C1416	U1302	U1176
C2465	C2283	G2283	G2283	G2256	G2075	A1970	G1793	G1640	U1530	C1416	U1302	U1176
C2466	C2283	G2283	G2283	G2257	G2076	A1971	G1793	G1640	U1530	C1416	U1302	U1176
C2467	C2283	G2283	G2283	G2258	G2077	A1972	G1793	G1640	U1530	C1416	U1302	U1176
C2468	C2283	G2283	G2283	G2259	G2078	A1973	G1793	G1640	U1530	C1416	U1302	U1176
C2469	C2283	G2283	G2283	G2260	G2079	A1974	G1793	G1640	U1530	C1416	U1302	U1176
C2470	C2283	G2283	G2283	G2261	G2080	A1975	G1793	G1640	U1530	C1416	U1302	U1176
C2471	C2											



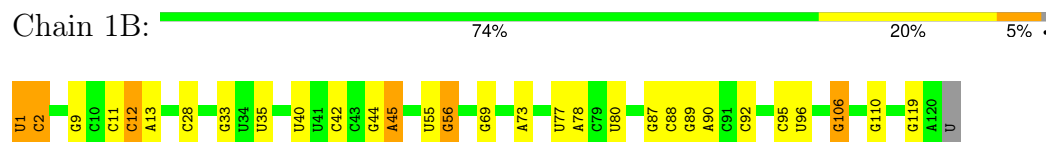
• Molecule 1: 23S Ribosomal RNA



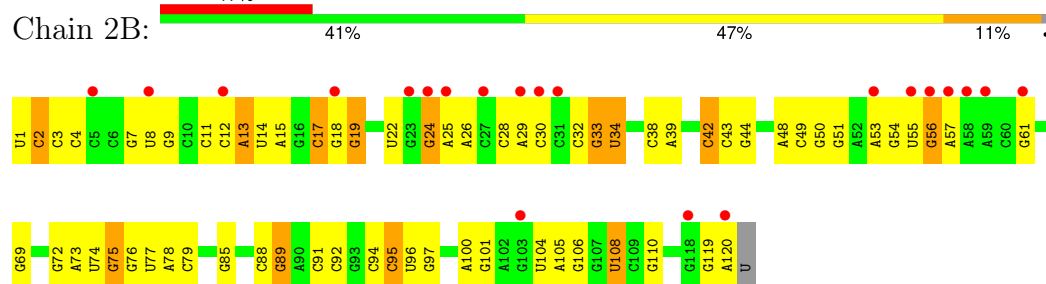




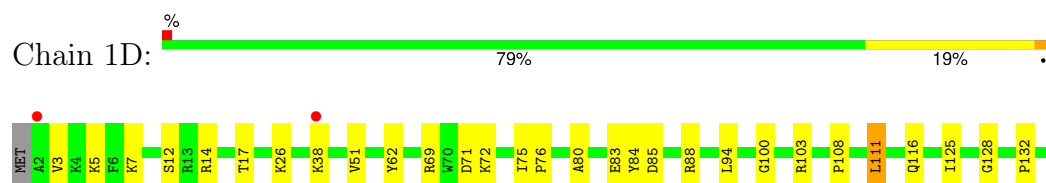
• Molecule 2: 5S Ribosomal RNA



• Molecule 2: 5S Ribosomal RNA

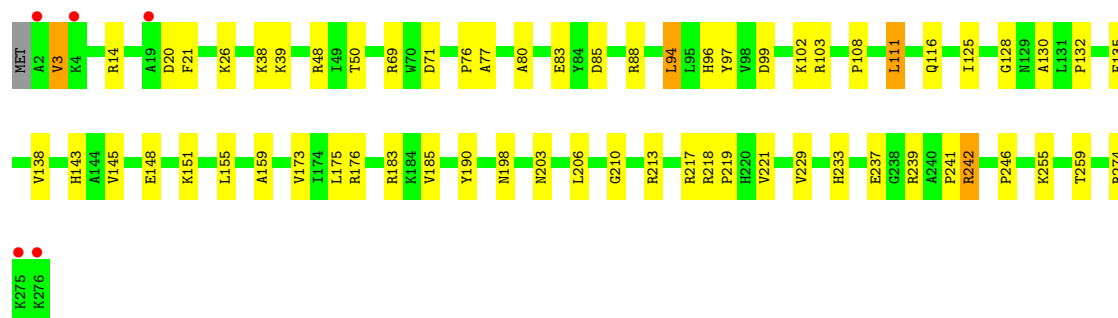
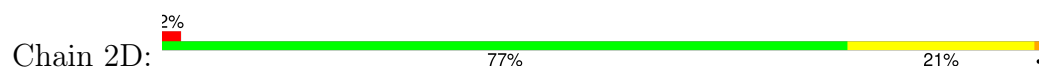


• Molecule 3: 50S ribosomal protein L2

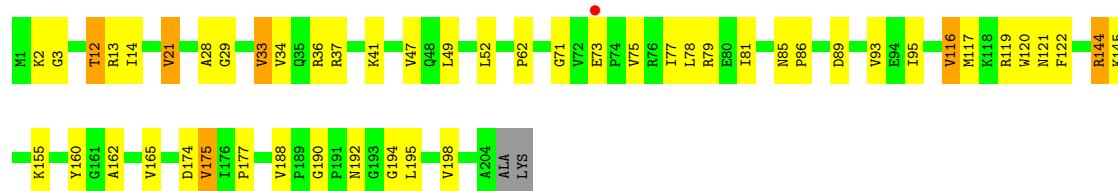
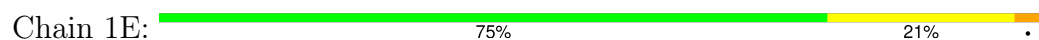




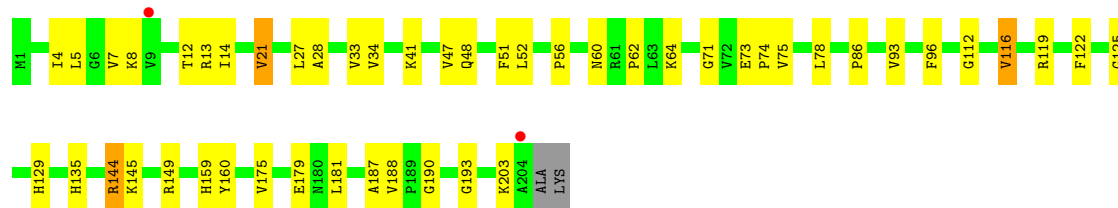
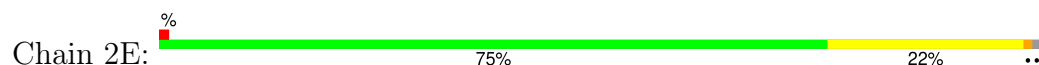
- Molecule 3: 50S ribosomal protein L2



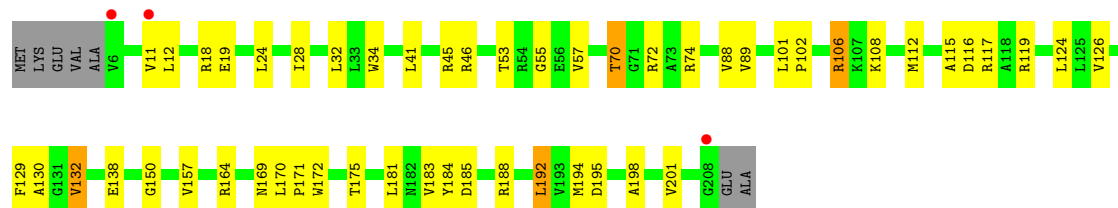
- Molecule 4: 50S ribosomal protein L3



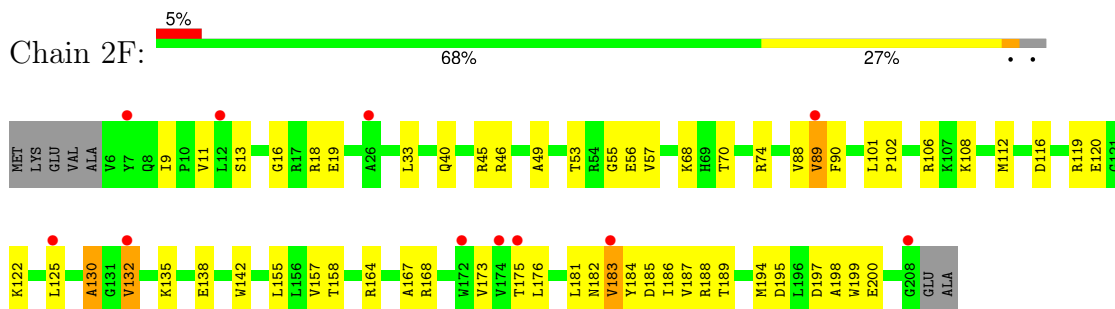
- Molecule 4: 50S ribosomal protein L3



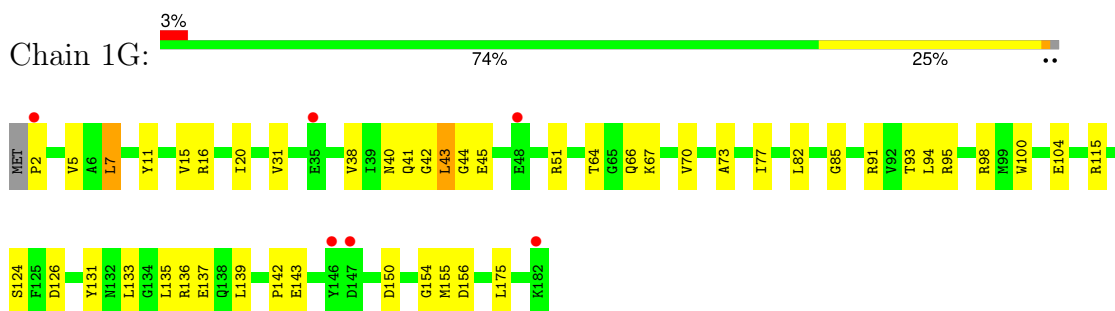
- Molecule 5: 50S ribosomal protein L4



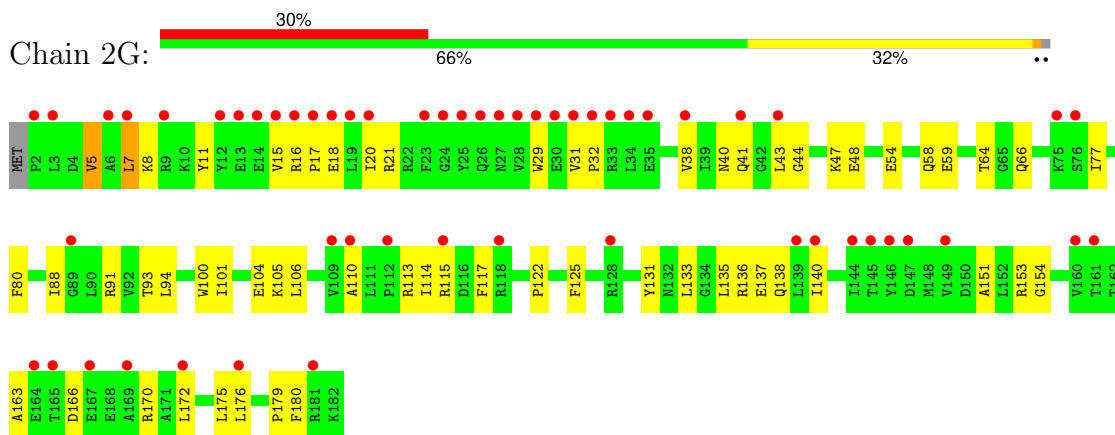
- Molecule 5: 50S ribosomal protein L4



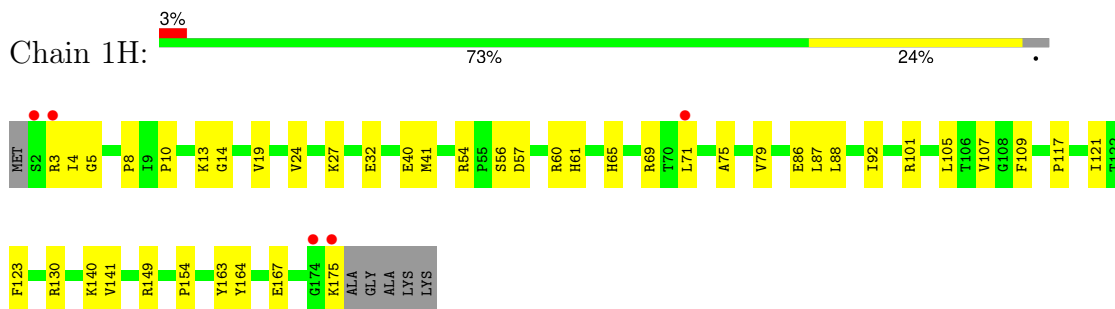
- Molecule 6: 50S ribosomal protein L5



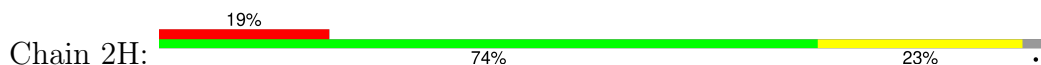
- Molecule 6: 50S ribosomal protein L5

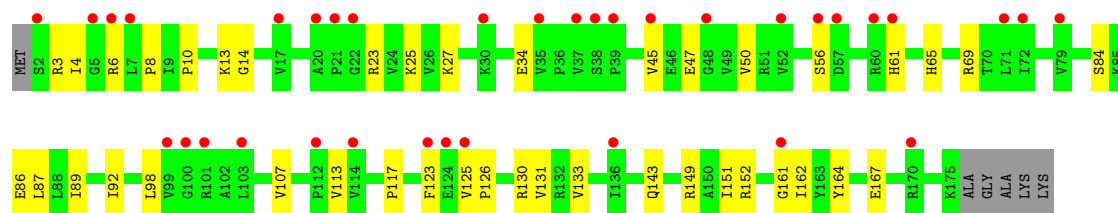


- Molecule 7: 50S ribosomal protein L6

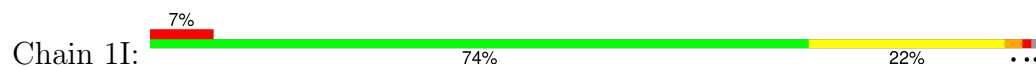


- Molecule 7: 50S ribosomal protein L6

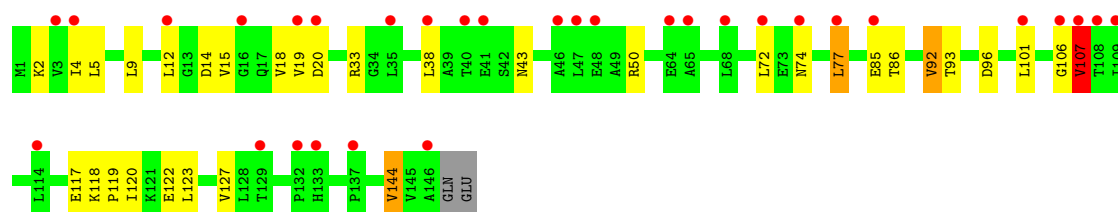
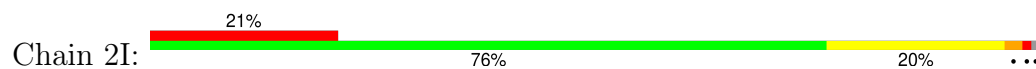




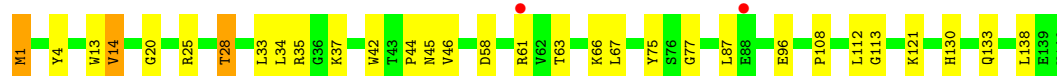
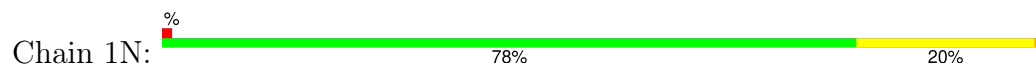
• Molecule 8: 50S ribosomal protein L9



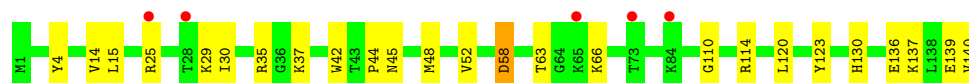
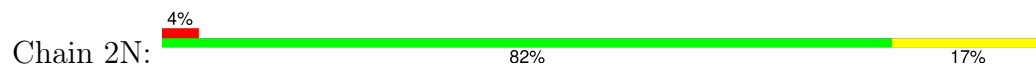
• Molecule 8: 50S ribosomal protein L9



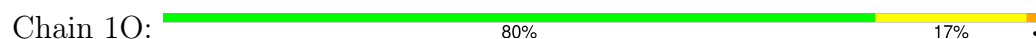
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13

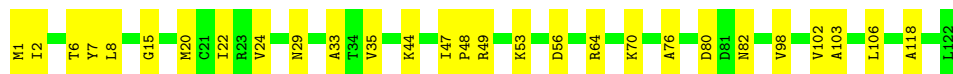


• Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14

Chain 2O:  77% 23%



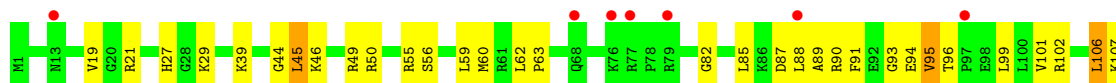
- Molecule 11: 50S ribosomal protein L15

Chain 1P:  4% 68% 29% . .



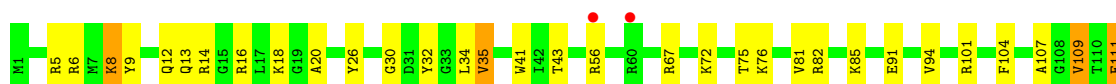
- Molecule 11: 50S ribosomal protein L15

Chain 2P:  5% 69% 28% . .



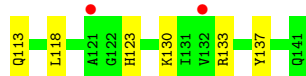
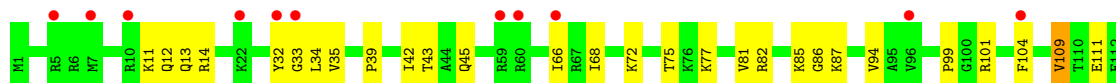
- Molecule 12: 50S ribosomal protein L16

Chain 1Q:  % 71% 26% .

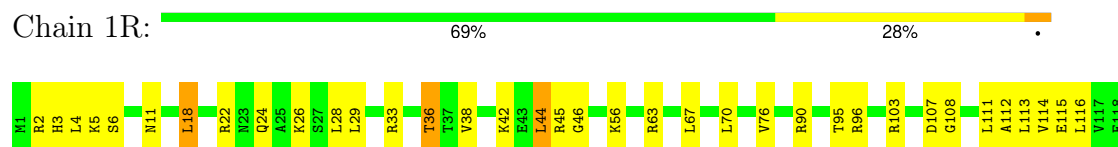


- Molecule 12: 50S ribosomal protein L16

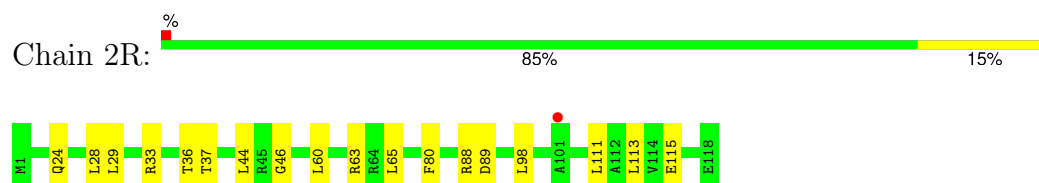
Chain 2Q:  9% 76% 23% .



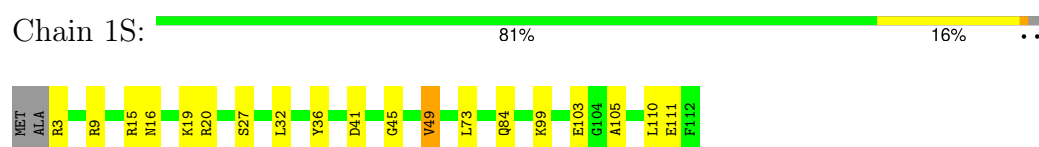
- Molecule 13: 50S ribosomal protein L17



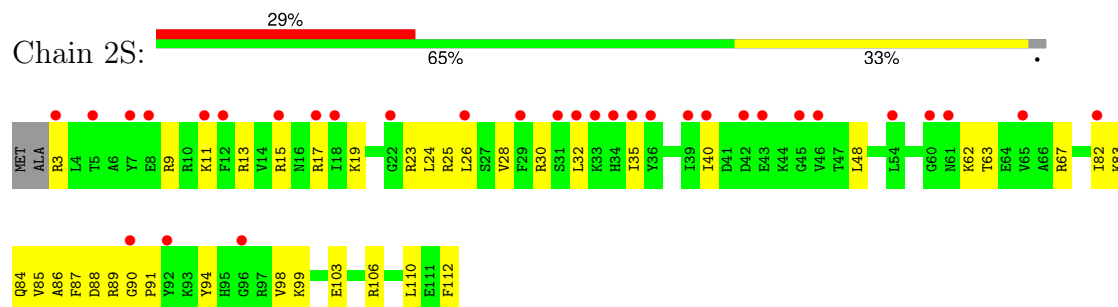
- Molecule 13: 50S ribosomal protein L17



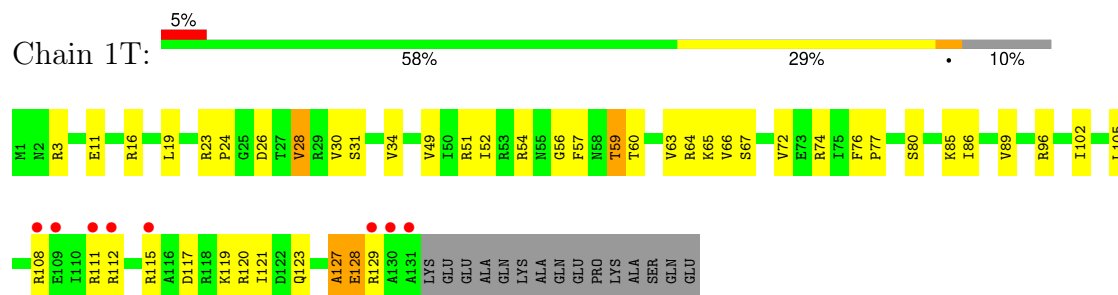
- Molecule 14: 50S ribosomal protein L18



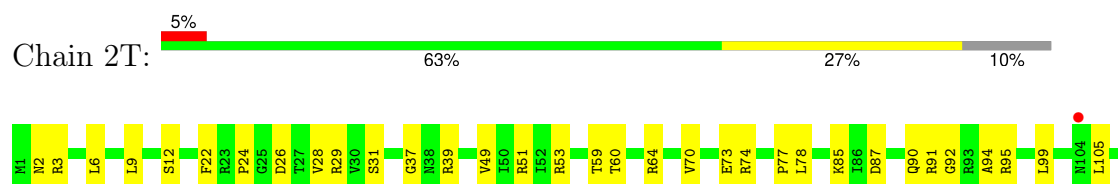
- Molecule 14: 50S ribosomal protein L18

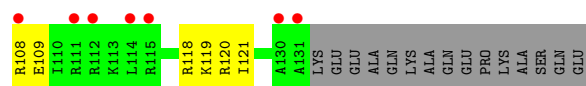


- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19

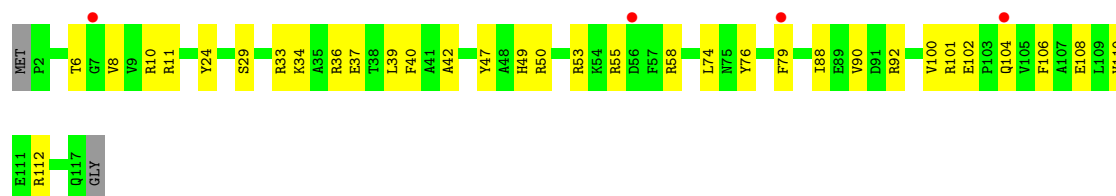




- Molecule 16: 50S ribosomal protein L20



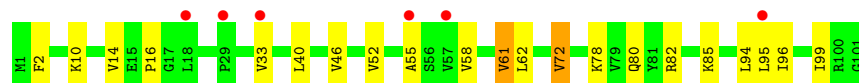
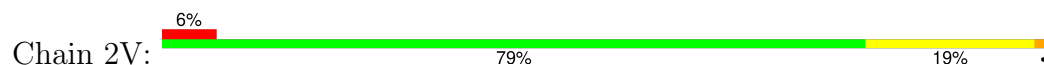
- Molecule 16: 50S ribosomal protein L20



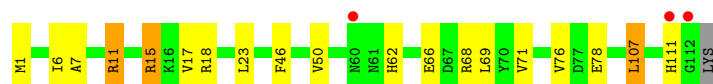
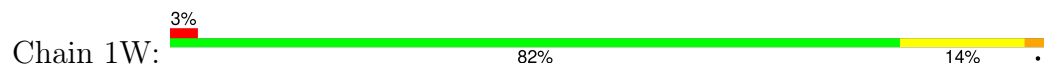
- Molecule 17: 50S ribosomal protein L21



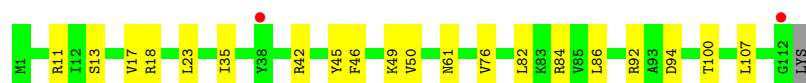
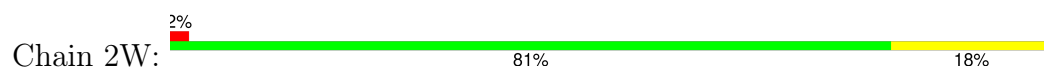
- Molecule 17: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L22



- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23

Chain 1X:  82% 15% ..



- Molecule 19: 50S ribosomal protein L23

Chain 2X:  6% 78% 21% .



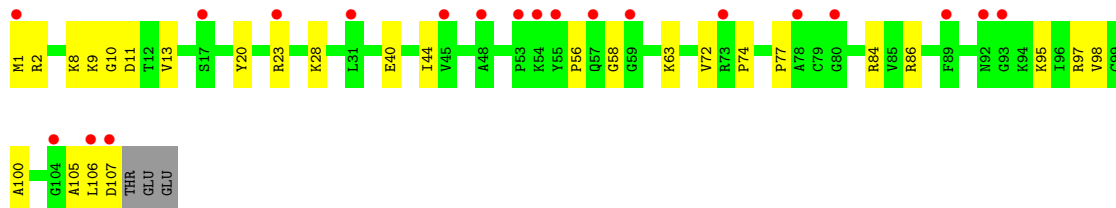
- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  3% 75% 21% ..

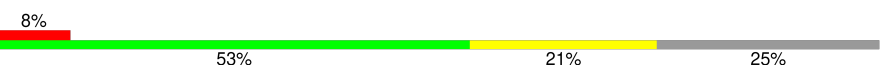


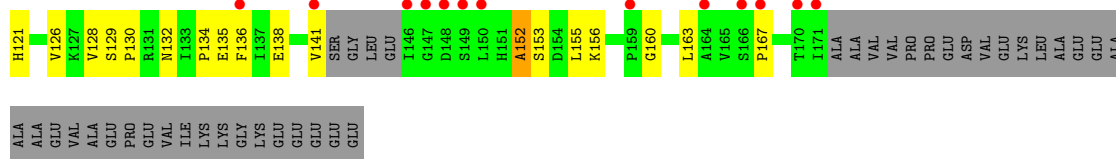
- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  18% 73% 25% .



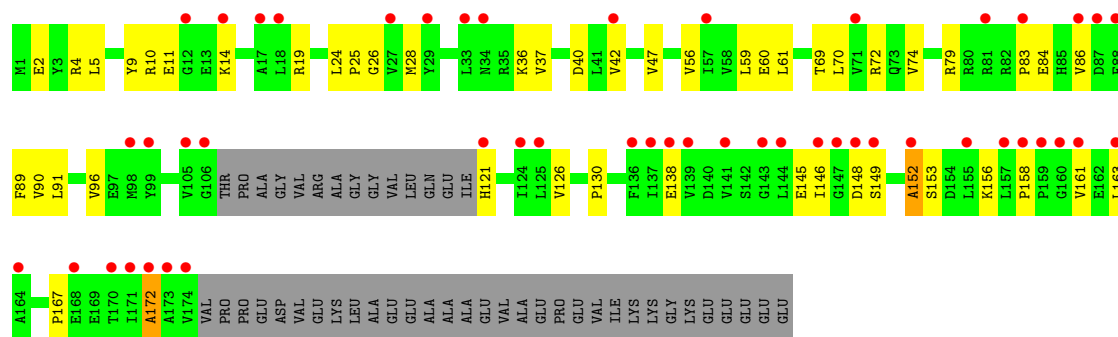
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  8% 53% 21% 25%

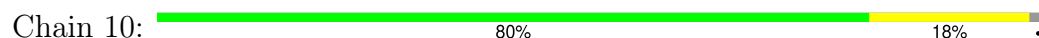


- Molecule 21: 50S ribosomal protein L25

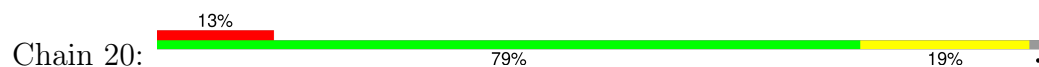
Chain 2Z:  24% 54% 23% 22%



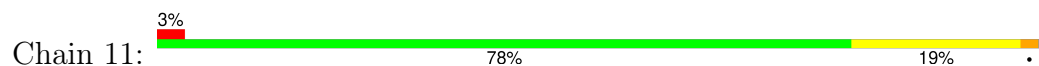
- Molecule 22: 50S ribosomal protein L27



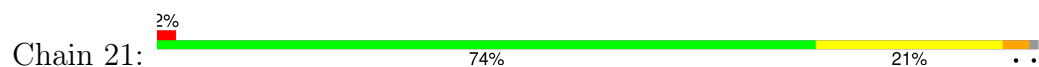
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



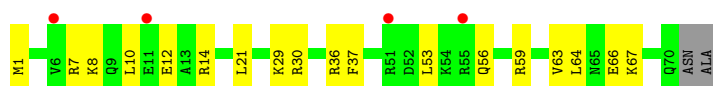
- Molecule 23: 50S ribosomal protein L28



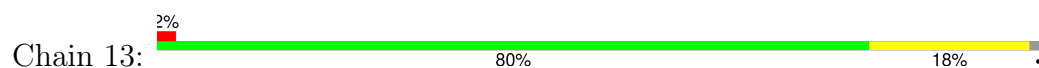
- Molecule 24: 50S ribosomal protein L29



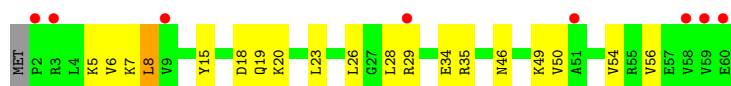
- Molecule 24: 50S ribosomal protein L29



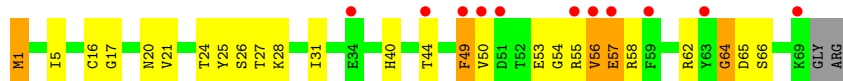
- Molecule 25: 50S ribosomal protein L30



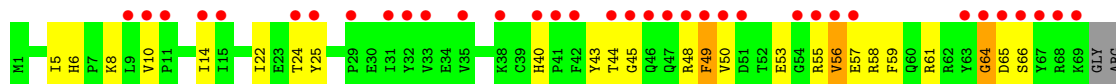
- Molecule 25: 50S ribosomal protein L30



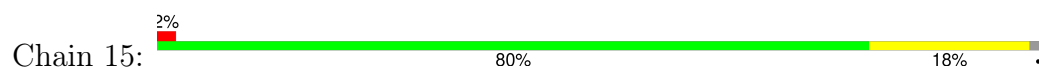
- Molecule 26: 50S ribosomal protein L31



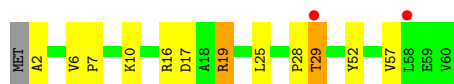
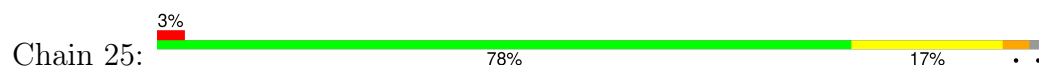
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

Chain 16:  80% 19%



- Molecule 28: 50S ribosomal protein L33

Chain 26:  78% 20%



- Molecule 29: 50S ribosomal protein L34

Chain 17:  2% 84% 10%



- Molecule 29: 50S ribosomal protein L34

Chain 27:  4% 71% 27%



- Molecule 30: 50S ribosomal protein L35

Chain 18:  57% 38%



- Molecule 30: 50S ribosomal protein L35

Chain 28:  2% 63% 34%



- Molecule 31: 50S ribosomal protein L36

Chain 19:  73% 24%



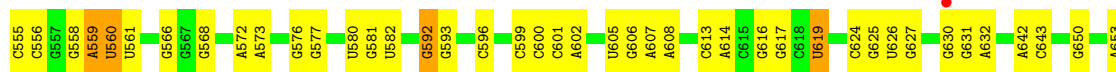
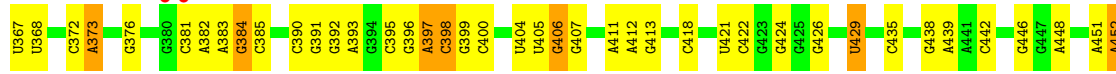
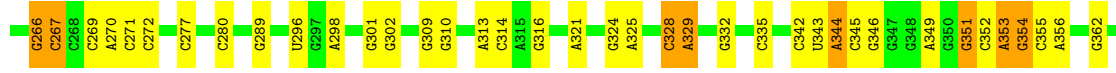
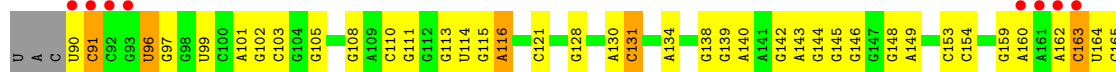
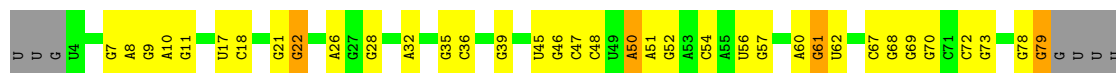
- Molecule 31: 50S ribosomal protein L36

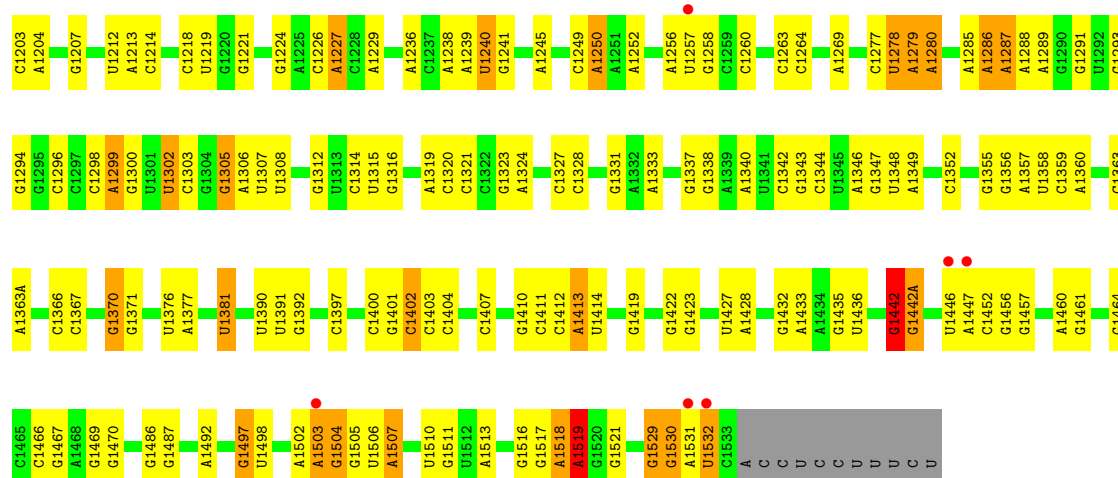
Chain 29:  78% 22%



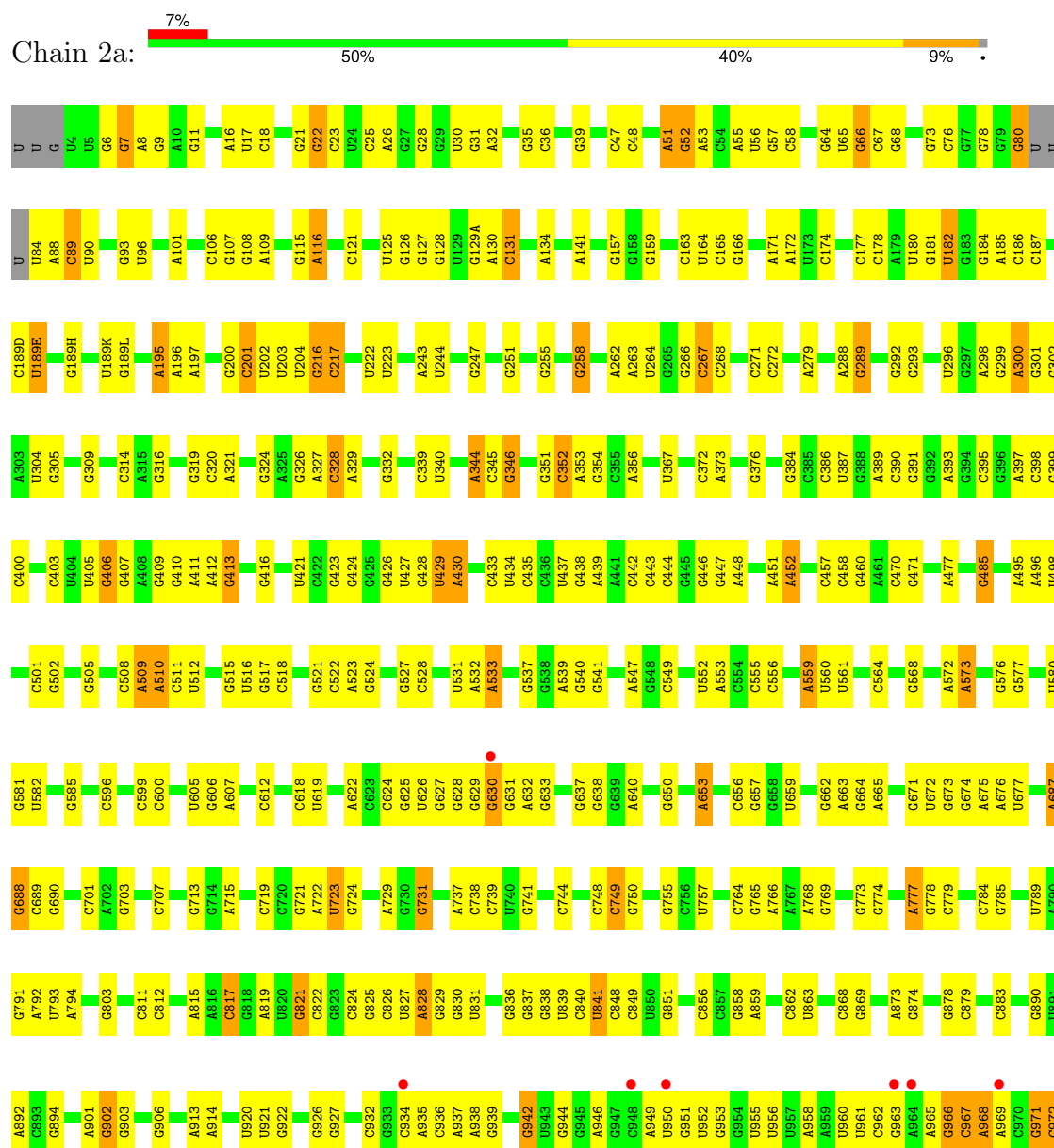
• Molecule 32: 16S Ribosomal RNA

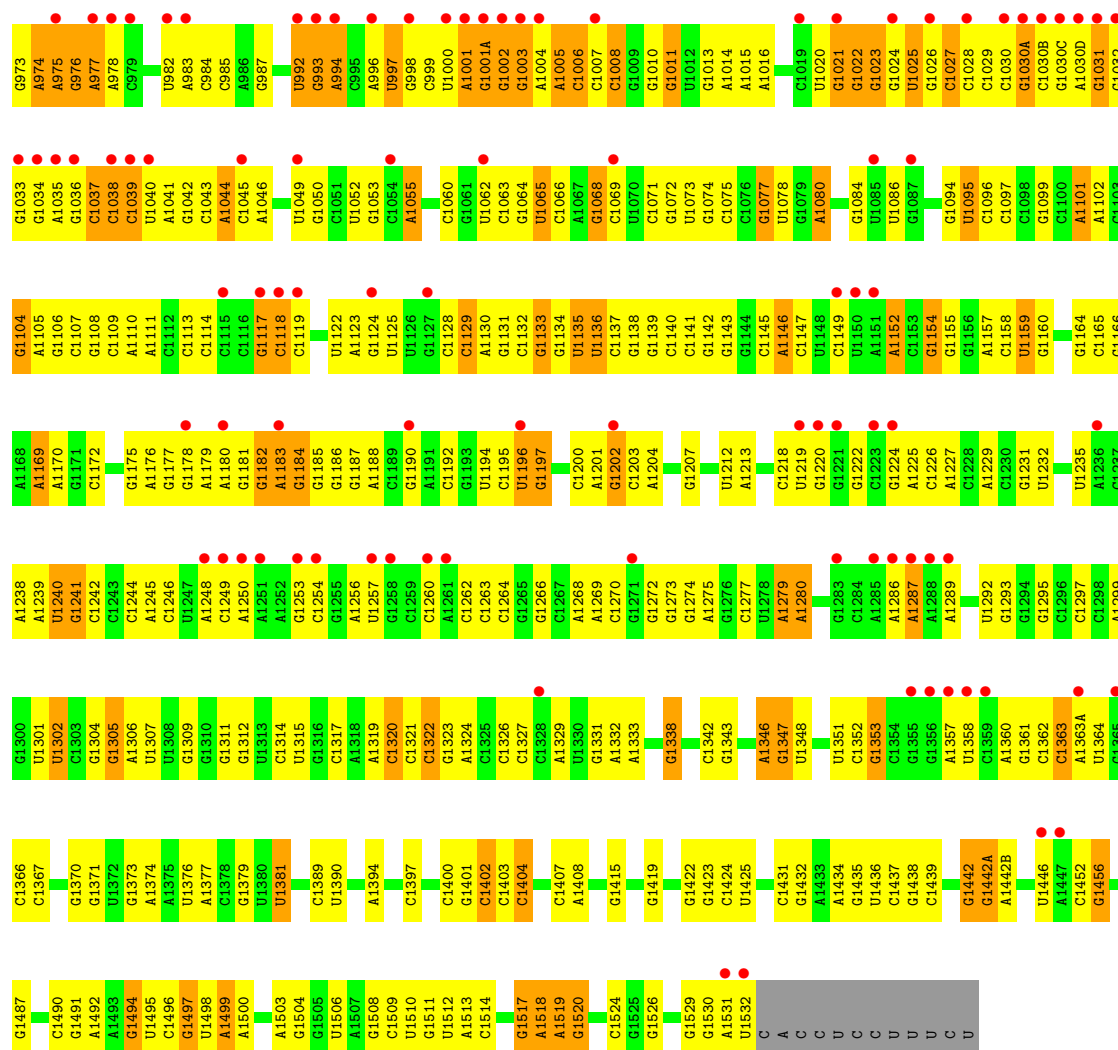
Chain 1a:  3% 57% 35% 7%





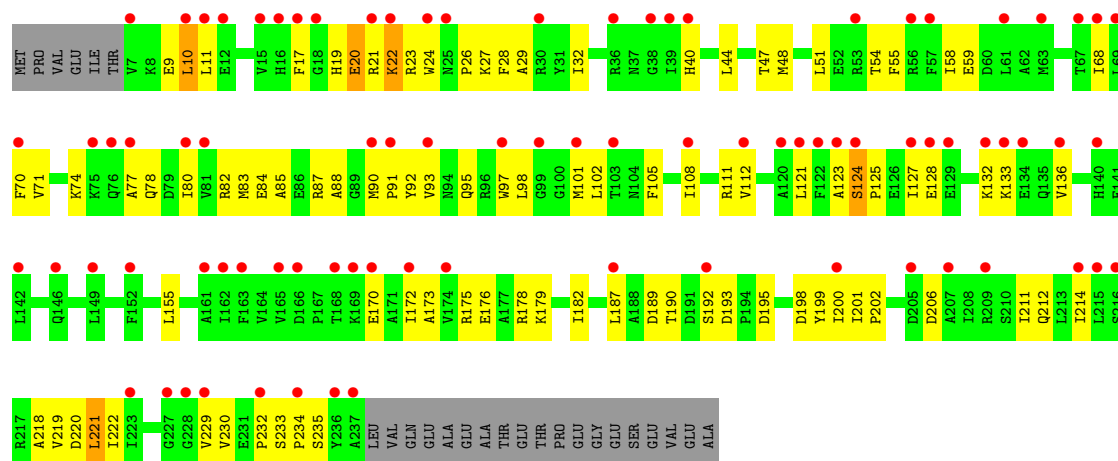
• Molecule 32: 16S Ribosomal RNA



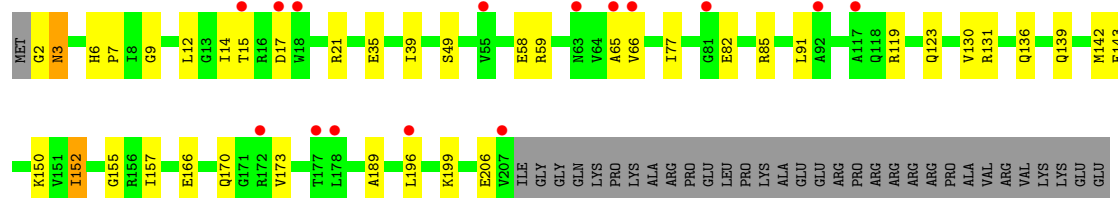


• Molecule 33: 30S ribosomal protein S2

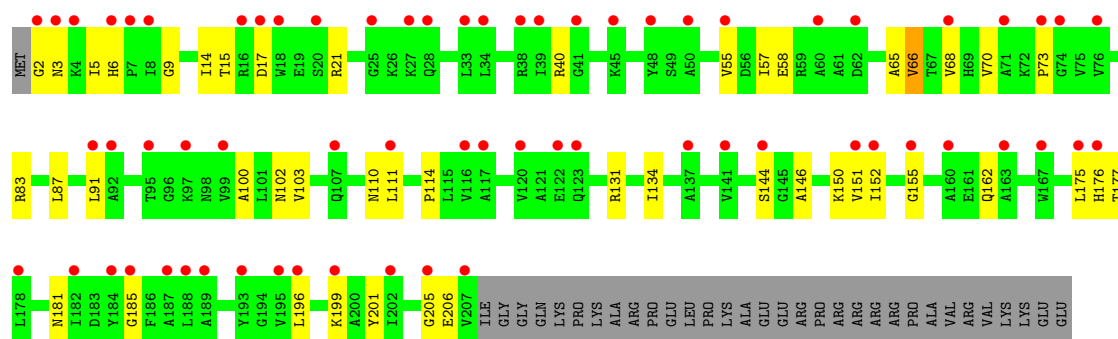




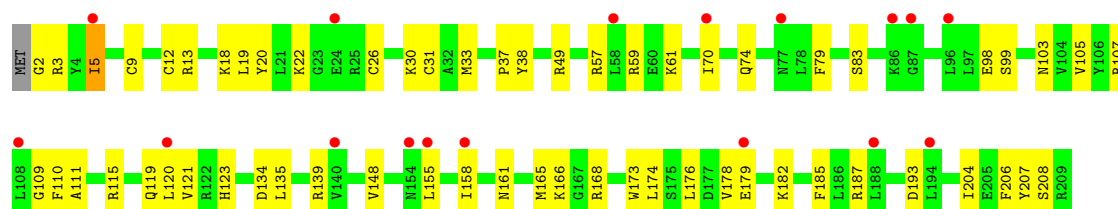
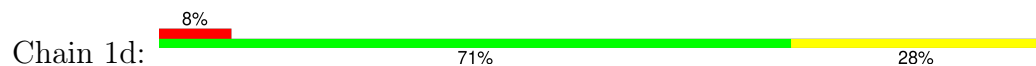
• Molecule 34: 30S ribosomal protein S3



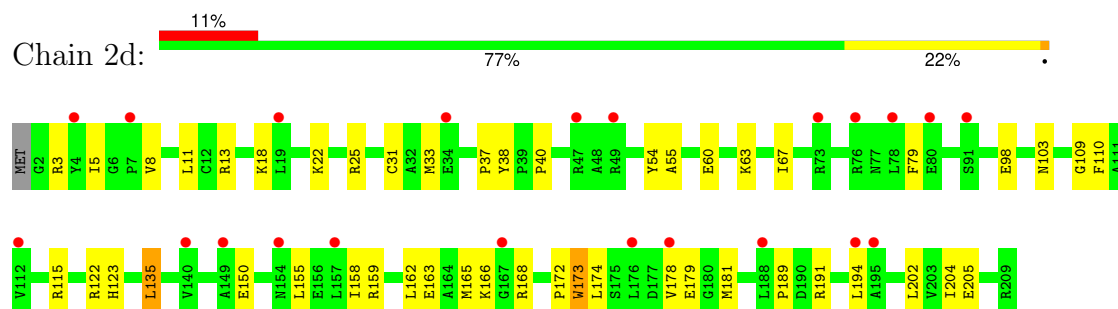
• Molecule 34: 30S ribosomal protein S3



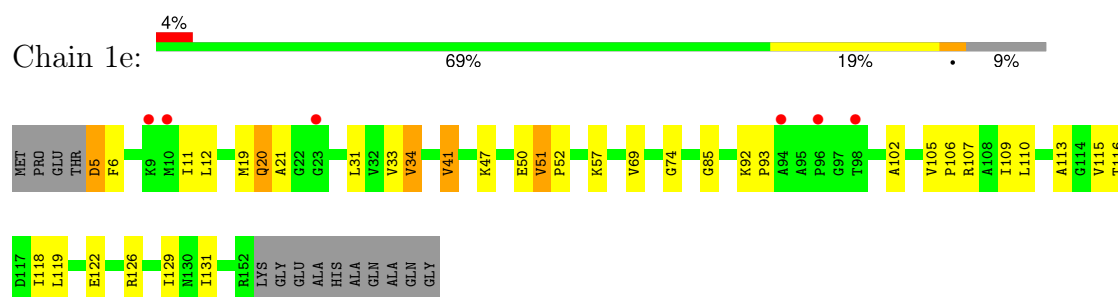
• Molecule 35: 30S ribosomal protein S4



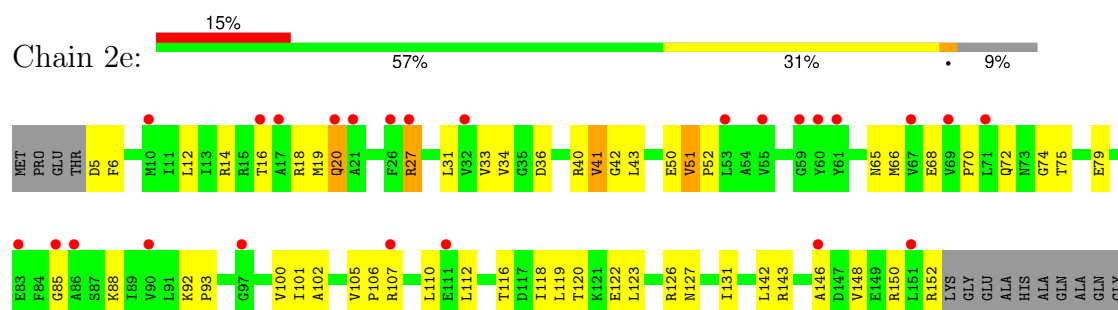
- Molecule 35: 30S ribosomal protein S4



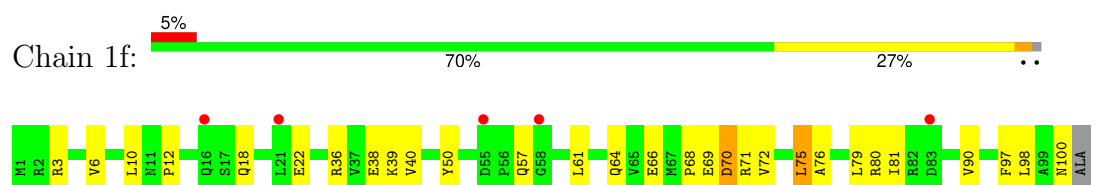
- Molecule 36: 30S ribosomal protein S5



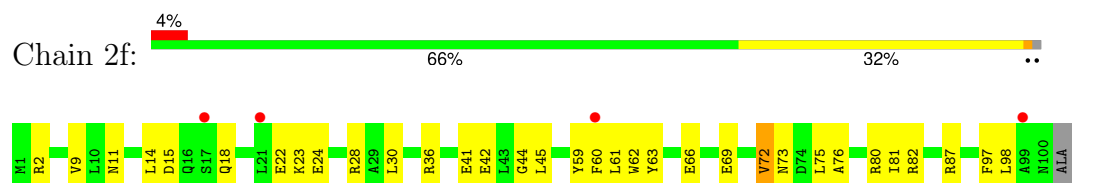
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6

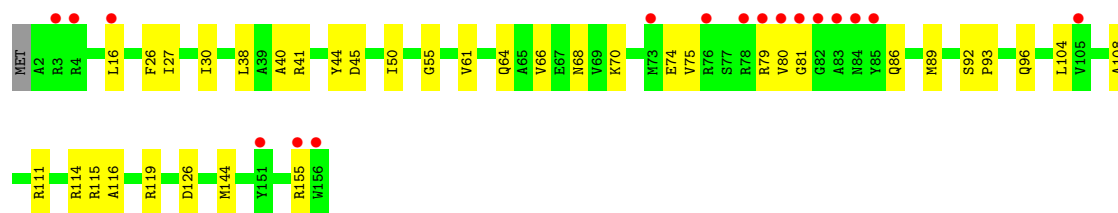


- Molecule 37: 30S ribosomal protein S6

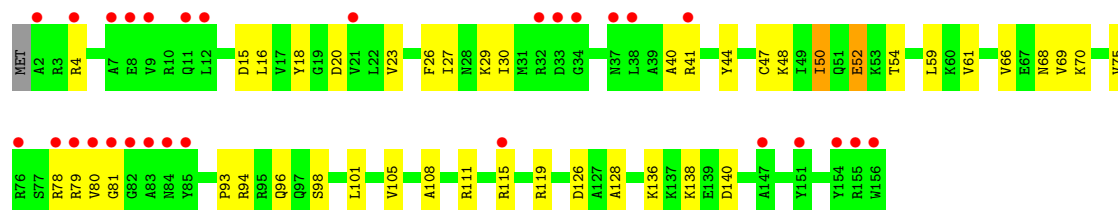


- Molecule 38: 30S ribosomal protein S7

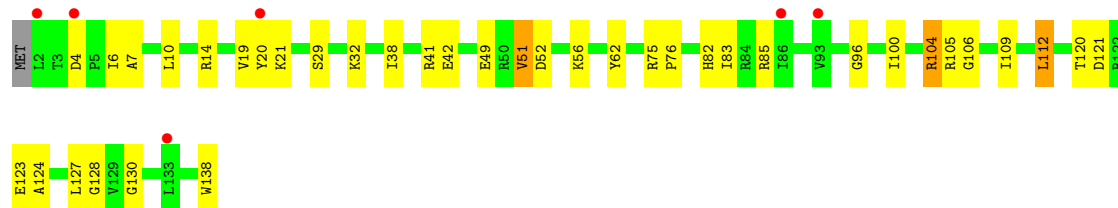
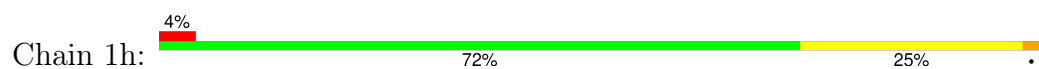




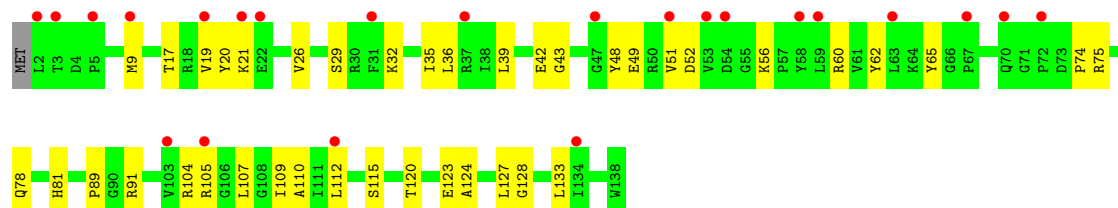
• Molecule 38: 30S ribosomal protein S7



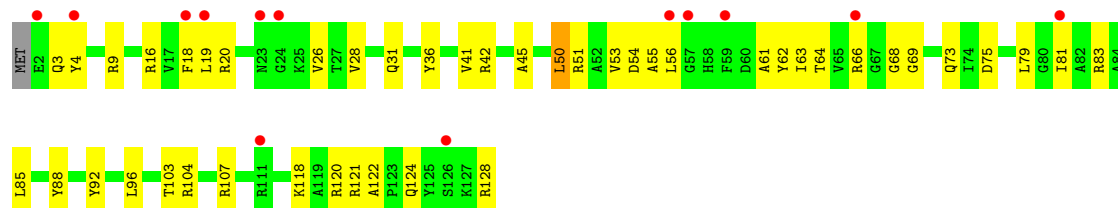
• Molecule 39: 30S ribosomal protein S8



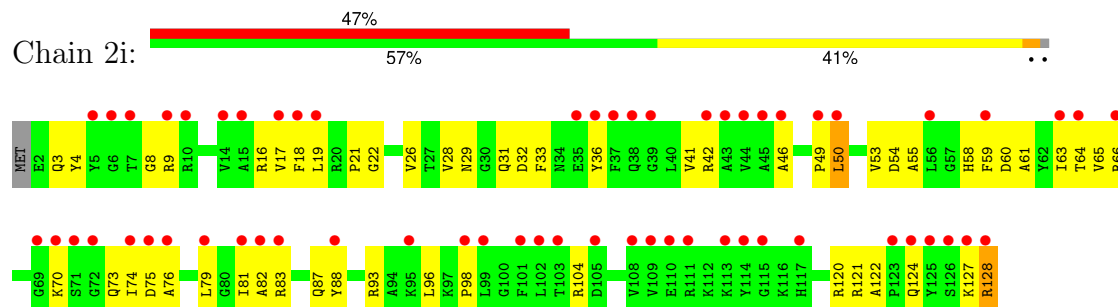
• Molecule 39: 30S ribosomal protein S8



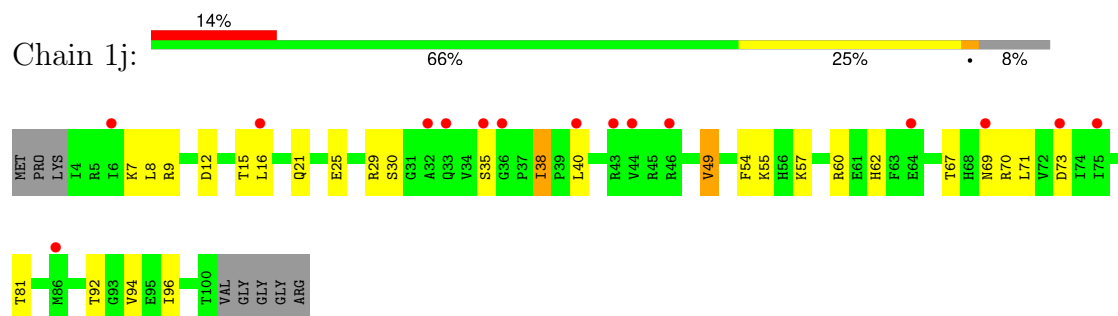
• Molecule 40: 30S ribosomal protein S9



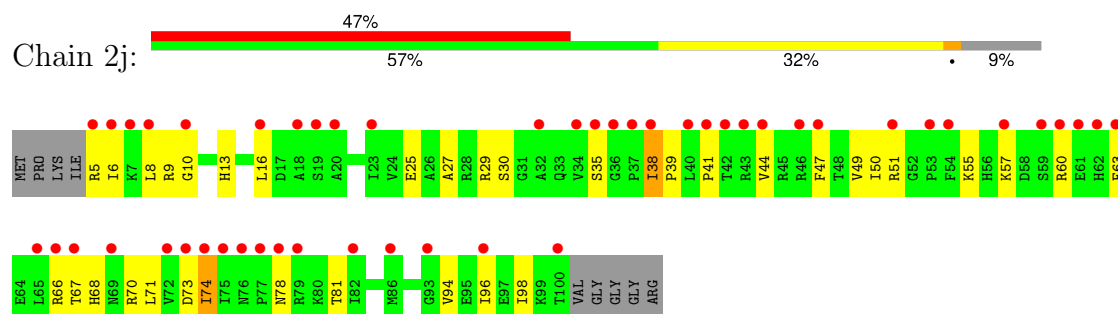
- Molecule 40: 30S ribosomal protein S9



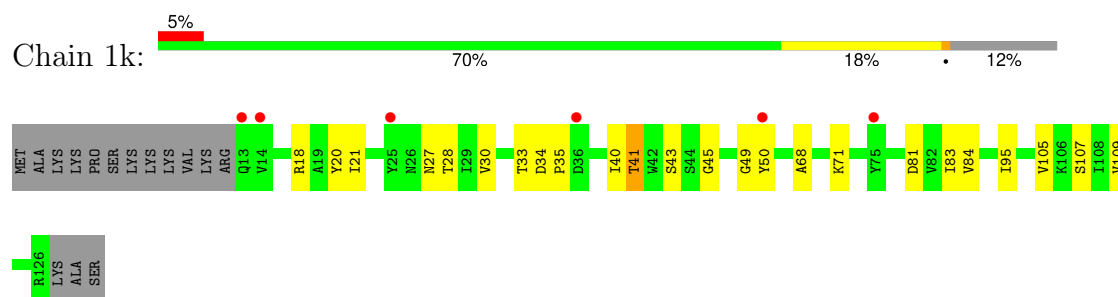
- Molecule 41: 30S ribosomal protein S10



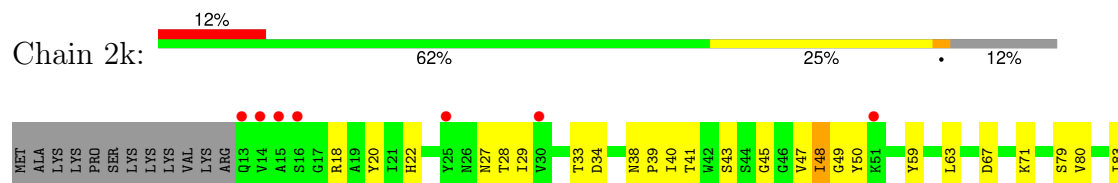
- Molecule 41: 30S ribosomal protein S10

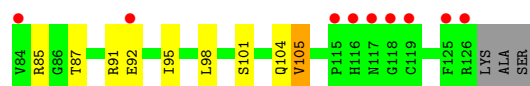


- Molecule 42: 30S ribosomal protein S11

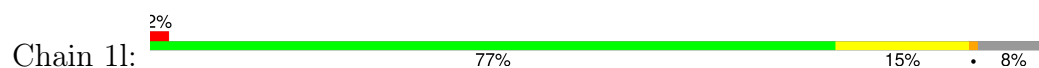


- Molecule 42: 30S ribosomal protein S11





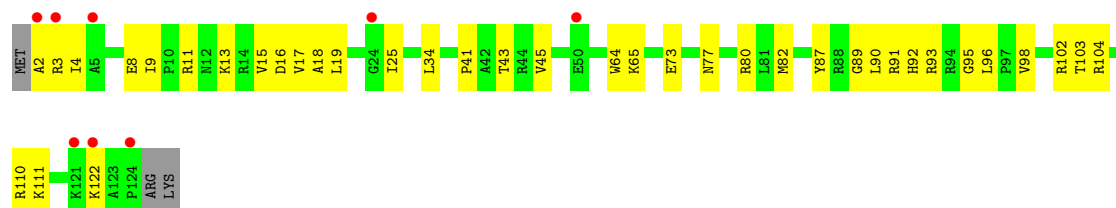
- Molecule 43: 30S ribosomal protein S12



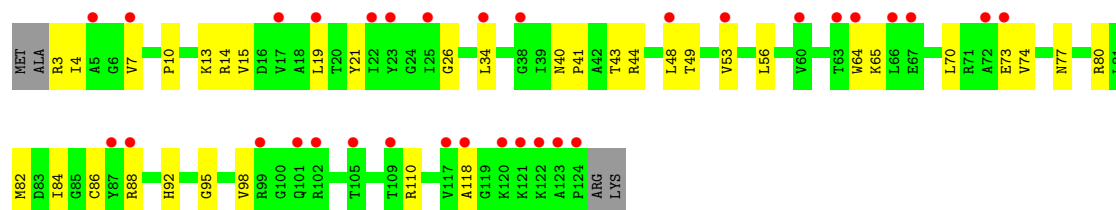
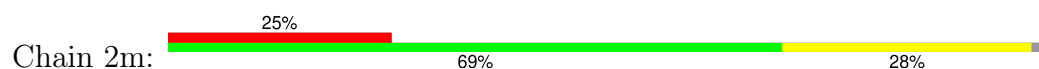
- Molecule 43: 30S ribosomal protein S12



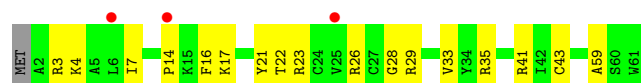
- Molecule 44: 30S ribosomal protein S13



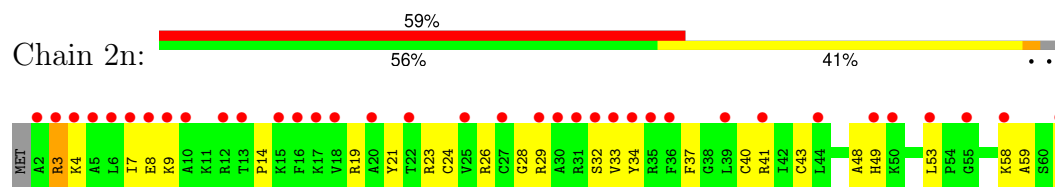
- Molecule 44: 30S ribosomal protein S13



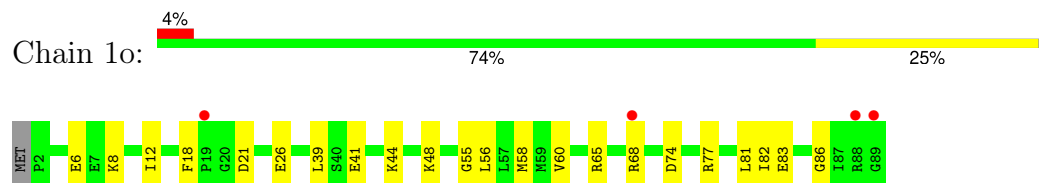
- Molecule 45: 30S ribosomal protein S14 type Z



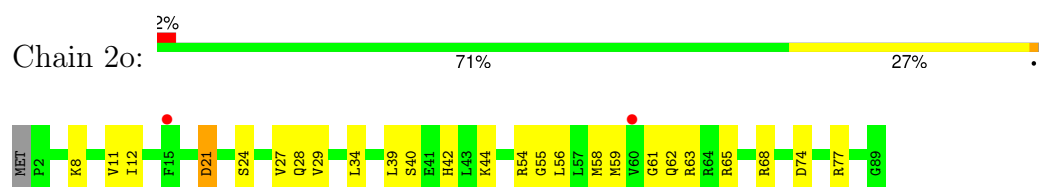
- Molecule 45: 30S ribosomal protein S14 type Z



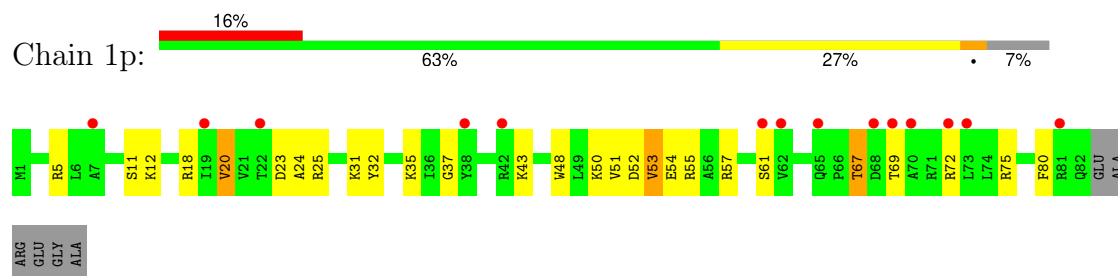
- Molecule 46: 30S ribosomal protein S15



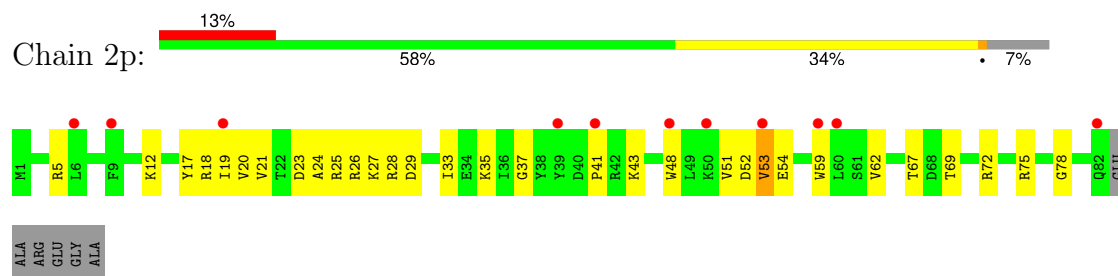
- Molecule 46: 30S ribosomal protein S15



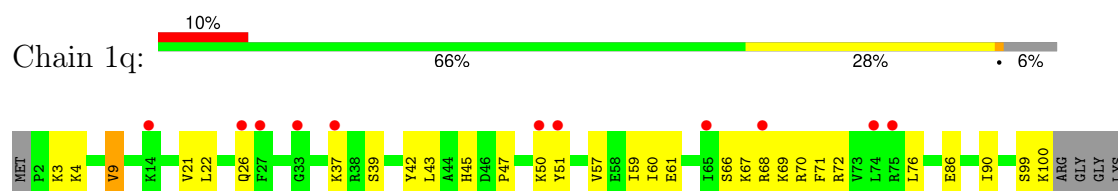
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16

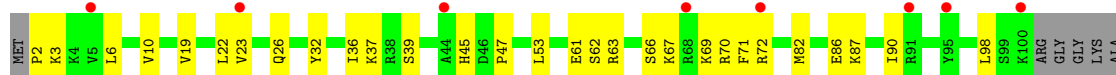


- Molecule 48: 30S ribosomal protein S17

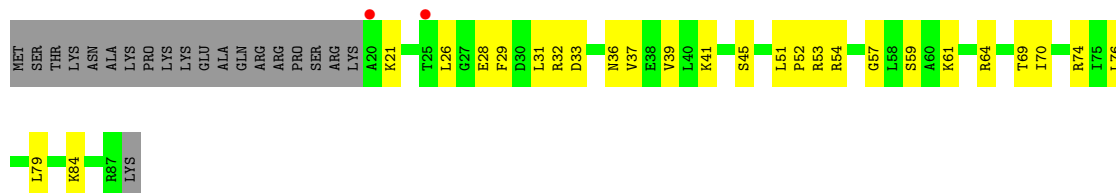


ALA

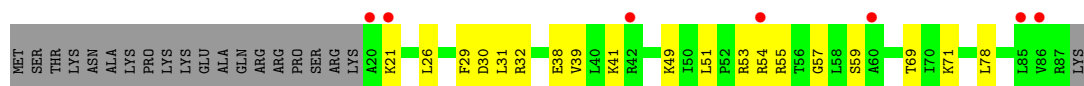
- Molecule 48: 30S ribosomal protein S17



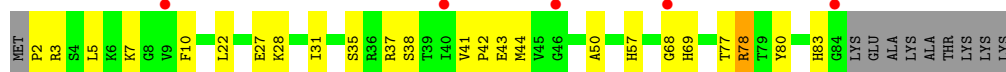
- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19

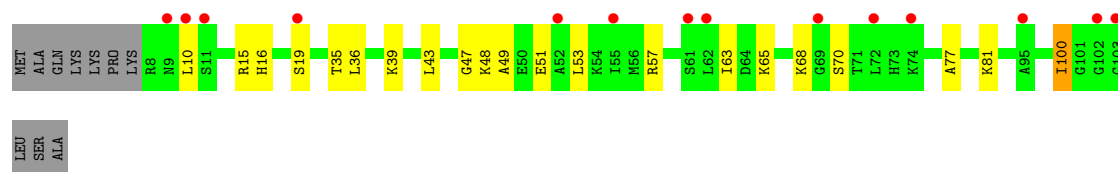


- Molecule 50: 30S ribosomal protein S19

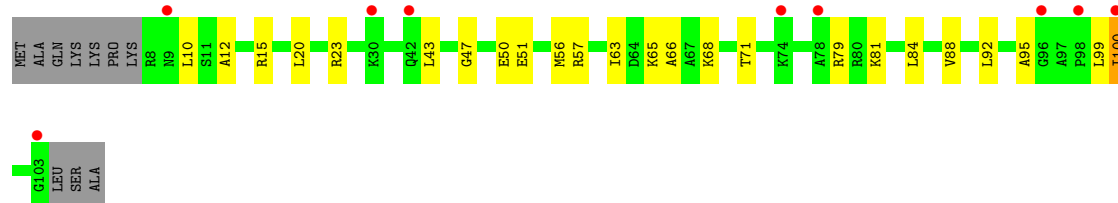


- Molecule 51: 30S ribosomal protein S20

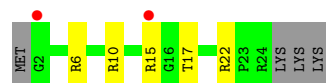




- Molecule 51: 30S ribosomal protein S20



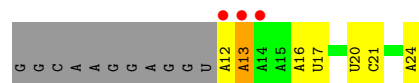
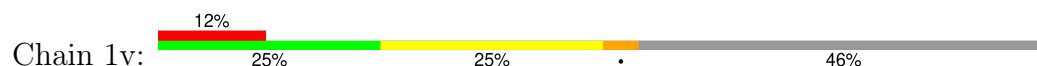
- Molecule 52: 30S ribosomal protein Thx



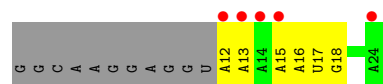
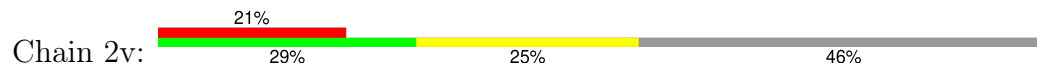
- Molecule 52: 30S ribosomal protein Thx



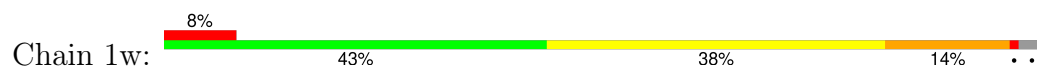
- Molecule 53: mRNA

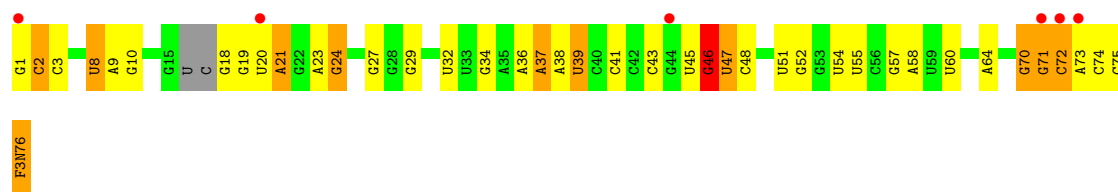


- Molecule 53: mRNA



- Molecule 54: A-site tRNA

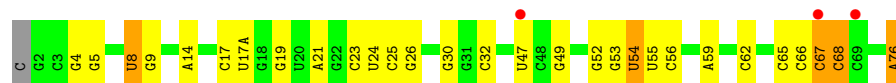




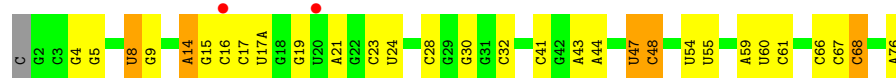
• Molecule 54: A-site tRNA



• Molecule 55: P-site tRNA



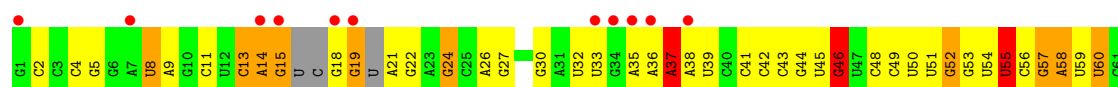
• Molecule 55: P-site tRNA

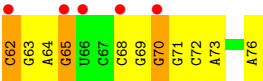


• Molecule 56: E-site tRNA



• Molecule 56: E-site tRNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.34Å 447.21Å 620.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.82 – 2.60 152.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (152.82-2.60) 98.3 (152.82-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.238 , 0.283 0.240 , 0.284	Depositor DCC
R_{free} test set	86837 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	298900	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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: 7MG, 4SU, ZN, PSU, K, MA6, 4OC, 2MG, OMG, SF4, 5MU, UR3, AQJ, MG, 2MU, 5MC, 2MA, M2G, F3N, MIA, 0TD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.27	0/69009	0.46	2/107712 (0.0%)
1	2A	0.21	0/67293	0.39	1/105034 (0.0%)
2	1B	0.23	0/2882	0.41	0/4494
2	2B	0.19	0/2879	0.36	0/4487
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.29	0/1592	0.53	0/2149
4	2E	0.21	0/1592	0.46	0/2149
5	1F	0.27	0/1619	0.51	0/2193
5	2F	0.20	0/1615	0.43	0/2188
6	1G	0.21	0/1454	0.45	0/1964
6	2G	0.18	0/1453	0.42	0/1963
7	1H	0.24	0/1356	0.42	0/1834
7	2H	0.18	0/1356	0.38	0/1834
8	1I	0.19	0/1112	0.45	0/1514
8	2I	0.19	0/1079	0.44	0/1475
9	1N	0.27	0/1144	0.48	0/1543
9	2N	0.19	0/1144	0.41	0/1543
10	1O	0.25	0/943	0.47	0/1269
10	2O	0.21	0/943	0.44	0/1269
11	1P	0.26	0/1152	0.49	0/1533
11	2P	0.22	0/1152	0.45	0/1533
12	1Q	0.28	0/1143	0.46	0/1527
12	2Q	0.19	0/1143	0.41	0/1527
13	1R	0.28	0/982	0.52	0/1312
13	2R	0.21	0/982	0.45	0/1312
14	1S	0.22	0/883	0.47	0/1176
14	2S	0.19	0/880	0.45	0/1172
15	1T	0.27	0/1105	0.47	0/1477
15	2T	0.21	0/1097	0.45	0/1468
16	1U	0.27	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.43	0/1301
17	1V	0.27	0/782	0.54	1/1049 (0.1%)
17	2V	0.18	0/782	0.42	0/1049
18	1W	0.26	0/897	0.46	0/1205
18	2W	0.22	0/897	0.40	0/1205
19	1X	0.26	0/764	0.50	0/1025
19	2X	0.21	0/764	0.41	0/1025
20	1Y	0.24	0/819	0.52	0/1095
20	2Y	0.21	0/819	0.45	0/1095
21	1Z	0.22	0/1267	0.46	0/1717
21	2Z	0.20	0/1299	0.46	0/1763
22	10	0.28	0/662	0.57	2/881 (0.2%)
22	20	0.22	0/662	0.43	0/881
23	11	0.26	0/762	0.47	0/1014
23	21	0.23	0/762	0.44	0/1014
24	12	0.25	0/590	0.44	0/781
24	22	0.20	0/590	0.41	0/781
25	13	0.26	0/474	0.44	0/635
25	23	0.19	0/469	0.42	0/630
26	14	0.28	0/565	0.61	0/761
26	24	0.27	0/545	0.61	1/737 (0.1%)
27	15	0.28	0/469	0.55	0/635
27	25	0.21	0/469	0.44	0/635
28	16	0.25	0/460	0.46	0/613
28	26	0.21	0/456	0.45	0/608
29	17	0.30	0/426	0.54	0/561
29	27	0.25	0/426	0.47	0/561
30	18	0.27	0/525	0.49	0/691
30	28	0.21	0/525	0.41	0/691
31	19	0.27	0/310	0.50	0/407
31	29	0.20	0/310	0.44	0/407
32	1a	0.20	0/35795	0.38	1/55864 (0.0%)
32	2a	0.19	0/35886	0.37	0/56005
33	1b	0.22	0/1881	0.47	0/2542
33	2b	0.20	0/1860	0.46	0/2518
34	1c	0.25	1/1572 (0.1%)	0.42	0/2126
34	2c	0.19	0/1566	0.41	0/2119
35	1d	0.20	0/1685	0.47	0/2262
35	2d	0.22	0/1704	0.46	0/2284
36	1e	0.20	0/1145	0.47	0/1543
36	2e	0.20	0/1149	0.45	0/1548
37	1f	0.20	0/823	0.42	0/1115
37	2f	0.19	0/829	0.38	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.39	0/1679
38	2g	0.18	0/1254	0.40	0/1683
39	1h	0.18	0/1108	0.41	0/1494
39	2h	0.18	0/1108	0.39	0/1494
40	1i	0.19	0/1002	0.48	0/1346
40	2i	0.20	0/997	0.47	0/1343
41	1j	0.21	0/722	0.47	0/982
41	2j	0.19	0/727	0.44	0/988
42	1k	0.24	0/844	0.44	0/1145
42	2k	0.17	0/848	0.38	0/1149
43	1l	0.21	0/937	0.43	0/1260
43	2l	0.21	0/937	0.46	0/1260
44	1m	0.22	0/969	0.45	0/1302
44	2m	0.21	0/961	0.46	0/1291
45	1n	0.20	0/501	0.42	0/664
45	2n	0.17	0/501	0.43	0/664
46	1o	0.19	0/739	0.39	0/985
46	2o	0.17	0/739	0.39	0/985
47	1p	0.22	0/697	0.46	0/939
47	2p	0.19	0/693	0.45	0/935
48	1q	0.20	0/836	0.43	0/1117
48	2q	0.19	0/836	0.42	0/1117
49	1r	0.20	0/560	0.40	0/746
49	2r	0.17	0/560	0.38	0/746
50	1s	0.21	0/667	0.48	0/900
50	2s	0.21	0/661	0.47	0/893
51	1t	0.21	0/730	0.46	0/965
51	2t	0.21	0/729	0.47	0/965
52	1u	0.18	0/203	0.44	0/266
52	2u	0.20	0/203	0.45	0/266
53	1v	0.20	0/310	0.34	0/480
53	2v	0.24	0/310	0.39	0/480
54	1w	0.24	0/1581	0.39	0/2458
54	2w	0.26	0/1531	0.40	0/2379
55	1x	0.26	0/1725	0.40	0/2689
55	2x	0.24	0/1725	0.38	0/2689
56	1y	0.28	0/1606	0.42	0/2497
56	2y	0.28	1/1583 (0.1%)	0.40	0/2459
All	All	0.23	2/316642 (0.0%)	0.42	8/474042 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	2P	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1c	173	VAL	C-N	6.16	1.48	1.33
56	2y	8	4SU	O3'-P	5.17	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1V	79	VAL	N-CA-C	-8.05	106.06	113.71
1	1A	2014	G	C2'-C3'-O3'	7.25	120.38	109.50
26	24	49	PHE	CB-CA-C	-7.25	107.16	115.79
1	2A	1992	G	C2'-C3'-O3'	5.62	117.93	109.50
22	10	41	ARG	CA-C-N	-5.51	113.45	121.44
22	10	41	ARG	C-N-CA	-5.51	113.45	121.44
1	1A	2014	G	P-O3'-C3'	5.39	128.28	120.20
32	1a	1442	G	P-O3'-C3'	5.11	125.84	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	2P	44	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31190	639	0
1	2A	60322	0	30415	721	0
2	1B	2577	0	1304	25	0
2	2B	2575	0	1302	43	0
3	1D	2136	0	2218	48	0
3	2D	2136	0	2218	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1559	0	1618	33	0
4	2E	1559	0	1618	32	0
5	1F	1584	0	1625	37	0
5	2F	1580	0	1619	41	0
6	1G	1429	0	1447	29	0
6	2G	1428	0	1438	52	0
7	1H	1330	0	1407	29	0
7	2H	1330	0	1407	23	0
8	1I	1097	0	1140	27	0
8	2I	1064	0	1082	21	0
9	1N	1117	0	1184	20	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	21	0
10	2O	933	0	996	26	0
11	1P	1135	0	1212	45	0
11	2P	1135	0	1211	33	0
12	1Q	1122	0	1179	30	0
12	2Q	1122	0	1179	24	0
13	1R	968	0	1033	24	0
13	2R	968	0	1033	11	0
14	1S	873	0	927	15	0
14	2S	870	0	923	28	0
15	1T	1091	0	1151	38	0
15	2T	1083	0	1136	32	0
16	1U	959	0	1019	24	0
16	2U	959	0	1018	25	0
17	1V	771	0	830	18	0
17	2V	771	0	830	13	0
18	1W	886	0	939	11	0
18	2W	886	0	940	12	0
19	1X	750	0	814	9	0
19	2X	750	0	813	14	0
20	1Y	806	0	881	17	0
20	2Y	806	0	881	21	0
21	1Z	1240	0	1240	26	0
21	2Z	1271	0	1273	31	0
22	10	653	0	674	14	0
22	20	653	0	674	15	0
23	11	755	0	826	17	0
23	21	755	0	826	19	0
24	12	588	0	643	16	0
24	22	588	0	643	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	469	0	518	6	0
25	23	464	0	514	14	0
26	14	552	0	533	24	0
26	24	532	0	503	21	0
27	15	455	0	465	11	0
27	25	455	0	465	10	0
28	16	453	0	473	6	0
28	26	449	0	469	8	0
29	17	418	0	466	4	0
29	27	418	0	467	8	0
30	18	517	0	582	21	0
30	28	517	0	582	21	0
31	19	307	0	335	7	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	419	0
32	2a	32327	0	16340	571	0
33	1b	1846	0	1867	58	0
33	2b	1825	0	1828	67	0
34	1c	1548	0	1535	23	0
34	2c	1542	0	1517	33	0
35	1d	1655	0	1672	47	0
35	2d	1674	0	1714	40	0
36	1e	1129	0	1185	27	0
36	2e	1133	0	1191	38	0
37	1f	810	0	804	19	0
37	2f	816	0	808	25	0
38	1g	1231	0	1238	26	0
38	2g	1235	0	1249	29	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	29	0
40	1i	983	0	986	32	0
40	2i	978	0	966	39	0
41	1j	709	0	650	20	0
41	2j	714	0	672	30	0
42	1k	829	0	825	14	0
42	2k	833	0	836	23	0
43	1l	932	0	981	19	0
43	2l	932	0	981	21	0
44	1m	958	0	1002	27	0
44	2m	950	0	988	26	0
45	1n	492	0	529	18	0
45	2n	492	0	529	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1o	728	0	760	16	0
46	2o	728	0	760	20	0
47	1p	681	0	697	24	0
47	2p	677	0	686	20	0
48	1q	823	0	891	26	0
48	2q	823	0	891	24	0
49	1r	555	0	618	21	0
49	2r	555	0	618	15	0
50	1s	652	0	662	20	0
50	2s	646	0	644	18	0
51	1t	728	0	798	17	0
51	2t	727	0	796	14	0
52	1u	199	0	208	4	0
52	2u	199	0	208	6	0
53	1v	277	0	140	5	0
53	2v	277	0	140	3	0
54	1w	1603	0	829	29	0
54	2w	1555	0	797	30	0
55	1x	1625	0	828	14	0
55	2x	1625	0	828	18	0
56	1y	1585	0	804	52	0
56	2y	1565	0	795	49	0
57	10	5	0	0	0	0
57	11	3	0	0	0	0
57	12	2	0	0	0	0
57	13	1	0	0	0	0
57	14	1	0	0	0	0
57	15	4	0	0	0	0
57	16	1	0	0	0	0
57	17	2	0	0	0	0
57	18	4	0	0	0	0
57	19	1	0	0	0	0
57	1A	1001	0	0	0	0
57	1B	31	0	0	0	0
57	1D	12	0	0	0	0
57	1E	10	0	0	0	0
57	1F	9	0	0	0	0
57	1G	5	0	0	0	0
57	1I	1	0	0	0	0
57	1N	7	0	0	0	0
57	1O	7	0	0	0	0
57	1P	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1Q	6	0	0	0	0
57	1R	3	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	4	0	0	0	0
57	1V	3	0	0	0	0
57	1W	6	0	0	0	0
57	1X	7	0	0	0	0
57	1Y	4	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	231	0	0	0	0
57	1b	2	0	0	0	0
57	1e	1	0	0	0	0
57	1f	1	0	0	0	0
57	1l	2	0	0	0	0
57	1n	2	0	0	0	0
57	1q	1	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1w	4	0	0	0	0
57	1x	11	0	0	0	0
57	1y	2	0	0	0	0
57	20	3	0	0	0	0
57	23	1	0	0	0	0
57	25	3	0	0	0	0
57	28	2	0	0	0	0
57	2A	687	0	0	0	0
57	2B	21	0	0	0	0
57	2D	8	0	0	0	0
57	2E	6	0	0	0	0
57	2F	6	0	0	0	0
57	2G	1	0	0	0	0
57	2O	1	0	0	0	0
57	2P	1	0	0	0	0
57	2Q	3	0	0	0	0
57	2R	2	0	0	0	0
57	2U	2	0	0	0	0
57	2V	2	0	0	0	0
57	2W	1	0	0	0	0
57	2X	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2a	201	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2g	1	0	0	0	0
57	2h	1	0	0	0	0
57	2j	2	0	0	0	0
57	2l	2	0	0	0	0
57	2q	3	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2w	4	0	0	0	0
57	2x	5	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	37	0	0	0	0
59	2A	37	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	10	7	0	0	0	0
62	11	2	0	0	1	0
62	12	4	0	0	1	0
62	13	3	0	0	0	0
62	14	1	0	0	0	0
62	15	4	0	0	0	0
62	17	4	0	0	0	0
62	18	8	0	0	0	0
62	19	1	0	0	0	0
62	1A	1610	0	0	79	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1B	40	0	0	1	0
62	1D	21	0	0	1	0
62	1E	19	0	0	5	0
62	1F	14	0	0	3	0
62	1G	5	0	0	0	0
62	1H	1	0	0	1	0
62	1I	2	0	0	0	0
62	1N	2	0	0	0	0
62	1O	5	0	0	0	0
62	1P	18	0	0	2	0
62	1Q	3	0	0	0	0
62	1R	6	0	0	0	0
62	1S	5	0	0	0	0
62	1T	6	0	0	0	0
62	1U	9	0	0	1	0
62	1V	4	0	0	0	0
62	1W	4	0	0	0	0
62	1X	5	0	0	0	0
62	1Y	3	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	276	0	0	14	0
62	1b	1	0	0	0	0
62	1e	1	0	0	0	0
62	1j	1	0	0	0	0
62	1k	1	0	0	0	0
62	1l	3	0	0	1	0
62	1q	1	0	0	0	0
62	1v	3	0	0	0	0
62	1w	6	0	0	0	0
62	1x	9	0	0	0	0
62	1y	1	0	0	0	0
62	20	3	0	0	0	0
62	21	3	0	0	0	0
62	22	1	0	0	0	0
62	25	3	0	0	0	0
62	27	4	0	0	1	0
62	28	4	0	0	1	0
62	29	1	0	0	0	0
62	2A	926	0	0	41	0
62	2B	10	0	0	0	0
62	2D	16	0	0	3	0
62	2E	10	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2F	5	0	0	0	0
62	2I	3	0	0	0	0
62	2N	1	0	0	0	0
62	2O	1	0	0	0	0
62	2P	10	0	0	0	0
62	2Q	1	0	0	0	0
62	2R	2	0	0	0	0
62	2T	2	0	0	0	0
62	2U	3	0	0	0	0
62	2V	1	0	0	1	0
62	2W	1	0	0	0	0
62	2X	3	0	0	1	0
62	2Z	2	0	0	0	0
62	2a	230	0	0	20	0
62	2d	2	0	0	0	0
62	2e	1	0	0	0	0
62	2f	1	0	0	0	0
62	2g	1	0	0	0	0
62	2i	2	0	0	0	0
62	2j	4	0	0	2	0
62	2l	3	0	0	1	0
62	2n	1	0	0	0	0
62	2o	1	0	0	1	0
62	2v	2	0	0	0	0
62	2w	1	0	0	0	0
62	2x	5	0	0	0	0
All	All	298900	0	196701	4241	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 9.

All (4241) 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:1128:U:H3	1:1A:1132:A:N6	1.45	1.13
56:2y:15:G:N2	56:2y:48:C:H42	1.50	1.10
56:2y:15:G:H22	56:2y:48:C:N4	1.51	1.06
1:1A:2160:C:N4	1:1A:2175:G:H1	1.57	1.02
32:2a:998:G:H1	32:2a:1043:C:H42	1.02	1.01
32:2a:999:C:N4	32:2a:1042:G:H1	1.57	1.00
1:1A:1099:C:N4	1:1A:1152:G:H1	1.59	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:1y:11:C:H42	56:1y:24:G:H1	1.10	0.97
32:1a:1133:G:H1	32:1a:1141:C:H42	1.13	0.96
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.46	0.96
1:1A:1128:U:O4	1:1A:1132:A:N1	1.96	0.96
32:2a:1008:C:H42	32:2a:1021:G:H1	1.04	0.96
32:2a:1164:G:H1	32:2a:1172:C:H42	1.08	0.96
1:2A:2138:C:H42	1:2A:2153:G:H1	1.01	0.96
1:2A:2139:C:H42	1:2A:2152:G:H1	0.97	0.95
32:2a:1262:C:H42	32:2a:1273:G:H1	1.13	0.94
1:2A:2139:C:N4	1:2A:2152:G:H1	1.64	0.94
32:2a:1132:C:H42	32:2a:1142:G:H1	0.94	0.93
32:1a:1008:C:N4	32:1a:1021:G:H1	1.66	0.93
56:1y:2:C:H42	56:1y:71:G:H1	0.98	0.92
32:2a:1029:C:C4	32:2a:1032:G:N1	2.39	0.91
32:2a:1132:C:N4	32:2a:1142:G:H1	1.68	0.91
12:1Q:12:GLN:HE21	12:1Q:72:LYS:HG3	1.36	0.91
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.50	0.91
22:10:10:THR:HG22	22:10:12:ASN:H	1.34	0.91
1:1A:2122:G:H1	1:1A:2211:U:H3	0.92	0.91
1:1A:2143:G:H1	1:1A:2199:C:H42	1.19	0.91
32:2a:1164:G:H1	32:2a:1172:C:N4	1.68	0.91
1:2A:2138:C:N4	1:2A:2153:G:H1	1.69	0.90
54:2w:76:F3N:H5'	54:2w:76:F3N:H8	1.51	0.90
32:1a:78:G:H1	32:1a:91:C:N4	1.69	0.90
32:1a:1008:C:H42	32:1a:1021:G:H1	0.93	0.90
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.36	0.89
56:1y:53:G:H1	56:1y:61:C:N4	1.69	0.89
56:1y:19:G:N2	56:1y:56:C:N3	2.20	0.88
56:1y:2:C:N4	56:1y:71:G:H1	1.70	0.88
32:2a:997:U:H3	32:2a:1044:A:H61	1.20	0.88
56:1y:53:G:H1	56:1y:61:C:H42	1.16	0.88
54:1w:1:G:O6	54:1w:72:C:N3	2.08	0.87
32:2a:64:G:H4'	32:2a:65:U:H3'	1.55	0.87
21:1Z:138:GLU:H	21:1Z:156:LYS:HZ1	1.24	0.86
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.09	0.86
32:2a:559:A:H4'	32:2a:560:U:H3'	1.55	0.86
54:1w:27:G:H1	54:1w:43:C:H42	1.21	0.86
32:1a:1027:C:N3	32:1a:1034:G:C6	2.44	0.85
1:2A:2319:G:H22	14:2S:3:ARG:HD2	1.41	0.85
32:2a:1381:U:H1'	38:2g:79:ARG:HD3	1.57	0.85
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.22	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:664:G:H22	32:1a:741:G:H1	1.23	0.85
3:1D:125:ILE:HB	37:1f:81:ILE:HD11	1.57	0.85
1:1A:1118:C:O2	1:1A:1138:C:N4	2.09	0.84
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.24	0.84
9:1N:20:GLY:HA2	9:1N:61:ARG:HD2	1.57	0.84
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.60	0.84
1:2A:1689:A:H62	1:2A:1698:A:H2	1.20	0.84
1:1A:1099:C:H42	1:1A:1152:G:H1	0.84	0.83
32:1a:376:G:H5''	47:1p:5:ARG:HG2	1.58	0.83
32:1a:79:G:H1	32:1a:90:U:H3	1.23	0.83
5:1F:108:LYS:HG2	5:1F:112:MET:HE2	1.60	0.83
32:2a:1008:C:N4	32:2a:1021:G:H1	1.76	0.83
13:2R:24:GLN:HB3	13:2R:44:LEU:HD11	1.61	0.83
10:2O:64:ARG:HH12	15:2T:70:VAL:HG21	1.44	0.82
32:2a:1075:C:OP1	33:2b:179:LYS:NZ	2.12	0.82
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.13	0.82
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.12	0.82
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.62	0.82
56:2y:14:A:H61	56:2y:21:A:H2	1.26	0.82
56:1y:19:G:H1	56:1y:56:C:H42	1.28	0.81
1:2A:271(K):U:O2	8:2I:50:ARG:NH2	2.13	0.81
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.63	0.81
32:2a:1013:G:N2	32:2a:1016:A:OP2	2.13	0.81
32:2a:998:G:H1	32:2a:1043:C:N4	1.76	0.81
1:2A:2138:C:N3	1:2A:2153:G:N2	2.28	0.81
1:1A:1070:G:OP2	62:1A:4144:HOH:O	1.99	0.81
32:2a:1183:A:H3'	32:2a:1184:G:H5''	1.62	0.81
1:1A:1018:A:OP2	62:1A:4152:HOH:O	1.97	0.80
2:2B:22:U:H3	2:2B:61:G:H1	1.28	0.80
56:2y:15:G:H22	56:2y:48:C:H42	0.83	0.80
56:2y:15:G:N1	56:2y:48:C:N3	2.28	0.80
32:2a:406:G:H5'	35:2d:5:ILE:HD11	1.62	0.80
1:2A:1529:G:H1	1:2A:1540:U:H3	1.29	0.80
32:2a:664:G:H22	32:2a:741:G:H1	1.27	0.80
5:2F:108:LYS:HG2	5:2F:112:MET:HE2	1.62	0.80
2:1B:42:C:N4	6:1G:91:ARG:HH12	1.80	0.79
7:2H:25:LYS:HB3	7:2H:27:LYS:HZ1	1.47	0.79
56:2y:55:PSU:HN1	56:2y:57:G:H5'	1.47	0.79
32:2a:987:G:H1	32:2a:1218:C:H42	1.27	0.79
1:1A:2160:C:N3	1:1A:2175:G:N2	2.30	0.79
32:1a:78:G:N2	32:1a:91:C:N3	2.31	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.16	0.79
1:1A:2121:U:H3	1:1A:2212:G:H1	1.30	0.79
1:1A:2331:G:H22	14:1S:3:ARG:HD2	1.48	0.79
22:10:11:ARG:O	22:10:14:ARG:NH2	2.13	0.79
32:1a:73:G:H1	32:1a:96:U:H3	1.28	0.78
56:1y:11:C:N4	56:1y:24:G:H1	1.81	0.78
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.16	0.78
32:2a:1262:C:N4	32:2a:1273:G:H1	1.80	0.78
12:2Q:77:LYS:NZ	12:2Q:86:GLY:O	2.17	0.78
1:2A:370:G:OP2	62:2A:3776:HOH:O	2.02	0.78
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.64	0.78
15:2T:39:ARG:NH2	32:2a:345:C:OP2	2.17	0.78
6:1G:41:GLN:NE2	6:1G:154:GLY:O	2.17	0.77
32:2a:975:A:H4'	32:2a:976:G:H5''	1.67	0.77
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.66	0.77
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.18	0.77
1:1A:211:A:OP1	62:1A:4155:HOH:O	2.02	0.77
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.15	0.77
2:2B:54:G:H21	6:2G:29:TRP:HZ2	1.31	0.77
32:2a:1351:U:H3	32:2a:1371:G:H1	1.31	0.77
32:1a:429:U:O2'	35:1d:22:LYS:NZ	2.17	0.77
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.65	0.77
1:2A:1204:A:H2	1:2A:1241:A:H62	1.32	0.77
32:2a:999:C:H42	32:2a:1042:G:H1	0.82	0.77
1:2A:1852:C:O2	1:2A:1890:A:N6	2.18	0.76
40:2i:16:ARG:HB2	40:2i:64:THR:HB	1.67	0.76
1:1A:2158:C:N4	1:1A:2177:G:C6	2.54	0.76
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.51	0.76
32:2a:1086:U:H3	32:2a:1099:G:H22	1.28	0.76
40:2i:55:ALA:HA	40:2i:58:HIS:HD2	1.49	0.76
56:2y:5:G:H1	56:2y:68:C:H42	1.33	0.76
32:1a:1027:C:C2	32:1a:1034:G:N1	2.53	0.76
2:2B:15:A:OP2	2:2B:69:G:N2	2.18	0.76
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.19	0.76
1:1A:2123:G:H1	1:1A:2210:C:N4	1.83	0.76
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.66	0.76
21:2Z:10:ARG:NH2	21:2Z:26:GLY:O	2.18	0.76
34:1c:6:HIS:HD2	34:1c:9:GLY:H	1.34	0.76
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.18	0.76
1:1A:1099:C:N3	1:1A:1152:G:N2	2.32	0.76
1:1A:1310:G:OP1	27:15:19:ARG:NH2	2.19	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1361:C:OP2	62:1A:4154:HOH:O	2.02	0.76
32:2a:999:C:N3	32:2a:1042:G:N2	2.33	0.76
1:1A:2614:A:OP1	62:1A:4153:HOH:O	2.02	0.76
3:2D:38:LYS:NZ	3:2D:39:LYS:O	2.18	0.76
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.19	0.76
1:1A:2123:G:N1	1:1A:2210:C:N4	2.34	0.75
54:1w:1:G:N1	54:1w:72:C:O2	2.18	0.75
32:2a:76:C:H42	32:2a:93:G:H1	1.34	0.75
32:2a:894:G:N7	62:2a:3332:HOH:O	2.19	0.75
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.68	0.75
1:2A:856:C:H2'	1:2A:857:C:H6	1.52	0.75
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.68	0.75
32:1a:159:G:N2	32:1a:162:A:OP2	2.20	0.75
41:1j:16:LEU:HD23	41:1j:70:ARG:HG2	1.68	0.75
1:2A:195:A:N7	62:2A:3705:HOH:O	2.18	0.75
1:2A:2807:G:N1	1:2A:2893:G:O6	2.18	0.75
32:1a:1133:G:H1	32:1a:1141:C:N4	1.85	0.75
56:2y:19:G:H1	56:2y:56:C:H42	1.34	0.75
1:1A:1093:G:H2'	1:1A:1156:G:H22	1.52	0.75
1:1A:7:G:H1	1:1A:2905:C:H42	1.35	0.75
1:1A:1120:G:O2'	1:1A:1121:C:OP1	2.05	0.75
1:1A:2160:C:H42	1:1A:2175:G:H1	0.79	0.75
1:2A:2793:G:H1	1:2A:2803:C:H42	1.33	0.74
1:2A:2867:G:OP2	15:2T:119:LYS:NZ	2.18	0.74
32:2a:134:A:N6	47:2p:25:ARG:HH12	1.85	0.74
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.32	0.74
56:1y:50:U:H3	56:1y:64:A:H2	1.34	0.74
32:2a:1224:G:H1	32:2a:1363:C:N4	1.85	0.74
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.69	0.74
1:1A:1139:G:H3'	1:1A:1140:U:H5''	1.70	0.74
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.21	0.74
56:1y:2:C:N3	56:1y:71:G:N2	2.33	0.74
56:1y:58:A:O2'	56:1y:59:U:OP1	2.06	0.74
3:2D:237:GLU:OE2	62:2D:401:HOH:O	2.05	0.74
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.69	0.74
1:1A:2152:U:O2'	1:1A:2180:A:N1	2.21	0.74
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.69	0.74
44:1m:73:GLU:O	44:1m:77:ASN:ND2	2.21	0.74
32:2a:1004:A:H5''	32:2a:1025:U:H5	1.53	0.74
32:2a:1029:C:N4	32:2a:1032:G:C6	2.55	0.74
1:1A:591:U:O4	62:1A:4152:HOH:O	2.05	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1360:A:OP2	45:1n:35:ARG:NH2	2.21	0.74
1:1A:929:G:H1	1:1A:940:C:H42	1.34	0.73
1:1A:71:U:OP1	62:1A:4156:HOH:O	2.05	0.73
1:1A:2205:C:H2'	1:1A:2206:G:H8	1.53	0.73
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.70	0.73
32:2a:974:A:OP2	45:2n:29:ARG:NH2	2.21	0.73
56:1y:19:G:H1	56:1y:56:C:N4	1.84	0.73
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.70	0.73
56:2y:58:A:O2'	56:2y:60:U:OP2	2.04	0.73
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.69	0.73
1:2A:740:U:OP2	62:2A:3777:HOH:O	2.06	0.73
33:2b:189:ASP:O	33:2b:192:SER:OG	2.06	0.73
33:1b:126:GLU:HG2	33:1b:127:ILE:HG12	1.70	0.73
32:2a:1240:U:N3	38:2g:30:ILE:O	2.18	0.73
1:1A:599:U:OP1	62:1A:4157:HOH:O	2.06	0.73
1:1A:2419:G:OP1	62:1A:4130:HOH:O	2.05	0.73
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	1.71	0.73
32:1a:975:A:H4'	32:1a:976:G:H5''	1.70	0.73
1:2A:599:G:N7	62:2A:3801:HOH:O	2.21	0.73
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.22	0.73
7:1H:86:GLU:OE2	7:1H:130:ARG:NH1	2.21	0.73
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.22	0.73
1:2A:1332:G:OP1	62:2A:3778:HOH:O	2.07	0.73
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.54	0.73
1:2A:1568:G:N7	62:2A:3799:HOH:O	2.21	0.72
56:2y:18:G:N2	56:2y:55:PSU:N3	2.37	0.72
56:2y:18:G:N2	56:2y:55:PSU:C4	2.57	0.72
1:1A:973:G:N7	62:1A:4194:HOH:O	2.21	0.72
32:2a:1040:U:H2'	32:2a:1041:A:H8	1.55	0.72
56:2y:19:G:N2	56:2y:56:C:N3	2.35	0.72
56:2y:4:C:H42	56:2y:69:G:H1	1.38	0.72
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.72	0.72
17:2V:78:LYS:O	62:2V:301:HOH:O	2.07	0.72
41:2j:8:LEU:HB2	41:2j:70:ARG:HB2	1.70	0.72
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.70	0.72
32:1a:1103:C:OP1	33:1b:96:ARG:NH2	2.23	0.72
20:2Y:20:TYR:HB3	20:2Y:23:ARG:HD2	1.71	0.72
1:2A:636:G:HO2'	1:2A:638:G:HO2'	1.38	0.72
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.08	0.72
39:2h:49:GLU:OE2	39:2h:62:TYR:OH	2.08	0.72
1:2A:1428:C:N4	1:2A:1570:A:OP2	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2123:G:N2	1:1A:2210:C:N3	2.36	0.71
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.23	0.71
32:2a:1262:C:N3	32:2a:1273:G:N2	2.36	0.71
1:1A:1114:G:N1	1:1A:1141:A:O2'	2.24	0.71
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.23	0.71
1:1A:2701:U:H4'	1:1A:2702:C:H5'	1.72	0.71
32:1a:78:G:N1	32:1a:91:C:N4	2.33	0.71
1:1A:242:C:OP2	30:18:5:LYS:NZ	2.21	0.71
1:1A:2518:U:H1'	54:1w:76:F3N:HD2	1.73	0.71
32:1a:1303:C:OP1	62:1a:3314:HOH:O	2.07	0.71
1:2A:527:C:N4	1:2A:2779:U:OP2	2.23	0.71
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.72	0.71
37:2f:24:GLU:HB3	37:2f:28:ARG:HH12	1.55	0.71
39:2h:29:SER:HB3	39:2h:32:LYS:HG3	1.71	0.71
1:2A:83:G:H1	1:2A:102:G:HO2'	1.38	0.71
32:1a:131:C:O2	32:1a:231:G:N2	2.19	0.71
4:2E:8:LYS:NZ	4:2E:190:GLY:O	2.22	0.71
32:2a:1028:C:C2	32:2a:1033:G:N1	2.59	0.71
32:1a:406:G:H5'	35:1d:5:ILE:HD11	1.71	0.71
34:1c:14:ILE:HG22	34:1c:15:THR:HG23	1.73	0.71
32:2a:1130:A:H4'	40:2i:3:GLN:HE22	1.55	0.71
44:1m:80:ARG:HH12	50:1s:69:HIS:HE1	1.39	0.70
48:1q:43:LEU:HD12	48:1q:68:ARG:HG2	1.73	0.70
21:2Z:138:GLU:H	21:2Z:156:LYS:HZ1	1.37	0.70
32:2a:987:G:H1	32:2a:1218:C:N4	1.89	0.70
56:1y:19:G:N1	56:1y:56:C:N4	2.32	0.70
1:2A:1951:U:OP1	62:2A:3779:HOH:O	2.09	0.70
32:2a:997:U:H3	32:2a:1044:A:N6	1.88	0.70
32:2a:1002:G:H2'	32:2a:1003:G:H8	1.56	0.70
17:1V:40:LEU:HB2	17:1V:46:VAL:HG22	1.73	0.70
32:1a:510:A:OP2	35:1d:49:ARG:NH1	2.24	0.70
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.24	0.70
1:1A:1116:A:N7	1:1A:1142:A:O2'	2.25	0.70
32:1a:1027:C:C2	32:1a:1034:G:C6	2.79	0.70
32:2a:944:G:OP2	62:2a:3322:HOH:O	2.09	0.70
32:1a:1095:U:OP2	62:1a:3315:HOH:O	2.09	0.70
33:1b:74:LYS:NZ	33:1b:206:ASP:OD1	2.23	0.70
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.24	0.70
1:1A:889:G:N7	62:1A:4219:HOH:O	2.24	0.70
1:2A:2166:G:O6	1:2A:2171:A:N6	2.25	0.70
43:2l:117:ARG:HG2	43:2l:122:THR:HB	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:26:GLN:HG2	48:2q:37:LYS:HG2	1.74	0.70
56:2y:11:C:N3	56:2y:24:G:O6	2.24	0.70
32:1a:67:C:H2'	32:1a:68:G:C8	2.27	0.70
48:1q:26:GLN:HG2	48:1q:37:LYS:HG2	1.74	0.70
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.25	0.70
56:2y:27:G:O6	56:2y:43:C:N3	2.25	0.70
32:2a:1113:C:H42	32:2a:1187:G:H1	1.40	0.70
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.74	0.70
1:1A:2725:A:N3	62:1A:4217:HOH:O	2.24	0.70
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	1.73	0.70
54:1w:27:G:H1	54:1w:43:C:N4	1.89	0.70
32:2a:1269:A:N1	32:2a:1312:G:O2'	2.23	0.69
1:1A:2143:G:H1	1:1A:2199:C:N4	1.90	0.69
32:1a:1086:U:H3	32:1a:1099:G:H22	1.38	0.69
1:1A:2158:C:N3	1:1A:2177:G:C2	2.60	0.69
33:1b:101:MET:HA	33:1b:108:ILE:HG21	1.74	0.69
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.25	0.69
1:2A:1269:A:OP1	62:2A:3780:HOH:O	2.10	0.69
32:1a:1001:A:H2'	32:1a:1001(A):G:C8	2.27	0.69
32:1a:1108:G:O6	62:1a:3315:HOH:O	2.09	0.69
22:20:51:VAL:HG22	22:20:81:VAL:HG23	1.74	0.69
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.22	0.69
56:2y:26:A:N1	56:2y:44:G:C6	2.60	0.69
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.26	0.69
1:2A:276:A:H5''	1:2A:277:C:H5'	1.74	0.69
1:2A:463:G:N7	62:2A:3816:HOH:O	2.26	0.69
46:2o:74:ASP:OD2	46:2o:77:ARG:NH1	2.25	0.69
1:1A:894:U:OP2	62:1A:4159:HOH:O	2.09	0.69
1:2A:2097:C:N3	1:2A:2192:G:O6	2.26	0.69
32:2a:983:A:N1	32:2a:1222:G:N2	2.41	0.69
32:2a:1311:G:H1	32:2a:1326:C:H42	1.41	0.69
50:2s:27:GLU:HB2	50:2s:28:LYS:HA	1.74	0.69
6:1G:7:LEU:HD13	6:1G:104:GLU:HA	1.75	0.69
1:2A:890:A:H2'	1:2A:892:G:C8	2.28	0.69
1:1A:1003:U:OP2	12:1Q:14:ARG:NH1	2.25	0.68
26:14:58:ARG:HH21	50:1s:68:GLY:HA3	1.58	0.68
1:2A:81:G:H21	20:2Y:1:MET:HE3	1.58	0.68
1:2A:1537:G:H2'	1:2A:1538:G:H8	1.56	0.68
4:2E:125:GLY:O	62:2E:401:HOH:O	2.11	0.68
32:2a:811:C:N4	62:2a:3333:HOH:O	2.25	0.68
1:1A:231:G:OP1	62:1A:4160:HOH:O	2.10	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.27	0.68
7:1H:101:ARG:NH2	7:1H:121:ILE:O	2.25	0.68
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.75	0.68
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.58	0.68
11:1P:138:LEU:HD23	11:1P:145:PRO:HG3	1.76	0.68
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.26	0.68
41:2j:98:ILE:O	62:2j:8101:HOH:O	2.11	0.68
1:1A:2718:G:N7	62:1A:4234:HOH:O	2.26	0.68
10:2O:49:ARG:HH22	32:2a:1423:G:H5'	1.58	0.68
12:2Q:68:ILE:HG22	12:2Q:101:ARG:HE	1.59	0.68
41:2j:16:LEU:HD23	41:2j:70:ARG:HG2	1.76	0.68
1:1A:928:G:H3'	1:1A:929:G:H8	1.57	0.68
4:2E:56:PRO:HG3	4:2E:74:PRO:HG2	1.75	0.68
32:2a:953:G:H5'	32:2a:965:A:H61	1.58	0.68
1:2A:2287:A:H62	1:2A:2344:U:H3	1.39	0.68
19:2X:44:GLU:OE1	62:2X:3101:HOH:O	2.12	0.68
32:2a:890:G:O2'	32:2a:906:G:O6	2.12	0.68
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.25	0.68
44:2m:19:LEU:HD21	44:2m:56:LEU:HD21	1.76	0.68
54:2w:14:A:H61	54:2w:21:A:H2	1.41	0.68
1:2A:2864:G:OP1	32:2a:1442(A):G:N2	2.27	0.68
1:1A:2530:A:OP2	62:1A:4161:HOH:O	2.10	0.67
30:18:28:GLY:O	30:18:36:LYS:NZ	2.27	0.67
1:2A:1153:C:OP2	62:2A:3784:HOH:O	2.12	0.67
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.27	0.67
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.75	0.67
41:2j:30:SER:O	41:2j:81:THR:OG1	2.11	0.67
1:2A:2022:U:OP1	62:2A:3782:HOH:O	2.11	0.67
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.28	0.67
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.57	0.67
10:1O:64:ARG:HH12	10:1O:100:GLY:HA3	1.60	0.67
2:2B:96:U:OP1	21:2Z:14:LYS:NZ	2.27	0.67
32:2a:998:G:N2	32:2a:1043:C:N3	2.38	0.67
32:2a:1133:G:H1	32:2a:1141:C:H42	1.40	0.67
1:1A:2205:C:H2'	1:1A:2206:G:C8	2.29	0.67
13:1R:24:GLN:HE22	13:1R:36:THR:HG21	1.59	0.67
34:1c:152:ILE:HB	34:1c:199:LYS:HB2	1.77	0.67
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.76	0.67
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.75	0.67
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.11	0.67
32:2a:1039:C:H2'	32:2a:1040:U:O4'	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:556:C:OP2	62:1A:4166:HOH:O	2.13	0.67
1:2A:730:C:OP2	62:2A:3785:HOH:O	2.13	0.67
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.28	0.67
3:2D:76:PRO:HB2	3:2D:116:GLN:HE21	1.59	0.67
32:2a:1244:C:H42	32:2a:1293:G:H1	1.42	0.67
1:1A:778:C:OP1	62:1A:4164:HOH:O	2.12	0.67
1:2A:2104:G:H1	1:2A:2185:C:H42	1.43	0.67
1:2A:2531:A:H61	1:2A:2662:A:H61	1.43	0.67
1:1A:1729:G:OP1	62:1A:4163:HOH:O	2.12	0.67
1:1A:2817:G:N1	1:1A:2902:G:O6	2.19	0.67
32:1a:446:G:H1	32:1a:488:C:H42	1.43	0.67
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.76	0.67
7:2H:23:ARG:NH1	7:2H:34:GLU:OE1	2.27	0.67
1:2A:271(H):G:HO2'	1:2A:271(I):G:H8	1.42	0.67
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.76	0.67
32:2a:429:U:O2'	35:2d:22:LYS:NZ	2.27	0.67
32:2a:573:A:N3	32:2a:883:C:O2'	2.26	0.67
32:2a:585:G:OP1	48:2q:37:LYS:NZ	2.23	0.67
32:2a:1266:G:N2	32:2a:1269:A:OP2	2.23	0.67
8:1I:5:LEU:HD23	8:1I:9:LEU:HD13	1.77	0.67
33:1b:98:LEU:H	33:1b:101:MET:HE3	1.59	0.67
32:2a:1314:C:N4	50:2s:2:PRO:O	2.28	0.67
47:2p:51:VAL:HG12	47:2p:53:VAL:H	1.60	0.67
1:1A:2518:U:OP1	4:1E:144:ARG:NH2	2.28	0.66
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.77	0.66
1:2A:469:G:OP2	62:2A:3781:HOH:O	2.11	0.66
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.76	0.66
6:2G:131:TYR:HE2	6:2G:133:LEU:HD23	1.58	0.66
41:2j:5:ARG:N	62:2j:8102:HOH:O	2.28	0.66
11:1P:42:SER:O	62:1P:3101:HOH:O	2.14	0.66
33:1b:19:HIS:NE2	33:1b:206:ASP:OD2	2.24	0.66
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.76	0.66
32:1a:79:G:N2	32:1a:90:U:O2	2.24	0.66
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.31	0.66
32:2a:1025:U:H3	32:2a:1036:G:H1	1.42	0.66
1:1A:331:G:N7	62:1A:4243:HOH:O	2.28	0.66
1:1A:2797:C:H1'	4:1E:37:ARG:HH12	1.59	0.66
32:1a:536:C:OP2	62:1a:3316:HOH:O	2.13	0.66
1:2A:277:C:H4'	1:2A:278:A:H8	1.60	0.66
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.77	0.66
8:2I:12:LEU:HD21	8:2I:19:VAL:HG21	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1224:G:H1	32:2a:1363:C:H42	1.42	0.66
55:2x:47:U:H3'	55:2x:48:C:H5'	1.77	0.66
32:1a:1145:C:O2	32:1a:1147:C:N4	2.28	0.66
32:2a:1028:C:N3	32:2a:1033:G:O6	2.29	0.66
32:2a:1224:G:OP1	62:2a:3323:HOH:O	2.14	0.66
1:1A:2164:C:N3	1:1A:2171:G:O6	2.29	0.66
33:1b:88:ALA:HB2	33:1b:219:VAL:HG13	1.76	0.66
36:1e:5:ASP:OD1	36:1e:5:ASP:N	2.27	0.66
6:2G:59:GLU:OE2	6:2G:153:ARG:NH1	2.27	0.66
25:23:18:ASP:OD1	25:23:19:GLN:N	2.29	0.66
1:1A:2717:A:N3	62:1A:4240:HOH:O	2.28	0.66
36:1e:11:ILE:N	36:1e:31:LEU:O	2.27	0.66
1:2A:963:U:OP2	62:2A:3713:HOH:O	2.13	0.66
1:2A:2744:G:N2	7:2H:143:GLN:OE1	2.29	0.66
6:2G:122:PRO:HG3	6:2G:180:PHE:HB3	1.76	0.66
33:2b:178:ARG:NH1	33:2b:198:ASP:OD1	2.28	0.66
10:1O:120:GLU:OE1	15:1T:67:SER:OG	2.13	0.66
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.31	0.66
1:2A:2127:G:N1	1:2A:2161:C:C2	2.63	0.66
30:28:30:ARG:O	62:28:201:HOH:O	2.13	0.66
32:1a:362:G:N7	62:1a:3328:HOH:O	2.29	0.66
33:1b:7:VAL:O	33:1b:217:ARG:NH2	2.27	0.66
39:1h:4:ASP:OD2	39:1h:85:ARG:NH1	2.27	0.66
56:1y:50:U:O4	56:1y:64:A:N1	2.29	0.66
1:2A:856:C:H2'	1:2A:857:C:C6	2.30	0.66
1:2A:956:G:OP2	12:2Q:14:ARG:NH2	2.27	0.66
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.31	0.66
33:2b:121:LEU:HG	33:2b:127:ILE:HG21	1.78	0.66
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.78	0.66
2:2B:48:A:OP2	14:2S:30:ARG:NH2	2.29	0.66
23:21:85:LEU:HD22	23:21:86:SER:H	1.61	0.66
43:1l:117:ARG:HG2	43:1l:122:THR:HB	1.77	0.65
56:1y:3:C:H42	56:1y:70:G:H1	1.42	0.65
1:2A:2518:A:OP2	62:2A:3786:HOH:O	2.13	0.65
13:1R:33:ARG:HH21	13:1R:113:LEU:HD22	1.60	0.65
32:2a:1145:C:H4'	32:2a:1146:A:H5'	1.79	0.65
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.12	0.65
26:24:64:GLY:O	26:24:66:SER:N	2.29	0.65
35:2d:191:ARG:NH1	35:2d:191:ARG:O	2.26	0.65
1:1A:943:C:N3	1:1A:944:C:N4	2.43	0.65
56:1y:49:C:N3	56:1y:65:G:O6	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:572:A:H61	17:1V:19:LYS:H	1.43	0.65
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.78	0.65
19:1X:35:THR:HG22	19:1X:38:GLU:HB2	1.78	0.65
32:1a:344:A:H5''	32:1a:345:C:H5	1.61	0.65
16:2U:6:THR:HG21	16:2U:10:ARG:HD3	1.77	0.65
1:1A:2812:A:H1'	1:1A:2904:U:H1'	1.79	0.65
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.79	0.65
32:1a:60:A:H4'	32:1a:61:G:H5'	1.78	0.65
1:2A:601:C:N4	62:2A:3834:HOH:O	2.30	0.65
1:2A:1009:A:OP2	9:2N:37:LYS:NZ	2.28	0.65
15:2T:108:ARG:NH1	32:2a:1432:G:OP2	2.29	0.65
33:2b:82:ARG:NH1	33:2b:92:TYR:OH	2.29	0.65
1:1A:1114:G:O2'	1:1A:1116:A:N7	2.27	0.65
4:2E:27:LEU:HD12	15:2T:6:LEU:HD21	1.79	0.65
5:1F:11:VAL:HB	5:1F:18:ARG:HB3	1.79	0.65
12:1Q:109:VAL:HG13	12:1Q:113:GLN:HB2	1.78	0.65
47:1p:51:VAL:HG12	47:1p:53:VAL:H	1.61	0.65
38:2g:44:TYR:HE2	40:2i:41:VAL:HG11	1.61	0.65
47:2p:69:THR:HA	47:2p:72:ARG:HG2	1.79	0.65
32:1a:1030(C):G:N7	32:1a:1031:G:N2	2.44	0.65
37:2f:42:GLU:OE2	37:2f:59:TYR:OH	2.12	0.65
1:1A:1140:U:H1'	1:1A:1143:U:C5	2.32	0.65
1:1A:1896:G:N2	1:1A:1899:A:OP2	2.27	0.65
32:1a:1027:C:C4	32:1a:1034:G:O6	2.50	0.65
1:2A:848:G:C2	1:2A:933:A:H1'	2.32	0.65
1:2A:2036:C:OP1	62:2A:3788:HOH:O	2.15	0.65
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.11	0.65
32:2a:1404:5MC:O2	32:2a:1519:MA6:O2'	2.14	0.65
1:1A:1740:U:H1'	3:1D:14:ARG:NH2	2.12	0.64
1:2A:1426:G:O2'	1:2A:1572:A:N6	2.28	0.64
32:2a:1124:G:H1	32:2a:1149:C:H42	1.46	0.64
42:2k:92:GLU:HA	42:2k:95:ILE:HD12	1.78	0.64
49:2r:51:LEU:HD22	49:2r:55:ARG:HD3	1.79	0.64
1:1A:1405:A:H2'	1:1A:1406:A:H5'	1.78	0.64
11:2P:93:GLY:H	11:2P:123:LEU:HD22	1.62	0.64
32:2a:1164:G:N2	32:2a:1172:C:N3	2.36	0.64
56:1y:53:G:N2	56:1y:61:C:N3	2.41	0.64
32:2a:389:A:O2'	62:2a:3325:HOH:O	2.15	0.64
32:2a:1101:A:N6	33:2b:176:GLU:OE2	2.31	0.64
50:2s:22:LEU:HB3	50:2s:27:GLU:HB3	1.79	0.64
1:2A:856:C:N4	62:2A:3706:HOH:O	2.25	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1434:A:H61	1:2A:1558:A:H62	1.43	0.64
32:2a:966:M2G:HM23	32:2a:967:5MC:H1'	1.77	0.64
32:1a:946:A:O2'	32:1a:1333:A:N3	2.27	0.64
1:2A:1783:A:OP1	62:2A:3777:HOH:O	2.15	0.64
1:1A:1133:G:H2'	1:1A:1135:G:C8	2.33	0.64
19:1X:1:MET:HE1	24:12:22:GLU:HA	1.79	0.64
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.80	0.64
14:2S:83:LYS:HG3	14:2S:84:GLN:H	1.63	0.64
1:1A:1827:U:H2'	1:1A:1828:C:C6	2.32	0.64
1:1A:2040:G:N3	16:1U:34:LYS:NZ	2.46	0.64
32:1a:1002:G:C5	32:1a:1003:G:H1'	2.32	0.64
34:1c:139:GLN:HE21	34:1c:143:GLU:HG3	1.62	0.64
1:2A:880:G:H2'	1:2A:881:G:H8	1.63	0.64
1:2A:2193:G:H2'	1:2A:2194:G:C8	2.33	0.64
32:2a:1178:G:OP1	40:2i:93:ARG:NH1	2.31	0.64
1:1A:288:U:OP2	62:1A:4170:HOH:O	2.15	0.64
1:1A:1105:G:N2	1:1A:1126:C:O2	2.31	0.64
1:1A:2772:G:N7	62:1A:4249:HOH:O	2.29	0.64
8:1I:72:LEU:C	8:1I:74:ASN:H	2.05	0.64
32:2a:1002:G:H1	32:2a:1038:C:H42	1.45	0.64
1:1A:625:G:O6	62:1A:4162:HOH:O	2.12	0.64
1:1A:1108:G:H1'	1:1A:1134:A:N7	2.12	0.64
32:1a:258:G:H2'	32:1a:259:G:H8	1.62	0.64
32:1a:1252:A:H61	32:1a:1285:A:H61	1.44	0.64
1:2A:1632:A:OP2	62:2A:3787:HOH:O	2.14	0.64
32:2a:55:A:OP1	62:2a:3324:HOH:O	2.15	0.64
1:1A:2127:C:H2'	1:1A:2128:G:H8	1.62	0.64
1:1A:2849:G:H5'	13:1R:46:GLY:HA2	1.80	0.64
33:1b:54:THR:HG21	33:1b:201:ILE:HD11	1.78	0.64
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.13	0.64
32:2a:1007:C:N3	32:2a:1022:G:O6	2.31	0.64
1:2A:1971:A:OP1	62:2A:3789:HOH:O	2.15	0.63
1:1A:1128:U:H3	1:1A:1132:A:H61	0.71	0.63
1:1A:1681:A:OP2	62:1A:4168:HOH:O	2.15	0.63
1:1A:2740:G:O2'	10:1O:70:LYS:NZ	2.31	0.63
32:1a:407:G:H5''	35:1d:115:ARG:HB3	1.80	0.63
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.63	0.63
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.32	0.63
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.79	0.63
22:20:10:THR:HG22	22:20:12:ASN:H	1.63	0.63
1:1A:23:G:OP1	1:1A:529:U:N3	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:77:ILE:HD13	4:1E:195:LEU:HD22	1.80	0.63
26:14:64:GLY:O	26:14:66:SER:N	2.31	0.63
1:2A:1778:U:OP1	62:2A:3790:HOH:O	2.15	0.63
41:2j:44:VAL:HG22	41:2j:66:ARG:HG2	1.79	0.63
15:1T:49:VAL:HG12	15:1T:63:VAL:HG22	1.80	0.63
32:2a:264:U:H4'	48:2q:63:ARG:HD2	1.80	0.63
1:1A:1114:G:H1	1:1A:1141:A:HO2'	1.43	0.63
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.31	0.63
11:2P:138:LEU:HD23	11:2P:145:PRO:HG3	1.81	0.63
43:2l:57:LYS:HG2	43:2l:67:THR:HG22	1.80	0.63
1:1A:2083:G:H5''	1:1A:2515:2MA:C2	2.29	0.63
1:2A:1466:G:HO2'	1:2A:1546:C:HO2'	1.42	0.63
1:2A:1803:A:O2'	3:2D:259:THR:HG21	1.98	0.63
1:2A:39:C:O2	5:2F:46:ARG:NH2	2.32	0.63
32:2a:972:C:OP2	41:2j:57:LYS:NZ	2.28	0.63
32:2a:1004:A:H5''	32:2a:1025:U:C5	2.33	0.63
32:2a:1029:C:C2	32:2a:1032:G:N2	2.67	0.63
1:1A:1202:A:OP1	16:1U:55:ARG:NH1	2.32	0.63
11:1P:106:LEU:HD13	11:1P:112:LEU:HD23	1.80	0.63
39:1h:124:ALA:O	39:1h:128:GLY:N	2.32	0.63
1:2A:2167:U:H2'	1:2A:2168:G:H21	1.64	0.63
1:2A:2299:G:H2'	1:2A:2300:G:C8	2.34	0.63
32:2a:1512:U:H2'	32:2a:1513:A:C8	2.34	0.63
56:2y:19:G:H1	56:2y:56:C:N4	1.95	0.63
32:1a:1027:C:O2	32:1a:1034:G:N1	2.31	0.62
33:1b:10:LEU:H	33:1b:48:MET:HE1	1.63	0.62
1:2A:1470:G:N2	1:2A:1520:G:OP2	2.32	0.62
1:2A:2011:U:O4	62:2A:3783:HOH:O	2.12	0.62
1:1A:181:C:OP1	62:1A:4172:HOH:O	2.16	0.62
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.80	0.62
13:1R:24:GLN:HB3	13:1R:44:LEU:HD11	1.80	0.62
56:1y:4:C:N3	56:1y:69:G:O6	2.32	0.62
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.17	0.62
36:2e:92:LYS:HB3	36:2e:119:LEU:HB2	1.81	0.62
47:2p:23:ASP:OD1	47:2p:24:ALA:N	2.32	0.62
1:1A:2877:G:OP2	15:1T:119:LYS:NZ	2.30	0.62
32:1a:1503:A:O2'	53:1v:13:A:N1	2.32	0.62
24:22:8:LYS:NZ	24:22:12:GLU:OE2	2.27	0.62
32:2a:1132:C:N3	32:2a:1142:G:N2	2.43	0.62
32:2a:1159:U:O4'	32:2a:1182:G:N2	2.33	0.62
33:2b:78:GLN:NE2	33:2b:95:GLN:OE1	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:30:SER:O	41:1j:81:THR:OG1	2.16	0.62
32:2a:677:U:H3	32:2a:713:G:H22	1.45	0.62
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.00	0.62
1:1A:2594:G:OP2	62:1A:4169:HOH:O	2.15	0.62
1:1A:2766:A:N3	31:19:15:LYS:NZ	2.47	0.62
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.30	0.62
32:1a:976:G:OP2	32:1a:1358:U:O2'	2.17	0.62
1:2A:83:G:N1	1:2A:102:G:O2'	2.26	0.62
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.80	0.62
36:2e:18:ARG:HD3	36:2e:27:ARG:HH12	1.65	0.62
1:1A:1087:C:H42	1:1A:1160:G:H1	1.48	0.62
1:1A:1108:G:H2'	1:1A:1109:G:C8	2.34	0.62
5:1F:164:ARG:HG3	5:1F:175:THR:OG1	1.99	0.62
1:2A:2300:G:N1	1:2A:2317:C:N3	2.48	0.62
8:1l:43:ASN:ND2	23:11:75:GLU:OE2	2.33	0.62
32:1a:1031:G:H2'	32:1a:1032:G:H8	1.64	0.62
37:1f:97:PHE:HB2	49:1r:32:ARG:NH1	2.14	0.62
32:2a:184:G:H2'	32:2a:185:A:H8	1.63	0.62
32:2a:299:G:O6	62:2a:3320:HOH:O	2.10	0.62
32:2a:376:G:H1	32:2a:387:U:H3	1.47	0.62
1:1A:313:A:N6	1:1A:375:G:O2'	2.33	0.62
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.82	0.62
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.81	0.62
1:2A:1721:G:N1	1:2A:1739:U:OP2	2.33	0.62
1:2A:2875:C:OP1	15:2T:3:ARG:NH1	2.25	0.62
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.82	0.62
32:2a:517:G:N2	32:2a:533:A:OP2	2.30	0.62
1:1A:24:G:O2'	18:1W:78:GLU:O	2.17	0.62
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.35	0.62
35:1d:33:MET:HE2	35:1d:33:MET:HA	1.81	0.62
35:1d:79:PHE:HE1	35:1d:204:ILE:HD13	1.65	0.62
32:2a:56:U:H2'	32:2a:57:G:C8	2.35	0.62
1:1A:2178:G:H2'	1:1A:2179:G:C4	2.35	0.62
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.82	0.62
21:1Z:129:SER:HB3	21:1Z:132:ASN:HD22	1.65	0.62
1:2A:1370:C:HO2'	1:2A:1811:G:HO2'	1.43	0.62
3:2D:132:PRO:HG2	3:2D:135:PHE:HD2	1.65	0.62
1:1A:1466:U:O2'	1:1A:1467:G:OP1	2.16	0.61
26:14:24:THR:OG1	26:14:25:TYR:N	2.33	0.61
1:2A:2572:A:C8	4:2E:144:ARG:HD2	2.34	0.61
1:1A:1785:C:H5	15:1T:96:ARG:HH21	1.46	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1864:U:O2'	1:1A:1991:A:N1	2.31	0.61
32:1a:343:U:O2'	32:1a:346:G:O6	2.15	0.61
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.33	0.61
32:2a:67:C:H2'	32:2a:68:G:C8	2.35	0.61
36:2e:110:LEU:HD13	36:2e:118:ILE:HD13	1.82	0.61
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	1.82	0.61
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.31	0.61
35:2d:166:LYS:NZ	35:2d:179:GLU:OE2	2.33	0.61
32:1a:376:G:O3'	47:1p:5:ARG:HD2	2.00	0.61
1:2A:453:C:OP1	62:2A:3792:HOH:O	2.16	0.61
1:1A:611:U:H2'	1:1A:612:C:C6	2.35	0.61
1:1A:1834:A:O2'	3:1D:259:THR:HG21	2.00	0.61
8:1I:38:LEU:HD12	8:1I:38:LEU:H	1.64	0.61
32:1a:1149:C:OP2	40:1i:9:ARG:NH2	2.33	0.61
38:2g:93:PRO:HA	38:2g:96:GLN:HG3	1.81	0.61
1:1A:484:G:O2'	1:1A:495:G:O6	2.17	0.61
16:1U:33:ARG:NH2	62:1U:301:HOH:O	2.34	0.61
21:1Z:91:LEU:HD23	21:1Z:130:PRO:HB3	1.83	0.61
32:1a:1312:G:H5'	50:1s:5:LEU:HD11	1.83	0.61
40:1i:42:ARG:NH2	40:1i:75:ASP:OD1	2.33	0.61
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.33	0.61
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.35	0.61
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.82	0.61
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.82	0.61
32:2a:344:A:H5''	32:2a:345:C:H5	1.66	0.61
41:2j:38:ILE:HG13	41:2j:71:LEU:HB3	1.81	0.61
1:1A:1440:U:OP1	62:1A:4174:HOH:O	2.16	0.61
32:1a:559:A:H4'	32:1a:560:U:H3'	1.83	0.61
1:2A:82:G:N1	1:2A:103:A:OP2	2.27	0.61
1:2A:2199:A:H5''	23:21:50:ARG:HH21	1.66	0.61
39:2h:124:ALA:O	39:2h:128:GLY:N	2.32	0.61
43:2l:78:GLN:NE2	62:2l:301:HOH:O	2.33	0.61
1:1A:1861:C:OP2	62:1A:4176:HOH:O	2.16	0.61
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.83	0.61
20:1Y:20:TYR:HB3	20:1Y:23:ARG:HD2	1.82	0.61
40:1i:79:LEU:HD22	40:1i:104:ARG:HB3	1.83	0.61
54:1w:29:G:H1	54:1w:41:C:H42	1.48	0.61
1:2A:2114:A:N6	1:2A:2119:A:H62	1.99	0.61
2:2B:24:G:N7	2:2B:56:G:H2'	2.16	0.61
5:2F:40:GLN:HE22	5:2F:182:ASN:HB2	1.65	0.61
6:2G:54:GLU:O	6:2G:58:GLN:N	2.29	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:49:ARG:NH2	32:2a:1422:G:O2'	2.34	0.61
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.83	0.61
32:2a:533:A:OP1	62:2a:3327:HOH:O	2.16	0.61
33:2b:77:ALA:HB2	33:2b:211:ILE:HD13	1.83	0.61
1:1A:233:A:OP2	30:18:11:LYS:NZ	2.33	0.61
1:1A:1451:U:H2'	1:1A:1452:U:C6	2.36	0.61
1:1A:2383:G:O6	62:1A:4167:HOH:O	2.14	0.61
33:1b:21:ARG:O	33:1b:23:ARG:N	2.34	0.61
1:2A:910:A:N3	1:2A:2264:C:O2'	2.33	0.61
1:2A:2142:C:N3	1:2A:2149:G:O6	2.33	0.61
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.65	0.61
49:2r:53:ARG:HH21	49:2r:59:SER:HA	1.66	0.61
1:1A:1313:U:OP1	62:1A:4171:HOH:O	2.16	0.61
1:2A:551:G:O2'	1:2A:1220:A:N3	2.29	0.61
1:2A:2313:C:O4'	6:2G:40:ASN:ND2	2.34	0.61
1:1A:964:A:N3	2:1B:80:U:O2'	2.33	0.60
1:2A:1613:G:H1	1:2A:1617:C:HO2'	1.46	0.60
1:2A:2136:C:H1'	1:2A:2137:C:H5'	1.83	0.60
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.82	0.60
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.82	0.60
32:2a:134:A:H61	47:2p:25:ARG:HH12	1.49	0.60
50:2s:70:LYS:HB2	50:2s:73:GLU:HG3	1.82	0.60
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.34	0.60
32:1a:1027:C:O2	32:1a:1034:G:C2	2.54	0.60
1:2A:625:G:N7	11:2P:107:LYS:NZ	2.43	0.60
2:2B:28:C:H2'	2:2B:29:A:H8	1.66	0.60
44:2m:15:VAL:HG21	44:2m:48:LEU:HD21	1.82	0.60
1:1A:2129:C:N4	1:1A:2204:G:H1	1.99	0.60
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.82	0.60
32:1a:1008:C:N3	32:1a:1021:G:N2	2.42	0.60
32:1a:1202:G:H1'	45:1n:29:ARG:HD2	1.83	0.60
38:1g:27:ILE:HD12	38:1g:40:ALA:HA	1.82	0.60
1:2A:880:G:H2'	1:2A:881:G:C8	2.37	0.60
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.37	0.60
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.34	0.60
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.83	0.60
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.34	0.60
32:2a:76:C:N4	32:2a:93:G:H1	1.99	0.60
1:1A:1101:G:N2	1:1A:1151:U:O2	2.34	0.60
1:1A:1123:A:H2	1:1A:1134:A:C2	2.18	0.60
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2164:C:O2	1:1A:2171:G:N1	2.29	0.60
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.34	0.60
1:1A:1151:U:H2'	1:1A:1152:G:H8	1.66	0.60
6:1G:67:LYS:HE3	26:14:5:ILE:HD12	1.83	0.60
1:2A:210:C:OP2	29:27:29:LYS:NZ	2.34	0.60
1:2A:2193:G:H2'	1:2A:2194:G:H8	1.67	0.60
32:2a:28:G:O2'	32:2a:296:U:OP1	2.18	0.60
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.15	0.60
40:2i:79:LEU:HD22	40:2i:104:ARG:HB3	1.83	0.60
1:1A:1584:G:H2'	1:1A:1585:G:H8	1.66	0.60
1:2A:409:C:OP1	62:2A:3791:HOH:O	2.16	0.60
12:2Q:12:GLN:HE21	12:2Q:72:LYS:HG3	1.67	0.60
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	1.84	0.60
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.36	0.60
32:2a:1204:A:OP1	45:2n:3:ARG:NH1	2.34	0.60
1:1A:1223:C:H2'	1:1A:1224:C:H6	1.67	0.60
37:1f:70:ASP:N	37:1f:70:ASP:OD1	2.32	0.60
1:2A:1190:G:N7	62:2A:3722:HOH:O	2.32	0.60
32:2a:1518:MA6:N6	32:2a:1519:MA6:H103	2.17	0.60
1:1A:1285:G:OP1	62:1A:4177:HOH:O	2.17	0.60
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.37	0.60
24:12:59:ARG:NH2	62:12:3101:HOH:O	2.34	0.60
32:1a:953:G:H5'	32:1a:965:A:H61	1.67	0.60
32:1a:1291:G:OP1	38:1g:41:ARG:NH2	2.34	0.60
21:2Z:74:VAL:HG22	21:2Z:86:VAL:HG12	1.83	0.60
32:2a:1004:A:H8	32:2a:1005:A:H4'	1.67	0.60
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	1.82	0.60
38:1g:64:GLN:HE21	38:1g:68:ASN:HD21	1.50	0.60
1:2A:2139:C:N3	1:2A:2152:G:N2	2.43	0.60
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.37	0.60
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.84	0.60
1:1A:1639:G:H2'	1:1A:1640:G:C8	2.37	0.60
32:1a:1027:C:N4	32:1a:1033:G:O6	2.35	0.60
56:1y:19:G:H4'	56:1y:20:U:OP2	2.02	0.60
56:1y:59:U:H3'	56:1y:60:U:C6	2.37	0.60
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.35	0.60
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.31	0.60
13:2R:24:GLN:HE22	13:2R:36:THR:HG21	1.67	0.60
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.84	0.60
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.83	0.60
34:2c:40:ARG:HG2	34:2c:55:VAL:HG11	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.34	0.60
1:1A:1210:G:H2'	1:1A:1211:U:C6	2.37	0.59
36:1e:122:GLU:O	36:1e:126:ARG:NH1	2.34	0.59
1:1A:260:A:N3	1:1A:395:C:O2'	2.32	0.59
1:1A:1232:G:H5''	17:1V:81:TYR:CE1	2.37	0.59
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.84	0.59
40:1i:51:ARG:HG2	40:1i:56:LEU:HD11	1.84	0.59
32:2a:659:U:OP2	46:2o:8:LYS:NZ	2.34	0.59
1:1A:848:G:O6	5:1F:53:THR:OG1	2.20	0.59
12:1Q:85:LYS:HD3	22:10:7:LEU:HD13	1.84	0.59
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.38	0.59
1:1A:89:U:H1'	1:1A:90:A:C8	2.36	0.59
1:1A:145:G:O6	62:1A:4165:HOH:O	2.12	0.59
11:1P:89:ALA:O	11:1P:121:LYS:NZ	2.33	0.59
32:1a:175:C:H2'	32:1a:176:C:H6	1.66	0.59
47:1p:35:LYS:HG2	47:1p:37:GLY:H	1.66	0.59
48:1q:45:HIS:CD2	48:1q:47:PRO:HG3	2.37	0.59
1:2A:385:C:O2'	1:2A:388:G:N2	2.35	0.59
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.02	0.59
32:2a:376:G:O3'	47:2p:5:ARG:HD2	2.03	0.59
32:2a:1029:C:C4	32:2a:1032:G:C2	2.90	0.59
42:2k:43:SER:HA	42:2k:47:VAL:HG21	1.85	0.59
50:1s:35:SER:OG	50:1s:38:SER:OG	2.17	0.59
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.83	0.59
32:2a:1002:G:H1	32:2a:1038:C:N4	2.00	0.59
39:2h:9:MET:HG3	39:2h:26:VAL:HG11	1.84	0.59
21:1Z:28:MET:HE3	21:1Z:37:VAL:HG11	1.84	0.59
32:1a:426:G:OP1	35:1d:38:TYR:OH	2.20	0.59
33:1b:230:VAL:HG22	33:1b:232:PRO:HD2	1.82	0.59
35:1d:166:LYS:HG2	35:1d:178:VAL:HG11	1.85	0.59
1:2A:752:A:H3'	29:27:1:MET:HE2	1.85	0.59
1:2A:1593:G:H2'	1:2A:1594:G:H8	1.67	0.59
32:2a:141:A:H1'	32:2a:182:U:O2	2.03	0.59
32:2a:309:G:O2'	32:2a:607:A:N1	2.35	0.59
32:2a:324:G:OP2	62:2a:3326:HOH:O	2.16	0.59
1:1A:661:G:O2'	1:1A:663:G:O2'	2.19	0.59
1:1A:786:G:OP1	62:1A:4173:HOH:O	2.16	0.59
56:1y:15:G:N2	56:1y:48:C:H42	2.01	0.59
9:2N:15:LEU:N	9:2N:136:GLU:O	2.34	0.59
1:1A:1233:U:H5'	17:1V:79:VAL:HG13	1.83	0.59
2:1B:28:C:OP1	14:1S:36:TYR:OH	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:115:ARG:HB3	6:1G:136:ARG:HH21	1.67	0.59
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.85	0.59
1:2A:1123:C:H1'	31:29:18:ARG:HH21	1.66	0.59
1:2A:2323:G:O6	1:2A:2332:U:N3	2.19	0.59
6:2G:41:GLN:HG3	6:2G:43:LEU:HD13	1.85	0.59
7:2H:3:ARG:NH2	7:2H:65:HIS:HB3	2.16	0.59
32:2a:1302:U:OP1	44:2m:13:LYS:NZ	2.34	0.59
34:2c:131:ARG:HH21	36:2e:50:GLU:HG3	1.68	0.59
21:1Z:138:GLU:H	21:1Z:156:LYS:NZ	1.98	0.59
32:1a:165:C:H2'	32:1a:166:G:H8	1.68	0.59
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.36	0.59
1:1A:2331:G:N2	14:1S:3:ARG:HD2	2.16	0.59
1:1A:2800:C:H1'	4:1E:62:PRO:HG3	1.85	0.59
7:1H:56:SER:HB3	7:1H:61:HIS:ND1	2.18	0.59
32:1a:46:G:O6	62:1a:3317:HOH:O	2.15	0.59
32:1a:164:U:H2'	32:1a:165:C:C6	2.38	0.59
38:2g:79:ARG:HG3	38:2g:80:VAL:H	1.68	0.59
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.85	0.59
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	1.83	0.59
1:1A:2162:C:O2	1:1A:2174:G:N2	2.35	0.58
32:1a:128:G:O2'	48:1q:3:LYS:NZ	2.35	0.58
8:2I:72:LEU:C	8:2I:74:ASN:H	2.10	0.58
33:2b:47:THR:HA	33:2b:202:PRO:HG2	1.83	0.58
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.85	0.58
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.38	0.58
33:1b:87:ARG:NH1	33:1b:233:SER:HB3	2.17	0.58
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.85	0.58
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.84	0.58
1:2A:2137:C:H2'	1:2A:2138:C:C6	2.38	0.58
3:2D:80:ALA:HB3	3:2D:94:LEU:HD23	1.84	0.58
32:2a:448:A:P	32:2a:485:G:H22	2.26	0.58
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.38	0.58
32:2a:1249:C:O2'	40:2i:73:GLN:NE2	2.35	0.58
34:2c:14:ILE:HG22	34:2c:15:THR:HG23	1.84	0.58
56:2y:13:C:N3	56:2y:22:G:O6	2.37	0.58
1:1A:387:G:H2'	1:1A:388:A:C8	2.38	0.58
1:1A:2156:A:H2	1:1A:2181:G:H4'	1.67	0.58
21:2Z:91:LEU:HD23	21:2Z:130:PRO:HB3	1.85	0.58
32:2a:1158:C:O2	32:2a:1181:G:N2	2.19	0.58
32:1a:142:G:H2'	32:1a:143:A:H8	1.68	0.58
34:1c:131:ARG:HH21	36:1e:50:GLU:HG3	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:36:ARG:NH2	37:1f:66:GLU:OE1	2.34	0.58
5:2F:132:VAL:HA	5:2F:138:GLU:HB3	1.84	0.58
32:2a:539:A:OP2	43:2l:115:LYS:NZ	2.37	0.58
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.84	0.58
40:2i:50:LEU:H	40:2i:50:LEU:HD13	1.68	0.58
56:2y:9:A:H5'	56:2y:46:7MG:N3	2.18	0.58
32:1a:811:C:N3	62:1a:3333:HOH:O	2.32	0.58
32:1a:1182:G:H4'	32:1a:1183:A:H5'	1.85	0.58
1:2A:2313:C:H5''	6:2G:91:ARG:HD3	1.85	0.58
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.85	0.58
3:2D:69:ARG:HE	3:2D:130:ALA:HB2	1.68	0.58
6:2G:41:GLN:NE2	6:2G:154:GLY:O	2.36	0.58
18:2W:35:ILE:HG23	27:25:28:PRO:HD2	1.85	0.58
33:2b:98:LEU:H	33:2b:101:MET:HE3	1.67	0.58
40:2i:31:GLN:HE21	40:2i:36:TYR:HD1	1.52	0.58
44:2m:80:ARG:HH12	50:2s:69:HIS:HE1	1.51	0.58
32:1a:662:G:H2'	32:1a:663:A:C8	2.37	0.58
47:1p:43:LYS:HG2	47:1p:48:TRP:CD2	2.38	0.58
49:1r:26:LEU:HD21	49:1r:39:VAL:HG13	1.86	0.58
1:2A:987:G:O2'	1:2A:1000:A:N3	2.32	0.58
1:2A:2756:U:H1'	1:2A:2757:A:H5''	1.85	0.58
32:2a:56:U:H2'	32:2a:57:G:H8	1.67	0.58
32:2a:942:G:H21	40:2i:124:GLN:NE2	2.01	0.58
32:2a:1029:C:N3	32:2a:1032:G:N2	2.51	0.58
32:2a:1159:U:OP1	33:2b:133:LYS:NZ	2.36	0.58
35:2d:173:TRP:CD2	35:2d:189:PRO:HG3	2.38	0.58
1:1A:1785:C:OP1	15:1T:96:ARG:NH1	2.37	0.58
13:1R:95:THR:HG22	13:1R:116:LEU:HD23	1.85	0.58
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.69	0.58
1:2A:1671:U:OP2	62:2A:3793:HOH:O	2.17	0.58
2:2B:14:U:O3'	2:2B:108:U:O2'	2.22	0.58
12:2Q:82:ARG:HB2	22:20:7:LEU:HD11	1.84	0.58
26:24:53:GLU:OE2	44:2m:65:LYS:NZ	2.31	0.58
1:1A:248:G:O2'	1:1A:646:A:O2'	2.18	0.58
1:1A:1782:C:HO2'	1:1A:2871:G:HO2'	1.48	0.58
7:1H:149:ARG:NH2	7:1H:167:GLU:OE2	2.35	0.58
32:1a:934:C:OP1	62:1a:3318:HOH:O	2.17	0.58
32:1a:1027:C:N3	32:1a:1034:G:O6	2.36	0.58
1:2A:2287:A:N6	1:2A:2344:U:H3	2.01	0.58
2:2B:49:C:H2'	2:2B:50:G:C8	2.39	0.58
32:2a:1111:A:N1	34:2c:177:THR:OG1	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:582:U:OP1	46:1o:68:ARG:NH2	2.33	0.58
55:1x:49:G:H1	55:1x:65:C:H42	1.52	0.58
1:2A:307:G:N1	1:2A:310:A:OP2	2.37	0.58
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.39	0.58
32:2a:1129:C:OP2	40:2i:66:ARG:NH1	2.37	0.58
1:1A:790:G:N7	62:1A:4266:HOH:O	2.33	0.58
1:1A:1108:G:H2'	1:1A:1109:G:H8	1.67	0.58
1:1A:1940:A:N6	62:1A:4283:HOH:O	2.34	0.58
1:1A:2346:G:H5'	14:1S:9:ARG:HG2	1.85	0.58
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.34	0.58
55:1x:52:G:H1	55:1x:62:C:H42	1.52	0.58
1:2A:574:C:N3	4:2E:145:LYS:NZ	2.52	0.58
1:2A:709:U:H2'	1:2A:710:G:C8	2.39	0.58
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.68	0.58
7:2H:25:LYS:HG2	7:2H:34:GLU:HG2	1.85	0.58
32:2a:656:C:O2	46:2o:28:GLN:NE2	2.36	0.58
32:2a:987:G:N2	32:2a:1218:C:N3	2.49	0.58
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.69	0.58
1:1A:1170:C:OP1	62:1A:4179:HOH:O	2.17	0.57
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.37	0.57
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.85	0.57
45:1n:21:TYR:HE1	45:1n:23:ARG:HE	1.51	0.57
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.28	0.57
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.39	0.57
12:2Q:81:VAL:HB	22:20:7:LEU:HD21	1.86	0.57
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.86	0.57
32:2a:1131:G:H1	32:2a:1143:G:H21	1.52	0.57
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.69	0.57
43:2l:26:ALA:HA	43:2l:64:TYR:HD2	1.69	0.57
1:1A:630:U:OP1	5:1F:102:PRO:HA	2.04	0.57
1:1A:1053:C:OP1	9:1N:35:ARG:NH1	2.37	0.57
1:1A:1452:U:H2'	1:1A:1453:C:C6	2.39	0.57
1:1A:2157:A:N6	1:1A:2178:G:O2'	2.37	0.57
1:1A:2227:G:H3'	1:1A:2228:G:C8	2.40	0.57
11:1P:47:ASP:OD2	11:1P:49:ARG:NH2	2.38	0.57
32:1a:153:C:H42	32:1a:168:G:H1	1.52	0.57
54:1w:18:G:H4'	54:1w:60:U:C5	2.39	0.57
32:2a:1133:G:H1	32:2a:1141:C:N4	2.02	0.57
1:1A:1712:A:H1'	10:1O:1:MET:HE3	1.85	0.57
32:1a:1249:C:O2'	40:1i:73:GLN:NE2	2.37	0.57
1:2A:1717:G:H1	1:2A:1745:C:H42	1.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.40	0.57
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	1.86	0.57
32:2a:304:U:H2'	32:2a:305:G:C8	2.39	0.57
32:2a:750:G:OP2	62:2a:3328:HOH:O	2.17	0.57
32:2a:984:C:H2'	32:2a:985:C:H6	1.68	0.57
32:1a:145:G:H1	32:1a:177:C:H42	1.51	0.57
32:1a:165:C:H2'	32:1a:166:G:C8	2.39	0.57
55:1x:4:G:H2'	55:1x:5:G:C8	2.39	0.57
10:2O:8:LEU:HD23	10:2O:82:ASN:HB3	1.86	0.57
32:2a:395:C:N4	62:2a:3351:HOH:O	2.36	0.57
43:2l:26:ALA:HA	43:2l:64:TYR:CD2	2.39	0.57
1:1A:2296:C:P	28:16:6:ARG:HG3	2.43	0.57
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.85	0.57
26:14:57:GLU:HB3	26:14:58:ARG:HD2	1.87	0.57
32:1a:396:G:O2'	32:1a:398:C:OP1	2.19	0.57
32:1a:1183:A:H3'	32:1a:1184:G:H5''	1.86	0.57
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.85	0.57
6:2G:32:PRO:HB2	6:2G:172:LEU:HD22	1.85	0.57
33:2b:51:LEU:HD23	33:2b:201:ILE:HD12	1.85	0.57
1:1A:660:C:O2'	1:1A:664:U:OP1	2.21	0.57
32:1a:600:C:H2'	32:1a:601:C:H6	1.68	0.57
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.38	0.57
1:2A:521:G:H2'	1:2A:522:G:H8	1.70	0.57
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	1.86	0.57
12:2Q:11:LYS:HD3	12:2Q:87:LYS:HD3	1.86	0.57
32:2a:195:A:OP2	62:2a:3329:HOH:O	2.17	0.57
44:2m:3:ARG:HG3	44:2m:4:ILE:H	1.70	0.57
47:2p:59:TRP:HA	47:2p:62:VAL:HG12	1.87	0.57
55:2x:23:C:H2'	55:2x:24:U:C6	2.39	0.57
1:1A:1814:A:N7	62:1A:4261:HOH:O	2.32	0.57
1:1A:2856:G:OP1	62:1A:4178:HOH:O	2.17	0.57
6:1G:150:ASP:OD1	6:1G:150:ASP:N	2.38	0.57
36:1e:110:LEU:HD13	36:1e:118:ILE:HD13	1.86	0.57
40:1i:79:LEU:HG	40:1i:83:ARG:HD2	1.86	0.57
1:2A:1693:U:H1'	3:2D:14:ARG:NH2	2.20	0.57
1:2A:1791:A:H5'	3:2D:206:LEU:HD12	1.86	0.57
33:2b:97:TRP:HH2	33:2b:176:GLU:CD	2.12	0.57
1:1A:880:U:O2	11:1P:55:ARG:NH2	2.33	0.57
1:1A:2127:C:H2'	1:1A:2128:G:C8	2.39	0.57
9:1N:1:MET:HE2	17:1V:12:TYR:HA	1.86	0.57
1:2A:2033:A:OP1	62:2A:3737:HOH:O	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:2r:53:ARG:HE	49:2r:59:SER:C	2.11	0.57
1:1A:2209:G:H2'	1:1A:2210:C:O4'	2.05	0.57
1:1A:2298:A:H4'	1:1A:2299:A:O4'	2.05	0.57
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.86	0.57
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.87	0.57
56:1y:55:PSU:C2	56:1y:57:G:H5'	2.39	0.57
1:2A:118:A:N3	1:2A:178:G:H1'	2.19	0.57
1:2A:288:C:H2'	1:2A:289:A:C8	2.40	0.57
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.37	0.57
4:1E:29:GLY:HA3	62:1E:401:HOH:O	2.05	0.57
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.87	0.57
35:1d:98:GLU:HA	35:1d:103:ASN:HD22	1.69	0.57
47:1p:57:ARG:O	47:1p:61:SER:N	2.35	0.57
1:2A:2398:U:H2'	1:2A:2399:G:C8	2.40	0.57
32:2a:637:G:H2'	32:2a:638:G:H8	1.69	0.57
32:2a:1028:C:O2	32:2a:1033:G:N1	2.37	0.57
32:2a:1135:U:H4'	32:2a:1136:U:H5	1.69	0.57
34:2c:6:HIS:HD2	34:2c:9:GLY:H	1.51	0.57
56:2y:5:G:H1	56:2y:68:C:N4	2.01	0.57
56:2y:8:4SU:S4	56:2y:14:A:N7	2.78	0.57
1:1A:1475:G:H2'	1:1A:1476:C:H6	1.69	0.56
3:1D:80:ALA:HB3	3:1D:94:LEU:HD23	1.86	0.56
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.23	0.56
15:2T:9:LEU:O	15:2T:12:SER:OG	2.14	0.56
1:1A:202:A:H2'	1:1A:203:G:O4'	2.05	0.56
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.40	0.56
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.04	0.56
1:2A:1827:C:C2'	1:2A:1828:G:H5'	2.35	0.56
1:2A:2171:A:H1'	1:2A:2172:U:C6	2.39	0.56
32:2a:413:G:H22	32:2a:429:U:H5''	1.69	0.56
32:2a:862:C:H2'	32:2a:863:U:H6	1.70	0.56
32:2a:1014:A:C2	32:2a:1219:U:H1'	2.40	0.56
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.04	0.56
33:2b:98:LEU:HD13	33:2b:108:ILE:HD11	1.86	0.56
34:2c:100:ALA:O	34:2c:102:ASN:ND2	2.37	0.56
36:2e:100:VAL:HG22	36:2e:118:ILE:HG22	1.87	0.56
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.86	0.56
1:1A:1633:A:H2'	1:1A:1634:C:C6	2.40	0.56
1:1A:2430:A:OP2	30:18:29:LYS:NZ	2.32	0.56
32:1a:130:A:O2'	32:1a:131:C:O5'	2.24	0.56
32:1a:1456:G:N2	51:1t:51:GLU:OE2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1521:G:N3	62:1a:3334:HOH:O	2.32	0.56
38:1g:93:PRO:HA	38:1g:96:GLN:HG3	1.88	0.56
1:2A:1219:G:H1	1:2A:1230:C:H42	1.54	0.56
1:2A:2576:G:O2'	1:2A:2579:C:OP2	2.19	0.56
5:2F:18:ARG:HG2	5:2F:19:GLU:H	1.70	0.56
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.86	0.56
28:26:10:LEU:HG	28:26:54:ILE:HG13	1.86	0.56
32:2a:674:G:OP1	37:2f:87:ARG:NH2	2.36	0.56
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.86	0.56
54:2w:3:C:N3	54:2w:70:G:N2	2.53	0.56
56:2y:27:G:N1	56:2y:43:C:O2	2.37	0.56
56:2y:62:C:H2'	56:2y:63:G:C8	2.39	0.56
2:1B:1:U:O2'	2:1B:2:C:OP1	2.20	0.56
32:1a:28:G:O2'	32:1a:296:U:OP1	2.22	0.56
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.70	0.56
51:1t:65:LYS:HA	51:1t:68:LYS:HD3	1.87	0.56
1:2A:646:A:H2'	1:2A:647:G:O4'	2.06	0.56
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.41	0.56
49:2r:21:LYS:NZ	49:2r:54:ARG:O	2.38	0.56
1:1A:609:A:N1	1:1A:856:G:O2'	2.35	0.56
32:1a:1360:A:H8	32:1a:1360:A:OP1	1.88	0.56
46:1o:26:GLU:OE2	46:1o:77:ARG:NE	2.29	0.56
1:2A:271(H):G:O2'	1:2A:271(I):G:H8	1.88	0.56
21:2Z:11:GLU:O	21:2Z:36:LYS:NZ	2.38	0.56
32:2a:301:G:H2'	32:2a:302:G:H8	1.70	0.56
37:2f:97:PHE:N	49:2r:30:ASP:OD1	2.38	0.56
49:2r:21:LYS:HE3	49:2r:57:GLY:HA2	1.87	0.56
1:1A:933:C:H4'	1:1A:933:C:OP1	2.06	0.56
1:1A:968:U:H2'	1:1A:969:C:C6	2.41	0.56
1:1A:1410:G:OP1	23:11:2:SER:HA	2.06	0.56
1:1A:2816:G:H2'	1:1A:2817:G:H8	1.71	0.56
20:1Y:17:SER:OG	20:1Y:71:LYS:NZ	2.39	0.56
35:1d:155:LEU:HB3	35:1d:158:ILE:HG12	1.87	0.56
41:1j:16:LEU:HD12	41:1j:94:VAL:HG22	1.86	0.56
56:1y:36:A:H2'	56:1y:37:MIA:O4'	2.05	0.56
1:2A:1142(A):A:H4'	9:2N:25:ARG:HH22	1.71	0.56
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.38	0.56
32:2a:1164:G:N1	32:2a:1172:C:N4	2.45	0.56
1:1A:248:G:HO2'	1:1A:646:A:HO2'	1.51	0.56
1:1A:287:G:N7	1:1A:448:U:H2'	2.20	0.56
1:1A:1128:U:C4	1:1A:1132:A:N1	2.74	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1451:U:H2'	1:1A:1452:U:H6	1.71	0.56
1:1A:1492:C:H2'	1:1A:1493:C:H6	1.71	0.56
3:1D:26:LYS:HB3	3:1D:83:GLU:HG2	1.88	0.56
6:1G:143:GLU:O	26:14:28:LYS:NZ	2.38	0.56
32:1a:1001:A:H2'	32:1a:1001(A):G:H8	1.69	0.56
32:1a:1518:MA6:N6	32:1a:1519:MA6:H103	2.19	0.56
40:1i:4:TYR:O	40:1i:19:LEU:N	2.23	0.56
54:1w:18:G:O2'	54:1w:57:G:N2	2.36	0.56
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.87	0.56
21:2Z:28:MET:HE3	21:2Z:37:VAL:HG11	1.86	0.56
1:1A:2311:G:H2'	1:1A:2312:G:H8	1.70	0.56
34:1c:82:GLU:OE1	34:1c:85:ARG:NH2	2.39	0.56
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.87	0.56
1:2A:984:A:H5''	1:2A:985:C:H5	1.70	0.56
1:2A:990:A:OP2	62:2A:3734:HOH:O	2.17	0.56
1:2A:1038:C:H42	1:2A:1117:G:H1	1.52	0.56
1:2A:1541:G:H3'	1:2A:1542:A:H2'	1.88	0.56
1:2A:2750:A:O2'	1:2A:2752:C:N4	2.35	0.56
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.87	0.56
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.21	0.56
1:1A:280:C:H2'	1:1A:281:G:H8	1.71	0.56
40:1i:121:ARG:NH1	40:1i:122:ALA:O	2.38	0.56
5:2F:164:ARG:HG3	5:2F:175:THR:OG1	2.06	0.56
8:2I:43:ASN:ND2	23:21:75:GLU:OE2	2.39	0.56
23:21:60:PHE:HE1	23:21:91:LYS:HG3	1.71	0.56
36:2e:88:LYS:HB3	36:2e:123:LEU:HB2	1.86	0.56
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.86	0.56
1:1A:325:G:OP2	20:1Y:84:ARG:NH2	2.39	0.56
1:1A:469:A:H1'	1:1A:1246:C:O4'	2.06	0.56
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.41	0.56
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.87	0.56
26:14:53:GLU:O	26:14:56:VAL:HG13	2.06	0.56
32:1a:67:C:H2'	32:1a:68:G:H8	1.70	0.56
1:2A:518:G:H2'	1:2A:519:U:C6	2.41	0.56
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.88	0.56
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.41	0.56
15:2T:105:LEU:HD22	15:2T:109:GLU:HB3	1.87	0.56
32:2a:180:U:O2	32:2a:196:A:N6	2.39	0.56
32:2a:1309:G:OP1	44:2m:88:ARG:NH2	2.36	0.56
24:12:51:ARG:HE	24:12:55:ARG:NH1	2.04	0.55
24:12:64:LEU:HD21	24:12:68:ARG:HE	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.41	0.55
32:2a:376:G:H5''	47:2p:5:ARG:CG	2.37	0.55
32:2a:580:U:H5''	46:2o:58:MET:HG2	1.87	0.55
32:2a:1029:C:N4	32:2a:1032:G:N1	2.53	0.55
32:2a:1304:G:OP2	62:2a:3330:HOH:O	2.18	0.55
34:2c:134:ILE:HG23	34:2c:151:VAL:HB	1.87	0.55
1:1A:436:C:OP1	62:1A:4180:HOH:O	2.18	0.55
1:1A:2686:G:H2'	1:1A:2687:A:C8	2.40	0.55
1:1A:2825:C:H5'	27:15:29:THR:HG21	1.88	0.55
15:1T:77:PRO:HB2	15:1T:80:SER:HB2	1.87	0.55
20:1Y:86:ARG:HB2	20:1Y:98:VAL:HG23	1.88	0.55
32:1a:390:C:H2'	32:1a:391:G:C8	2.41	0.55
49:1r:53:ARG:HH21	49:1r:59:SER:HA	1.70	0.55
6:2G:138:GLN:NE2	6:2G:151:ALA:O	2.37	0.55
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.71	0.55
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.88	0.55
32:2a:501:C:H2'	32:2a:502:G:H8	1.70	0.55
32:2a:828:A:H2'	32:2a:829:G:O4'	2.06	0.55
32:2a:1101:A:N7	33:2b:175:ARG:NH2	2.55	0.55
41:2j:10:GLY:HA3	41:2j:16:LEU:HD11	1.88	0.55
47:2p:43:LYS:HG2	47:2p:48:TRP:CD2	2.41	0.55
50:2s:80:TYR:O	50:2s:82:GLY:N	2.38	0.55
1:1A:1102:G:N2	1:1A:1148:C:OP2	2.32	0.55
1:1A:2699:U:H2'	1:1A:2700:U:O4'	2.06	0.55
26:14:53:GLU:OE2	44:1m:65:LYS:NZ	2.39	0.55
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.21	0.55
32:1a:1349:A:H5''	40:1i:121:ARG:HB2	1.88	0.55
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.42	0.55
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.89	0.55
56:1y:15:G:H22	56:1y:48:C:H42	1.54	0.55
1:2A:861:A:N3	2:2B:79:C:O2'	2.36	0.55
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.71	0.55
32:2a:1008:C:N3	32:2a:1021:G:N2	2.43	0.55
36:2e:74:GLY:HA3	36:2e:116:THR:HG22	1.88	0.55
49:2r:26:LEU:HD21	49:2r:39:VAL:HG13	1.88	0.55
54:2w:25:C:H2'	54:2w:26:A:H5'	1.88	0.55
1:1A:965:G:N2	1:1A:2281:A:OP2	2.39	0.55
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.42	0.55
1:1A:2129:C:H42	1:1A:2204:G:H1	1.54	0.55
28:26:2:ALA:HB1	28:26:6:ARG:O	2.06	0.55
32:2a:267:C:OP1	48:2q:67:LYS:HD3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:10:LEU:H	33:2b:48:MET:HE1	1.71	0.55
33:2b:91:PRO:HG2	33:2b:155:LEU:HD13	1.87	0.55
1:1A:2410:U:H2'	1:1A:2411:G:H8	1.72	0.55
35:1d:166:LYS:NZ	35:1d:179:GLU:OE2	2.39	0.55
36:1e:11:ILE:HG21	36:1e:105:VAL:HG13	1.88	0.55
49:1r:21:LYS:HE3	49:1r:57:GLY:HA2	1.88	0.55
1:2A:994:C:O2'	1:2A:996:A:OP1	2.18	0.55
5:2F:195:ASP:HB2	5:2F:198:ALA:H	1.72	0.55
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.06	0.55
39:2h:19:VAL:HG23	39:2h:21:LYS:HG2	1.89	0.55
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.88	0.55
25:13:8:LEU:HD13	25:13:31:LEU:HD23	1.89	0.55
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.22	0.55
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.42	0.55
14:2S:15:ARG:HB3	14:2S:19:LYS:NZ	2.21	0.55
32:2a:107:G:N7	51:2t:15:ARG:NH2	2.54	0.55
1:1A:1586:G:H2'	1:1A:1587:U:O4'	2.07	0.55
1:1A:2614:A:N6	55:1x:76:A:H2'	2.22	0.55
1:2A:422:A:H2'	1:2A:423:A:C8	2.42	0.55
1:2A:2138:C:N4	1:2A:2153:G:N1	2.33	0.55
1:2A:2285:C:OP2	28:26:6:ARG:HD3	2.07	0.55
6:2G:5:VAL:HG13	6:2G:8:LYS:HB3	1.89	0.55
7:1H:121:ILE:HD11	7:1H:140:LYS:HG2	1.89	0.55
8:1I:61:ARG:NH1	8:1I:64:GLU:OE1	2.40	0.55
32:1a:381:C:H2'	32:1a:382:A:O4'	2.07	0.55
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.88	0.55
2:2B:54:G:N2	6:2G:29:TRP:HZ2	2.02	0.55
15:2T:59:THR:HG23	15:2T:78:LEU:HB3	1.86	0.55
32:2a:345:C:H5'	32:2a:346:G:C5	2.42	0.55
1:1A:662:A:OP1	11:1P:133:SER:OG	2.21	0.55
32:1a:45:U:H2'	32:1a:46:G:C8	2.42	0.55
32:1a:1227:A:OP2	44:1m:111:LYS:NZ	2.40	0.55
1:2A:1425:G:H2'	1:2A:1426:G:O4'	2.07	0.55
1:2A:1918:A:O2'	1:2A:1920:4OC:N4	2.40	0.55
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.89	0.55
6:2G:47:LYS:HG3	6:2G:48:GLU:N	2.21	0.55
32:2a:165:C:H2'	32:2a:166:G:H8	1.72	0.55
32:2a:803:G:OP1	62:2a:3331:HOH:O	2.18	0.55
32:2a:1029:C:N3	32:2a:1032:G:C2	2.75	0.55
1:1A:2325:C:H4'	6:1G:91:ARG:HD3	1.89	0.55
32:1a:624:C:H5'	47:1p:11:SER:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:975:A:H5'	32:1a:975:A:H8	1.72	0.55
32:1a:1278:U:H5'	32:1a:1279:A:O4'	2.07	0.55
39:1h:20:TYR:HE2	39:1h:75:ARG:HD2	1.72	0.55
43:1l:70:ILE:HG12	43:1l:100:ILE:HD12	1.89	0.55
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.07	0.55
1:2A:922:U:O2'	22:20:29:GLN:NE2	2.40	0.55
32:2a:301:G:H2'	32:2a:302:G:C8	2.42	0.55
32:2a:811:C:O2'	32:2a:901:A:N1	2.34	0.55
32:2a:1114:C:H42	32:2a:1186:G:H1	1.55	0.55
32:2a:1235:U:O2'	32:2a:1305:G:O5'	2.24	0.55
32:2a:1319:A:H61	32:2a:1361:G:H21	1.54	0.55
54:2w:43:C:H2'	54:2w:44:G:C8	2.42	0.55
56:2y:8:4SU:H1'	56:2y:48:C:H1'	1.88	0.55
1:1A:791:G:OP1	62:1A:4183:HOH:O	2.18	0.54
1:1A:1378:G:OP1	62:1A:4154:HOH:O	2.18	0.54
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.21	0.54
1:1A:2874:G:OP1	15:1T:119:LYS:HD2	2.06	0.54
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.88	0.54
33:1b:97:TRP:HH2	33:1b:176:GLU:CD	2.14	0.54
35:1d:121:VAL:O	35:1d:134:ASP:HA	2.07	0.54
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.42	0.54
9:2N:137:LYS:NZ	9:2N:139:GLU:OE2	2.40	0.54
32:2a:390:C:H2'	32:2a:391:G:C8	2.42	0.54
32:2a:393:A:OP2	47:2p:12:LYS:NZ	2.23	0.54
32:2a:830:G:N2	32:2a:856:C:O2	2.20	0.54
32:2a:1074:G:O2'	32:2a:1101:A:N1	2.39	0.54
32:2a:1302:U:OP2	44:2m:21:TYR:OH	2.12	0.54
37:2f:36:ARG:NH2	37:2f:66:GLU:OE1	2.39	0.54
56:2y:26:A:N1	56:2y:44:G:O6	2.40	0.54
1:1A:1515:C:H2'	1:1A:1516:A:H8	1.73	0.54
42:1k:18:ARG:HB2	42:1k:33:THR:OG1	2.07	0.54
32:2a:181:G:N2	32:2a:182:U:O4	2.34	0.54
32:2a:184:G:H2'	32:2a:185:A:C8	2.41	0.54
32:2a:582:U:OP1	46:2o:68:ARG:NH2	2.33	0.54
34:2c:155:GLY:HA3	34:2c:196:LEU:HD23	1.90	0.54
42:2k:33:THR:HG22	42:2k:39:PRO:HA	1.88	0.54
1:1A:839:G:N3	1:1A:2094:G:O2'	2.33	0.54
1:1A:2054:G:OP2	1:1A:2466:G:O2'	2.21	0.54
15:1T:30:VAL:HG22	15:1T:86:ILE:HG12	1.88	0.54
17:1V:52:VAL:HG23	17:1V:55:ALA:HB3	1.89	0.54
1:2A:2297:C:O2	1:2A:2333:A:N6	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2308:G:O2'	1:2A:2310:A:N7	2.37	0.54
4:2E:149:ARG:O	62:2E:402:HOH:O	2.18	0.54
7:2H:25:LYS:NZ	7:2H:34:GLU:OE2	2.39	0.54
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	1.90	0.54
32:2a:1158:C:N4	32:2a:1181:G:O6	2.31	0.54
38:2g:15:ASP:OD1	38:2g:20:ASP:N	2.37	0.54
32:1a:164:U:H2'	32:1a:165:C:H6	1.73	0.54
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.08	0.54
38:1g:89:MET:SD	38:1g:155:ARG:HB2	2.47	0.54
1:2A:652(C):G:N2	1:2A:653:A:H1'	2.23	0.54
20:2Y:56:PRO:C	20:2Y:58:GLY:H	2.15	0.54
32:2a:662:G:H2'	32:2a:663:A:C8	2.42	0.54
32:2a:976:G:N2	32:2a:1363:C:OP2	2.39	0.54
54:2w:3:C:N4	54:2w:70:G:N1	2.54	0.54
1:1A:2158:C:N4	1:1A:2177:G:N1	2.55	0.54
32:1a:555:C:H2'	32:1a:556:C:C6	2.43	0.54
32:1a:1203:C:P	45:1n:3:ARG:HH11	2.31	0.54
45:1n:4:LYS:HA	45:1n:7:ILE:HG22	1.89	0.54
1:2A:7:G:H2'	1:2A:8:A:C8	2.42	0.54
1:2A:8:A:H2'	1:2A:9:U:H6	1.71	0.54
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.08	0.54
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.21	0.54
14:2S:11:LYS:HG3	14:2S:91:PRO:HD3	1.90	0.54
32:2a:537:G:H5''	43:2l:113:ARG:NH1	2.22	0.54
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.73	0.54
32:2a:1274:G:N2	32:2a:1275:A:N7	2.56	0.54
32:2a:1518:MA6:H8	32:2a:1518:MA6:O5'	2.07	0.54
54:2w:45:U:H5''	54:2w:46:7MG:OP2	2.06	0.54
1:1A:1221:G:H1'	1:1A:1222:A:H5''	1.89	0.54
1:1A:1694:G:OP1	62:1A:4127:HOH:O	2.18	0.54
32:1a:56:U:H2'	32:1a:57:G:C8	2.42	0.54
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.43	0.54
32:2a:66:G:H8	32:2a:66:G:OP1	1.91	0.54
32:2a:1124:G:H1	32:2a:1149:C:N4	2.05	0.54
36:2e:102:ALA:HB3	36:2e:107:ARG:HB2	1.90	0.54
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.41	0.54
1:1A:2297:C:OP2	28:16:6:ARG:HD3	2.06	0.54
33:1b:119:GLU:O	33:1b:123:ALA:N	2.39	0.54
1:2A:1827:C:H2'	1:2A:1828:G:H5'	1.89	0.54
1:2A:2129:C:N4	1:2A:2159:G:H1	2.06	0.54
12:2Q:109:VAL:HG13	12:2Q:113:GLN:HB2	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:6:G:H4'	32:2a:298:A:H4'	1.89	0.54
33:2b:24:TRP:CD1	33:2b:24:TRP:H	2.26	0.54
1:1A:407:U:H2'	1:1A:408:G:H8	1.73	0.54
1:1A:1827:U:H2'	1:1A:1828:C:H6	1.72	0.54
1:1A:2410:U:H2'	1:1A:2411:G:C8	2.42	0.54
1:1A:2854:G:O6	62:1A:4175:HOH:O	2.16	0.54
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.42	0.54
56:1y:7:A:H2'	56:1y:49:C:OP2	2.07	0.54
1:2A:122:G:OP1	1:2A:149:A:O2'	2.26	0.54
1:2A:878:A:N6	1:2A:899:A:O2'	2.40	0.54
2:2B:94:C:H2'	2:2B:95:C:H6	1.71	0.54
10:2O:7:TYR:CE1	10:2O:20:MET:HB2	2.42	0.54
25:23:6:VAL:HG22	25:23:56:VAL:HG13	1.89	0.54
56:1y:34:G:H2'	56:1y:35:A:C8	2.42	0.54
1:2A:1920:4OC:HM22	1:2A:1921:G:H5'	1.89	0.54
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.73	0.54
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.73	0.54
32:2a:689:C:H2'	32:2a:690:G:O4'	2.08	0.54
32:2a:1239:A:H62	32:2a:1299:A:N6	2.05	0.54
32:2a:1338:G:H21	55:2x:41:C:H1'	1.72	0.54
37:2f:60:PHE:HE2	49:2r:78:LEU:HD21	1.73	0.54
56:2y:4:C:N4	56:2y:69:G:H1	2.06	0.54
56:2y:51:U:H2'	56:2y:52:G:O4'	2.08	0.54
15:1T:54:ARG:HA	15:1T:59:THR:HB	1.89	0.54
19:1X:60:ARG:NH1	29:17:47:ARG:HH22	2.05	0.54
31:19:1:MET:HE2	31:19:33:LYS:HE3	1.89	0.54
32:1a:1391:U:O2'	32:1a:1532:U:OP2	2.22	0.54
32:1a:1457:G:H5''	51:1t:35:THR:HG21	1.89	0.54
56:1y:51:U:H3	56:1y:63:G:H1	1.55	0.54
1:2A:307:G:H21	1:2A:330:A:N6	2.05	0.54
1:2A:816:C:O2'	1:2A:932:G:O6	2.26	0.54
32:2a:606:G:H1'	32:2a:632:A:H61	1.73	0.54
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.08	0.54
32:2a:1239:A:H4'	32:2a:1240:U:H5'	1.89	0.54
1:1A:273:G:N2	8:1I:50:ARG:HH12	2.06	0.53
10:1O:20:MET:HE3	10:1O:44:LYS:HE3	1.89	0.53
12:1Q:16:ARG:HH21	12:1Q:18:LYS:HD3	1.73	0.53
1:2A:637:A:OP1	11:2P:133:SER:OG	2.22	0.53
1:2A:1688:U:H1'	1:2A:1701:A:C6	2.43	0.53
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.90	0.53
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1104:G:H2'	32:2a:1105:A:O4'	2.09	0.53
33:2b:178:ARG:HH22	39:2h:74:PRO:HB3	1.73	0.53
35:2d:98:GLU:HA	35:2d:103:ASN:ND2	2.23	0.53
1:1A:1492:C:H2'	1:1A:1493:C:C6	2.44	0.53
5:1F:74:ARG:HG2	62:1F:410:HOH:O	2.08	0.53
44:1m:82:MET:HE2	44:1m:92:HIS:HB3	1.90	0.53
56:1y:7:A:O2'	56:1y:49:C:H5'	2.08	0.53
28:26:14:THR:O	28:26:17:LYS:NZ	2.42	0.53
32:2a:255:G:OP1	48:2q:69:LYS:NZ	2.39	0.53
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.41	0.53
55:2x:23:C:H2'	55:2x:24:U:H6	1.73	0.53
1:1A:932:C:C4	1:1A:933:C:H1'	2.43	0.53
1:1A:2359:C:H2'	1:1A:2360:U:C6	2.43	0.53
20:1Y:97:ARG:HH11	20:1Y:107:ASP:C	2.17	0.53
23:11:50:ARG:NH1	62:11:201:HOH:O	2.42	0.53
32:1a:456:C:H2'	32:1a:457:C:H6	1.72	0.53
1:2A:1826:G:H4'	3:2D:242:ARG:NH2	2.23	0.53
1:2A:2109:U:H5''	1:2A:2149:G:H21	1.73	0.53
3:2D:108:PRO:HG2	3:2D:111:LEU:HG	1.91	0.53
32:2a:8:A:N6	35:2d:205:GLU:O	2.40	0.53
32:2a:1001:A:H2'	32:2a:1001(A):G:H5''	1.90	0.53
40:2i:19:LEU:HD21	40:2i:81:ILE:HD12	1.89	0.53
43:2l:11:VAL:HG11	48:2q:36:ILE:HG21	1.90	0.53
1:1A:1800:G:O2'	1:1A:1980:C:OP1	2.18	0.53
5:1F:28:ILE:HD13	5:1F:119:ARG:HH21	1.74	0.53
32:1a:880:C:H5''	43:1l:12:ARG:HH12	1.72	0.53
47:1p:52:ASP:O	47:1p:54:GLU:N	2.42	0.53
1:2A:2155:G:H2'	1:2A:2156:G:H5'	1.91	0.53
32:2a:1028:C:N3	32:2a:1033:G:C6	2.77	0.53
37:2f:22:GLU:OE1	37:2f:82:ARG:HG2	2.09	0.53
1:1A:2365:G:N7	62:1A:4285:HOH:O	2.34	0.53
1:1A:2603:C:H2'	1:1A:2604:G:C8	2.43	0.53
1:2A:13:A:O2'	1:2A:15:G:N7	2.34	0.53
1:2A:1587:A:H2'	1:2A:1588:C:C6	2.44	0.53
1:2A:1803:A:HO2'	3:2D:259:THR:HG21	1.72	0.53
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.42	0.53
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.44	0.53
2:2B:92:C:OP1	21:2Z:79:ARG:NH1	2.41	0.53
38:2g:27:ILE:HD12	38:2g:40:ALA:HA	1.90	0.53
38:2g:70:LYS:HB3	38:2g:96:GLN:NE2	2.24	0.53
56:2y:11:C:O2	56:2y:24:G:N1	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1077:G:H5''	31:19:8:LYS:HE3	1.90	0.53
1:1A:1911:A:H2'	1:1A:1912:A:C8	2.44	0.53
1:1A:1959:A:H1'	1:1A:1961:5MU:H72	1.90	0.53
1:1A:2096:U:H2'	1:1A:2097:U:C6	2.43	0.53
1:1A:2450:U:OP1	62:1A:4181:HOH:O	2.18	0.53
21:1Z:74:VAL:HG22	21:1Z:86:VAL:HG12	1.89	0.53
46:1o:82:ILE:O	46:1o:86:GLY:N	2.41	0.53
48:1q:67:LYS:HA	48:1q:70:ARG:HH12	1.74	0.53
51:1t:43:LEU:O	51:1t:47:GLY:N	2.41	0.53
6:2G:179:PRO:HG3	26:24:43:TYR:CZ	2.44	0.53
10:2O:7:TYR:HE1	10:2O:20:MET:HB2	1.73	0.53
32:2a:1202:G:H1'	45:2n:29:ARG:HD2	1.89	0.53
1:2A:568:U:H5'	1:2A:945:A:N1	2.24	0.53
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.23	0.53
1:2A:586:A:H5'	5:2F:89:VAL:HG21	1.90	0.53
1:2A:776:G:N2	1:2A:2241:A:OP1	2.40	0.53
1:2A:945:A:OP2	62:2A:3795:HOH:O	2.19	0.53
1:1A:174:U:H2'	1:1A:175:G:C8	2.44	0.53
1:1A:1296:G:N7	11:1P:18:ARG:NH2	2.57	0.53
1:1A:1785:C:H5	15:1T:96:ARG:NH2	2.05	0.53
7:1H:41:MET:HE2	7:1H:65:HIS:HA	1.90	0.53
22:20:27:GLU:HB2	22:20:69:PHE:HD2	1.74	0.53
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.42	0.53
32:2a:409:G:H1	32:2a:433:C:H42	1.56	0.53
32:2a:1497:G:H1'	32:2a:1518:MA6:H2	1.90	0.53
46:2o:29:VAL:HG13	46:2o:63:ARG:HG3	1.90	0.53
13:1R:2:ARG:HG2	13:1R:5:LYS:HB2	1.90	0.53
1:2A:1533:G:H2'	1:2A:1536:C:H42	1.73	0.53
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.09	0.53
6:2G:77:ILE:HG22	6:2G:80:PHE:H	1.74	0.53
6:2G:131:TYR:CE2	6:2G:133:LEU:HD23	2.43	0.53
32:2a:328:C:H4'	32:2a:329:A:H5'	1.90	0.53
32:2a:581:G:OP1	46:2o:61:GLY:HA3	2.09	0.53
43:2l:124:LYS:HD2	43:2l:125:PRO:HD2	1.91	0.53
1:1A:561:A:H2'	1:1A:562:C:C6	2.44	0.53
32:1a:134:A:N6	47:1p:25:ARG:HH12	2.06	0.53
37:1f:69:GLU:O	37:1f:72:VAL:HG12	2.08	0.53
1:2A:384:U:H2'	1:2A:385:C:H6	1.74	0.53
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.74	0.53
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.91	0.53
35:2d:173:TRP:CD1	35:2d:173:TRP:H	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	1.90	0.53
36:2e:93:PRO:HG2	39:2h:105:ARG:NH2	2.24	0.53
39:2h:51:VAL:HG12	39:2h:52:ASP:H	1.74	0.53
50:2s:63:THR:OG1	50:2s:65:ASN:OD1	2.27	0.53
1:1A:2018:C:H4'	1:1A:2019:G:OP1	2.09	0.52
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.44	0.52
32:1a:258:G:H2'	32:1a:259:G:C8	2.44	0.52
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.43	0.52
1:2A:8:A:H2'	1:2A:9:U:C6	2.44	0.52
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.27	0.52
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.40	0.52
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.36	0.52
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.33	0.52
42:2k:41:THR:HG21	42:2k:71:LYS:HB2	1.89	0.52
1:1A:1342:G:OP1	1:1A:2721:G:O2'	2.19	0.52
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.44	0.52
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.41	0.52
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.90	0.52
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.92	0.52
50:1s:77:THR:HG23	50:1s:78:ARG:HG2	1.92	0.52
1:2A:300:A:H1'	1:2A:319:C:H1'	1.91	0.52
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.44	0.52
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.42	0.52
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	1.90	0.52
1:1A:969:C:C4'	22:10:29:GLN:HE21	2.21	0.52
1:1A:2185:C:OP1	1:1A:2187:G:N1	2.42	0.52
1:1A:2816:G:H2'	1:1A:2817:G:C8	2.43	0.52
9:1N:4:TYR:HB2	16:1U:101:ARG:HH12	1.74	0.52
32:1a:791:G:N2	32:1a:1497:G:O3'	2.42	0.52
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.91	0.52
1:2A:81:G:N2	20:2Y:1:MET:HE3	2.25	0.52
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.14	0.52
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.44	0.52
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.35	0.52
5:2F:13:SER:OG	5:2F:16:GLY:O	2.27	0.52
9:2N:4:TYR:HB2	16:2U:101:ARG:HH12	1.75	0.52
24:22:63:VAL:O	24:22:67:LYS:HG2	2.09	0.52
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	1.90	0.52
47:2p:18:ARG:HD3	47:2p:35:LYS:HD3	1.91	0.52
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.91	0.52
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.89	0.52
32:1a:277:C:H5''	48:1q:68:ARG:NH2	2.23	0.52
32:1a:592:G:H2'	32:1a:593:G:H8	1.73	0.52
1:2A:997:G:OP2	16:2U:58:ARG:NH1	2.42	0.52
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.25	0.52
1:2A:1670:C:O2	4:2E:129:HIS:NE2	2.35	0.52
4:2E:135:HIS:NE2	62:2E:404:HOH:O	2.34	0.52
21:2Z:4:ARG:NH2	21:2Z:60:GLU:OE2	2.42	0.52
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.90	0.52
33:2b:87:ARG:NH1	33:2b:233:SER:HB3	2.24	0.52
35:2d:18:LYS:HE2	35:2d:31:CYS:SG	2.49	0.52
35:2d:33:MET:HA	35:2d:33:MET:HE2	1.92	0.52
1:1A:7:G:H2'	1:1A:8:A:C8	2.44	0.52
1:1A:650:G:O6	11:1P:107:LYS:NZ	2.39	0.52
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.91	0.52
13:1R:38:VAL:HG22	13:1R:112:ALA:HB2	1.91	0.52
32:1a:1355:G:H2'	32:1a:1356:G:H8	1.74	0.52
33:1b:155:LEU:HD21	33:1b:159:PRO:HG3	1.90	0.52
40:1i:64:THR:HG22	40:1i:66:ARG:HH22	1.74	0.52
1:2A:571:A:N6	1:2A:2499:C:O3'	2.43	0.52
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.23	0.52
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.42	0.52
32:2a:447:G:O6	32:2a:485:G:O2'	2.16	0.52
40:2i:17:VAL:HG11	40:2i:81:ILE:HA	1.92	0.52
1:1A:519:G:H4'	18:1W:6:ILE:HB	1.92	0.52
1:1A:721:G:O2'	5:1F:74:ARG:HD3	2.10	0.52
1:1A:1716:A:H5''	1:1A:2562:G:OP1	2.09	0.52
1:1A:2175:G:H2'	1:1A:2176:G:H8	1.75	0.52
1:2A:307:G:H21	1:2A:330:A:H62	1.58	0.52
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.45	0.52
1:2A:2144:U:O2'	1:2A:2147:G:O6	2.21	0.52
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.45	0.52
3:2D:132:PRO:HG2	3:2D:135:PHE:CD2	2.45	0.52
8:2I:9:LEU:HD23	8:2I:12:LEU:HD13	1.92	0.52
26:24:58:ARG:HG3	50:2s:65:ASN:HA	1.92	0.52
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.45	0.52
33:2b:101:MET:HA	33:2b:108:ILE:HG21	1.90	0.52
39:2h:20:TYR:HE2	39:2h:75:ARG:HD2	1.74	0.52
1:1A:303:C:H42	1:1A:385:G:H1	1.58	0.52
1:1A:323:A:N1	1:1A:346:A:O2'	2.43	0.52
1:1A:1144:A:H2'	1:1A:1145:G:H5'	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1218:G:O2'	1:1A:1219:A:O5'	2.27	0.52
3:1D:132:PRO:HD3	3:1D:190:TYR:CZ	2.45	0.52
32:1a:1028:C:C2	32:1a:1029:C:H1'	2.45	0.52
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.10	0.52
32:1a:1280:A:OP1	41:1j:7:LYS:NZ	2.38	0.52
32:1a:1355:G:H2'	32:1a:1356:G:C8	2.45	0.52
1:2A:2206:G:H5''	1:2A:2207:G:C5	2.45	0.52
1:2A:2502:G:H5''	1:2A:2503:2MA:H5''	1.92	0.52
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	1.91	0.52
32:2a:222:U:H2'	32:2a:223:U:C6	2.45	0.52
45:2n:29:ARG:HD3	45:2n:40:CYS:SG	2.50	0.52
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.10	0.52
55:2x:15:G:H2'	55:2x:59:A:N1	2.24	0.52
8:1I:12:LEU:HD21	8:1I:19:VAL:HG21	1.92	0.52
12:1Q:76:LYS:HB3	12:1Q:91:GLU:HG3	1.90	0.52
32:1a:344:A:H5''	32:1a:345:C:C5	2.44	0.52
32:1a:404:U:H2'	32:1a:405:U:C6	2.45	0.52
44:1m:102:ARG:HH21	44:1m:104:ARG:HD3	1.73	0.52
56:1y:49:C:H42	56:1y:64:A:H61	1.58	0.52
1:2A:900:A:O2'	1:2A:901:A:OP1	2.26	0.52
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.10	0.52
1:2A:2130:U:H4'	1:2A:2133:G:H4'	1.91	0.52
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.45	0.52
32:2a:1004:A:N6	32:2a:1037:C:C2	2.78	0.52
37:2f:24:GLU:HB3	37:2f:28:ARG:NH1	2.23	0.52
44:2m:34:LEU:HD13	44:2m:41:PRO:HA	1.91	0.52
54:2w:11:C:H2'	54:2w:12:U:H6	1.73	0.52
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.92	0.52
19:1X:94:GLY:HA3	19:1X:95:LEU:HG	1.92	0.52
32:1a:309:G:O2'	32:1a:607:A:N1	2.43	0.52
32:1a:452:A:H4'	47:1p:72:ARG:NH2	2.25	0.52
33:1b:19:HIS:CD2	33:1b:20:GLU:HG3	2.45	0.52
1:2A:134:C:H42	1:2A:145:G:H1	1.58	0.52
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.45	0.52
32:2a:438:G:N1	32:2a:495:A:OP2	2.26	0.52
32:2a:1007:C:O2	32:2a:1022:G:N1	2.41	0.52
51:2t:50:GLU:HG3	51:2t:100:ILE:HD13	1.91	0.52
54:2w:4:C:H42	54:2w:69:G:H1	1.56	0.52
55:2x:4:G:H2'	55:2x:5:G:C8	2.45	0.52
2:1B:87:G:N2	2:1B:90:A:OP2	2.34	0.52
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2033:A:O2'	1:2A:2035:G:OP2	2.23	0.52
1:2A:2474:C:H5''	1:2A:2475:C:OP2	2.10	0.52
9:2N:63:THR:OG1	9:2N:66:LYS:NZ	2.41	0.52
32:2a:51:A:N1	32:2a:314:C:O2'	2.43	0.52
32:2a:501:C:H2'	32:2a:502:G:C8	2.45	0.52
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.74	0.52
39:2h:42:GLU:HG2	39:2h:109:ILE:HD13	1.92	0.52
41:2j:25:GLU:O	41:2j:29:ARG:HG2	2.09	0.52
54:2w:51:U:H2'	54:2w:52:G:H8	1.75	0.52
56:2y:15:G:O6	56:2y:48:C:O2	2.28	0.52
56:2y:36:A:H2'	56:2y:37:MIA:O4'	2.10	0.52
2:1B:88:C:H2'	2:1B:89:G:O4'	2.09	0.51
32:1a:302:G:O2'	32:1a:556:C:H5''	2.10	0.51
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.42	0.51
32:1a:1159:U:OP1	33:1b:133:LYS:NZ	2.43	0.51
56:1y:11:C:N3	56:1y:24:G:N2	2.52	0.51
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.45	0.51
1:2A:2104:G:H1	1:2A:2185:C:N4	2.08	0.51
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.92	0.51
32:2a:1024:G:H2'	32:2a:1025:U:H5''	1.91	0.51
32:2a:1080:A:H5'	36:2e:16:THR:HG21	1.91	0.51
1:1A:2247:G:H2'	1:1A:2248:C:C6	2.45	0.51
1:1A:2840:G:N7	62:1A:4287:HOH:O	2.34	0.51
32:1a:1227:A:OP1	50:1s:80:TYR:OH	2.19	0.51
33:1b:98:LEU:HG	33:1b:101:MET:HE3	1.93	0.51
46:1o:26:GLU:HG3	46:1o:81:LEU:HD22	1.92	0.51
56:1y:59:U:H3'	56:1y:60:U:H6	1.74	0.51
1:2A:1409:C:H2'	1:2A:1410:G:C8	2.45	0.51
1:2A:2117:A:N6	1:2A:2166:G:O6	2.42	0.51
1:2A:2206:G:H5''	1:2A:2207:G:C6	2.45	0.51
1:2A:2612:C:OP2	27:25:2:ALA:N	2.43	0.51
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.45	0.51
32:2a:299:G:H8	32:2a:299:G:O5'	1.94	0.51
32:2a:1326:C:OP1	52:2u:17:THR:OG1	2.25	0.51
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.46	0.51
12:1Q:5:ARG:HG3	12:1Q:6:ARG:HG2	1.91	0.51
32:1a:253:U:OP1	48:1q:67:LYS:NZ	2.37	0.51
32:1a:1030(C):G:H2'	32:1a:1030(D):A:H8	1.76	0.51
34:1c:17:ASP:CG	34:1c:21:ARG:HH21	2.18	0.51
49:1r:21:LYS:NZ	49:1r:54:ARG:O	2.44	0.51
1:2A:245:G:O6	30:28:8:LYS:NZ	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.92	0.51
36:2e:6:PHE:HB3	36:2e:34:VAL:HG22	1.93	0.51
45:2n:23:ARG:HD2	45:2n:28:GLY:O	2.09	0.51
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.74	0.51
7:1H:40:GLU:CD	7:1H:60:ARG:HH12	2.19	0.51
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.41	0.51
13:1R:24:GLN:NE2	13:1R:36:THR:HG21	2.24	0.51
32:1a:266:G:H2'	32:1a:266:G:N3	2.25	0.51
32:1a:335:C:O2'	32:1a:1433:A:N3	2.40	0.51
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.10	0.51
33:1b:22:LYS:HA	33:1b:40:HIS:HE1	1.75	0.51
49:1r:33:ASP:OD2	49:1r:36:ASN:HB2	2.10	0.51
1:2A:289:A:H2'	1:2A:290:G:O4'	2.11	0.51
1:2A:639:U:H2'	1:2A:640:C:C6	2.45	0.51
1:2A:1251:C:OP1	16:2U:10:ARG:HG3	2.10	0.51
1:2A:1315:C:OP2	62:2A:3778:HOH:O	2.19	0.51
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.46	0.51
11:2P:62:LEU:O	30:28:13:ARG:NH1	2.36	0.51
20:2Y:11:ASP:OD2	20:2Y:97:ARG:NH2	2.43	0.51
1:1A:2153:G:H5''	1:1A:2154:U:H3'	1.91	0.51
5:1F:126:VAL:HG21	5:1F:129:PHE:CZ	2.45	0.51
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.43	0.51
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.91	0.51
32:1a:1030(B):C:H2'	32:1a:1030(C):G:H5'	1.91	0.51
33:1b:80:ILE:HD13	33:1b:211:ILE:HG22	1.93	0.51
1:2A:854:G:H2'	1:2A:855:G:H8	1.75	0.51
1:2A:1466:G:O2'	1:2A:1546:C:O2'	2.14	0.51
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.46	0.51
33:2b:9:GLU:O	33:2b:11:LEU:N	2.43	0.51
42:2k:98:LEU:O	42:2k:101:SER:OG	2.28	0.51
1:1A:936:C:O2'	1:1A:937:A:O4'	2.28	0.51
1:1A:1093:G:O2'	1:1A:1094:A:O5'	2.25	0.51
1:1A:1219:A:H4'	1:1A:1220:U:OP1	2.11	0.51
1:1A:2604:G:OP1	62:1A:4187:HOH:O	2.19	0.51
6:1G:66:GLN:OE1	6:1G:98:ARG:NE	2.39	0.51
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.26	0.51
1:2A:271(F):C:H42	1:2A:271(R):G:H1	1.57	0.51
1:2A:1341:U:OP1	1:2A:1397:U:N3	2.41	0.51
33:2b:70:PHE:HD2	33:2b:85:ALA:HB2	1.75	0.51
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.93	0.51
1:1A:1102:G:H5''	1:1A:1103:A:O4'	2.08	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1218:G:H22	1:1A:1222:A:P	2.33	0.51
1:1A:2564:2MU:H2'	1:1A:2566:U:OP2	2.10	0.51
32:1a:608:A:OP2	62:1a:3319:HOH:O	2.19	0.51
32:1a:748:C:H4'	32:1a:749:C:O5'	2.11	0.51
32:1a:1124:G:N7	32:1a:1145:C:O2'	2.43	0.51
32:1a:1136:U:H5''	32:1a:1137:C:C5	2.45	0.51
32:2a:457:C:H2'	32:2a:458:C:C6	2.46	0.51
33:2b:48:MET:HA	33:2b:51:LEU:HD12	1.93	0.51
56:2y:50:U:H3	56:2y:64:A:H61	1.58	0.51
2:1B:1:U:H2'	2:1B:2:C:H6	1.76	0.51
39:1h:29:SER:HB3	39:1h:32:LYS:HG3	1.92	0.51
1:2A:400:G:N7	62:2A:3861:HOH:O	2.34	0.51
1:2A:784:A:OP1	62:2A:3756:HOH:O	2.18	0.51
1:2A:1155:A:OP1	16:2U:55:ARG:HD2	2.10	0.51
2:2B:28:C:H2'	2:2B:29:A:C8	2.45	0.51
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.44	0.51
6:2G:136:ARG:HG3	6:2G:137:GLU:HG3	1.92	0.51
18:2W:86:LEU:N	18:2W:94:ASP:O	2.40	0.51
32:2a:689:C:OP1	42:2k:27:ASN:ND2	2.44	0.51
33:2b:212:GLN:NE2	33:2b:235:SER:HA	2.26	0.51
41:2j:8:LEU:HD22	41:2j:96:ILE:HG22	1.91	0.51
54:2w:8:4SU:S4	54:2w:13:C:O2'	2.53	0.51
54:2w:9:A:O2'	54:2w:10:G:N7	2.43	0.51
1:1A:999:G:H5''	12:1Q:13:GLN:HB3	1.93	0.51
2:1B:9:G:O6	62:1B:3101:HOH:O	2.17	0.51
3:1D:180:GLY:HA3	3:1D:275:LYS:HB2	1.93	0.51
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.46	0.51
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.31	0.51
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.46	0.51
2:2B:18:G:H2'	2:2B:19:G:C8	2.46	0.51
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.25	0.51
8:2I:123:LEU:HA	8:2I:144:VAL:HG23	1.91	0.51
32:2a:821:G:H2'	32:2a:822:C:C6	2.46	0.51
34:2c:5:ILE:HD13	41:2j:51:ARG:HH12	1.76	0.51
35:2d:8:VAL:HA	35:2d:11:LEU:HD13	1.92	0.51
36:2e:142:LEU:O	36:2e:143:ARG:NH1	2.39	0.51
1:1A:603:C:H1'	62:1A:5102:HOH:O	2.11	0.51
1:1A:831:A:N6	3:1D:229:VAL:HG11	2.26	0.51
1:1A:909:G:O2'	2:1B:78:A:N3	2.44	0.51
1:1A:927:G:N2	1:1A:944:C:N3	2.59	0.51
3:1D:237:GLU:OE2	62:1D:401:HOH:O	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1089:G:H1	32:1a:1096:C:H42	1.59	0.51
1:2A:557:U:O2	9:2N:45:ASN:HB2	2.11	0.51
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.11	0.51
1:2A:2695:C:H2'	1:2A:2696:U:H6	1.76	0.51
23:21:59:THR:O	23:21:91:LYS:NZ	2.40	0.51
26:24:55:ARG:O	26:24:56:VAL:HB	2.10	0.51
32:2a:1244:C:N4	32:2a:1293:G:H1	2.07	0.51
33:2b:124:SER:N	33:2b:125:PRO:HD3	2.26	0.51
56:2y:71:G:H2'	56:2y:72:C:C6	2.46	0.51
1:1A:1614:A:OP2	3:1D:84:TYR:OH	2.28	0.50
5:1F:18:ARG:HG2	5:1F:19:GLU:H	1.76	0.50
42:1k:81:ASP:OD1	42:1k:107:SER:OG	2.26	0.50
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.75	0.50
1:2A:191:A:H2'	1:2A:192:C:C6	2.46	0.50
1:2A:800:A:H8	1:2A:800:A:OP1	1.94	0.50
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.45	0.50
1:2A:2733:A:N1	4:2E:203:LYS:HA	2.26	0.50
6:2G:64:THR:HG22	6:2G:94:LEU:HD11	1.92	0.50
17:2V:80:GLN:HA	17:2V:82:ARG:NH1	2.26	0.50
32:2a:515:G:N7	62:2a:3345:HOH:O	2.32	0.50
32:2a:1500:A:H5''	32:2a:1508:G:H5''	1.93	0.50
35:2d:98:GLU:HA	35:2d:103:ASN:HD22	1.75	0.50
37:2f:61:LEU:HD23	37:2f:63:TYR:OH	2.11	0.50
21:1Z:5:LEU:HD11	21:1Z:44:PHE:HA	1.93	0.50
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.76	0.50
33:1b:209:ARG:HA	33:1b:212:GLN:HB3	1.94	0.50
34:1c:155:GLY:HA3	34:1c:196:LEU:HD23	1.93	0.50
36:1e:113:ALA:HB3	36:1e:115:VAL:HG23	1.94	0.50
1:2A:1308:A:H2'	1:2A:1309:G:O4'	2.11	0.50
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.12	0.50
3:2D:3:VAL:HG21	3:2D:203:ASN:HB2	1.93	0.50
5:2F:11:VAL:HB	5:2F:18:ARG:HB3	1.92	0.50
10:2O:64:ARG:NH1	15:2T:70:VAL:HG21	2.22	0.50
32:2a:1224:G:N2	32:2a:1363:C:N3	2.50	0.50
32:2a:1229:A:O2'	55:2x:30:G:OP1	2.27	0.50
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	1.92	0.50
32:2a:1360:A:H8	32:2a:1360:A:OP1	1.95	0.50
38:2g:78:ARG:HG2	38:2g:79:ARG:H	1.76	0.50
1:1A:572:A:N6	17:1V:19:LYS:H	2.08	0.50
1:1A:923:C:H2'	1:1A:924:U:O4'	2.11	0.50
1:1A:1014:U:H2'	1:1A:1015:C:C6	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1057:G:OP1	16:1U:77:SER:OG	2.29	0.50
1:1A:1223:C:H2'	1:1A:1224:C:C6	2.46	0.50
1:1A:1515:C:H2'	1:1A:1516:A:C8	2.45	0.50
1:1A:2479:C:H4'	12:1Q:123:HIS:CD2	2.46	0.50
4:1E:14:ILE:HG13	4:1E:21:VAL:HG13	1.92	0.50
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.93	0.50
32:1a:551:U:H2'	32:1a:552:U:C6	2.46	0.50
32:1a:560:U:H5'	32:1a:566:G:N2	2.26	0.50
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.39	0.50
32:1a:1221:G:O3'	50:1s:77:THR:OG1	2.26	0.50
56:1y:5:G:H1'	56:1y:69:G:C2	2.47	0.50
1:2A:400:G:O6	62:2A:3796:HOH:O	2.19	0.50
1:2A:576:U:H2'	1:2A:577:G:C8	2.46	0.50
1:2A:1912:A:O2'	32:2a:1494:G:O2'	2.28	0.50
13:2R:33:ARG:HH21	13:2R:113:LEU:HD22	1.77	0.50
15:2T:92:GLY:O	15:2T:120:ARG:NH2	2.44	0.50
32:2a:722:A:C8	32:2a:724:G:H1'	2.45	0.50
32:2a:1007:C:N3	32:2a:1022:G:C6	2.79	0.50
34:2c:73:PRO:HB3	34:2c:103:VAL:HG11	1.92	0.50
38:2g:47:CYS:HA	38:2g:50:ILE:HG22	1.92	0.50
1:1A:387:G:H2'	1:1A:388:A:H8	1.76	0.50
1:1A:721:G:H1'	5:1F:74:ARG:HD3	1.92	0.50
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.47	0.50
1:1A:2885:C:OP1	15:1T:3:ARG:NH1	2.42	0.50
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.93	0.50
6:1G:115:ARG:HB3	6:1G:136:ARG:NH2	2.27	0.50
1:2A:1364:G:P	23:21:3:LYS:HG3	2.51	0.50
4:2E:8:LYS:O	4:2E:193:GLY:N	2.38	0.50
19:2X:36:LYS:HG2	19:2X:54:VAL:HB	1.93	0.50
20:2Y:86:ARG:HD2	20:2Y:100:ALA:HA	1.94	0.50
32:2a:1175:G:H2'	32:2a:1176:A:H8	1.74	0.50
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.92	0.50
42:2k:79:SER:HA	42:2k:104:GLN:HB3	1.92	0.50
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.92	0.50
51:2t:63:ILE:HG21	51:2t:81:LYS:HG3	1.93	0.50
1:1A:236:G:H4'	1:1A:413:G:C5	2.46	0.50
1:1A:305:G:H1'	1:1A:384:G:N2	2.26	0.50
1:1A:1410:G:OP2	23:11:3:LYS:HG3	2.12	0.50
1:1A:2158:C:N3	1:1A:2177:G:N2	2.59	0.50
23:11:77:ALA:HB1	23:11:82:LEU:HD11	1.94	0.50
32:1a:102:G:H2'	32:1a:103:C:C6	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.12	0.50
51:1t:57:ARG:HH22	51:1t:100:ILE:HD12	1.77	0.50
1:2A:833:U:O2	11:2P:55:ARG:NH2	2.44	0.50
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.11	0.50
2:2B:104:U:O2'	21:2Z:72:ARG:HG2	2.12	0.50
6:2G:47:LYS:NZ	6:2G:80:PHE:O	2.35	0.50
32:2a:973:G:H3'	32:2a:974:A:H5''	1.93	0.50
32:2a:1031:G:H2'	32:2a:1032:G:H8	1.74	0.50
35:2d:155:LEU:HB3	35:2d:158:ILE:HG12	1.93	0.50
1:1A:932:C:H3'	1:1A:933:C:C4'	2.42	0.50
1:1A:1159:U:H2'	1:1A:1160:G:C8	2.46	0.50
1:1A:1845:G:H4'	3:1D:51:VAL:HG21	1.93	0.50
3:1D:76:PRO:HB2	3:1D:116:GLN:HE21	1.77	0.50
5:1F:195:ASP:CB	5:1F:198:ALA:H	2.25	0.50
11:1P:101:VAL:HG21	11:1P:108:LYS:HG2	1.93	0.50
32:1a:1366:C:O2'	41:1j:60:ARG:NH1	2.43	0.50
48:1q:59:ILE:HD12	48:1q:71:PHE:HD2	1.76	0.50
1:2A:768:G:O2'	1:2A:1379:A:N1	2.41	0.50
1:2A:1713:U:H2'	1:2A:1714:G:H8	1.76	0.50
1:2A:2129:C:H42	1:2A:2159:G:H1	1.57	0.50
1:2A:2721:A:OP1	62:2A:3794:HOH:O	2.19	0.50
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.46	0.50
10:2O:29:ASN:N	10:2O:29:ASN:OD1	2.44	0.50
19:2X:11:PRO:HD3	24:22:37:PHE:CD1	2.47	0.50
20:2Y:86:ARG:HB2	20:2Y:98:VAL:HG23	1.93	0.50
21:2Z:24:LEU:HD12	21:2Z:25:PRO:HD2	1.92	0.50
32:2a:216:G:H2'	32:2a:217:C:C6	2.46	0.50
32:2a:1263:C:H2'	32:2a:1264:C:C6	2.47	0.50
33:2b:19:HIS:CD2	33:2b:20:GLU:HG3	2.47	0.50
38:2g:115:ARG:O	38:2g:119:ARG:HG3	2.12	0.50
39:2h:51:VAL:HG21	39:2h:60:ARG:HG3	1.94	0.50
1:1A:847:A:H8	1:1A:847:A:OP1	1.95	0.50
1:1A:1115:A:H1'	1:1A:1142:A:H4'	1.92	0.50
1:1A:1140:U:H3	1:1A:1142:A:H3'	1.75	0.50
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.19	0.50
26:14:64:GLY:C	26:14:66:SER:H	2.20	0.50
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.94	0.50
44:1m:92:HIS:CE1	44:1m:98:VAL:HG21	2.46	0.50
1:2A:2116:G:O2'	1:2A:2117:A:N3	2.44	0.50
1:2A:2126:A:H4'	1:2A:2127:G:OP1	2.12	0.50
1:2A:2875:C:O2'	15:2T:2:ASN:OD1	2.20	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:128:G:O2'	48:2q:3:LYS:NZ	2.43	0.50
32:2a:1065:U:OP2	32:2a:1190:G:N2	2.45	0.50
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.94	0.50
1:1A:481:C:N3	1:1A:499:G:H5'	2.27	0.50
1:1A:1360:C:OP1	62:1A:4154:HOH:O	2.19	0.50
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.12	0.50
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.93	0.50
1:2A:652(C):G:H22	1:2A:653:A:H1'	1.76	0.50
1:2A:2167:U:H2'	1:2A:2168:G:N2	2.27	0.50
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.12	0.50
1:2A:2532:G:C6	1:2A:2533:A:C6	3.00	0.50
8:2I:2:LYS:HG2	8:2I:20:ASP:OD1	2.12	0.50
21:2Z:138:GLU:H	21:2Z:156:LYS:NZ	2.08	0.50
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.12	0.50
33:2b:219:VAL:HA	33:2b:222:ILE:HD12	1.94	0.50
2:1B:9:G:OP1	14:1S:15:ARG:HD3	2.12	0.50
8:1I:123:LEU:HA	8:1I:144:VAL:HG23	1.94	0.50
32:1a:616:G:H2'	32:1a:617:G:H8	1.76	0.50
32:1a:741:G:H2'	32:1a:742:G:O4'	2.12	0.50
32:1a:1075:C:OP1	33:1b:179:LYS:NZ	2.28	0.50
32:1a:1133:G:N2	32:1a:1141:C:N3	2.52	0.50
35:1d:70:ILE:HD11	35:1d:74:GLN:HB3	1.93	0.50
1:2A:1166:C:H2'	1:2A:1167:U:C6	2.46	0.50
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	1.94	0.50
32:2a:868:C:H2'	32:2a:869:G:O4'	2.11	0.50
32:2a:1239:A:H62	32:2a:1299:A:H62	1.57	0.50
35:2d:166:LYS:HG2	35:2d:178:VAL:HG11	1.94	0.50
1:1A:1324:A:OP1	13:1R:36:THR:HG23	2.12	0.49
1:1A:2156:A:OP2	1:1A:2179:G:N2	2.45	0.49
1:1A:2541:G:N7	31:19:31:LYS:NZ	2.58	0.49
1:1A:2584:A:N7	4:1E:144:ARG:HD2	2.27	0.49
3:1D:132:PRO:HG2	3:1D:135:PHE:CD2	2.46	0.49
32:1a:256:U:H2'	32:1a:257:G:C8	2.47	0.49
32:1a:1316:G:H5''	45:1n:17:LYS:NZ	2.26	0.49
47:1p:69:THR:HA	47:1p:72:ARG:HG2	1.94	0.49
49:1r:70:ILE:HG23	49:1r:79:LEU:HD13	1.94	0.49
54:1w:1:G:C6	54:1w:72:C:N3	2.80	0.49
1:2A:601:C:O2'	1:2A:605:C:H5''	2.12	0.49
1:2A:2532:G:H2'	1:2A:2533:A:C8	2.47	0.49
26:24:64:GLY:C	26:24:66:SER:H	2.20	0.49
32:2a:821:G:H2'	32:2a:822:C:H6	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2y:62:C:H2'	56:2y:63:G:H8	1.74	0.49
17:1V:60:GLU:HB2	17:1V:97:LYS:HD3	1.94	0.49
30:18:26:LYS:HG2	30:18:46:ARG:O	2.12	0.49
32:1a:160:A:H8	32:1a:160:A:OP1	1.95	0.49
43:1l:34:ARG:NH1	62:1l:8101:HOH:O	2.45	0.49
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.46	0.49
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.94	0.49
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.47	0.49
1:2A:2864:G:OP1	15:2T:119:LYS:HD2	2.12	0.49
19:2X:46:ALA:O	24:22:30:ARG:NH2	2.46	0.49
26:24:14:ILE:HB	26:24:22:ILE:HB	1.94	0.49
32:2a:540:G:H2'	32:2a:541:G:O4'	2.12	0.49
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.10	0.49
32:2a:1113:C:N4	32:2a:1187:G:H1	2.08	0.49
32:2a:1286:A:H2'	32:2a:1287:A:H4'	1.94	0.49
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.27	0.49
38:2g:68:ASN:ND2	38:2g:128:ALA:O	2.45	0.49
38:2g:94:ARG:NH1	38:2g:98:SER:OG	2.45	0.49
41:2j:16:LEU:HD12	41:2j:94:VAL:HG22	1.94	0.49
55:2x:47:U:H3'	55:2x:48:C:C5'	2.42	0.49
1:1A:320:C:O3'	20:1Y:95:LYS:NZ	2.40	0.49
1:1A:2034:G:OP1	18:1W:11:ARG:NH2	2.45	0.49
32:1a:62:U:OP1	32:1a:385:C:O2'	2.29	0.49
32:1a:715:A:H2'	32:1a:716:A:C8	2.47	0.49
32:1a:1239:A:H62	32:1a:1299:A:H62	1.60	0.49
54:1w:2:C:O2	54:1w:71:G:N1	2.45	0.49
1:2A:597:U:H2'	1:2A:598:G:C8	2.47	0.49
1:2A:2344:U:OP1	28:26:37:ARG:HD3	2.12	0.49
1:2A:2478:A:C2	1:2A:2529:G:H2'	2.47	0.49
20:2Y:98:VAL:HG12	20:2Y:105:ALA:HA	1.94	0.49
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.94	0.49
32:2a:21:G:H2'	32:2a:22:G:C8	2.47	0.49
32:2a:116:A:OP1	62:2a:3305:HOH:O	2.19	0.49
32:2a:327:A:H1'	32:2a:329:A:O4'	2.12	0.49
32:2a:994:A:O2'	45:2n:8:GLU:HG2	2.12	0.49
32:2a:1311:G:H1	32:2a:1326:C:N4	2.08	0.49
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.26	0.49
34:2c:58:GLU:H	34:2c:65:ALA:HB3	1.76	0.49
37:2f:41:GLU:HB2	37:2f:62:TRP:HB3	1.93	0.49
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.47	0.49
54:2w:67:C:H2'	54:2w:68:C:C6	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2x:8:4SU:O5'	55:2x:8:4SU:H6	2.12	0.49
1:1A:27:G:N2	1:1A:537:G:H1'	2.27	0.49
1:1A:572:A:H61	17:1V:19:LYS:N	2.11	0.49
1:1A:889:G:H2'	1:1A:890:G:O4'	2.12	0.49
1:1A:2183:C:O2'	1:1A:2184:G:H5''	2.12	0.49
1:1A:2549:U:H2'	1:1A:2550:C:C6	2.48	0.49
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.95	0.49
12:1Q:81:VAL:HB	22:10:7:LEU:HD21	1.95	0.49
30:18:31:HIS:CE1	30:18:32:LEU:HD22	2.48	0.49
32:1a:545:C:O2'	32:1a:549:C:OP1	2.31	0.49
48:1q:45:HIS:O	48:1q:47:PRO:HD3	2.13	0.49
1:2A:108:U:H2'	1:2A:109:G:C8	2.47	0.49
1:2A:579:G:H2'	1:2A:580:C:C6	2.48	0.49
1:2A:1178:C:O2	1:2A:1178:C:H2'	2.12	0.49
1:2A:2156:G:O5'	1:2A:2156:G:H8	1.95	0.49
1:2A:2379:G:O2'	14:2S:17:ARG:NH2	2.45	0.49
17:2V:80:GLN:HA	17:2V:82:ARG:HH12	1.76	0.49
32:2a:279:A:C5	48:2q:98:LEU:HD23	2.48	0.49
32:2a:410:G:N7	35:2d:22:LYS:NZ	2.58	0.49
32:2a:878:G:H5''	39:2h:89:PRO:HB2	1.95	0.49
34:2c:87:LEU:O	34:2c:91:LEU:N	2.44	0.49
40:2i:18:PHE:O	40:2i:61:ALA:HA	2.12	0.49
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.45	0.49
4:1E:175:VAL:O	4:1E:177:PRO:HD3	2.12	0.49
10:1O:104:ARG:CZ	15:1T:34:VAL:HG21	2.42	0.49
32:1a:216:G:H2'	32:1a:217:C:C6	2.47	0.49
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.44	0.49
32:1a:448:A:OP2	32:1a:485:G:N2	2.27	0.49
32:1a:486:U:H2'	32:1a:487:A:C8	2.48	0.49
32:1a:921:U:O2	36:1e:19:MET:HB2	2.12	0.49
32:1a:1202:G:O3'	45:1n:3:ARG:NH1	2.43	0.49
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.77	0.49
37:1f:50:TYR:OH	49:1r:74:ARG:O	2.25	0.49
44:1m:95:GLY:O	44:1m:110:ARG:HG2	2.12	0.49
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.12	0.49
15:2T:31:SER:HB2	15:2T:85:LYS:HG2	1.93	0.49
16:2U:102:GLU:HG3	17:2V:2:PHE:CZ	2.47	0.49
23:21:40:ARG:NH2	23:21:42:GLN:HG2	2.28	0.49
32:2a:564:C:O2'	39:2h:91:ARG:NH1	2.33	0.49
32:2a:1402:4OC:H2'	32:2a:1403:C:O4'	2.12	0.49
40:2i:8:GLY:HA3	40:2i:76:ALA:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.47	0.49
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.10	0.49
16:1U:104:GLN:HE21	16:1U:105:VAL:HG23	1.77	0.49
32:1a:524:G:H2'	32:1a:525:C:C6	2.47	0.49
55:1x:67:C:C2'	55:1x:68:C:H5'	2.42	0.49
1:2A:887:A:H4'	1:2A:888:C:C5	2.48	0.49
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.12	0.49
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.12	0.49
1:2A:2392:A:OP2	30:28:31:HIS:NE2	2.46	0.49
32:2a:339:C:H2'	32:2a:340:U:C6	2.47	0.49
1:1A:1900:G:H2'	1:1A:1901:C:C6	2.48	0.49
18:1W:1:MET:HE2	18:1W:62:HIS:HB3	1.94	0.49
24:12:22:GLU:HG3	24:12:64:LEU:HD11	1.94	0.49
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.48	0.49
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.28	0.49
33:1b:28:PHE:CD2	33:1b:190:THR:HA	2.48	0.49
47:1p:23:ASP:OD1	47:1p:24:ALA:N	2.45	0.49
1:2A:1291:C:H2'	1:2A:1292:U:C6	2.48	0.49
11:2P:19:VAL:HG12	11:2P:27:HIS:HB3	1.94	0.49
17:2V:61:VAL:HA	17:2V:94:LEU:HD23	1.95	0.49
32:2a:984:C:H2'	32:2a:985:C:C6	2.47	0.49
33:2b:17:PHE:HA	33:2b:44:LEU:HD11	1.94	0.49
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.94	0.49
1:1A:174:U:H2'	1:1A:175:G:H8	1.76	0.49
1:1A:831:A:C6	3:1D:229:VAL:HG11	2.48	0.49
1:1A:1847:G:H3'	3:1D:62:TYR:CE1	2.48	0.49
1:1A:2149:G:N2	1:1A:2195:A:O2'	2.46	0.49
15:1T:16:ARG:HH21	15:1T:19:LEU:HD21	1.78	0.49
25:13:16:PRO:HB2	25:13:18:ASP:OD1	2.12	0.49
26:14:40:HIS:O	26:14:44:THR:HG22	2.13	0.49
27:15:8:LYS:O	27:15:9:LYS:HD2	2.13	0.49
32:1a:383:A:C5	32:1a:384:G:H1'	2.48	0.49
32:1a:526:C:P	43:1l:91:LYS:HE3	2.53	0.49
46:1o:6:GLU:OE1	46:1o:6:GLU:N	2.39	0.49
1:2A:527:C:H4'	1:2A:528:A:H5'	1.95	0.49
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.13	0.49
1:2A:1291:C:H2'	1:2A:1292:U:H6	1.77	0.49
1:2A:2080:G:OP1	23:21:35:THR:OG1	2.28	0.49
3:2D:26:LYS:HB3	3:2D:83:GLU:HG2	1.94	0.49
32:2a:998:G:N1	32:2a:1043:C:N4	2.47	0.49
32:2a:1013:G:O2'	32:2a:1015:A:N7	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:2l:117:ARG:NH2	43:2l:124:LYS:HD3	2.26	0.49
54:2w:61:C:H2'	54:2w:62:C:C6	2.48	0.49
1:1A:764:G:H2'	1:1A:765:A:O4'	2.13	0.49
1:1A:1117:G:O2'	1:1A:1135:G:H2'	2.12	0.49
1:1A:1284:G:OP2	62:1A:4190:HOH:O	2.20	0.49
1:1A:2178:G:H2'	1:1A:2179:G:N3	2.28	0.49
21:1Z:101:PRO:HG2	21:1Z:135:GLU:O	2.12	0.49
26:14:26:SER:OG	26:14:27:THR:N	2.46	0.49
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.48	0.49
32:1a:167:G:H2'	32:1a:168:G:C8	2.48	0.49
32:1a:971:G:N1	32:1a:1363(A):A:OP2	2.38	0.49
32:1a:1401:G:C2	32:1a:1402:4OC:H1'	2.48	0.49
1:2A:1800:C:P	3:2D:183:ARG:HH12	2.35	0.49
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.47	0.49
11:1P:47:ASP:CG	11:1P:49:ARG:HH21	2.20	0.49
12:1Q:20:ALA:HB2	21:1Z:79:ARG:HG3	1.93	0.49
15:1T:56:GLY:O	15:1T:59:THR:HG22	2.12	0.49
16:1U:27:LEU:HB3	16:1U:31:SER:HB3	1.95	0.49
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.45	0.49
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.47	0.49
51:1t:49:ALA:O	51:1t:53:LEU:HG	2.13	0.49
54:1w:71:G:H2'	54:1w:71:G:N3	2.28	0.49
1:2A:116:C:H2'	1:2A:117:G:O4'	2.13	0.49
1:2A:247:G:H4'	1:2A:386:G:C5	2.48	0.49
1:2A:797:C:H2'	1:2A:798:G:O4'	2.12	0.49
1:2A:868:U:C4	1:2A:869:G:N7	2.81	0.49
1:2A:1384:A:N3	1:2A:1405:U:H1'	2.28	0.49
1:2A:2127:G:H2'	1:2A:2128:C:C6	2.47	0.49
12:2Q:45:GLN:OE1	12:2Q:45:GLN:N	2.45	0.49
32:2a:952:U:H2'	32:2a:953:G:H8	1.78	0.49
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.48	0.49
41:2j:63:PHE:CE1	45:2n:58:LYS:HG2	2.48	0.49
44:2m:14:ARG:HG3	44:2m:44:ARG:NH1	2.27	0.49
1:1A:1110:C:H2'	1:1A:1111:U:H5'	1.95	0.48
1:1A:1904:C:H2'	1:1A:1905:G:O4'	2.13	0.48
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.52	0.48
7:1H:41:MET:HE1	7:1H:54:ARG:HB3	1.94	0.48
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	1.95	0.48
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.13	0.48
22:10:43:THR:O	22:10:43:THR:HG23	2.12	0.48
32:1a:974:A:H8	32:1a:974:A:OP1	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.95	0.48
54:1w:36:A:N6	54:1w:37:MIA:H121	2.28	0.48
55:1x:67:C:H2'	55:1x:68:C:H5'	1.95	0.48
1:2A:2119:A:O2'	1:2A:2120:G:H5''	2.13	0.48
4:2E:12:THR:HG22	4:2E:13:ARG:H	1.78	0.48
32:2a:7:G:O2'	36:2e:120:THR:O	2.31	0.48
37:2f:2:ARG:CZ	37:2f:69:GLU:HG2	2.43	0.48
1:1A:1359:U:H5''	62:1A:4245:HOH:O	2.13	0.48
32:1a:373:A:O2'	32:1a:451:A:N7	2.46	0.48
32:1a:946:A:H2'	32:1a:947:G:C8	2.47	0.48
32:1a:1507:A:OP2	53:1v:13:A:N6	2.42	0.48
36:1e:51:VAL:HG23	36:1e:52:PRO:HD3	1.95	0.48
1:2A:521:G:H2'	1:2A:522:G:C8	2.48	0.48
1:2A:975(A):G:H1'	1:2A:990:A:C2	2.48	0.48
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.95	0.48
26:24:59:PHE:CD2	50:2s:64:GLU:HB3	2.48	0.48
32:2a:629:G:H2'	32:2a:630:G:O4'	2.12	0.48
33:2b:170:GLU:HG3	33:2b:173:ALA:HB3	1.95	0.48
1:1A:223:C:H2'	1:1A:224:U:C6	2.49	0.48
1:1A:637:U:H5'	1:1A:640:A:N6	2.29	0.48
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.47	0.48
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.49	0.48
32:1a:601:C:H2'	32:1a:602:A:C8	2.48	0.48
32:1a:1004:A:C6	32:1a:1037:C:N3	2.81	0.48
33:1b:212:GLN:O	33:1b:216:SER:OG	2.23	0.48
39:1h:49:GLU:OE2	39:1h:62:TYR:OH	2.25	0.48
54:1w:9:A:O2'	54:1w:10:G:N7	2.46	0.48
56:1y:3:C:N4	56:1y:70:G:H1	2.09	0.48
1:2A:2134:A:O2'	1:2A:2135:A:OP1	2.31	0.48
1:2A:2316:C:H2'	1:2A:2317:C:C6	2.48	0.48
2:2B:72:G:O2'	2:2B:105:A:N6	2.46	0.48
2:2B:89:G:OP2	2:2B:89:G:H8	1.97	0.48
5:2F:125:LEU:HD21	5:2F:199:TRP:CD2	2.48	0.48
7:2H:4:ILE:O	7:2H:69:ARG:HD2	2.14	0.48
32:2a:1071:C:H42	32:2a:1104:G:H1	1.60	0.48
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.13	0.48
51:2t:50:GLU:HB2	51:2t:99:LEU:HD22	1.95	0.48
54:2w:26:A:H2'	54:2w:27:G:H8	1.79	0.48
1:1A:2117:C:H2'	1:1A:2118:U:O4'	2.14	0.48
1:1A:2193:A:O2'	1:1A:2194:U:H5''	2.14	0.48
1:1A:2348:A:H61	22:10:43:THR:CG2	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.47	0.48
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.13	0.48
45:1n:23:ARG:HD2	45:1n:28:GLY:O	2.12	0.48
50:1s:3:ARG:NH2	50:1s:7:LYS:HE2	2.29	0.48
56:1y:49:C:N4	56:1y:64:A:H61	2.12	0.48
1:2A:2292:C:H4'	1:2A:2375:G:H4'	1.96	0.48
10:2O:49:ARG:NH2	32:2a:1422:G:O3'	2.47	0.48
12:2Q:43:THR:HG22	12:2Q:94:VAL:HG12	1.95	0.48
32:2a:17:U:H2'	32:2a:18:C:C6	2.49	0.48
32:2a:824:C:H2'	32:2a:825:G:C8	2.48	0.48
44:2m:3:ARG:N	44:2m:7:VAL:O	2.47	0.48
45:2n:4:LYS:HA	45:2n:7:ILE:HG22	1.96	0.48
48:2q:86:GLU:O	48:2q:90:ILE:HG12	2.13	0.48
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.78	0.48
54:2w:9:A:H8	54:2w:11:C:H41	1.61	0.48
1:1A:1546:G:O2'	3:1D:100:GLY:O	2.26	0.48
15:1T:120:ARG:HA	15:1T:123:GLN:HG2	1.96	0.48
20:1Y:98:VAL:HG12	20:1Y:105:ALA:HA	1.95	0.48
23:11:60:PHE:HE1	23:11:91:LYS:HG3	1.78	0.48
32:1a:175:C:H2'	32:1a:176:C:C6	2.46	0.48
32:1a:539:A:OP2	43:1l:115:LYS:NZ	2.46	0.48
32:1a:631:G:H2'	32:1a:632:A:H8	1.78	0.48
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	1.95	0.48
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.94	0.48
1:2A:81:G:H2'	1:2A:82:G:O4'	2.14	0.48
1:2A:1010:A:N3	1:2A:1153:C:H1'	2.28	0.48
1:2A:1022:G:N2	1:2A:1023:U:O4	2.45	0.48
1:2A:1159:U:H2'	1:2A:1160:G:H8	1.77	0.48
1:2A:1501:C:H2'	1:2A:1502:C:H6	1.78	0.48
1:2A:1993:U:OP2	62:2A:3797:HOH:O	2.19	0.48
1:2A:2073:C:HO2'	1:2A:2598:A:HO2'	1.58	0.48
11:2P:128:HIS:NE2	11:2P:148:LEU:HD11	2.29	0.48
32:2a:1064:G:H4'	32:2a:1065:U:O5'	2.13	0.48
1:1A:656:A:OP1	11:1P:65:ARG:NE	2.46	0.48
1:1A:1314:A:H2'	1:1A:1315:A:O4'	2.13	0.48
1:1A:1921:G:N3	1:1A:1921:G:H2'	2.27	0.48
15:1T:108:ARG:NH1	32:1a:1432:G:OP2	2.47	0.48
17:1V:80:GLN:HA	17:1V:82:ARG:HH12	1.78	0.48
27:15:16:ARG:HG3	27:15:17:ASP:N	2.28	0.48
33:1b:80:ILE:HD11	33:1b:212:GLN:HA	1.95	0.48
36:1e:47:LYS:O	36:1e:57:LYS:NZ	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:29:G:H1	54:1w:41:C:N4	2.11	0.48
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.46	0.48
1:2A:1501:C:H2'	1:2A:1502:C:C6	2.49	0.48
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.48	0.48
6:2G:113:ARG:HD3	6:2G:140:ILE:O	2.14	0.48
11:2P:59:LEU:HD22	11:2P:60:MET:HE2	1.96	0.48
14:2S:25:ARG:CG	14:2S:40:ILE:HB	2.44	0.48
14:2S:28:VAL:HG13	14:2S:35:ILE:HD11	1.96	0.48
16:2U:74:LEU:HD13	16:2U:79:PHE:HB2	1.96	0.48
24:22:21:LEU:HB2	24:22:64:LEU:HD12	1.94	0.48
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.28	0.48
32:2a:1154:G:H2'	32:2a:1155:G:H8	1.77	0.48
32:2a:1403:C:H1'	32:2a:1500:A:N1	2.29	0.48
35:2d:162:LEU:HD22	35:2d:181:MET:HG2	1.96	0.48
37:2f:69:GLU:O	37:2f:72:VAL:HG12	2.13	0.48
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.96	0.48
55:2x:67:C:H2'	55:2x:68:C:H5'	1.96	0.48
1:1A:776:G:C6	3:1D:208:LYS:HB2	2.49	0.48
1:1A:1699:A:N6	13:1R:11:ASN:OD1	2.46	0.48
32:1a:613:C:H2'	32:1a:614:A:C8	2.47	0.48
32:1a:1002:G:N7	32:1a:1003:G:H1'	2.28	0.48
32:1a:1194:U:H2'	32:1a:1195:C:C6	2.49	0.48
32:1a:1390:U:H2'	32:1a:1391:U:C6	2.49	0.48
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.48	0.48
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.94	0.48
1:2A:375:C:H2'	1:2A:376:C:C6	2.49	0.48
1:2A:686:G:N2	1:2A:788:A:H61	2.12	0.48
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.13	0.48
1:2A:2313:C:C1'	6:2G:40:ASN:HD22	2.27	0.48
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.14	0.48
2:2B:119:G:H2'	2:2B:120:A:C8	2.48	0.48
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.94	0.48
32:2a:936:C:H2'	32:2a:937:A:O4'	2.14	0.48
35:2d:173:TRP:CE3	35:2d:189:PRO:HG3	2.49	0.48
40:2i:50:LEU:HD12	40:2i:81:ILE:HG12	1.95	0.48
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.46	0.48
43:2l:53:ARG:HB3	43:2l:69:TYR:HE1	1.79	0.48
1:1A:1108:G:H5''	1:1A:1116:A:O2'	2.13	0.48
13:1R:18:LEU:HD21	13:1R:22:ARG:NH1	2.29	0.48
25:13:5:LYS:HG3	25:13:36:VAL:HG22	1.96	0.48
32:1a:26:A:N6	32:1a:558:G:O2'	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1029:C:H41	32:1a:1030(A):G:N2	2.11	0.48
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.49	0.48
54:1w:2:C:N3	54:1w:71:G:O6	2.47	0.48
56:1y:15:G:H22	56:1y:48:C:N4	2.10	0.48
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.14	0.48
1:2A:2659:G:N2	1:2A:2662:A:OP2	2.47	0.48
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.96	0.48
30:28:14:VAL:HG22	30:28:24:ALA:HB2	1.96	0.48
31:29:1:MET:HE2	31:29:33:LYS:HG2	1.95	0.48
32:2a:416:G:H1	32:2a:427:U:H3	1.62	0.48
32:2a:946:A:O2'	32:2a:1333:A:N3	2.36	0.48
32:2a:1152:A:OP1	41:2j:70:ARG:NH2	2.46	0.48
33:2b:71:VAL:HA	33:2b:93:VAL:HG23	1.96	0.48
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.29	0.48
35:2d:33:MET:HE2	35:2d:37:PRO:HA	1.95	0.48
1:1A:327:U:H2'	1:1A:328:G:C8	2.49	0.48
1:1A:569:G:N2	1:1A:572:A:OP1	2.47	0.48
1:1A:931:C:H2'	1:1A:932:C:H4'	1.95	0.48
1:1A:1055:A:OP2	62:1A:4120:HOH:O	2.19	0.48
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	1.95	0.48
5:1F:116:ASP:OD2	5:1F:117:ARG:NH1	2.47	0.48
7:1H:87:LEU:HD23	7:1H:164:TYR:HA	1.96	0.48
18:1W:18:ARG:NH2	18:1W:76:VAL:O	2.46	0.48
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.95	0.48
24:12:35:LEU:HD12	24:12:53:LEU:HD12	1.96	0.48
32:1a:755:G:OP2	46:1o:65:ARG:HD3	2.13	0.48
32:1a:1065:U:H4'	32:1a:1066:C:O5'	2.14	0.48
32:1a:1142:G:H2'	32:1a:1143:G:O4'	2.13	0.48
42:1k:18:ARG:NH2	42:1k:35:PRO:O	2.47	0.48
1:2A:398:G:OP1	1:2A:2090:G:O2'	2.30	0.48
1:2A:1786:A:H1'	1:2A:1938:A:H61	1.77	0.48
1:2A:2025:C:H2'	1:2A:2026:C:C6	2.48	0.48
1:2A:2075:U:OP2	1:2A:2238:G:O2'	2.28	0.48
24:22:10:LEU:HB3	24:22:14:ARG:NH1	2.28	0.48
32:2a:106:C:N4	62:2a:3367:HOH:O	2.47	0.48
32:2a:296:U:O2'	32:2a:556:C:O2	2.25	0.48
32:2a:1123:A:C2	41:2j:39:PRO:HD2	2.49	0.48
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.47	0.48
38:2g:66:VAL:HG12	38:2g:70:LYS:HE3	1.96	0.48
41:2j:9:ARG:O	41:2j:16:LEU:HD11	2.13	0.48
54:2w:76:F3N:H5''	54:2w:76:F3N:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:794:U:O2	1:1A:2036:A:H1'	2.13	0.48
1:1A:1478:C:H2'	1:1A:1479:U:O4'	2.14	0.48
1:1A:2045:G:H5'	1:1A:2629:C:H4'	1.96	0.48
7:1H:109:PHE:O	62:1H:5001:HOH:O	2.20	0.48
10:1O:80:ASP:OD2	15:1T:64:ARG:NH2	2.46	0.48
32:1a:189(F):U:H3	48:1q:72:ARG:HH12	1.60	0.48
32:1a:310:G:H4'	47:1p:31:LYS:HE3	1.94	0.48
32:1a:404:U:H2'	32:1a:405:U:H6	1.79	0.48
32:1a:1414:U:H3	32:1a:1486:G:H1	1.62	0.48
38:1g:70:LYS:HB3	38:1g:96:GLN:NE2	2.29	0.48
38:1g:79:ARG:HG3	38:1g:80:VAL:H	1.78	0.48
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.26	0.48
1:2A:1363:C:O2'	1:2A:1809:A:N3	2.43	0.48
1:2A:1434:A:N6	1:2A:1558:A:H62	2.11	0.48
1:2A:1919:A:H3'	1:2A:1920:4OC:H6	1.96	0.48
1:2A:2331:G:O2'	1:2A:2336:A:N1	2.41	0.48
1:2A:2335:A:C8	1:2A:2337:G:C5	3.02	0.48
6:2G:122:PRO:HB3	6:2G:170:ARG:NH1	2.29	0.48
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.60	0.48
12:2Q:111:GLU:OE1	12:2Q:133:ARG:NH2	2.46	0.48
25:23:26:LEU:O	25:23:35:ARG:NE	2.47	0.48
34:2c:17:ASP:CG	34:2c:21:ARG:HH21	2.22	0.48
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	1.96	0.48
42:2k:59:TYR:CE1	42:2k:63:LEU:HD21	2.49	0.48
56:2y:11:C:N3	56:2y:24:G:C6	2.82	0.48
1:1A:265:U:H2'	1:1A:266:C:C6	2.50	0.47
1:1A:762:G:C2	46:1o:56:LEU:HD21	2.48	0.47
1:1A:858:U:H2'	11:1P:21:ARG:HA	1.96	0.47
1:1A:2156:A:N3	1:1A:2181:G:O2'	2.38	0.47
2:1B:13:A:N1	2:1B:69:G:O2'	2.46	0.47
3:1D:152:GLY:O	3:1D:154:LYS:HG2	2.14	0.47
4:1E:190:GLY:HA3	62:1E:414:HOH:O	2.14	0.47
32:1a:342:C:H2'	32:1a:343:U:O4'	2.14	0.47
33:1b:35:GLU:OE2	33:1b:38:GLY:HA2	2.13	0.47
38:1g:108:ALA:O	38:1g:111:ARG:HB2	2.14	0.47
40:1i:4:TYR:N	40:1i:19:LEU:O	2.47	0.47
49:1r:52:PRO:HB2	49:1r:54:ARG:HG2	1.96	0.47
54:1w:27:G:N2	54:1w:43:C:N3	2.56	0.47
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	1.96	0.47
1:2A:1186:G:H2'	1:2A:1187:G:O4'	2.14	0.47
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2337:G:H2'	1:2A:2338:G:H8	1.78	0.47
6:2G:115:ARG:H	6:2G:136:ARG:HH22	1.62	0.47
32:2a:109:A:C6	32:2a:326:G:C6	3.02	0.47
32:2a:501:C:H1'	32:2a:549:C:H1'	1.96	0.47
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.14	0.47
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.79	0.47
33:2b:28:PHE:CD2	33:2b:190:THR:HA	2.49	0.47
33:2b:201:ILE:HG21	33:2b:214:ILE:HG21	1.96	0.47
44:2m:10:PRO:HG2	44:2m:13:LYS:HD2	1.96	0.47
44:2m:73:GLU:O	44:2m:77:ASN:ND2	2.44	0.47
1:1A:57:G:O2'	1:1A:72:A:N1	2.43	0.47
1:1A:831:A:O4'	3:1D:227:ASN:ND2	2.48	0.47
1:1A:1654:A:H1'	1:1A:1656:A:OP2	2.14	0.47
1:1A:1807:G:OP2	62:1A:4188:HOH:O	2.20	0.47
1:1A:2145:G:H1	1:1A:2197:C:H42	1.61	0.47
1:1A:2175:G:H2'	1:1A:2176:G:C8	2.49	0.47
1:1A:2346:G:N2	14:1S:16:ASN:OD1	2.40	0.47
1:1A:2658:C:H2'	1:1A:2659:U:O4'	2.14	0.47
3:1D:132:PRO:HG2	3:1D:135:PHE:HD2	1.78	0.47
22:10:10:THR:HG22	22:10:12:ASN:N	2.16	0.47
32:1a:353:A:H5'	32:1a:353:A:H8	1.79	0.47
32:1a:631:G:H2'	32:1a:632:A:C8	2.49	0.47
33:1b:51:LEU:HD23	33:1b:201:ILE:HD12	1.95	0.47
48:1q:26:GLN:HE21	48:1q:37:LYS:HD3	1.79	0.47
1:2A:500:G:N2	1:2A:502:A:H3'	2.29	0.47
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.49	0.47
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.30	0.47
1:2A:2784:C:H2'	1:2A:2785:C:C6	2.48	0.47
1:2A:2886:G:H2'	1:2A:2887:U:C6	2.49	0.47
3:2D:274:ARG:N	62:2D:403:HOH:O	2.46	0.47
32:2a:1049:U:C5	32:2a:1201:A:H5'	2.49	0.47
39:2h:36:LEU:HD23	39:2h:39:LEU:HD22	1.95	0.47
45:2n:21:TYR:HE1	45:2n:23:ARG:HE	1.62	0.47
46:2o:39:LEU:HD22	46:2o:56:LEU:HB2	1.96	0.47
47:2p:21:VAL:HG13	47:2p:33:ILE:HB	1.96	0.47
56:2y:63:G:H2'	56:2y:64:A:O4'	2.14	0.47
1:1A:740:C:HO2'	1:1A:1399:A:HO2'	1.62	0.47
26:14:54:GLY:O	26:14:56:VAL:HA	2.14	0.47
33:1b:142:LEU:HA	33:1b:145:LEU:HB2	1.95	0.47
35:1d:109:GLY:HA3	35:1d:165:MET:HG3	1.96	0.47
56:1y:5:G:H1'	56:1y:69:G:N2	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:380:U:H4'	23:21:16:ASN:O	2.14	0.47
1:2A:518:G:H4'	18:2W:18:ARG:NE	2.30	0.47
1:2A:657:U:H2'	1:2A:658:C:C6	2.49	0.47
1:2A:813:U:H2'	1:2A:814:C:C6	2.49	0.47
1:2A:880:G:N2	1:2A:898:C:O2	2.47	0.47
1:2A:990:A:H1'	1:2A:1156:A:N3	2.29	0.47
1:2A:1836:C:H2'	1:2A:1837:C:H6	1.79	0.47
1:2A:2206:G:H3'	1:2A:2207:G:N7	2.28	0.47
12:2Q:35:VAL:HG13	12:2Q:130:LYS:HB3	1.96	0.47
15:2T:29:ARG:HB3	15:2T:87:ASP:HB2	1.95	0.47
30:28:26:LYS:HD2	30:28:48:PHE:CD2	2.50	0.47
32:2a:130:A:O2'	32:2a:131:C:O5'	2.26	0.47
32:2a:1320:C:O4'	50:2s:73:GLU:HG2	2.15	0.47
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	1.95	0.47
48:2q:62:SER:HB3	48:2q:72:ARG:NH1	2.29	0.47
55:2x:16:C:H4'	55:2x:60:U:H1'	1.94	0.47
1:1A:280:C:H2'	1:1A:281:G:C8	2.50	0.47
1:1A:2204:G:H2'	1:1A:2205:C:C6	2.50	0.47
32:1a:382:A:H2'	32:1a:383:A:C8	2.49	0.47
32:1a:523:A:H61	43:1l:92:0TD:CG	2.27	0.47
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.32	0.47
33:1b:107:THR:O	33:1b:110:GLN:HB3	2.13	0.47
40:1i:18:PHE:CD2	40:1i:62:TYR:HD2	2.33	0.47
42:1k:41:THR:OG1	42:1k:71:LYS:HD3	2.13	0.47
1:2A:2125:G:H21	1:2A:2173:A:H62	1.61	0.47
10:2O:7:TYR:CE1	10:2O:44:LYS:HG3	2.49	0.47
17:2V:14:VAL:HB	17:2V:96:ILE:HG13	1.96	0.47
32:2a:1154:G:H2'	32:2a:1155:G:C8	2.49	0.47
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.49	0.47
56:2y:8:4SU:C2	56:2y:14:A:H62	2.27	0.47
56:2y:19:G:N1	56:2y:56:C:N4	2.52	0.47
1:1A:2190:G:H8	1:1A:2192:A:N7	2.12	0.47
1:1A:2486:C:H5''	1:1A:2487:C:OP2	2.15	0.47
32:1a:1054:C:C4	54:1w:34:G:H1'	2.47	0.47
39:1h:96:GLY:O	39:1h:100:ILE:HG13	2.14	0.47
41:1j:12:ASP:O	41:1j:15:THR:OG1	2.29	0.47
51:1t:36:LEU:HA	51:1t:39:LYS:HB3	1.97	0.47
1:2A:142:A:N1	1:2A:1595:G:O2'	2.43	0.47
1:2A:795:C:H2'	1:2A:796:C:C6	2.49	0.47
1:2A:1529:G:N2	1:2A:1540:U:O2	2.42	0.47
1:2A:1971:A:C4	3:2D:241:PRO:HD3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2127:G:O6	1:2A:2161:C:C4	2.68	0.47
5:2F:183:VAL:O	5:2F:187:VAL:HG23	2.14	0.47
32:2a:399:G:H2'	32:2a:400:C:C6	2.50	0.47
32:2a:1158:C:N3	32:2a:1181:G:N1	2.36	0.47
33:2b:102:LEU:HD23	33:2b:182:ILE:HD12	1.97	0.47
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.29	0.47
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.24	0.47
37:2f:45:LEU:HD12	37:2f:59:TYR:HD1	1.79	0.47
41:2j:50:ILE:HA	41:2j:60:ARG:HG2	1.96	0.47
1:1A:223:C:H2'	1:1A:224:U:H6	1.78	0.47
1:1A:1027:A:OP1	62:1A:4192:HOH:O	2.20	0.47
1:1A:1700:G:H3'	13:1R:2:ARG:HD3	1.97	0.47
1:1A:1834:A:H4'	3:1D:259:THR:HG23	1.96	0.47
8:1I:130:TYR:CE2	8:1I:132:PRO:HB3	2.49	0.47
32:1a:376:G:OP2	47:1p:67:THR:HG21	2.14	0.47
1:2A:635:C:H2'	1:2A:636:G:O4'	2.14	0.47
2:2B:33:G:C6	2:2B:34:U:C4	3.03	0.47
8:2I:5:LEU:HD23	8:2I:9:LEU:HD13	1.96	0.47
15:2T:26:ASP:O	15:2T:49:VAL:HG22	2.14	0.47
32:2a:789:U:O2'	32:2a:791:G:N7	2.35	0.47
32:2a:1509:C:H2'	32:2a:1510:U:O4'	2.14	0.47
37:2f:15:ASP:OD1	37:2f:18:GLN:N	2.31	0.47
40:2i:22:GLY:HA3	40:2i:60:ASP:OD2	2.14	0.47
1:1A:407:U:H2'	1:1A:408:G:C8	2.50	0.47
1:1A:1375:U:H3'	1:1A:1376:C:H6	1.80	0.47
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.14	0.47
1:1A:1733:C:H2'	1:1A:1734:G:O4'	2.15	0.47
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.50	0.47
1:1A:2145:G:H2'	1:1A:2146:G:H8	1.78	0.47
1:1A:2550:C:H2'	1:1A:2551:C:H6	1.78	0.47
1:1A:2617:PSU:OP2	62:1A:4189:HOH:O	2.20	0.47
1:1A:2672:A:N7	7:1H:175:LYS:NZ	2.62	0.47
6:1G:40:ASN:HB3	6:1G:156:ASP:HB2	1.97	0.47
8:1I:103:ARG:HG3	8:1I:104:GLN:H	1.79	0.47
10:1O:49:ARG:NH2	32:1a:1423:G:H5'	2.30	0.47
19:1X:95:LEU:HD23	19:1X:95:LEU:HA	1.69	0.47
30:18:31:HIS:ND1	30:18:32:LEU:HD13	2.30	0.47
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.97	0.47
32:1a:715:A:OP1	32:1a:805:C:O2'	2.29	0.47
32:1a:1298:C:C4	38:1g:114:ARG:HD2	2.49	0.47
35:1d:57:ARG:NH2	36:1e:107:ARG:HH11	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:40:LEU:HB2	41:1j:69:ASN:HB3	1.96	0.47
51:1t:63:ILE:HG22	51:1t:77:ALA:HB1	1.96	0.47
55:1x:4:G:H2'	55:1x:5:G:H8	1.79	0.47
56:1y:54:5MU:H2'	56:1y:55:PSU:C4	2.50	0.47
1:2A:236:C:H2'	1:2A:237:C:C6	2.50	0.47
1:2A:959:A:N3	1:2A:2457:U:O2'	2.43	0.47
1:2A:1265:A:OP2	62:2A:3758:HOH:O	2.20	0.47
1:2A:1999:C:H5''	1:2A:2723:C:O2'	2.15	0.47
1:2A:2366:A:H2'	1:2A:2367:G:O4'	2.15	0.47
1:2A:2893:G:H5''	1:2A:2894:G:O4'	2.15	0.47
14:2S:94:TYR:CZ	14:2S:99:LYS:HG3	2.49	0.47
16:2U:88:ILE:HG22	16:2U:90:VAL:HG23	1.97	0.47
25:23:15:TYR:O	25:23:20:LYS:HE3	2.14	0.47
32:2a:625:G:H2'	32:2a:626:U:C6	2.49	0.47
32:2a:631:G:H2'	32:2a:632:A:C8	2.50	0.47
32:2a:1029:C:C4	32:2a:1032:G:C6	2.99	0.47
32:2a:1055:A:H62	32:2a:1200:C:H42	1.63	0.47
32:2a:1194:U:H2'	32:2a:1195:C:C6	2.50	0.47
32:2a:1314:C:H2'	32:2a:1315:U:C6	2.49	0.47
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.49	0.47
35:2d:31:CYS:SG	35:2d:33:MET:HB2	2.54	0.47
36:2e:148:VAL:O	36:2e:152:ARG:HG2	2.14	0.47
38:2g:50:ILE:HD11	38:2g:61:VAL:HG11	1.97	0.47
40:2i:96:LEU:H	40:2i:98:PRO:HD2	1.80	0.47
42:2k:20:TYR:CE1	42:2k:83:ILE:HD12	2.50	0.47
54:2w:68:C:H2'	54:2w:69:G:H8	1.80	0.47
56:2y:69:G:H2'	56:2y:70:G:O4'	2.14	0.47
1:1A:217:A:H8	1:1A:218:A:H5'	1.79	0.47
1:1A:384:G:H2'	1:1A:385:G:C8	2.49	0.47
1:1A:1403:U:H2'	1:1A:1404:G:O4'	2.15	0.47
1:1A:1696:G:O2'	13:1R:107:ASP:OD2	2.31	0.47
1:1A:2143:G:N2	1:1A:2199:C:N3	2.52	0.47
20:1Y:86:ARG:HG3	20:1Y:100:ALA:HB2	1.95	0.47
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.97	0.47
32:1a:486:U:H2'	32:1a:487:A:H8	1.79	0.47
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.15	0.47
33:1b:97:TRP:HZ2	33:1b:102:LEU:HD13	1.80	0.47
42:1k:20:TYR:CE1	42:1k:83:ILE:HD12	2.50	0.47
44:1m:15:VAL:HG23	44:1m:43:THR:O	2.14	0.47
1:2A:484:C:H2'	1:2A:485:C:C6	2.50	0.47
1:2A:2376:A:H2'	1:2A:2377:A:O4'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:132:PRO:HA	3:2D:190:TYR:HA	1.97	0.47
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.95	0.47
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.15	0.47
32:2a:748:C:H4'	32:2a:749:C:O5'	2.15	0.47
1:1A:282:G:H2'	1:1A:283:G:O4'	2.15	0.47
1:1A:895:G:H2'	1:1A:896:A:C8	2.50	0.47
1:1A:944:C:N4	1:1A:945:A:H62	2.13	0.47
1:1A:1375:U:H5''	1:1A:1376:C:H5	1.80	0.47
1:1A:1631:C:O2'	1:1A:1632:A:O5'	2.23	0.47
1:1A:2508:C:OP2	12:1Q:82:ARG:HD3	2.15	0.47
1:1A:2880:C:H2'	1:1A:2881:C:O4'	2.15	0.47
11:1P:112:LEU:HD13	11:1P:114:ILE:HD11	1.97	0.47
32:1a:108:G:H1	51:1t:15:ARG:HG2	1.80	0.47
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.50	0.47
39:1h:7:ALA:HB2	39:1h:85:ARG:HG3	1.96	0.47
48:1q:61:GLU:HA	48:1q:71:PHE:CD1	2.49	0.47
54:1w:3:C:H42	54:1w:70:G:H1	1.63	0.47
1:2A:27:G:N2	1:2A:512:G:H1'	2.30	0.47
1:2A:484:C:H2'	1:2A:485:C:H6	1.79	0.47
1:2A:495:G:N3	18:2W:61:ASN:ND2	2.63	0.47
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.97	0.47
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.97	0.47
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.50	0.47
4:2E:48:GLN:NE2	4:2E:78:LEU:HD23	2.29	0.47
6:2G:114:ILE:HB	6:2G:117:PHE:HB2	1.97	0.47
21:2Z:5:LEU:HD12	21:2Z:47:VAL:HG21	1.97	0.47
32:2a:992:U:H5''	32:2a:993:G:C4	2.50	0.47
32:2a:1165:C:H2'	32:2a:1166:G:O4'	2.13	0.47
20:1Y:28:LYS:NZ	20:1Y:64:GLU:OE1	2.33	0.47
32:1a:17:U:H2'	32:1a:18:C:C6	2.50	0.47
32:1a:881:G:OP2	43:1l:12:ARG:NH2	2.48	0.47
37:1f:97:PHE:CD2	49:1r:31:LEU:HD12	2.50	0.47
38:1g:70:LYS:HB3	38:1g:96:GLN:HE21	1.79	0.47
50:1s:41:VAL:HG12	50:1s:44:MET:HG3	1.97	0.47
6:2G:7:LEU:HD23	6:2G:100:TRP:HE3	1.80	0.47
32:2a:84:U:H4'	32:2a:89:C:C4	2.50	0.47
32:2a:452:A:H4'	47:2p:72:ARG:NH2	2.30	0.47
32:2a:837:G:H1	32:2a:849:C:H42	1.64	0.47
35:2d:150:GLU:OE1	35:2d:150:GLU:N	2.44	0.47
36:2e:5:ASP:N	36:2e:5:ASP:OD1	2.48	0.47
47:2p:75:ARG:O	47:2p:78:GLY:N	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2y:37:MIA:H2'	56:2y:38:A:O4'	2.15	0.47
3:1D:159:ALA:HB1	3:1D:198:ASN:O	2.16	0.46
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.50	0.46
11:1P:49:ARG:HG2	30:18:60:LEU:HD12	1.98	0.46
20:1Y:7:VAL:HG21	20:1Y:72:VAL:HG12	1.96	0.46
32:1a:21:G:H2'	32:1a:22:G:C8	2.49	0.46
32:1a:660:G:H2'	32:1a:661:G:O4'	2.15	0.46
32:1a:835:U:OP1	49:1r:64:ARG:NH2	2.41	0.46
43:1l:26:ALA:HA	43:1l:64:TYR:HD2	1.80	0.46
1:2A:102:G:OP1	24:22:7:ARG:NH2	2.48	0.46
1:2A:514:A:N3	1:2A:581:C:O2'	2.37	0.46
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.51	0.46
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.79	0.46
1:2A:2316:C:H2'	1:2A:2317:C:H6	1.80	0.46
5:2F:130:ALA:H	5:2F:142:TRP:CD1	2.33	0.46
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.97	0.46
32:2a:413:G:H1'	32:2a:428:G:H21	1.79	0.46
32:2a:723:U:O2'	32:2a:724:G:H5'	2.15	0.46
32:2a:1129:C:H1'	32:2a:1130:A:N7	2.30	0.46
32:2a:1190:G:OP1	34:2c:5:ILE:N	2.49	0.46
32:2a:1279:A:P	41:2j:9:ARG:HH21	2.39	0.46
36:2e:79:GLU:OE1	39:2h:104:ARG:HA	2.14	0.46
1:1A:600:G:O2'	1:1A:1300:A:OP1	2.31	0.46
1:1A:2146:G:H2'	1:1A:2147:G:O4'	2.16	0.46
1:1A:2177:G:H5'	1:1A:2178:G:OP2	2.15	0.46
1:1A:2490:A:OP2	31:19:2:LYS:NZ	2.28	0.46
4:1E:3:GLY:HA2	4:1E:198:VAL:O	2.15	0.46
4:1E:121:ASN:ND2	62:1E:404:HOH:O	2.42	0.46
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.96	0.46
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.50	0.46
11:1P:27:HIS:HB2	62:1P:3111:HOH:O	2.14	0.46
12:1Q:35:VAL:HA	12:1Q:101:ARG:O	2.15	0.46
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.48	0.46
1:2A:142(A):C:H2'	1:2A:143:G:C8	2.50	0.46
1:2A:277:C:H4'	1:2A:278:A:C8	2.46	0.46
1:2A:1328:G:H2'	1:2A:1330:C:C4	2.50	0.46
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.15	0.46
29:27:24:THR:O	29:27:28:ARG:HG3	2.16	0.46
32:2a:446:G:H2'	32:2a:447:G:O4'	2.14	0.46
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.50	0.46
55:2x:17:C:H5'	55:2x:61:C:OP1	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:24:G:H2'	1:1A:25:U:O4'	2.16	0.46
1:1A:83:A:H5''	20:1Y:8:LYS:HE3	1.96	0.46
1:1A:1587:U:H2'	1:1A:1588:G:O4'	2.16	0.46
5:1F:89:VAL:O	62:1F:401:HOH:O	2.21	0.46
5:1F:195:ASP:HB3	5:1F:198:ALA:H	1.80	0.46
7:1H:4:ILE:O	7:1H:69:ARG:HD2	2.15	0.46
10:1O:104:ARG:NH1	10:1O:122:LEU:OXT	2.48	0.46
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.33	0.46
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.62	0.46
32:1a:166:G:H2'	32:1a:167:G:C8	2.51	0.46
37:1f:75:LEU:O	37:1f:79:LEU:HG	2.15	0.46
38:1g:92:SER:O	38:1g:96:GLN:HG2	2.16	0.46
43:1l:113:ARG:HB2	43:1l:122:THR:HG21	1.98	0.46
1:2A:581:C:OP1	16:2U:33:ARG:HG2	2.16	0.46
1:2A:724:U:H2'	1:2A:725:G:O4'	2.15	0.46
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.16	0.46
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.15	0.46
10:2O:102:VAL:HB	10:2O:106:LEU:HD12	1.97	0.46
12:2Q:32:TYR:HE1	12:2Q:133:ARG:HE	1.63	0.46
14:2S:15:ARG:O	14:2S:19:LYS:HG3	2.15	0.46
16:2U:102:GLU:OE1	16:2U:104:GLN:NE2	2.37	0.46
32:2a:443:C:H2'	32:2a:444:C:C6	2.50	0.46
32:2a:955:U:O2'	50:2s:83:HIS:HD2	1.98	0.46
1:1A:602:G:O2'	1:1A:2041:A:OP1	2.30	0.46
1:1A:957:A:H2'	12:1Q:9:TYR:OH	2.16	0.46
1:1A:2203:G:O2'	1:1A:2204:G:OP1	2.32	0.46
15:1T:111:ARG:NH2	32:1a:1464:G:OP2	2.49	0.46
32:1a:690:G:C6	32:1a:691:G:C6	3.04	0.46
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.97	0.46
32:1a:1367:C:H5'	41:1j:60:ARG:NH1	2.31	0.46
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.44	0.46
39:1h:120:THR:H	39:1h:123:GLU:HB2	1.79	0.46
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.41	0.46
54:1w:1:G:N1	54:1w:72:C:C2	2.76	0.46
1:2A:137:C:H42	1:2A:143:G:H1	1.64	0.46
1:2A:1491:G:O4'	3:2D:99:ASP:HB3	2.15	0.46
16:2U:34:LYS:HA	16:2U:34:LYS:HD3	1.70	0.46
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.49	0.46
56:2y:55:PSU:HN1	56:2y:57:G:C5'	2.22	0.46
1:1A:8:A:H2'	1:1A:9:U:C6	2.51	0.46
1:1A:449:A:H2'	1:1A:450:A:C8	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:469:A:N7	5:1F:45:ARG:HG2	2.31	0.46
1:1A:645:G:H5'	1:1A:645:G:N3	2.30	0.46
1:1A:662:A:H2'	11:1P:117:GLU:OE1	2.15	0.46
12:1Q:43:THR:HG22	12:1Q:94:VAL:HG12	1.98	0.46
14:1S:41:ASP:O	14:1S:45:GLY:N	2.49	0.46
16:1U:108:GLU:O	16:1U:112:ARG:HG2	2.15	0.46
26:14:20:ASN:OD1	26:14:21:VAL:N	2.48	0.46
32:1a:765:G:N1	32:1a:812:C:O2'	2.44	0.46
32:1a:1289:A:P	52:1u:10:ARG:HH22	2.38	0.46
33:1b:204:ASN:OD1	33:1b:206:ASP:N	2.46	0.46
35:1d:107:ARG:HD2	35:1d:173:TRP:CH2	2.51	0.46
38:1g:41:ARG:O	38:1g:45:ASP:HB2	2.16	0.46
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.16	0.46
13:2R:88:ARG:NH2	13:2R:89:ASP:OD1	2.49	0.46
15:2T:22:PHE:HA	15:2T:91:ARG:HH12	1.81	0.46
25:23:7:LYS:HB2	25:23:34:GLU:HG2	1.96	0.46
32:2a:127:G:N2	48:2q:61:GLU:OE2	2.44	0.46
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.16	0.46
33:2b:124:SER:H	33:2b:125:PRO:HD3	1.81	0.46
36:2e:31:LEU:HD22	36:2e:43:LEU:HD11	1.97	0.46
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.15	0.46
54:2w:33:U:O2'	54:2w:35:A:N7	2.47	0.46
1:1A:1857:G:O2'	3:1D:242:ARG:NH2	2.49	0.46
1:1A:2830:A:OP2	13:1R:2:ARG:NH2	2.48	0.46
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.63	0.46
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.97	0.46
32:1a:356:A:N3	32:1a:368:U:O2'	2.44	0.46
32:1a:411:A:OP2	35:1d:30:LYS:HD3	2.15	0.46
43:1l:8:ASN:O	43:1l:12:ARG:HB2	2.15	0.46
45:1n:14:PRO:HG2	45:1n:16:PHE:O	2.16	0.46
1:2A:171:G:H2'	1:2A:172:C:C6	2.50	0.46
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.30	0.46
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.15	0.46
1:2A:1848:A:C4	1:2A:1849:G:C8	3.04	0.46
1:2A:2398:U:H2'	1:2A:2399:G:H8	1.79	0.46
1:2A:2422:A:O4'	56:2y:76:A:N6	2.48	0.46
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.46	0.46
14:2S:85:VAL:HG11	14:2S:110:LEU:HD23	1.96	0.46
32:2a:35:G:H2'	32:2a:36:C:C6	2.51	0.46
32:2a:405:U:H5''	32:2a:495:A:H2	1.79	0.46
32:2a:524:G:H8	32:2a:524:G:OP1	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1401:G:OP1	53:2v:18:G:O2'	2.26	0.46
32:2a:1438:G:H2'	32:2a:1439:C:C6	2.50	0.46
33:2b:55:PHE:O	33:2b:59:GLU:N	2.33	0.46
34:2c:150:LYS:HE3	34:2c:152:ILE:HD11	1.98	0.46
1:1A:737:G:H2'	1:1A:738:C:C6	2.51	0.46
1:1A:1857:G:H4'	3:1D:242:ARG:CZ	2.45	0.46
1:1A:2346:G:H21	14:1S:16:ASN:CG	2.23	0.46
11:1P:2:LYS:HG2	11:1P:3:LEU:H	1.81	0.46
32:1a:1342:C:H2'	32:1a:1343:G:C8	2.51	0.46
34:1c:6:HIS:CD2	34:1c:9:GLY:H	2.24	0.46
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.98	0.46
1:2A:1662:C:O2'	1:2A:2687:U:OP1	2.31	0.46
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.16	0.46
62:2A:3981:HOH:O	5:2F:68:LYS:HE2	2.14	0.46
32:2a:25:C:H2'	32:2a:26:A:C8	2.51	0.46
32:2a:80:G:N1	32:2a:90:U:O2	2.49	0.46
32:2a:438:G:H4'	35:2d:123:HIS:ND1	2.31	0.46
55:2x:67:C:C2'	55:2x:68:C:H5'	2.44	0.46
1:1A:27:G:C2	1:1A:537:G:N3	2.83	0.46
1:1A:1189:A:OP1	9:1N:25:ARG:NH2	2.49	0.46
1:1A:1974:A:C6	1:1A:1975:A:N1	2.84	0.46
1:1A:2142:G:C2'	1:1A:2143:G:H5'	2.45	0.46
1:1A:2353:G:N7	62:1A:4300:HOH:O	2.36	0.46
1:1A:2585:C:N4	54:1w:75:C:O2'	2.49	0.46
4:1E:2:LYS:HB2	4:1E:95:ILE:HD12	1.98	0.46
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.51	0.46
15:1T:127:ALA:C	15:1T:129:ARG:H	2.23	0.46
23:11:3:LYS:HB2	23:11:61:ARG:HH22	1.79	0.46
23:11:78:LYS:HA	23:11:78:LYS:HD3	1.79	0.46
32:1a:110:C:H2'	32:1a:111:G:O4'	2.15	0.46
34:1c:150:LYS:HE3	34:1c:152:ILE:HD11	1.98	0.46
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.97	0.46
36:1e:93:PRO:HG2	39:1h:105:ARG:NH2	2.31	0.46
44:1m:11:ARG:C	44:1m:13:LYS:H	2.24	0.46
1:2A:271(U):G:H2'	1:2A:271(V):G:H8	1.80	0.46
1:2A:557:U:H2'	1:2A:558:G:H8	1.80	0.46
1:2A:760:G:H2'	1:2A:761:A:O4'	2.15	0.46
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.16	0.46
1:2A:1309:G:O2'	1:2A:1611:C:O2'	2.20	0.46
10:2O:49:ARG:NH2	32:2a:1423:G:H5'	2.27	0.46
19:2X:35:THR:HG23	19:2X:38:GLU:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:40:HIS:HB3	26:24:43:TYR:HD2	1.81	0.46
32:2a:707:C:OP1	42:2k:85:ARG:NH1	2.49	0.46
32:2a:938:A:C6	32:2a:939:G:C5	3.04	0.46
32:2a:1490:C:H2'	32:2a:1491:G:C8	2.51	0.46
34:2c:111:LEU:HD21	34:2c:144:SER:O	2.16	0.46
37:2f:97:PHE:HB2	49:2r:32:ARG:NH1	2.31	0.46
1:1A:297:C:H2'	1:1A:298:G:C8	2.51	0.46
1:1A:624:C:O2'	1:1A:628:C:OP1	2.29	0.46
1:1A:1120:G:HO2'	1:1A:1121:C:P	2.36	0.46
1:1A:1793:A:H2'	62:1A:5449:HOH:O	2.16	0.46
1:1A:2190:G:C8	1:1A:2192:A:N7	2.84	0.46
5:1F:34:TRP:CH2	11:1P:8:PRO:HB3	2.51	0.46
7:1H:19:VAL:HG22	7:1H:24:VAL:HG12	1.97	0.46
32:1a:262:A:C6	32:1a:263:A:C6	3.03	0.46
32:1a:539:A:H2'	32:1a:540:G:C8	2.50	0.46
32:1a:724:G:H2'	32:1a:725:G:H8	1.80	0.46
32:1a:736:C:H2'	32:1a:737:A:H8	1.81	0.46
32:1a:955:U:O2'	50:1s:83:HIS:HD2	1.99	0.46
32:1a:1226:C:H4'	50:1s:80:TYR:OH	2.16	0.46
35:1d:98:GLU:HA	35:1d:103:ASN:ND2	2.31	0.46
41:1j:54:PHE:O	41:1j:55:LYS:HG2	2.16	0.46
42:1k:84:VAL:HG21	42:1k:95:ILE:HD11	1.97	0.46
48:1q:4:LYS:O	48:1q:60:ILE:HA	2.16	0.46
1:2A:647:G:H8	1:2A:647:G:O5'	1.99	0.46
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.51	0.46
1:2A:2250:G:OP1	12:2Q:85:LYS:NZ	2.47	0.46
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.16	0.46
5:2F:40:GLN:OE1	5:2F:184:TYR:HB2	2.16	0.46
24:22:1:MET:SD	24:22:56:GLN:NE2	2.89	0.46
32:2a:131:C:O2'	32:2a:262:A:N3	2.41	0.46
32:2a:585:G:N3	32:2a:879:C:H4'	2.31	0.46
33:2b:21:ARG:O	33:2b:23:ARG:N	2.49	0.46
33:2b:68:ILE:H	33:2b:90:MET:HE3	1.81	0.46
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.98	0.46
38:2g:108:ALA:O	38:2g:111:ARG:HB2	2.16	0.46
42:2k:59:TYR:CE2	42:2k:63:LEU:HD11	2.51	0.46
51:2t:20:LEU:O	51:2t:23:ARG:HG2	2.16	0.46
1:1A:940:C:H2'	1:1A:941:U:O4'	2.16	0.46
1:1A:956:A:H62	12:1Q:12:GLN:HA	1.81	0.46
1:1A:1997:G:H2'	1:1A:1998:U:O4'	2.16	0.46
1:1A:2139:A:O2'	1:1A:2140:U:H5''	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2596:U:H2'	1:1A:2597:U:C6	2.51	0.46
1:1A:2691:A:H5'	4:1E:165:VAL:HG21	1.98	0.46
7:1H:27:LYS:HE3	7:1H:32:GLU:OE1	2.16	0.46
13:1R:33:ARG:HG2	13:1R:115:GLU:CB	2.46	0.46
24:12:54:LYS:HB3	24:12:54:LYS:HE2	1.79	0.46
30:18:63:PRO:HG2	30:18:64:TYR:CD2	2.51	0.46
32:1a:1293:G:H2'	32:1a:1294:G:C8	2.51	0.46
42:1k:43:SER:HB3	42:1k:68:ALA:HB2	1.97	0.46
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	1.98	0.46
46:1o:74:ASP:OD2	46:1o:77:ARG:HB2	2.16	0.46
1:2A:1028:A:H2	1:2A:2486:G:N3	2.14	0.46
1:2A:1169:G:H1	1:2A:1180:C:H42	1.63	0.46
7:2H:87:LEU:HD23	7:2H:164:TYR:HA	1.97	0.46
16:2U:76:TYR:HH	16:2U:92:ARG:HE	1.56	0.46
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.50	0.46
32:2a:437:U:H5'	35:2d:155:LEU:HD21	1.98	0.46
32:2a:1289:A:N1	32:2a:1371:G:O2'	2.41	0.46
32:2a:1357:A:O2'	45:2n:34:TYR:HE1	1.99	0.46
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.51	0.46
33:2b:24:TRP:HZ3	33:2b:29:ALA:HB2	1.81	0.46
34:2c:114:PRO:HA	34:2c:185:GLY:HA3	1.97	0.46
48:2q:45:HIS:NE2	48:2q:47:PRO:HG3	2.31	0.46
1:1A:174:U:H4'	1:1A:207:A:H4'	1.97	0.45
1:1A:599:U:H2'	1:1A:600:G:C8	2.52	0.45
1:1A:905:U:O2	1:1A:2280:A:H2'	2.16	0.45
1:1A:1525:G:H2'	1:1A:1526:G:H8	1.81	0.45
1:1A:2697:G:P	15:1T:51:ARG:HH12	2.39	0.45
1:1A:2802:C:H1'	1:1A:2901:A:H2	1.81	0.45
9:1N:45:ASN:OD1	9:1N:46:VAL:HG23	2.16	0.45
12:1Q:34:LEU:HB2	12:1Q:118:LEU:HD22	1.98	0.45
26:14:58:ARG:HD3	44:1m:80:ARG:NH1	2.31	0.45
32:1a:545:C:H2'	32:1a:546:G:O4'	2.16	0.45
32:1a:1054:C:C5	54:1w:34:G:H1'	2.51	0.45
32:1a:1312:G:N7	50:1s:2:PRO:HD2	2.31	0.45
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.80	0.45
1:2A:29:U:H2'	1:2A:30:G:C8	2.51	0.45
1:2A:444:C:H4'	5:2F:49:ALA:HB2	1.98	0.45
1:2A:1821:A:H2'	1:2A:1822:G:C8	2.51	0.45
1:2A:2127:G:H2'	1:2A:2128:C:H6	1.81	0.45
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.51	0.45
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.51	0.45
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.50	0.45
8:2I:86:THR:HG22	8:2I:122:GLU:OE1	2.16	0.45
18:2W:45:TYR:CZ	18:2W:49:LYS:HE2	2.50	0.45
32:2a:181:G:H4'	32:2a:182:U:H5'	1.97	0.45
32:2a:421:U:O2'	32:2a:423:G:N7	2.49	0.45
32:2a:1014:A:H2	32:2a:1219:U:H1'	1.80	0.45
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.16	0.45
47:2p:52:ASP:O	47:2p:54:GLU:N	2.49	0.45
1:1A:215:G:H21	1:1A:217:A:H62	1.63	0.45
1:1A:273:G:H21	8:1I:50:ARG:HH12	1.64	0.45
1:1A:1639:G:H2'	1:1A:1640:G:H8	1.77	0.45
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.15	0.45
9:1N:67:LEU:HD23	9:1N:87:LEU:HD22	1.98	0.45
32:1a:553:A:H5''	43:1l:24:VAL:HG21	1.97	0.45
32:1a:730:G:C5	32:1a:731:G:H1'	2.51	0.45
32:1a:736:C:H2'	32:1a:737:A:C8	2.51	0.45
32:1a:840:C:H4'	32:1a:841:U:OP1	2.16	0.45
38:1g:86:GLN:HE22	56:1y:32:PSU:H4'	1.81	0.45
38:1g:115:ARG:O	38:1g:119:ARG:HG3	2.16	0.45
40:1i:16:ARG:HB2	40:1i:64:THR:HB	1.98	0.45
56:1y:15:G:N1	56:1y:48:C:N3	2.63	0.45
1:2A:524:U:H2'	1:2A:525:U:C6	2.52	0.45
1:2A:829:A:N7	1:2A:2247:A:O2'	2.48	0.45
1:2A:1182:A:H2'	1:2A:1183:G:C8	2.50	0.45
1:2A:1540:U:H2'	1:2A:1541:G:O4'	2.16	0.45
1:2A:1616:A:O2'	62:2A:3800:HOH:O	2.21	0.45
1:2A:2102:U:H3	1:2A:2187:G:H1	1.65	0.45
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.52	0.45
2:2B:55:U:H2'	2:2B:56:G:O4'	2.16	0.45
6:2G:15:VAL:HG21	6:2G:176:LEU:HD23	1.98	0.45
14:2S:48:LEU:HD23	14:2S:82:ILE:HD11	1.97	0.45
17:2V:52:VAL:HG23	17:2V:55:ALA:HB3	1.96	0.45
32:2a:376:G:H5''	47:2p:5:ARG:HG2	1.97	0.45
32:2a:1499:A:H1'	32:2a:1520:G:H5'	1.98	0.45
36:2e:41:VAL:O	36:2e:66:MET:HA	2.15	0.45
46:2o:55:GLY:O	46:2o:59:MET:HG3	2.17	0.45
1:1A:843:C:H2'	1:1A:844:C:C6	2.52	0.45
1:1A:1053:C:H5''	9:1N:35:ARG:HH11	1.82	0.45
1:1A:1830:G:N7	3:1D:179:SER:OG	2.42	0.45
1:1A:2389:A:H2'	1:1A:2390:A:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2697:G:H5'	10:1O:68:GLU:OE2	2.16	0.45
14:1S:99:LYS:HE2	14:1S:103:GLU:OE2	2.16	0.45
19:1X:40:LYS:HG3	19:1X:51:VAL:HB	1.97	0.45
23:11:13:ILE:HD11	23:11:42:GLN:OE1	2.16	0.45
23:11:53:VAL:HG22	23:11:74:VAL:HG13	1.98	0.45
26:14:49:PHE:HD1	26:14:49:PHE:HA	1.71	0.45
32:1a:280:C:N3	48:1q:39:SER:N	2.63	0.45
32:1a:926:G:C6	32:1a:1505:G:C6	3.05	0.45
32:1a:998:G:H1	32:1a:1043:C:H42	1.64	0.45
32:1a:1529:G:H4'	32:1a:1530:G:OP2	2.16	0.45
38:1g:50:ILE:HD11	38:1g:61:VAL:HG11	1.98	0.45
38:1g:66:VAL:HG12	38:1g:70:LYS:HE3	1.97	0.45
48:1q:66:SER:OG	48:1q:69:LYS:HB2	2.17	0.45
54:1w:58:A:O2'	54:1w:60:U:OP2	2.33	0.45
56:1y:54:5MU:H2'	56:1y:55:PSU:C5	2.51	0.45
1:2A:26:G:H1'	1:2A:515:A:H61	1.80	0.45
1:2A:764:A:H5'	3:2D:210:GLY:CA	2.47	0.45
1:2A:942:G:OP2	11:2P:39:LYS:NZ	2.48	0.45
1:2A:1416:G:O2'	1:2A:1417:C:OP2	2.25	0.45
1:2A:1422:G:C1'	1:2A:1495:A:H61	2.29	0.45
1:2A:1656:C:H2'	1:2A:1657:C:C6	2.52	0.45
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.51	0.45
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.17	0.45
1:2A:2564:A:OP1	1:2A:2648:C:O2'	2.24	0.45
4:2E:7:VAL:HG12	4:2E:27:LEU:HB3	1.97	0.45
5:2F:53:THR:HG22	5:2F:56:GLU:CD	2.41	0.45
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.51	0.45
32:2a:637:G:H2'	32:2a:638:G:C8	2.51	0.45
32:2a:739:C:O2'	46:2o:42:HIS:ND1	2.46	0.45
40:2i:79:LEU:HG	40:2i:83:ARG:HD2	1.97	0.45
40:2i:127:LYS:O	40:2i:128:ARG:HG2	2.16	0.45
54:2w:51:U:H2'	54:2w:52:G:C8	2.51	0.45
1:1A:141:C:H2'	1:1A:142:G:O4'	2.17	0.45
1:1A:1059:C:OP2	62:1A:4195:HOH:O	2.21	0.45
1:1A:1269:G:N2	1:1A:1272:A:OP2	2.40	0.45
1:1A:1627:A:H5'	1:1A:1628:G:OP2	2.17	0.45
2:1B:95:C:H2'	2:1B:96:U:C6	2.51	0.45
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.17	0.45
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	1.98	0.45
29:17:34:ARG:NH1	29:17:39:ARG:HG2	2.31	0.45
32:1a:110:C:O2'	47:1p:25:ARG:O	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:142:G:H2'	32:1a:143:A:C8	2.50	0.45
32:1a:270:A:H2'	32:1a:271:C:C6	2.51	0.45
32:1a:328:C:H4'	32:1a:329:A:H5'	1.98	0.45
32:1a:1342:C:H2'	32:1a:1343:G:H8	1.81	0.45
40:1i:3:GLN:CD	40:1i:20:ARG:HH21	2.24	0.45
1:2A:78:A:H2'	1:2A:79:G:H8	1.81	0.45
3:2D:96:HIS:CD2	3:2D:102:LYS:HG2	2.52	0.45
13:2R:36:THR:HG22	13:2R:37:THR:N	2.32	0.45
14:2S:88:ASP:OD1	14:2S:90:GLY:N	2.48	0.45
21:2Z:126:VAL:HG11	21:2Z:161:VAL:HG23	1.98	0.45
23:21:83:GLU:OE1	23:21:83:GLU:N	2.50	0.45
32:2a:824:C:H2'	32:2a:825:G:H8	1.82	0.45
32:2a:1329:A:H5''	44:2m:26:GLY:N	2.31	0.45
34:2c:111:LEU:HD22	34:2c:146:ALA:HB2	1.98	0.45
36:2e:148:VAL:HG21	39:2h:107:LEU:HD22	1.98	0.45
43:2l:10:LEU:HB3	48:2q:32:TYR:CE2	2.51	0.45
1:1A:831:A:OP1	1:1A:2600:G:H5''	2.16	0.45
1:1A:1312:G:O5'	18:1W:15:ARG:NH2	2.49	0.45
1:1A:2710:U:H2'	1:1A:2711:C:C6	2.51	0.45
5:1F:172:TRP:CD1	5:1F:172:TRP:H	2.35	0.45
6:1G:7:LEU:HD23	6:1G:100:TRP:CE3	2.51	0.45
11:1P:59:LEU:HD23	30:18:13:ARG:HD2	1.98	0.45
32:1a:7:G:H5'	32:1a:298:A:O4'	2.17	0.45
32:1a:50:A:H1'	32:1a:52:G:C8	2.52	0.45
32:1a:1316:G:N1	32:1a:1319:A:OP2	2.50	0.45
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.52	0.45
41:1j:57:LYS:HE2	41:1j:60:ARG:NH2	2.32	0.45
42:1k:34:ASP:HB3	42:1k:40:ILE:HD11	1.98	0.45
43:1l:28:LYS:HB2	43:1l:33:ARG:HH21	1.81	0.45
1:2A:330:A:H2	1:2A:1210:A:O2'	2.00	0.45
1:2A:686:G:H21	1:2A:788:A:H61	1.64	0.45
1:2A:817:C:H2'	1:2A:818:G:O4'	2.17	0.45
1:2A:2141:G:O6	1:2A:2150:U:O2	2.34	0.45
1:2A:2888:C:H2'	1:2A:2889:C:H6	1.82	0.45
14:2S:67:ARG:NH2	14:2S:103:GLU:OE1	2.47	0.45
32:2a:11:G:H1	32:2a:23:C:H42	1.64	0.45
32:2a:25:C:H2'	32:2a:26:A:H8	1.81	0.45
32:2a:619:U:C2	35:2d:135:LEU:HD22	2.52	0.45
32:2a:1309:G:H1'	44:2m:74:VAL:HG22	1.98	0.45
37:2f:11:ASN:HB3	37:2f:14:LEU:HG	1.99	0.45
46:2o:21:ASP:OD2	46:2o:24:SER:OG	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:23:A:H2'	54:2w:24:G:C8	2.52	0.45
1:1A:265:U:H2'	1:1A:266:C:H6	1.82	0.45
1:1A:1117:G:N3	1:1A:1135:G:O2'	2.50	0.45
1:1A:2145:G:H2'	1:1A:2146:G:C8	2.52	0.45
1:1A:2504:U:H2'	1:1A:2505:U:C6	2.52	0.45
9:1N:14:VAL:HG22	9:1N:138:LEU:HG	1.99	0.45
10:1O:49:ARG:HH22	32:1a:1423:G:H5'	1.80	0.45
12:1Q:32:TYR:HE1	12:1Q:133:ARG:HE	1.65	0.45
15:1T:112:ARG:HG3	15:1T:115:ARG:HH21	1.82	0.45
30:18:23:VAL:HG22	30:18:47:LYS:HB3	1.98	0.45
32:1a:1442:G:O2'	32:1a:1442(A):G:H5'	2.16	0.45
39:1h:42:GLU:HG2	39:1h:109:ILE:HD13	1.98	0.45
41:1j:21:GLN:O	41:1j:25:GLU:HG2	2.17	0.45
47:1p:75:ARG:HA	47:1p:80:PHE:HD2	1.82	0.45
51:1t:16:HIS:O	51:1t:19:SER:OG	2.31	0.45
1:2A:1371:G:H2'	1:2A:1372:U:H5	1.82	0.45
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.52	0.45
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.82	0.45
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.16	0.45
1:2A:2334:G:O6	22:20:74:ARG:NH1	2.32	0.45
1:2A:2842:G:H1	1:2A:2875:C:H42	1.65	0.45
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.50	0.45
15:2T:90:GLN:OE1	15:2T:121:ILE:HD11	2.15	0.45
16:2U:24:TYR:HB2	16:2U:29:SER:HB3	1.98	0.45
21:2Z:149:SER:OG	21:2Z:172:ALA:O	2.21	0.45
32:2a:300:A:O2'	32:2a:564:C:N3	2.39	0.45
32:2a:521:G:H4'	43:2l:73:GLU:HG2	1.98	0.45
32:2a:1122:U:H2'	32:2a:1123:A:H8	1.82	0.45
32:2a:1224:G:N2	32:2a:1363:C:C2	2.76	0.45
32:2a:1343:G:O2'	40:2i:121:ARG:HD2	2.17	0.45
33:2b:24:TRP:H	33:2b:24:TRP:HD1	1.63	0.45
33:2b:27:LYS:HD3	33:2b:195:ASP:OD2	2.17	0.45
34:2c:68:VAL:HB	34:2c:102:ASN:O	2.17	0.45
38:2g:23:VAL:O	38:2g:27:ILE:HG12	2.16	0.45
44:2m:84:ILE:HG13	44:2m:86:CYS:H	1.81	0.45
55:2x:43:A:H2'	55:2x:44:A:C8	2.51	0.45
1:1A:636:G:N2	1:1A:640:A:O2'	2.49	0.45
1:1A:807:G:H2'	1:1A:808:A:O4'	2.17	0.45
1:1A:1093:G:C2'	1:1A:1156:G:H22	2.27	0.45
1:1A:1100:A:C6	1:1A:1101:G:C6	3.05	0.45
1:1A:1971:G:C6	1:1A:1972:G:C6	3.05	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2129:C:N3	1:1A:2204:G:N2	2.62	0.45
1:1A:2279:A:H5''	1:1A:2280:A:H5'	1.98	0.45
15:1T:127:ALA:O	15:1T:128:GLU:HG2	2.16	0.45
16:1U:97:ASP:OD1	16:1U:101:ARG:NH1	2.50	0.45
25:13:7:LYS:HA	25:13:33:GLN:O	2.16	0.45
32:1a:393:A:OP2	47:1p:12:LYS:NZ	2.29	0.45
32:1a:737:A:H2'	32:1a:738:C:C6	2.52	0.45
36:1e:20:GLN:NE2	36:1e:21:ALA:O	2.50	0.45
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.98	0.45
37:1f:97:PHE:CE2	49:1r:31:LEU:HD12	2.51	0.45
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.52	0.45
1:2A:1321:A:H2'	1:2A:1322:A:O4'	2.16	0.45
1:2A:1515:G:H2'	1:2A:1516:C:C6	2.52	0.45
1:2A:1914:C:H2'	1:2A:1915:5MU:O4'	2.17	0.45
1:2A:2191:G:C2	1:2A:2192:G:H1'	2.52	0.45
1:2A:2554:U:H2'	1:2A:2555:U:C6	2.51	0.45
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.51	0.45
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.99	0.45
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.98	0.45
18:2W:18:ARG:NH2	18:2W:76:VAL:O	2.49	0.45
26:24:50:VAL:HG11	44:2m:64:TRP:C	2.41	0.45
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.32	0.45
32:2a:553:A:H5''	43:2l:24:VAL:HG21	1.98	0.45
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.51	0.45
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.82	0.45
32:2a:1134:G:H2'	32:2a:1134:G:N3	2.30	0.45
54:2w:11:C:H2'	54:2w:12:U:C6	2.50	0.45
1:1A:830:A:H1'	1:1A:1810:U:O4'	2.17	0.45
1:1A:1410:G:P	23:11:3:LYS:HG3	2.57	0.45
3:1D:72:LYS:HB3	3:1D:75:ILE:HD12	1.98	0.45
10:1O:7:TYR:HE1	10:1O:20:MET:HB2	1.82	0.45
11:1P:52:GLU:HG2	30:18:57:ARG:HH22	1.81	0.45
14:1S:105:ALA:O	14:1S:110:LEU:HB2	2.17	0.45
32:1a:1015:A:N3	32:1a:1218:C:O2'	2.43	0.45
32:1a:1240:U:H1'	38:1g:38:LEU:HD21	1.98	0.45
32:1a:1402:4OC:H2'	32:1a:1403:C:O4'	2.17	0.45
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.99	0.45
1:2A:171:G:H2'	1:2A:172:C:H6	1.82	0.45
1:2A:531:C:H4'	1:2A:532:A:H5''	1.97	0.45
1:2A:588:U:H2'	1:2A:589:C:C6	2.51	0.45
1:2A:848:G:H2'	1:2A:849:A:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.51	0.45
1:2A:1683:C:H2'	1:2A:1684:C:C6	2.52	0.45
1:2A:2155:G:H5'	1:2A:2155:G:H8	1.82	0.45
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.81	0.45
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.50	0.45
42:2k:48:ILE:HD12	42:2k:63:LEU:HB2	1.98	0.45
56:2y:18:G:C2	56:2y:55:PSU:C4	3.04	0.45
1:1A:364:A:H2'	1:1A:365:G:O4'	2.17	0.45
1:1A:1572:G:C6	1:1A:1573:G:C2	3.05	0.45
1:1A:1868:C:OP1	32:1a:784:C:H4'	2.17	0.45
1:1A:2518:U:O2'	54:1w:76:F3N:H4'	2.17	0.45
1:1A:2735:G:OP2	62:1A:4196:HOH:O	2.21	0.45
2:1B:55:U:H2'	2:1B:56:G:O4'	2.16	0.45
21:1Z:128:VAL:HG23	21:1Z:160:GLY:O	2.16	0.45
32:1a:192:U:H2'	32:1a:193:C:H6	1.82	0.45
32:1a:599:C:H4'	39:1h:130:GLY:C	2.42	0.45
32:1a:1460:A:H2'	32:1a:1461:G:O4'	2.16	0.45
32:1a:1466:C:H2'	32:1a:1467:G:O4'	2.17	0.45
56:1y:8:4SU:H1'	56:1y:48:C:H1'	1.99	0.45
56:1y:43:C:H2'	56:1y:44:G:O4'	2.15	0.45
1:2A:27:G:O2'	1:2A:28:A:OP2	2.27	0.45
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.52	0.45
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.49	0.45
1:2A:2471:C:H2'	1:2A:2472:G:O4'	2.17	0.45
1:2A:2572:A:N7	4:2E:144:ARG:HD2	2.32	0.45
2:2B:78:A:H2'	2:2B:79:C:O4'	2.17	0.45
8:2I:77:LEU:HD11	8:2I:101:LEU:HB2	1.98	0.45
11:2P:99:LEU:HA	11:2P:102:ARG:HE	1.81	0.45
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.99	0.45
32:2a:55:A:OP2	32:2a:352:C:N4	2.49	0.45
32:2a:955:U:H2'	32:2a:956:U:O4'	2.17	0.45
32:2a:1030(B):C:H2'	32:2a:1030(C):G:O4'	2.17	0.45
32:2a:1268:A:O2'	52:2u:19:GLY:HA2	2.17	0.45
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.99	0.45
1:1A:237:G:OP1	62:1A:4197:HOH:O	2.21	0.45
1:1A:1074:A:N6	1:1A:1171:G:H2'	2.32	0.45
1:1A:1653:C:H4'	1:1A:1654:A:O5'	2.16	0.45
1:1A:2623:U:C4	27:15:3:LYS:HG2	2.52	0.45
2:1B:1:U:H2'	2:1B:2:C:C6	2.51	0.45
8:1I:72:LEU:C	8:1I:74:ASN:N	2.72	0.45
9:1N:121:LYS:HG2	9:1N:130:HIS:NE2	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:875:C:O2'	39:1h:14:ARG:HD2	2.16	0.45
35:1d:59:ARG:HD3	35:1d:59:ARG:HA	1.76	0.45
36:1e:31:LEU:HD11	36:1e:129:ILE:HA	1.99	0.45
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.99	0.45
1:2A:848:G:N2	1:2A:933:A:H1'	2.32	0.45
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.32	0.45
6:2G:18:GLU:HA	6:2G:21:ARG:HG2	1.99	0.45
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.17	0.45
12:2Q:12:GLN:HG3	12:2Q:72:LYS:HZ2	1.82	0.45
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.99	0.45
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.17	0.45
32:2a:920:U:H2'	32:2a:921:U:C6	2.52	0.45
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.16	0.45
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.17	0.45
38:2g:26:PHE:CE2	38:2g:30:ILE:HD11	2.52	0.45
40:2i:32:ASP:OD1	40:2i:33:PHE:N	2.50	0.45
48:2q:6:LEU:HB3	48:2q:23:VAL:HG21	1.99	0.45
48:2q:45:HIS:CD2	48:2q:47:PRO:HG3	2.52	0.45
1:1A:1384:G:O2'	1:1A:1439:A:N1	2.39	0.44
8:1I:38:LEU:HD13	23:11:75:GLU:OE1	2.18	0.44
13:1R:103:ARG:HD3	13:1R:108:GLY:O	2.17	0.44
26:14:50:VAL:HG11	44:1m:65:LYS:N	2.32	0.44
38:1g:111:ARG:NH2	38:1g:126:ASP:OD2	2.43	0.44
40:1i:50:LEU:HD12	40:1i:81:ILE:HG12	1.98	0.44
47:1p:52:ASP:HB3	47:1p:55:ARG:HB2	1.99	0.44
48:1q:67:LYS:O	48:1q:68:ARG:HB3	2.17	0.44
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.52	0.44
1:2A:355:G:H2'	1:2A:356:G:C8	2.52	0.44
1:2A:857:C:H1'	22:20:26:TYR:HE1	1.82	0.44
1:2A:918:A:C5	1:2A:919:G:H1'	2.52	0.44
1:2A:924:C:H2'	1:2A:925:C:C6	2.52	0.44
1:2A:1022:G:N2	1:2A:1142(A):A:H2	2.03	0.44
1:2A:1184:G:H5'	25:23:29:ARG:NH2	2.32	0.44
1:2A:1200:C:H2'	1:2A:1201:C:C6	2.52	0.44
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.18	0.44
1:2A:1795:C:O2	3:2D:255:LYS:NZ	2.40	0.44
1:2A:2126:A:N6	1:2A:2163:C:H5'	2.32	0.44
3:2D:20:ASP:OD1	3:2D:21:PHE:N	2.50	0.44
20:2Y:1:MET:HG2	20:2Y:2:ARG:H	1.82	0.44
26:24:40:HIS:HB3	26:24:43:TYR:CD2	2.52	0.44
32:2a:126:G:OP1	32:2a:605:U:O2'	2.27	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:4:TYR:O	40:2i:19:LEU:N	2.39	0.44
52:2u:6:ARG:NH2	52:2u:15:ARG:HH22	2.15	0.44
1:1A:185:A:H2'	1:1A:185:A:N3	2.32	0.44
1:1A:390:G:H2'	1:1A:391:G:C8	2.52	0.44
1:1A:1051:C:O2'	9:1N:28:THR:HG21	2.17	0.44
1:1A:1569:U:H2'	1:1A:1570:G:C8	2.51	0.44
6:1G:43:LEU:HA	6:1G:45:GLU:OE1	2.16	0.44
9:1N:63:THR:OG1	9:1N:66:LYS:NZ	2.51	0.44
35:1d:99:SER:HB3	35:1d:139:ARG:HG3	1.99	0.44
1:2A:1919:A:N1	32:2a:1495:U:O2'	2.41	0.44
2:2B:55:U:H1'	6:2G:29:TRP:HE1	1.82	0.44
13:2R:24:GLN:NE2	13:2R:36:THR:HG21	2.31	0.44
32:2a:552:U:H4'	43:2l:86:ARG:HD2	1.99	0.44
35:2d:63:LYS:O	35:2d:67:ILE:HG13	2.16	0.44
39:2h:112:LEU:HB3	39:2h:133:LEU:HD23	1.99	0.44
51:2t:84:LEU:O	51:2t:88:VAL:HG23	2.17	0.44
1:1A:469:A:N6	5:1F:41:LEU:O	2.43	0.44
1:1A:2198:A:H2'	1:1A:2199:C:C6	2.52	0.44
1:1A:2623:U:H6	1:1A:2623:U:H5'	1.83	0.44
1:1A:2797:C:H1'	4:1E:37:ARG:NH1	2.29	0.44
4:1E:192:ASN:HB3	15:1T:3:ARG:NH2	2.32	0.44
13:1R:56:LYS:NZ	13:1R:90:ARG:O	2.51	0.44
13:1R:63:ARG:O	13:1R:67:LEU:HB2	2.17	0.44
15:1T:117:ASP:O	15:1T:121:ILE:HG13	2.17	0.44
16:1U:17:ILE:HD13	16:1U:17:ILE:HA	1.79	0.44
32:1a:392:G:H2'	32:1a:393:A:C8	2.52	0.44
32:1a:953:G:H2'	32:1a:954:G:O4'	2.17	0.44
38:1g:74:GLU:HG2	38:1g:75:VAL:N	2.32	0.44
52:1u:6:ARG:HH21	52:1u:15:ARG:HH12	1.64	0.44
1:2A:652(A):A:C3'	1:2A:652(B):A:H5'	2.47	0.44
1:2A:711:G:H1	1:2A:720:C:H42	1.66	0.44
1:2A:1665:A:H1'	10:2O:1:MET:HE3	1.98	0.44
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.53	0.44
1:2A:1709:U:H2'	1:2A:1710:C:H6	1.82	0.44
3:2D:242:ARG:HH11	3:2D:242:ARG:HG3	1.83	0.44
11:2P:49:ARG:NH1	30:28:61:LEU:HD23	2.31	0.44
22:20:10:THR:HG22	22:20:11:ARG:N	2.33	0.44
32:2a:115:G:H4'	32:2a:116:A:O5'	2.17	0.44
32:2a:316:G:OP2	32:2a:351:G:O2'	2.28	0.44
32:2a:580:U:H2'	32:2a:581:G:O4'	2.17	0.44
32:2a:996:A:H2'	32:2a:997:U:O4'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:2r:38:GLU:HA	49:2r:41:LYS:HE2	1.99	0.44
1:1A:1045:U:OP2	62:1A:4198:HOH:O	2.21	0.44
1:1A:1139:G:H3'	1:1A:1140:U:C5'	2.45	0.44
3:1D:108:PRO:HG2	3:1D:111:LEU:HG	1.98	0.44
11:1P:63:PRO:HD3	30:18:27:THR:HG22	2.00	0.44
11:1P:95:VAL:HG13	11:1P:125:VAL:HA	1.98	0.44
32:1a:138:G:H2'	32:1a:139:G:O4'	2.18	0.44
37:1f:3:ARG:NE	37:1f:38:GLU:OE2	2.50	0.44
39:1h:19:VAL:HG23	39:1h:21:LYS:HG2	2.00	0.44
39:1h:112:LEU:HD11	39:1h:124:ALA:HB2	2.00	0.44
52:1u:17:THR:O	52:1u:22:ARG:NH1	2.48	0.44
1:2A:1263:U:H1'	27:25:10:LYS:HG3	1.98	0.44
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.46	0.44
1:2A:2378:A:H4'	14:2S:23:ARG:NH1	2.33	0.44
3:2D:242:ARG:HD3	3:2D:246:PRO:HG3	1.99	0.44
6:2G:170:ARG:HH22	6:2G:180:PHE:HB2	1.82	0.44
14:2S:9:ARG:O	14:2S:13:ARG:HG3	2.17	0.44
22:20:69:PHE:CE1	22:20:79:VAL:HG22	2.52	0.44
32:2a:413:G:H1'	32:2a:428:G:N2	2.33	0.44
32:2a:1077:G:H5'	32:2a:1078:U:OP2	2.17	0.44
32:2a:1122:U:H2'	32:2a:1123:A:C8	2.52	0.44
32:2a:1292:U:OP2	38:2g:41:ARG:NH2	2.50	0.44
54:2w:24:G:C6	54:2w:25:C:C4	3.06	0.44
1:1A:327:U:H2'	1:1A:328:G:H8	1.82	0.44
1:1A:1122:C:H4'	1:1A:1123:A:OP1	2.16	0.44
1:1A:1699:A:O2'	1:1A:1700:G:H5'	2.18	0.44
1:1A:2362:C:OP2	62:1A:4193:HOH:O	2.21	0.44
3:1D:5:LYS:HG2	3:1D:17:THR:HG22	1.98	0.44
6:1G:136:ARG:HG3	6:1G:137:GLU:HG3	1.99	0.44
20:1Y:11:ASP:OD2	20:1Y:97:ARG:NH2	2.48	0.44
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.17	0.44
24:12:10:LEU:HB3	24:12:14:ARG:NH1	2.33	0.44
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.53	0.44
32:1a:1239:A:H62	32:1a:1299:A:N6	2.15	0.44
37:1f:39:LYS:H	37:1f:64:GLN:HB3	1.82	0.44
39:1h:104:ARG:C	39:1h:106:GLY:H	2.26	0.44
40:1i:50:LEU:HB2	40:1i:55:ALA:HB3	1.99	0.44
1:2A:140:G:N2	1:2A:1596:A:H4'	2.32	0.44
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.18	0.44
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.47	0.44
1:2A:2478:A:O2'	1:2A:2536:G:N2	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:94:GLU:OE2	11:2P:124:LYS:NZ	2.50	0.44
30:28:23:VAL:HG22	30:28:47:LYS:HB3	2.00	0.44
32:2a:624:C:H2'	32:2a:625:G:H8	1.82	0.44
32:2a:841:U:C5	32:2a:848:C:H1'	2.52	0.44
32:2a:1129:C:H42	32:2a:1143:G:H1	1.64	0.44
33:2b:22:LYS:HA	33:2b:40:HIS:HE1	1.82	0.44
37:2f:23:LYS:HB3	37:2f:23:LYS:HE2	1.86	0.44
38:2g:69:VAL:HA	38:2g:138:LYS:HD3	1.99	0.44
40:2i:42:ARG:NH2	40:2i:75:ASP:OD1	2.51	0.44
45:2n:59:ALA:HB1	45:2n:61:TRP:HZ3	1.83	0.44
1:1A:1117:G:OP1	1:1A:1117:G:H3'	2.17	0.44
1:1A:2283:G:OP1	22:10:18:ALA:HB1	2.17	0.44
10:1O:49:ARG:NH2	32:1a:1422:G:O3'	2.48	0.44
18:1W:66:GLU:HA	18:1W:69:LEU:HD12	1.99	0.44
32:1a:267:C:OP1	48:1q:67:LYS:HD3	2.18	0.44
32:1a:880:C:OP1	43:1l:8:ASN:ND2	2.43	0.44
32:1a:1034:G:C2	32:1a:1035:A:H1'	2.53	0.44
34:1c:39:ILE:HG23	34:1c:91:LEU:HD11	1.98	0.44
35:1d:12:CYS:SG	35:1d:19:LEU:HB2	2.57	0.44
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.53	0.44
44:1m:16:ASP:OD1	44:1m:16:ASP:N	2.49	0.44
1:2A:307:G:N2	1:2A:310:A:O5'	2.47	0.44
2:2B:25:A:H2'	2:2B:26:A:O4'	2.17	0.44
2:2B:94:C:H2'	2:2B:95:C:C6	2.50	0.44
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.98	0.44
14:2S:15:ARG:HB3	14:2S:19:LYS:HZ1	1.83	0.44
18:2W:82:LEU:HD22	18:2W:84:ARG:HH22	1.82	0.44
27:25:25:LEU:HD23	27:25:25:LEU:HA	1.85	0.44
32:2a:186:C:H2'	32:2a:187:C:C6	2.53	0.44
32:2a:189(D):C:H2'	32:2a:189(E):U:O4'	2.17	0.44
32:2a:292:G:N7	32:2a:293:G:H1'	2.33	0.44
32:2a:950:U:H2'	32:2a:951:G:C8	2.52	0.44
32:2a:967:5MC:H2'	32:2a:968:A:N7	2.33	0.44
32:2a:971:G:P	32:2a:1231:G:H21	2.39	0.44
33:2b:24:TRP:CZ3	33:2b:26:PRO:HA	2.53	0.44
33:2b:27:LYS:HD2	33:2b:193:ASP:OD1	2.18	0.44
34:2c:5:ILE:HD11	45:2n:49:HIS:HE1	1.82	0.44
36:2e:131:ILE:HD13	36:2e:131:ILE:HA	1.90	0.44
40:2i:49:PRO:HB3	40:2i:82:ALA:HB2	2.00	0.44
43:2l:34:ARG:HG3	43:2l:105:TYR:CE2	2.52	0.44
1:1A:1821:C:O2'	3:1D:209:ALA:HB2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:44:G:OP2	26:14:1:MET:N	2.40	0.44
16:1U:32:PHE:CZ	16:1U:36:ARG:HD2	2.52	0.44
28:16:39:TYR:HB2	28:16:46:HIS:CE1	2.53	0.44
32:1a:8:A:N7	35:1d:208:SER:OG	2.36	0.44
32:1a:72:C:H2'	32:1a:73:G:C8	2.53	0.44
32:1a:986:A:H2'	32:1a:987:G:O4'	2.17	0.44
32:1a:1226:C:H2'	44:1m:103:THR:HB	2.00	0.44
32:1a:1366:C:HO2'	41:1j:60:ARG:HH12	1.63	0.44
33:1b:219:VAL:HA	33:1b:222:ILE:HD12	1.99	0.44
45:1n:26:ARG:HD3	45:1n:43:CYS:HB3	1.98	0.44
56:1y:18:G:O2'	56:1y:19:G:H5'	2.18	0.44
56:1y:47:U:H2'	56:1y:50:U:OP1	2.18	0.44
1:2A:2166:G:H2'	1:2A:2167:U:C6	2.52	0.44
1:2A:2680:C:H1'	4:2E:187:ALA:HB1	1.99	0.44
1:2A:2793:G:H1	1:2A:2803:C:N4	2.09	0.44
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.83	0.44
5:2F:181:LEU:HD11	5:2F:186:ILE:HD11	2.00	0.44
18:2W:13:SER:O	18:2W:17:VAL:HG23	2.18	0.44
32:2a:52:G:H2'	32:2a:53:A:C8	2.53	0.44
32:2a:108:G:P	32:2a:326:G:H22	2.41	0.44
32:2a:958:A:N3	32:2a:985:C:O2'	2.37	0.44
32:2a:1241:G:H2'	32:2a:1242:C:H6	1.82	0.44
37:2f:97:PHE:CD2	49:2r:31:LEU:HD12	2.53	0.44
48:2q:26:GLN:HE21	48:2q:37:LYS:HD3	1.82	0.44
54:2w:36:A:H2'	54:2w:37:MIA:H8	1.99	0.44
1:1A:661:G:OP1	11:1P:132:LYS:NZ	2.39	0.44
1:1A:2831:A:OP2	62:1A:4143:HOH:O	2.21	0.44
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.53	0.44
15:1T:102:ILE:HA	15:1T:105:LEU:HG	2.00	0.44
17:1V:80:GLN:HA	17:1V:82:ARG:NH1	2.32	0.44
32:1a:501:C:H2'	32:1a:502:G:C8	2.52	0.44
32:1a:1001(A):G:H2'	32:1a:1002:G:O4'	2.17	0.44
54:1w:21:A:N6	54:1w:46:7MG:C4	2.86	0.44
56:1y:58:A:H2'	56:1y:60:U:H5	1.83	0.44
1:2A:322:A:H5'	1:2A:340:A:H1'	1.99	0.44
11:2P:96:THR:H	11:2P:99:LEU:HD21	1.82	0.44
12:2Q:39:PRO:HB3	12:2Q:99:PRO:HD3	1.99	0.44
18:2W:11:ARG:HA	18:2W:100:THR:HG22	1.99	0.44
32:2a:84:U:H4'	32:2a:89:C:N4	2.32	0.44
32:2a:434:U:H2'	32:2a:435:C:C6	2.53	0.44
32:2a:731:G:OP1	32:2a:766:A:H1'	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:977:A:H2'	32:2a:978:A:H5''	1.98	0.44
32:2a:1013:G:H2'	32:2a:1015:A:OP2	2.17	0.44
32:2a:1169:A:H2'	32:2a:1170:A:C8	2.53	0.44
37:2f:76:ALA:O	37:2f:80:ARG:HG3	2.18	0.44
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.83	0.44
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.82	0.44
1:1A:1320:A:N3	1:1A:1343:C:H1'	2.32	0.44
1:1A:1346:U:H4'	1:1A:1347:A:H5'	1.99	0.44
2:1B:40:U:O4	26:14:1:MET:N	2.39	0.44
11:1P:36:LYS:HA	11:1P:41:ARG:HH12	1.83	0.44
16:1U:47:TYR:HA	16:1U:50:ARG:NH2	2.32	0.44
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.52	0.44
42:1k:45:GLY:O	42:1k:50:TYR:HB2	2.18	0.44
56:1y:68:C:N3	56:1y:69:G:C8	2.86	0.44
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.52	0.44
1:2A:2096:U:H3	1:2A:2193:G:H1	1.65	0.44
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.51	0.44
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.18	0.44
24:22:53:LEU:HD23	24:22:53:LEU:HA	1.84	0.44
26:24:24:THR:OG1	26:24:25:TYR:N	2.41	0.44
32:2a:271:C:H2'	32:2a:272:C:H6	1.83	0.44
32:2a:942:G:C2	32:2a:1342:C:C2	3.05	0.44
32:2a:1436:U:H2'	32:2a:1437:C:O4'	2.18	0.44
33:2b:59:GLU:HB2	33:2b:221:LEU:HD21	1.99	0.44
35:2d:159:ARG:O	35:2d:163:GLU:N	2.50	0.44
36:2e:72:GLN:O	36:2e:75:THR:HG22	2.18	0.44
48:2q:61:GLU:HA	48:2q:71:PHE:CD1	2.53	0.44
54:2w:26:A:H2'	54:2w:27:G:C8	2.52	0.44
1:1A:602:G:H2'	1:1A:603:C:C6	2.53	0.43
1:1A:1068:G:C5	1:1A:1185:C:C4	3.06	0.43
1:1A:1314:A:C2	1:1A:2035:A:C4	3.06	0.43
1:1A:1945:U:H2'	1:1A:1946:C:C6	2.53	0.43
1:1A:2142:G:H2'	1:1A:2143:G:H5'	2.00	0.43
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.53	0.43
3:1D:183:ARG:HG3	3:1D:184:LYS:N	2.32	0.43
8:1I:79:ILE:HG22	8:1I:81:VAL:HG13	2.00	0.43
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.99	0.43
32:1a:1028:C:N4	32:1a:1029:C:C2	2.86	0.43
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.53	0.43
39:1h:38:ILE:HG12	39:1h:41:ARG:HH21	1.83	0.43
39:1h:82:HIS:HB3	39:1h:138:TRP:CE2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:588:U:H1'	5:2F:90:PHE:CG	2.53	0.43
1:2A:594:U:H2'	1:2A:595:C:C6	2.53	0.43
1:2A:774:A:H2'	1:2A:774:A:N3	2.33	0.43
1:2A:1484:G:N2	1:2A:1506:C:H1'	2.34	0.43
1:2A:1549:C:H2'	1:2A:1550:C:C6	2.53	0.43
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.17	0.43
1:2A:2126:A:C2	1:2A:2127:G:H1'	2.53	0.43
1:2A:2152:G:H8	1:2A:2152:G:O5'	2.00	0.43
1:2A:2327:A:H2'	1:2A:2328:A:H8	1.83	0.43
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.18	0.43
21:2Z:121:HIS:N	21:2Z:172:ALA:HB2	2.32	0.43
32:2a:16:A:N3	32:2a:1080:A:O2'	2.45	0.43
32:2a:687:A:H4'	32:2a:688:G:O5'	2.18	0.43
32:2a:892:A:O2'	32:2a:1415:G:H4'	2.19	0.43
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.33	0.43
36:2e:68:GLU:HG3	36:2e:70:PRO:HD3	1.99	0.43
56:2y:33:U:H2'	56:2y:35:A:OP2	2.18	0.43
1:1A:1246:C:H2'	1:1A:1247:C:C6	2.53	0.43
1:1A:1765:U:H2'	1:1A:1766:G:O4'	2.18	0.43
1:1A:2141:A:C5	1:1A:2192:A:C2	3.06	0.43
1:1A:2622:C:H1'	62:1A:4329:HOH:O	2.18	0.43
1:1A:2705:A:H2'	1:1A:2706:G:H8	1.82	0.43
1:1A:2825:C:C5'	27:15:29:THR:HG21	2.48	0.43
4:1E:117:MET:HE2	4:1E:117:MET:HB3	1.75	0.43
7:1H:75:ALA:O	7:1H:79:VAL:HG22	2.18	0.43
16:1U:46:ALA:O	16:1U:50:ARG:HG3	2.18	0.43
24:12:25:VAL:HG13	24:12:57:ILE:HG23	1.99	0.43
26:14:50:VAL:HG11	44:1m:64:TRP:C	2.43	0.43
28:16:13:CYS:SG	28:16:47:THR:HG21	2.58	0.43
32:1a:72:C:N3	32:1a:97:G:O6	2.51	0.43
32:1a:324:G:N7	62:1a:3338:HOH:O	2.35	0.43
32:1a:831:U:H2'	32:1a:832:C:C6	2.53	0.43
36:1e:102:ALA:HB3	36:1e:107:ARG:HB2	2.00	0.43
37:1f:100:ASN:C	49:1r:28:GLU:HG2	2.43	0.43
43:1l:28:LYS:HG3	43:1l:62:SER:HB2	2.00	0.43
55:1x:23:C:H2'	55:1x:24:U:C6	2.53	0.43
1:2A:443:A:N7	5:2F:45:ARG:HG2	2.33	0.43
1:2A:1341:U:H3'	1:2A:1397:U:O2	2.18	0.43
2:2B:100:A:H3'	2:2B:101:G:H8	1.83	0.43
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.99	0.43
6:2G:135:LEU:O	6:2G:154:GLY:HA3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:200:G:H2'	32:2a:201:C:O4'	2.17	0.43
32:2a:1015:A:H2'	32:2a:1016:A:C8	2.53	0.43
32:2a:1104:G:H4'	33:2b:111:ARG:HH21	1.83	0.43
32:2a:1183:A:O2'	32:2a:1185:G:OP2	2.36	0.43
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.53	0.43
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.83	0.43
32:2a:1389:C:H2'	32:2a:1390:U:O4'	2.18	0.43
50:2s:15:LEU:HD13	50:2s:33:THR:HB	1.98	0.43
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.53	0.43
1:1A:2021:C:H4'	1:1A:2736:C:O2	2.18	0.43
1:1A:2077:C:OP1	27:15:8:LYS:NZ	2.51	0.43
1:1A:2204:G:O2'	1:1A:2205:C:O4'	2.28	0.43
1:1A:2257:U:O2'	1:1A:2448:G:OP2	2.26	0.43
1:1A:2798:C:OP1	4:1E:41:LYS:NZ	2.49	0.43
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.82	0.43
12:1Q:26:TYR:O	12:1Q:67:ARG:NH1	2.46	0.43
32:1a:72:C:H2'	32:1a:73:G:H8	1.83	0.43
32:1a:153:C:N4	32:1a:168:G:H1	2.15	0.43
32:1a:395:C:H2'	32:1a:396:G:H8	1.83	0.43
33:1b:189:ASP:OD1	33:1b:189:ASP:N	2.47	0.43
39:1h:121:ASP:OD1	39:1h:121:ASP:N	2.48	0.43
40:1i:31:GLN:HE21	40:1i:36:TYR:HB2	1.82	0.43
47:1p:37:GLY:HA3	47:1p:50:LYS:O	2.18	0.43
1:2A:513:A:H2	1:2A:582:G:H4'	1.82	0.43
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.33	0.43
1:2A:2841:C:H2'	1:2A:2842:G:C8	2.53	0.43
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.19	0.43
9:2N:4:TYR:HB2	16:2U:101:ARG:NH1	2.33	0.43
15:2T:2:ASN:O	15:2T:6:LEU:HD13	2.18	0.43
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG22	2.18	0.43
26:24:40:HIS:O	26:24:44:THR:HG22	2.18	0.43
32:2a:784:C:H2'	32:2a:785:G:O4'	2.18	0.43
32:2a:1326:C:H2'	32:2a:1327:C:C6	2.54	0.43
38:2g:18:TYR:CD1	38:2g:59:LEU:HD22	2.54	0.43
39:2h:110:ALA:O	39:2h:120:THR:HA	2.18	0.43
48:2q:22:LEU:HD11	48:2q:39:SER:HB2	2.01	0.43
1:1A:2040:G:H2'	1:1A:2041:A:O4'	2.18	0.43
1:1A:2125:C:O2	1:1A:2209:G:N2	2.52	0.43
6:1G:7:LEU:HD23	6:1G:100:TRP:HE3	1.83	0.43
24:12:32:LEU:O	24:12:36:ARG:HG3	2.19	0.43
32:1a:421:U:OP2	32:1a:422:C:N4	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:79:LEU:O	40:1i:83:ARG:HG3	2.18	0.43
41:1j:9:ARG:O	41:1j:16:LEU:HD11	2.18	0.43
1:2A:721:C:H2'	1:2A:722:A:C8	2.54	0.43
1:2A:877:U:O2'	1:2A:900:A:N6	2.52	0.43
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.33	0.43
1:2A:2726:U:O2'	1:2A:2727:G:H8	2.00	0.43
5:2F:120:GLU:HB2	5:2F:122:LYS:HG2	2.00	0.43
7:2H:125:VAL:HG12	7:2H:131:VAL:HG22	1.99	0.43
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	2.00	0.43
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD23	2.00	0.43
32:2a:460:G:N1	32:2a:471:G:OP2	2.42	0.43
32:2a:1002:G:N3	32:2a:1003:G:C8	2.87	0.43
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.51	0.43
32:2a:1122:U:N3	32:2a:1123:A:N7	2.66	0.43
32:2a:1184:G:OP1	32:2a:1184:G:H3'	2.18	0.43
32:2a:1277:C:O2'	32:2a:1279:A:H1'	2.17	0.43
32:2a:1394:A:H8	32:2a:1394:A:OP1	2.01	0.43
33:2b:55:PHE:CE1	33:2b:218:ALA:HA	2.54	0.43
42:2k:18:ARG:HB2	42:2k:33:THR:OG1	2.17	0.43
51:2t:65:LYS:HA	51:2t:68:LYS:HD3	2.00	0.43
1:1A:1830:G:O2'	3:1D:181:GLU:OE2	2.26	0.43
1:1A:2045:G:H4'	1:1A:2629:C:O3'	2.19	0.43
1:1A:2357:G:N3	1:1A:2393:C:H2'	2.34	0.43
1:1A:2592:U:OP1	62:1A:4199:HOH:O	2.21	0.43
2:1B:11:C:OP2	2:1B:12:C:N4	2.41	0.43
16:1U:83:LEU:HD12	16:1U:113:ALA:HB2	2.00	0.43
32:1a:392:G:H2'	32:1a:393:A:H8	1.83	0.43
32:1a:850:U:H2'	32:1a:851:G:H5''	1.99	0.43
32:1a:1028:C:C4	32:1a:1029:C:C2	3.07	0.43
32:1a:1101:A:N6	33:1b:176:GLU:OE2	2.51	0.43
1:2A:27:G:HO2'	1:2A:28:A:P	2.40	0.43
1:2A:570:G:H2'	1:2A:2030:A:C5	2.53	0.43
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.54	0.43
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.53	0.43
2:2B:50:G:OP1	14:2S:63:THR:N	2.50	0.43
2:2B:50:G:OP2	14:2S:62:LYS:HB2	2.19	0.43
6:2G:115:ARG:HB3	6:2G:136:ARG:HH21	1.84	0.43
19:2X:27:THR:HA	19:2X:79:ALA:O	2.19	0.43
25:23:6:VAL:O	25:23:34:GLU:HA	2.19	0.43
32:2a:811:C:N3	62:2a:3350:HOH:O	2.36	0.43
32:2a:838:G:H2'	32:2a:839:U:H2'	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1069:C:H4'	32:2a:1192:C:O2	2.18	0.43
32:2a:1106:G:H2'	32:2a:1107:C:H6	1.83	0.43
32:2a:1123:A:N3	41:2j:39:PRO:HD2	2.32	0.43
32:2a:1176:A:H2'	32:2a:1177:G:O4'	2.17	0.43
32:2a:1196:U:H3	34:2c:162:GLN:HE22	1.65	0.43
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.54	0.43
41:2j:27:ALA:HB1	41:2j:74:ILE:HD13	2.00	0.43
1:1A:134:G:O6	62:1A:4191:HOH:O	2.20	0.43
1:1A:471:C:N4	1:1A:472:G:C6	2.87	0.43
1:1A:646:A:OP2	11:1P:108:LYS:NZ	2.47	0.43
1:1A:1117:G:H1'	1:1A:1135:G:H2'	1.99	0.43
1:1A:1217:G:H3'	1:1A:1218:G:H5'	2.01	0.43
1:1A:2327:G:H2'	1:1A:2328:C:C6	2.53	0.43
11:1P:128:HIS:NE2	11:1P:148:LEU:HD11	2.33	0.43
32:1a:222:U:H2'	32:1a:223:U:C6	2.53	0.43
44:1m:90:LEU:HD23	44:1m:93:ARG:HD2	1.99	0.43
44:1m:122:LYS:HA	44:1m:122:LYS:HD2	1.85	0.43
48:1q:99:SER:OG	48:1q:100:LYS:N	2.52	0.43
1:2A:479:A:N3	1:2A:481:G:H5''	2.33	0.43
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.83	0.43
1:2A:2111:C:H6	1:2A:2111:C:OP2	2.02	0.43
1:2A:2734:A:H2'	1:2A:2735:G:O4'	2.18	0.43
1:2A:2869:G:C2	1:2A:2870:C:C2	3.06	0.43
6:2G:115:ARG:H	6:2G:136:ARG:NH2	2.16	0.43
14:2S:99:LYS:HE2	14:2S:103:GLU:OE2	2.19	0.43
23:21:81:LYS:HB3	23:21:81:LYS:HE2	1.68	0.43
26:24:8:LYS:HE3	26:24:10:VAL:HG12	2.01	0.43
32:2a:410:G:OP2	35:2d:25:ARG:HD2	2.19	0.43
32:2a:1027:C:H42	32:2a:1035:A:H2	1.67	0.43
32:2a:1097:C:O2'	32:2a:1169:A:N3	2.40	0.43
38:2g:16:LEU:HD22	40:2i:41:VAL:O	2.18	0.43
42:2k:80:VAL:HG23	42:2k:105:VAL:HA	2.00	0.43
44:2m:49:THR:O	44:2m:53:VAL:HG23	2.18	0.43
46:2o:68:ARG:NH1	62:2o:101:HOH:O	2.50	0.43
51:2t:43:LEU:O	51:2t:47:GLY:N	2.50	0.43
54:2w:68:C:H2'	54:2w:69:G:C8	2.52	0.43
1:1A:1463:C:H2'	1:1A:1464:G:O4'	2.19	0.43
1:1A:1472:G:O2'	1:1A:1619:A:N6	2.45	0.43
1:1A:1847:G:O2'	1:1A:1848:G:OP2	2.34	0.43
1:1A:2661:U:H2'	1:1A:2662:U:C6	2.53	0.43
3:1D:242:ARG:HD3	3:1D:246:PRO:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:135:ASP:O	12:1Q:139:GLU:HG3	2.18	0.43
14:1S:15:ARG:O	14:1S:19:LYS:HG3	2.18	0.43
20:1Y:37:VAL:HG21	20:1Y:72:VAL:HG21	2.01	0.43
26:14:64:GLY:C	26:14:66:SER:N	2.77	0.43
30:18:30:ARG:HA	30:18:30:ARG:HD3	1.77	0.43
32:1a:10:A:H2'	32:1a:11:G:C8	2.54	0.43
32:1a:148:G:H2'	32:1a:149:A:C8	2.54	0.43
32:1a:395:C:H2'	32:1a:396:G:C8	2.53	0.43
32:1a:473:G:H2'	32:1a:474:G:H8	1.83	0.43
36:1e:131:ILE:HD13	36:1e:131:ILE:HA	1.91	0.43
1:2A:918:A:O2'	2:2B:97:G:N2	2.47	0.43
1:2A:1022:G:N2	1:2A:1142(A):A:C2	2.83	0.43
1:2A:1252:G:C2	1:2A:1253:A:C2	3.07	0.43
1:2A:1742:G:H2'	1:2A:1743:C:O4'	2.17	0.43
1:2A:1792:G:O2'	1:2A:1830:C:OP1	2.35	0.43
1:2A:2103:C:C2'	1:2A:2104:G:H5'	2.49	0.43
1:2A:2335:A:O2'	1:2A:2336:A:OP2	2.36	0.43
6:2G:115:ARG:HB3	6:2G:136:ARG:NH2	2.34	0.43
7:2H:117:PRO:HG3	7:2H:123:PHE:CD2	2.54	0.43
11:2P:45:LEU:HD23	11:2P:46:LYS:O	2.19	0.43
13:2R:33:ARG:HG2	13:2R:115:GLU:HB3	2.01	0.43
32:2a:302:G:O2'	32:2a:556:C:H5''	2.18	0.43
32:2a:522:C:H2'	32:2a:523:A:O4'	2.18	0.43
32:2a:657:G:H4'	46:2o:28:GLN:HG2	2.01	0.43
32:2a:721:G:H4'	32:2a:722:A:O4'	2.18	0.43
32:2a:1220:G:O3'	50:2s:36:ARG:HD3	2.19	0.43
32:2a:1280:A:H5'	41:2j:41:PRO:HD2	2.00	0.43
32:2a:1317:C:N4	45:2n:19:ARG:HH21	2.17	0.43
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.34	0.43
33:2b:55:PHE:HA	33:2b:58:ILE:HB	2.00	0.43
36:2e:12:LEU:HD21	36:2e:14:ARG:HB2	2.00	0.43
36:2e:36:ASP:OD1	36:2e:40:ARG:HB2	2.19	0.43
44:2m:92:HIS:NE2	44:2m:98:VAL:HG21	2.34	0.43
1:1A:26:G:C6	1:1A:27:G:N1	2.87	0.43
1:1A:419:C:OP1	62:1A:4180:HOH:O	2.21	0.43
1:1A:582:G:H22	16:1U:49:HIS:CE1	2.36	0.43
1:1A:2311:G:H2'	1:1A:2312:G:C8	2.50	0.43
1:1A:2829:G:H2'	1:1A:2831:A:N7	2.34	0.43
12:1Q:8:LYS:HG2	12:1Q:9:TYR:CE2	2.53	0.43
20:1Y:7:VAL:HG21	20:1Y:72:VAL:CG1	2.49	0.43
31:19:32:HIS:O	31:19:34:GLN:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:69:G:H2'	32:1a:70:G:C8	2.53	0.43
35:1d:3:ARG:O	35:1d:5:ILE:HG22	2.18	0.43
43:1l:26:ALA:HA	43:1l:64:TYR:CD2	2.54	0.43
55:1x:17:C:OP2	55:1x:17(A):U:O2'	2.30	0.43
1:2A:150:C:H2'	1:2A:151:C:C6	2.54	0.43
1:2A:392:C:H5''	1:2A:409:C:H5''	2.01	0.43
1:2A:870:A:C2	1:2A:908:C:C2	3.07	0.43
1:2A:1848:A:H2'	1:2A:1849:G:H8	1.84	0.43
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.54	0.43
1:2A:2275:C:H6	1:2A:2275:C:H5'	1.84	0.43
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.54	0.43
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.81	0.43
6:2G:43:LEU:HB3	6:2G:44:GLY:H	1.73	0.43
15:2T:64:ARG:HG3	15:2T:73:GLU:HG2	2.01	0.43
29:27:20:ALA:N	62:27:102:HOH:O	2.45	0.43
32:2a:901:A:C5	32:2a:902:G:H1'	2.54	0.43
32:2a:1038:C:C2	32:2a:1039:C:C5	3.07	0.43
32:2a:1195:C:H2'	32:2a:1197:G:O4'	2.18	0.43
32:2a:1353:G:H5''	62:2a:3416:HOH:O	2.19	0.43
36:2e:101:ILE:O	36:2e:120:THR:OG1	2.35	0.43
39:2h:78:GLN:O	39:2h:81:HIS:NE2	2.52	0.43
53:2v:12:A:N3	53:2v:12:A:H2'	2.33	0.43
1:1A:34:C:H5''	1:1A:35:G:OP2	2.18	0.43
1:1A:821:A:H2'	1:1A:821:A:N3	2.33	0.43
1:1A:1102:G:H2'	1:1A:1149:A:H61	1.83	0.43
1:1A:2698:G:OP2	62:1A:4200:HOH:O	2.21	0.43
7:1H:54:ARG:NH2	7:1H:57:ASP:OD1	2.43	0.43
12:1Q:111:GLU:OE1	12:1Q:133:ARG:NH2	2.51	0.43
32:1a:1277:C:O2'	32:1a:1279:A:H8	2.01	0.43
54:1w:51:U:H2'	54:1w:52:G:C8	2.53	0.43
1:2A:903:C:H2'	1:2A:904:C:C6	2.53	0.43
1:2A:2020:A:O2'	1:2A:2021:C:H5'	2.19	0.43
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.18	0.43
1:2A:2127:G:O6	1:2A:2161:C:N3	2.52	0.43
1:2A:2600:A:H2'	1:2A:2601:C:C6	2.53	0.43
2:2B:11:C:H3'	2:2B:12:C:H6	1.84	0.43
3:2D:145:VAL:HB	3:2D:155:LEU:HB2	2.01	0.43
8:2I:106:GLY:O	8:2I:107:VAL:HG23	2.19	0.43
9:2N:42:TRP:CH2	9:2N:44:PRO:HB3	2.54	0.43
26:24:57:GLU:CB	26:24:58:ARG:HD2	2.49	0.43
30:28:62:LEU:HB3	30:28:65:GLU:CG	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:509:A:H5'	35:2d:54:TYR:HD2	1.83	0.43
32:2a:627:G:H2'	32:2a:628:G:C8	2.53	0.43
32:2a:1040:U:H2'	32:2a:1041:A:C8	2.44	0.43
32:2a:1225:A:H2'	32:2a:1226:C:C5	2.54	0.43
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.83	0.43
1:1A:589:U:OP1	11:1P:29:LYS:NZ	2.41	0.43
1:1A:633:G:H2'	1:1A:634:C:C6	2.54	0.43
1:1A:1136:U:C4	1:1A:1148:C:O2	2.72	0.43
1:1A:1402:G:N7	62:1A:4295:HOH:O	2.35	0.43
1:1A:1423:G:H2'	62:1A:5137:HOH:O	2.18	0.43
1:1A:1431:G:O2'	1:1A:1442:U:O2	2.29	0.43
1:1A:1517:G:H5''	1:1A:1518:A:OP1	2.19	0.43
1:1A:2761:A:H5'	7:1H:4:ILE:HD12	2.00	0.43
1:1A:2828:G:O2'	1:1A:2829:G:H5'	2.19	0.43
13:1R:26:LYS:HE2	13:1R:70:LEU:O	2.19	0.43
32:1a:313:A:H2'	32:1a:314:C:C6	2.54	0.43
33:1b:87:ARG:HH21	33:1b:219:VAL:HB	1.83	0.43
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.19	0.43
1:2A:362:U:O2'	1:2A:363:G:H5'	2.19	0.43
1:2A:773:U:O2'	3:2D:48:ARG:HD3	2.19	0.43
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.19	0.43
1:2A:2153:G:C2	1:2A:2154:G:C5	3.07	0.43
1:2A:2284:C:P	28:26:6:ARG:HG3	2.59	0.43
1:2A:2784:C:H2'	1:2A:2785:C:H6	1.82	0.43
2:2B:75:G:H5'	2:2B:76:G:OP2	2.19	0.43
24:22:63:VAL:HA	24:22:66:GLU:OE1	2.19	0.43
29:27:9:ARG:HH21	29:27:47:ARG:HD3	1.83	0.43
30:28:30:ARG:HA	30:28:30:ARG:HD3	1.78	0.43
32:2a:127:G:HO2'	48:2q:2:PRO:N	2.16	0.43
32:2a:913:A:OP1	43:2l:46:LYS:NZ	2.49	0.43
32:2a:1005:A:H2	32:2a:1026:G:N7	2.17	0.43
32:2a:1027:C:N4	32:2a:1036:G:O6	2.50	0.43
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	2.00	0.43
45:2n:32:SER:OG	45:2n:41:ARG:HB3	2.19	0.43
1:1A:346:A:OP2	5:1F:169:ASN:HB2	2.18	0.42
1:1A:861:C:H2'	1:1A:862:C:H6	1.83	0.42
1:1A:1195:G:H2'	1:1A:1196:C:C6	2.54	0.42
1:1A:1411:A:O2'	23:11:11:ARG:NH1	2.52	0.42
1:1A:1453:C:O5'	1:1A:1453:C:H6	2.02	0.42
1:1A:1848:G:OP1	3:1D:88:ARG:NH2	2.50	0.42
1:1A:2182:G:C6	1:1A:2183:C:N4	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2579:G:H2'	1:1A:2580:C:C6	2.54	0.42
7:1H:40:GLU:OE1	7:1H:60:ARG:NH1	2.52	0.42
8:1I:2:LYS:HG2	8:1I:20:ASP:OD1	2.19	0.42
10:1O:79:PHE:CD1	15:1T:72:VAL:HG22	2.54	0.42
11:1P:95:VAL:HA	11:1P:99:LEU:HD21	2.01	0.42
21:1Z:45:ASP:O	21:1Z:49:ARG:HG2	2.18	0.42
32:1a:189(F):U:H3	48:1q:72:ARG:NH1	2.17	0.42
32:1a:406:G:H5'	35:1d:5:ILE:CD1	2.43	0.42
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.34	0.42
32:1a:1314:C:H2'	32:1a:1315:U:C6	2.54	0.42
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.54	0.42
33:1b:72:GLY:HA3	33:1b:81:VAL:HG21	2.01	0.42
47:1p:20:VAL:HG23	47:1p:35:LYS:HA	2.01	0.42
1:2A:902:C:H2'	1:2A:903:C:C6	2.54	0.42
1:2A:1422:G:H1'	1:2A:1495:A:H61	1.84	0.42
2:2B:39:A:C6	2:2B:44:G:C6	3.07	0.42
9:2N:29:LYS:HD2	9:2N:140:VAL:HB	2.01	0.42
32:2a:344:A:H5''	32:2a:345:C:C5	2.51	0.42
32:2a:764:C:H2'	32:2a:765:G:O4'	2.19	0.42
32:2a:1109:C:H5''	62:2a:3344:HOH:O	2.18	0.42
33:2b:105:PHE:HA	33:2b:108:ILE:HG22	2.00	0.42
56:2y:9:A:O3'	56:2y:45:U:O2'	2.35	0.42
1:1A:701:A:H2	1:1A:702:A:C2	2.37	0.42
1:1A:762:G:H2'	1:1A:763:A:O4'	2.19	0.42
1:1A:932:C:N4	1:1A:933:C:O2	2.52	0.42
1:1A:1584:G:H2'	1:1A:1585:G:C8	2.50	0.42
1:1A:2023:A:H2'	1:1A:2024:G:C8	2.54	0.42
1:1A:2343:G:O2'	22:10:43:THR:HG22	2.19	0.42
5:1F:32:LEU:HD13	5:1F:112:MET:HE1	2.01	0.42
8:1I:106:GLY:O	8:1I:107:VAL:HG23	2.19	0.42
15:1T:11:GLU:CD	15:1T:57:PHE:HB3	2.44	0.42
16:1U:86:ALA:HB2	16:1U:116:ALA:HB2	2.00	0.42
28:16:6:ARG:HH21	28:16:24:GLU:CD	2.27	0.42
32:1a:10:A:OP2	36:1e:126:ARG:HD2	2.18	0.42
32:1a:642:A:C5	32:1a:643:C:C4	3.08	0.42
32:1a:973:G:H3'	32:1a:974:A:H5''	2.01	0.42
32:1a:977:A:H1'	32:1a:982:U:O4	2.19	0.42
32:1a:1381:U:O2'	38:1g:79:ARG:HD3	2.20	0.42
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.78	0.42
38:1g:16:LEU:HD21	40:1i:45:ALA:HB2	2.00	0.42
50:1s:31:ILE:O	50:1s:50:ALA:N	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:41:VAL:HG22	50:1s:42:PRO:HD2	2.01	0.42
54:1w:46:7MG:H3'	54:1w:47:U:H5''	2.00	0.42
1:2A:7:G:H2'	1:2A:8:A:H8	1.82	0.42
1:2A:37:C:H4'	1:2A:451:C:OP1	2.20	0.42
1:2A:150:C:H2'	1:2A:151:C:H6	1.84	0.42
1:2A:184:C:H2'	1:2A:185:U:C6	2.54	0.42
1:2A:643:A:C8	28:26:44:ARG:NH1	2.87	0.42
1:2A:1306:C:C2	1:2A:1623:G:C2	3.07	0.42
2:2B:17:C:H2'	2:2B:18:G:O4'	2.19	0.42
6:2G:11:TYR:HA	6:2G:15:VAL:HB	2.01	0.42
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	2.00	0.42
10:2O:98:VAL:HG23	10:2O:118:ALA:HA	2.01	0.42
33:2b:97:TRP:CZ3	33:2b:172:ILE:HG22	2.54	0.42
33:2b:230:VAL:HG22	33:2b:232:PRO:HD2	2.01	0.42
36:2e:51:VAL:HG23	36:2e:52:PRO:HD3	2.01	0.42
44:2m:10:PRO:CG	44:2m:13:LYS:HD2	2.49	0.42
48:2q:10:VAL:HG13	48:2q:19:VAL:HB	2.01	0.42
51:2t:66:ALA:O	51:2t:71:THR:HB	2.19	0.42
1:1A:93:G:N2	24:12:47:ASN:OD1	2.47	0.42
1:1A:2088:C:H5''	62:1A:5169:HOH:O	2.17	0.42
1:1A:2407:C:O2'	23:11:30:VAL:HG22	2.20	0.42
1:1A:2569:G:H2'	1:1A:2570:C:C6	2.54	0.42
62:1A:4704:HOH:O	30:18:42:ARG:HD2	2.18	0.42
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	2.00	0.42
16:1U:34:LYS:HA	16:1U:34:LYS:HD3	1.69	0.42
32:1a:35:G:H2'	32:1a:36:C:C6	2.53	0.42
32:1a:90:U:O2'	32:1a:91:C:OP1	2.32	0.42
32:1a:344:A:H4'	32:1a:345:C:OP2	2.19	0.42
32:1a:964:A:N3	32:1a:969:A:O2'	2.49	0.42
46:1o:8:LYS:O	46:1o:12:ILE:HG13	2.19	0.42
46:1o:39:LEU:HD22	46:1o:56:LEU:HB2	2.01	0.42
56:1y:38:A:H2'	56:1y:39:PSU:O4'	2.18	0.42
1:2A:571:A:H1'	1:2A:573:G:H5''	2.02	0.42
1:2A:952:G:C6	1:2A:966:G:C6	3.08	0.42
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.52	0.42
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.33	0.42
4:2E:60:ASN:O	4:2E:64:LYS:HB2	2.20	0.42
14:2S:24:LEU:O	14:2S:86:ALA:N	2.50	0.42
21:2Z:145:GLU:H	21:2Z:148:ASP:HB2	1.85	0.42
23:21:67:ILE:N	23:21:68:PRO:HD2	2.34	0.42
26:24:5:ILE:HG13	26:24:6:HIS:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:612:C:O2	32:2a:629:G:N2	2.52	0.42
32:2a:1029:C:C5	32:2a:1032:G:N1	2.85	0.42
32:2a:1033:G:H2'	32:2a:1034:G:H8	1.84	0.42
32:2a:1182:G:H4'	32:2a:1183:A:H5'	2.00	0.42
32:2a:1306:A:H2'	32:2a:1307:U:O4'	2.19	0.42
34:2c:152:ILE:HB	34:2c:199:LYS:HB2	2.01	0.42
40:2i:4:TYR:HD1	40:2i:87:GLN:HG2	1.85	0.42
1:1A:207:A:C2	1:1A:224:U:H4'	2.53	0.42
1:1A:215:G:N2	1:1A:217:A:H62	2.18	0.42
1:1A:354:A:HO2'	1:1A:355:A:H8	1.66	0.42
1:1A:953:U:H4'	12:1Q:101:ARG:HH22	1.84	0.42
1:1A:1576:G:H2'	1:1A:1577:C:O4'	2.19	0.42
1:1A:2078:G:H2'	1:1A:2078:G:N3	2.35	0.42
1:1A:2482:G:O6	1:1A:2488:A:O2'	2.30	0.42
1:1A:2545:A:H2'	1:1A:2546:A:O4'	2.19	0.42
1:1A:2639:G:O2'	1:1A:2794:A:N1	2.48	0.42
1:1A:2867:G:N2	1:1A:2870:A:OP2	2.44	0.42
8:1I:72:LEU:O	8:1I:74:ASN:N	2.48	0.42
17:1V:34:GLU:HB3	17:1V:56:SER:HB2	2.02	0.42
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD21	2.00	0.42
24:12:1:MET:SD	24:12:56:GLN:NE2	2.92	0.42
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.17	0.42
32:1a:1038:C:O2'	32:1a:1039:C:H5'	2.20	0.42
32:1a:1245:A:C2	32:1a:1293:G:C2	3.08	0.42
32:1a:1289:A:OP1	52:1u:10:ARG:NH2	2.50	0.42
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.55	0.42
33:1b:68:ILE:H	33:1b:90:MET:CE	2.32	0.42
35:1d:107:ARG:HD2	35:1d:173:TRP:HH2	1.84	0.42
38:1g:66:VAL:O	38:1g:70:LYS:HG3	2.19	0.42
39:1h:6:ILE:HB	39:1h:85:ARG:NH1	2.34	0.42
39:1h:20:TYR:CE2	39:1h:75:ARG:HB3	2.54	0.42
40:1i:96:LEU:HD23	40:1i:96:LEU:HA	1.85	0.42
42:1k:20:TYR:CZ	42:1k:83:ILE:HD12	2.55	0.42
42:1k:21:ILE:HG12	42:1k:30:VAL:HG22	2.02	0.42
1:2A:184:C:H2'	1:2A:185:U:H6	1.84	0.42
1:2A:271(P):C:H2'	1:2A:271(Q):G:O4'	2.18	0.42
1:2A:493:G:H2'	1:2A:494:G:O4'	2.19	0.42
1:2A:1484:G:H2'	1:2A:1485:G:H8	1.84	0.42
10:2O:80:ASP:OD2	15:2T:64:ARG:NH2	2.53	0.42
11:2P:95:VAL:HA	11:2P:99:LEU:HD21	2.00	0.42
20:2Y:97:ARG:HH11	20:2Y:107:ASP:C	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	2.01	0.42
32:2a:67:C:H2'	32:2a:68:G:H8	1.80	0.42
32:2a:195:A:N3	32:2a:222:U:O2'	2.38	0.42
32:2a:599:C:H2'	32:2a:600:C:C6	2.54	0.42
32:2a:1279:A:H5''	32:2a:1280:A:OP1	2.19	0.42
32:2a:1305:G:C2	32:2a:1331:G:N3	2.87	0.42
39:2h:35:ILE:O	39:2h:39:LEU:HD13	2.18	0.42
1:1A:559:U:H2'	1:1A:560:C:C6	2.54	0.42
1:1A:1073:A:C2	1:1A:2500:A:H5'	2.55	0.42
1:1A:1452:U:H2'	1:1A:1453:C:H6	1.85	0.42
1:1A:2161:C:C2	1:1A:2175:G:N2	2.88	0.42
1:1A:2205:C:O2'	1:1A:2206:G:OP1	2.36	0.42
4:1E:162:ALA:HB3	62:1E:407:HOH:O	2.20	0.42
5:1F:72:ARG:HE	5:1F:72:ARG:HB3	1.65	0.42
11:1P:2:LYS:HG2	11:1P:3:LEU:N	2.34	0.42
12:1Q:112:GLU:HG3	12:1Q:113:GLN:N	2.34	0.42
26:14:62:ARG:HA	26:14:62:ARG:HD3	1.69	0.42
32:1a:435:C:O5'	32:1a:435:C:H6	2.03	0.42
32:1a:944:G:O6	32:1a:1337:G:H8	2.01	0.42
32:1a:1307:U:H2'	32:1a:1308:U:C6	2.54	0.42
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.53	0.42
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.85	0.42
33:1b:47:THR:HA	33:1b:202:PRO:HG2	2.00	0.42
36:1e:41:VAL:HG11	36:1e:109:ILE:HG23	2.02	0.42
1:2A:1157:G:C6	1:2A:1158:C:C4	3.07	0.42
1:2A:1378:A:O2'	1:2A:1379:A:H5''	2.20	0.42
1:2A:1916:A:N1	32:2a:1408:A:O2'	2.43	0.42
1:2A:2109:U:O2'	1:2A:2110:G:H5'	2.19	0.42
1:2A:2124:G:C5	1:2A:2125:G:H1'	2.55	0.42
1:2A:2307:G:H8	1:2A:2307:G:OP1	2.03	0.42
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.43	0.42
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	2.00	0.42
13:2R:98:LEU:HB2	13:2R:113:LEU:HD11	2.01	0.42
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.55	0.42
32:2a:949:A:H61	32:2a:1232:U:H3	1.66	0.42
32:2a:1004:A:C2	32:2a:1038:C:C4	3.08	0.42
33:2b:32:ILE:HD13	33:2b:40:HIS:CD2	2.55	0.42
38:2g:26:PHE:O	38:2g:30:ILE:HG13	2.20	0.42
40:2i:29:ASN:ND2	40:2i:65:VAL:O	2.43	0.42
42:2k:59:TYR:O	42:2k:63:LEU:HG	2.19	0.42
42:2k:87:THR:HA	42:2k:91:ARG:NH1	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:77:THR:HG23	50:2s:78:ARG:HG2	2.00	0.42
1:1A:181:C:O2'	1:1A:849:A:N3	2.50	0.42
1:1A:753:A:OP1	3:1D:7:LYS:HE3	2.19	0.42
1:1A:1093:G:H2'	1:1A:1156:G:N2	2.27	0.42
1:1A:1769:G:H2'	1:1A:1770:A:H8	1.83	0.42
1:1A:1820:A:H2'	1:1A:1821:C:O4'	2.20	0.42
1:1A:2249:G:H5''	1:1A:2250:G:OP1	2.20	0.42
1:1A:2584:A:C8	4:1E:144:ARG:HD2	2.53	0.42
1:1A:2859:U:O4	15:1T:23:ARG:NH1	2.34	0.42
6:1G:73:ALA:HB3	6:1G:85:GLY:H	1.85	0.42
7:1H:3:ARG:HD2	7:1H:3:ARG:HA	1.73	0.42
11:1P:81:GLN:OE1	11:1P:107:LYS:N	2.46	0.42
32:1a:114:U:H1'	32:1a:353:A:H1'	2.01	0.42
32:1a:452:A:H4'	47:1p:72:ARG:HH21	1.84	0.42
32:1a:674:G:H2'	32:1a:675:A:C8	2.55	0.42
32:1a:1302:U:C5	44:1m:17:VAL:HG11	2.54	0.42
32:1a:1367:C:O2'	41:1j:62:HIS:HE1	2.02	0.42
32:1a:1502:A:H5'	32:1a:1504:G:N7	2.34	0.42
34:1c:123:GLN:HE22	34:1c:136:GLN:NE2	2.17	0.42
35:1d:9:CYS:O	35:1d:13:ARG:HG3	2.20	0.42
46:1o:41:GLU:OE2	46:1o:44:LYS:NZ	2.34	0.42
49:1r:37:VAL:O	49:1r:41:LYS:HG2	2.20	0.42
1:2A:11:G:H2'	1:2A:12:U:H5'	2.01	0.42
1:2A:320:A:H4'	1:2A:322:A:N7	2.34	0.42
1:2A:372:G:O2'	1:2A:400:G:O6	2.35	0.42
1:2A:566:U:H2'	1:2A:567:A:O4'	2.20	0.42
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.54	0.42
1:2A:1803:A:H4'	3:2D:259:THR:HG23	2.01	0.42
1:2A:2801(A):A:N3	1:2A:2895:U:O2'	2.40	0.42
10:2O:7:TYR:HD1	10:2O:7:TYR:HA	1.74	0.42
16:2U:108:GLU:O	16:2U:112:ARG:HG2	2.20	0.42
20:2Y:9:LYS:HD2	20:2Y:28:LYS:O	2.20	0.42
25:23:18:ASP:OD1	25:23:19:GLN:HG3	2.19	0.42
26:24:48:ARG:HD3	26:24:48:ARG:HA	1.70	0.42
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.55	0.42
32:2a:509:A:H2'	32:2a:510:A:C8	2.54	0.42
32:2a:715:A:H1'	32:2a:777:A:N1	2.35	0.42
32:2a:858:G:O6	32:2a:869:G:H3'	2.20	0.42
32:2a:1064:G:N2	32:2a:1190:G:H2'	2.35	0.42
32:2a:1097:C:H1'	32:2a:1170:A:H1'	2.01	0.42
32:2a:1117:G:H21	32:2a:1180:A:H1'	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:109:GLY:HA3	35:2d:165:MET:SD	2.59	0.42
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	2.01	0.42
53:2v:16:A:H2'	53:2v:17:U:O4'	2.20	0.42
54:2w:3:C:N4	54:2w:70:G:C6	2.86	0.42
1:1A:505:A:N3	1:1A:507:G:H5''	2.34	0.42
32:1a:676:A:H2'	32:1a:677:U:C6	2.54	0.42
32:1a:1004:A:H5'	32:1a:1024:G:O6	2.19	0.42
32:1a:1089:G:H1	32:1a:1096:C:N4	2.17	0.42
32:1a:1229:A:O2'	55:1x:30:G:OP1	2.35	0.42
32:1a:1371:G:O3'	40:1i:69:GLY:HA3	2.19	0.42
32:1a:1456:G:O2'	51:1t:39:LYS:HE3	2.20	0.42
33:1b:24:TRP:HZ3	33:1b:29:ALA:HB2	1.85	0.42
33:1b:91:PRO:HG2	33:1b:155:LEU:HD13	2.02	0.42
42:1k:68:ALA:HA	42:1k:71:LYS:HD2	2.02	0.42
50:1s:43:GLU:OE1	50:1s:43:GLU:N	2.52	0.42
1:2A:288:C:H2'	1:2A:289:A:H8	1.81	0.42
1:2A:296:C:H2'	1:2A:297:C:C6	2.55	0.42
1:2A:910:A:N1	1:2A:2277:G:H1'	2.35	0.42
1:2A:1376:C:H2'	1:2A:1377:G:O4'	2.20	0.42
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.55	0.42
1:2A:1529:G:C6	1:2A:1530:C:N4	2.88	0.42
1:2A:2061:G:OP1	5:2F:68:LYS:NZ	2.50	0.42
1:2A:2140:C:H2'	1:2A:2141:G:H5'	2.01	0.42
1:2A:2317:C:N4	1:2A:2318:G:O6	2.52	0.42
1:2A:2571:C:H5''	1:2A:2572:A:H5''	2.02	0.42
2:2B:30:C:OP2	14:2S:32:LEU:HD11	2.19	0.42
3:2D:175:LEU:HD12	3:2D:185:VAL:HG21	2.02	0.42
6:2G:16:ARG:CZ	6:2G:31:VAL:HG11	2.50	0.42
17:2V:10:LYS:HE2	17:2V:10:LYS:HB2	1.91	0.42
32:2a:1072:G:C6	32:2a:1073:U:C4	3.08	0.42
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.55	0.42
43:2l:113:ARG:HH21	43:2l:116:SER:HB2	1.85	0.42
46:2o:40:SER:O	46:2o:44:LYS:HG3	2.19	0.42
56:2y:41:C:H2'	56:2y:42:C:C6	2.54	0.42
1:1A:365:G:N7	62:1A:4305:HOH:O	2.36	0.42
1:1A:1074:A:N3	1:1A:2498:G:O2'	2.50	0.42
1:1A:1090:G:H5'	1:1A:1091:A:OP2	2.20	0.42
1:1A:2830:A:C5	13:1R:4:LEU:HD11	2.55	0.42
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	2.01	0.42
10:1O:24:VAL:HA	10:1O:39:ILE:HG22	2.01	0.42
23:11:2:SER:HB3	23:11:46:LEU:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:79:G:C2	32:1a:91:C:C2	3.08	0.42
32:1a:938:A:C6	32:1a:939:G:C5	3.08	0.42
32:1a:1321:C:O2'	50:1s:77:THR:HG21	2.20	0.42
33:1b:212:GLN:NE2	33:1b:235:SER:HA	2.35	0.42
35:1d:187:ARG:NH1	35:1d:193:ASP:OD2	2.45	0.42
1:2A:118:A:C8	1:2A:119:A:C8	3.08	0.42
1:2A:747:U:O2'	18:2W:92:ARG:NH1	2.53	0.42
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.84	0.42
1:2A:2168:G:H8	1:2A:2170:A:N7	2.18	0.42
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	2.02	0.42
5:2F:33:LEU:HD11	5:2F:112:MET:HB2	2.02	0.42
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.20	0.42
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CD1	2.55	0.42
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.54	0.42
25:23:23:LEU:HD12	25:23:50:VAL:HG11	2.00	0.42
32:2a:258:G:H1	32:2a:268:C:H42	1.68	0.42
32:2a:675:A:H2'	32:2a:676:A:O4'	2.20	0.42
32:2a:825:G:H2'	32:2a:826:C:C6	2.55	0.42
32:2a:1101:A:H4'	32:2a:1102:A:O5'	2.20	0.42
32:2a:1203:C:H2'	32:2a:1204:A:C8	2.52	0.42
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.34	0.42
1:1A:138:G:N3	62:1A:4151:HOH:O	2.52	0.42
1:1A:1085:G:O2'	1:1A:1086:C:H5'	2.20	0.42
1:1A:1375:U:H5''	1:1A:1376:C:C5	2.54	0.42
1:1A:1566:U:H2'	1:1A:1567:G:O4'	2.20	0.42
1:1A:2168:C:H4'	1:1A:2169:G:C4	2.55	0.42
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.34	0.42
6:1G:135:LEU:HB2	6:1G:155:MET:HG2	2.02	0.42
12:1Q:35:VAL:HG13	12:1Q:130:LYS:HB3	2.01	0.42
12:1Q:41:TRP:HB3	12:1Q:94:VAL:HG21	2.02	0.42
13:1R:45:ARG:HE	13:1R:45:ARG:HB2	1.65	0.42
32:1a:256:U:H2'	32:1a:257:G:H8	1.84	0.42
32:1a:674:G:H2'	32:1a:675:A:H8	1.84	0.42
32:1a:738:C:H2'	32:1a:739:C:C6	2.55	0.42
32:1a:1048:G:OP1	45:1n:3:ARG:HB3	2.19	0.42
32:1a:1149:C:O2'	32:1a:1280:A:N1	2.48	0.42
32:1a:1516:G:N1	32:1a:1519:MA6:OP2	2.49	0.42
33:1b:40:HIS:CB	33:1b:190:THR:HG21	2.50	0.42
37:1f:18:GLN:O	37:1f:22:GLU:HG2	2.19	0.42
41:1j:62:HIS:HB3	45:1n:59:ALA:HB3	2.01	0.42
51:1t:10:LEU:HA	51:1t:10:LEU:HD12	1.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:1y:18:G:C2	56:1y:57:G:C6	3.08	0.42
56:1y:20:U:H4'	56:1y:21:A:OP1	2.19	0.42
1:2A:55:G:H2'	1:2A:56:A:H8	1.85	0.42
1:2A:533:G:H2'	1:2A:534:U:O4'	2.19	0.42
1:2A:559:G:H22	16:2U:49:HIS:CE1	2.38	0.42
1:2A:1388:G:H4'	1:2A:1525:G:O2'	2.20	0.42
1:2A:1447:G:H2'	1:2A:1448:G:O4'	2.20	0.42
1:2A:1548:C:H2'	1:2A:1549:C:H6	1.85	0.42
1:2A:1857:G:C6	1:2A:1858:G:N1	2.88	0.42
1:2A:2164:C:H5''	1:2A:2165:G:OP2	2.20	0.42
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.20	0.42
23:21:3:LYS:HB3	23:21:4:VAL:H	1.63	0.42
28:26:34:LEU:HB2	28:26:51:GLU:HB2	2.02	0.42
32:2a:157:G:H1	32:2a:164:U:H3	1.67	0.42
41:2j:16:LEU:HB3	41:2j:70:ARG:HG3	2.01	0.42
42:2k:67:ASP:OD1	42:2k:71:LYS:HE3	2.20	0.42
43:2l:70:ILE:HD13	43:2l:77:LEU:HD12	2.02	0.42
55:2x:66:C:H2'	55:2x:67:C:O4'	2.20	0.42
1:1A:234:G:O5'	11:1P:73:GLY:HA2	2.19	0.42
11:1P:124:LYS:HA	11:1P:144:GLU:HB3	2.02	0.42
18:1W:68:ARG:HH11	18:1W:111:HIS:HA	1.85	0.42
32:1a:261:U:H2'	32:1a:263:A:OP2	2.20	0.42
32:1a:418:C:H1'	32:1a:540:G:O2'	2.20	0.42
32:1a:1518:MA6:C6	32:1a:1519:MA6:H103	2.50	0.42
34:1c:35:GLU:CD	34:1c:59:ARG:HH22	2.28	0.42
35:1d:110:PHE:CE1	35:1d:148:VAL:HG23	2.54	0.42
41:1j:49:VAL:HG23	45:1n:41:ARG:HD2	2.02	0.42
44:1m:15:VAL:O	44:1m:19:LEU:HD13	2.20	0.42
51:1t:63:ILE:HG21	51:1t:81:LYS:HG3	2.01	0.42
56:1y:53:G:N1	56:1y:61:C:N4	2.48	0.42
1:2A:1179:C:H2'	1:2A:1180:C:C6	2.54	0.42
1:2A:1828:G:OP2	1:2A:1828:G:H8	2.03	0.42
1:2A:1952:A:N3	10:2O:22:ILE:HD12	2.35	0.42
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.53	0.42
2:2B:13:A:N1	2:2B:69:G:O2'	2.42	0.42
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.20	0.42
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.60	0.42
16:2U:39:LEU:HA	16:2U:42:ALA:HB3	2.01	0.42
25:23:46:ASN:O	25:23:50:VAL:HG22	2.20	0.42
30:28:31:HIS:ND1	30:28:32:LEU:HD13	2.35	0.42
32:2a:288:A:H2'	32:2a:289:G:H4'	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1332:A:H2'	32:2a:1333:A:C8	2.55	0.42
33:2b:132:LYS:O	33:2b:136:VAL:HG23	2.19	0.42
34:2c:175:LEU:HD21	34:2c:201:TYR:CE1	2.55	0.42
38:2g:48:LYS:O	38:2g:52:GLU:HG3	2.20	0.42
2:1B:1:U:HO2'	2:1B:2:C:P	2.42	0.41
4:1E:120:TRP:CD1	4:1E:155:LYS:HB3	2.55	0.41
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	2.00	0.41
17:1V:85:LYS:HE2	17:1V:85:LYS:HB2	1.81	0.41
32:1a:163:C:H2'	32:1a:164:U:C6	2.55	0.41
32:1a:727:G:N2	32:1a:730:G:OP2	2.41	0.41
32:1a:987:G:N2	32:1a:1219:U:O2	2.52	0.41
35:1d:161:ASN:O	35:1d:165:MET:HG2	2.20	0.41
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	2.02	0.41
40:1i:19:LEU:HD23	40:1i:19:LEU:HA	1.86	0.41
1:2A:250:G:C6	1:2A:251:A:C6	3.07	0.41
1:2A:746:A:H2'	1:2A:2612:C:H5''	2.02	0.41
1:2A:900:A:HO2'	1:2A:901:A:P	2.43	0.41
1:2A:1508:A:H5'	1:2A:1509(A):A:C8	2.55	0.41
1:2A:2619:C:H2'	1:2A:2620:C:H6	1.85	0.41
1:2A:2817:G:O2'	1:2A:2836:U:O2	2.29	0.41
7:2H:84:SER:HA	7:2H:133:VAL:O	2.19	0.41
10:2O:2:ILE:O	10:2O:33:ALA:N	2.40	0.41
32:2a:93:G:C6	32:2a:96:U:C4	3.08	0.41
32:2a:386:C:H2'	32:2a:387:U:O4'	2.19	0.41
32:2a:653:A:O4'	39:2h:56:LYS:HE2	2.20	0.41
32:2a:723:U:HO2'	32:2a:724:G:H5'	1.85	0.41
32:2a:744:C:O2'	32:2a:851:G:N2	2.52	0.41
32:2a:962:C:H2'	32:2a:963:G:C8	2.56	0.41
32:2a:1016:A:O5'	32:2a:1016:A:H8	2.02	0.41
32:2a:1023:G:H8	32:2a:1023:G:OP2	2.03	0.41
32:2a:1272:G:H2'	32:2a:1273:G:O4'	2.19	0.41
32:2a:1360:A:H2'	32:2a:1361:G:C8	2.55	0.41
37:2f:98:LEU:HA	49:2r:29:PHE:O	2.20	0.41
38:2g:136:LYS:O	38:2g:140:ASP:HB2	2.20	0.41
39:2h:120:THR:H	39:2h:123:GLU:HB2	1.84	0.41
43:2l:28:LYS:HG3	43:2l:62:SER:HB2	2.02	0.41
44:2m:118:ALA:HB2	55:2x:28:C:H4'	2.01	0.41
48:2q:87:LYS:HE3	48:2q:87:LYS:HB2	1.94	0.41
54:2w:72:C:H2'	54:2w:73:A:H8	1.85	0.41
1:1A:313:A:H2'	1:1A:314:G:O4'	2.20	0.41
1:1A:402:C:H2'	1:1A:403:C:C6	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:861:C:H2'	1:1A:862:C:C6	2.56	0.41
1:1A:1207:C:O2'	17:1V:8:GLY:HA2	2.20	0.41
1:1A:1410:G:N7	23:11:3:LYS:HD2	2.35	0.41
1:1A:1540:A:H2	1:1A:1626:A:H1'	1.85	0.41
1:1A:1715:A:H4'	1:1A:1716:A:O5'	2.21	0.41
1:1A:2136:A:N6	1:1A:2141:A:H62	2.19	0.41
1:1A:2444:A:H2'	1:1A:2445:A:C8	2.55	0.41
2:1B:45:A:O4'	6:1G:95:ARG:NH1	2.53	0.41
4:1E:33:VAL:HG12	4:1E:89:ASP:O	2.19	0.41
11:1P:1:MET:HE3	11:1P:1:MET:HB3	1.95	0.41
32:1a:356:A:N7	62:1a:3339:HOH:O	2.36	0.41
32:1a:509:A:N3	32:1a:543:C:O2'	2.43	0.41
34:1c:119:ARG:O	34:1c:123:GLN:N	2.49	0.41
39:1h:20:TYR:CZ	39:1h:76:PRO:HD2	2.55	0.41
42:1k:109:VAL:HG21	49:1r:84:LYS:HD3	2.02	0.41
44:1m:91:ARG:NH2	44:1m:96:LEU:HB3	2.34	0.41
46:1o:82:ILE:HG13	46:1o:83:GLU:N	2.35	0.41
56:1y:72:C:H2'	56:1y:73:A:C8	2.56	0.41
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	2.01	0.41
1:2A:93:G:H2'	1:2A:94:C:C6	2.55	0.41
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.55	0.41
1:2A:825:C:H4'	1:2A:2428:G:N7	2.35	0.41
1:2A:1523:U:H2'	1:2A:1524:G:C8	2.55	0.41
1:2A:1530:C:H42	1:2A:1539:G:H1	1.66	0.41
1:2A:1581:G:C6	1:2A:1582:C:C4	3.08	0.41
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.21	0.41
1:2A:2390:U:P	30:28:35:GLN:HE22	2.43	0.41
1:2A:2787:C:H2'	1:2A:2788:C:H6	1.85	0.41
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.84	0.41
7:2H:89:ILE:HD11	7:2H:131:VAL:HG23	2.02	0.41
7:2H:152:ARG:HG3	7:2H:161:GLY:HA2	2.02	0.41
16:2U:47:TYR:HA	16:2U:50:ARG:NH2	2.35	0.41
32:2a:7:G:H5'	32:2a:298:A:O4'	2.19	0.41
32:2a:978:A:O2'	32:2a:1322:C:N3	2.45	0.41
32:2a:1038:C:H2'	32:2a:1039:C:H5'	2.02	0.41
34:2c:181:ASN:N	34:2c:205:GLY:O	2.34	0.41
35:2d:110:PHE:CD1	35:2d:162:LEU:HD11	2.55	0.41
37:2f:44:GLY:HA2	37:2f:59:TYR:CE1	2.55	0.41
39:2h:17:THR:HA	39:2h:65:TYR:OH	2.19	0.41
39:2h:48:TYR:HA	39:2h:60:ARG:O	2.20	0.41
54:2w:23:A:C6	54:2w:24:G:C6	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2y:64:A:H3'	56:2y:65:G:H8	1.86	0.41
1:1A:1035:G:OP2	25:13:11:SER:OG	2.33	0.41
1:1A:1091:A:O2'	1:1A:1093:G:C5	2.71	0.41
1:1A:1292:A:O2'	62:1A:4158:HOH:O	2.08	0.41
4:1E:194:GLY:HA3	62:1E:414:HOH:O	2.20	0.41
6:1G:98:ARG:CZ	26:14:1:MET:HE2	2.49	0.41
15:1T:31:SER:HB2	15:1T:85:LYS:HG2	2.02	0.41
21:1Z:30:ASN:HA	21:1Z:89:PHE:HE1	1.85	0.41
21:1Z:126:VAL:HG12	21:1Z:128:VAL:HB	2.02	0.41
32:1a:580:U:H2'	32:1a:581:G:O4'	2.20	0.41
32:1a:1144:G:C6	32:1a:1145:C:N4	2.88	0.41
32:1a:1288:A:N3	32:1a:1352:C:O2'	2.47	0.41
32:1a:1296:C:H4'	32:1a:1302:U:C4	2.55	0.41
32:1a:1359:C:OP1	45:1n:22:THR:OG1	2.32	0.41
35:1d:33:MET:CE	35:1d:37:PRO:HA	2.50	0.41
53:1v:20:U:H2'	53:1v:21:C:C6	2.55	0.41
56:1y:64:A:C2	56:1y:65:G:C5	3.08	0.41
1:2A:530:G:C5	1:2A:2022:U:H5''	2.55	0.41
1:2A:2095:C:C4	1:2A:2096:U:C4	3.09	0.41
1:2A:2136:C:HO2'	1:2A:2137:C:H6	1.65	0.41
1:2A:2182:G:H2'	1:2A:2183:C:C6	2.55	0.41
1:2A:2340:G:H2'	1:2A:2341:G:H8	1.85	0.41
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.19	0.41
4:2E:5:LEU:HD12	4:2E:51:PHE:HB2	2.02	0.41
26:24:59:PHE:C	26:24:61:ARG:H	2.29	0.41
32:2a:429:U:H1'	32:2a:430:A:H5''	2.01	0.41
32:2a:537:G:H5''	43:2l:113:ARG:HH12	1.85	0.41
32:2a:618:C:O2	32:2a:622:A:N6	2.54	0.41
32:2a:768:A:H5'	32:2a:1524:C:H1'	2.01	0.41
32:2a:1362:C:H2'	32:2a:1363:C:H5''	2.01	0.41
32:2a:1424:C:H2'	32:2a:1425:U:O4'	2.19	0.41
34:2c:57:ILE:HG12	34:2c:66:VAL:HG22	2.02	0.41
39:2h:20:TYR:CE2	39:2h:75:ARG:HD2	2.52	0.41
1:1A:94:G:H4'	24:12:45:SER:O	2.20	0.41
1:1A:604:C:OP1	16:1U:33:ARG:HG2	2.20	0.41
1:1A:1099:C:N4	1:1A:1152:G:N1	2.38	0.41
1:1A:1508:G:H2'	1:1A:1509:C:H6	1.86	0.41
1:1A:2118:U:H3	1:1A:2215:G:H1	1.69	0.41
7:1H:8:PRO:O	7:1H:10:PRO:HD3	2.21	0.41
7:1H:88:LEU:HD23	7:1H:130:ARG:HG3	2.01	0.41
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:18:62:LEU:HB3	30:18:65:GLU:HG3	2.01	0.41
32:1a:113:G:O4'	32:1a:354:G:H4'	2.20	0.41
32:1a:325:A:OP2	51:1t:70:SER:OG	2.24	0.41
32:1a:1005:A:O2'	32:1a:1036:G:N2	2.53	0.41
44:1m:89:GLY:O	44:1m:93:ARG:HG3	2.19	0.41
55:1x:53:G:H3'	55:1x:54:5MU:H73	2.03	0.41
1:2A:192:C:O2'	1:2A:802:A:N3	2.48	0.41
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.43	0.41
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.20	0.41
1:2A:2828:C:H2'	1:2A:2829:C:C6	2.56	0.41
7:2H:86:GLU:OE2	7:2H:130:ARG:HD2	2.20	0.41
7:2H:149:ARG:HA	7:2H:162:ILE:HG21	2.03	0.41
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.86	0.41
11:2P:59:LEU:HD23	30:28:13:ARG:HD2	2.02	0.41
16:2U:36:ARG:HH21	16:2U:40:PHE:HZ	1.69	0.41
19:2X:60:ARG:HH22	29:27:47:ARG:HH22	1.66	0.41
32:2a:125:U:H2'	32:2a:126:G:C8	2.55	0.41
32:2a:177:C:H2'	32:2a:178:C:C6	2.55	0.41
32:2a:627:G:H2'	32:2a:628:G:H8	1.85	0.41
32:2a:815:A:O4'	32:2a:817:C:N4	2.53	0.41
32:2a:992:U:H5''	32:2a:993:G:C5	2.55	0.41
32:2a:997:U:O2	32:2a:1044:A:N1	2.54	0.41
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.21	0.41
35:2d:13:ARG:NH2	35:2d:40:PRO:HA	2.35	0.41
50:2s:28:LYS:HE2	50:2s:46:GLY:C	2.45	0.41
1:1A:1650:C:H5''	62:1A:4957:HOH:O	2.20	0.41
1:1A:2603:C:H2'	1:1A:2604:G:H8	1.84	0.41
4:1E:144:ARG:HB3	4:1E:145:LYS:H	1.53	0.41
5:1F:70:THR:HG23	62:1F:402:HOH:O	2.19	0.41
10:1O:2:ILE:HG23	10:1O:6:THR:HG21	2.02	0.41
17:1V:95:LEU:HD22	17:1V:97:LYS:HD2	2.03	0.41
21:1Z:9:TYR:OH	21:1Z:61:LEU:HD23	2.21	0.41
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.53	0.41
26:14:16:CYS:SG	26:14:17:GLY:N	2.94	0.41
32:1a:185:A:N3	51:1t:81:LYS:NZ	2.68	0.41
32:1a:1133:G:H2'	32:1a:1134:G:O4'	2.19	0.41
32:1a:1305:G:O2'	32:1a:1306:A:OP2	2.30	0.41
32:1a:1370:G:O6	62:1a:3320:HOH:O	2.20	0.41
34:1c:6:HIS:HA	34:1c:7:PRO:HD3	1.96	0.41
35:1d:31:CYS:SG	35:1d:33:MET:HB2	2.60	0.41
1:2A:1133:U:O2'	1:2A:1137:G:OP1	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1218:C:H42	1:2A:1231:G:H1	1.69	0.41
1:2A:1669:A:O3'	1:2A:2549:G:H5''	2.21	0.41
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.03	0.41
1:2A:2410:G:C2	1:2A:2411:A:H1'	2.56	0.41
1:2A:2623:G:OP1	1:2A:2826:A:O2'	2.27	0.41
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.21	0.41
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.21	0.41
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.20	0.41
19:2X:3:THR:HG21	24:22:29:LYS:HD3	2.01	0.41
20:2Y:28:LYS:HD2	20:2Y:40:GLU:OE1	2.20	0.41
30:28:63:PRO:HG2	30:28:64:TYR:CD2	2.56	0.41
32:2a:319:G:H2'	32:2a:320:C:O4'	2.21	0.41
32:2a:509:A:H5''	35:2d:55:ALA:HB2	2.01	0.41
32:2a:555:C:H2'	32:2a:556:C:C6	2.56	0.41
32:2a:841:U:H5	32:2a:848:C:H1'	1.85	0.41
32:2a:1028:C:C4	32:2a:1033:G:O6	2.74	0.41
32:2a:1253:G:H2'	32:2a:1254:C:C6	2.55	0.41
32:2a:1326:C:H2'	32:2a:1327:C:H6	1.85	0.41
36:2e:152:ARG:HB2	39:2h:43:GLY:O	2.20	0.41
44:2m:95:GLY:O	44:2m:110:ARG:HG2	2.19	0.41
1:1A:1001:G:OP2	12:1Q:14:ARG:NH2	2.54	0.41
1:1A:1108:G:H1'	1:1A:1134:A:C8	2.55	0.41
1:1A:1527:G:C6	1:1A:1528:U:N3	2.88	0.41
1:1A:1897:C:H2'	1:1A:1898:A:O4'	2.20	0.41
1:1A:2366:G:H2'	1:1A:2367:C:H6	1.86	0.41
8:1I:2:LYS:HA	8:1I:19:VAL:O	2.20	0.41
8:1I:135:GLU:C	8:1I:137:PRO:HD3	2.46	0.41
14:1S:32:LEU:HD23	14:1S:32:LEU:HA	1.91	0.41
32:1a:551:U:H2'	32:1a:552:U:H6	1.85	0.41
32:1a:605:U:H2'	32:1a:606:G:O4'	2.21	0.41
32:1a:626:U:H2'	32:1a:627:G:C8	2.55	0.41
32:1a:814:A:H2'	32:1a:816:A:H5''	2.02	0.41
49:1r:74:ARG:HG3	49:1r:79:LEU:HB2	2.01	0.41
49:1r:76:LEU:HD12	49:1r:76:LEU:HA	1.77	0.41
1:2A:458:G:O2'	1:2A:469:G:O6	2.23	0.41
1:2A:794:G:H2'	1:2A:795:C:C6	2.55	0.41
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.50	0.41
3:2D:213:ARG:HD2	3:2D:217:ARG:O	2.21	0.41
4:2E:27:LEU:HD12	15:2T:6:LEU:CD2	2.50	0.41
7:2H:3:ARG:HG2	7:2H:6:ARG:HH11	1.85	0.41
21:2Z:36:LYS:HB2	21:2Z:36:LYS:HE3	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:64:GLY:C	26:24:66:SER:N	2.79	0.41
27:25:52:TYR:HB3	27:25:57:VAL:HG21	2.02	0.41
32:2a:373:A:O2'	32:2a:451:A:N7	2.54	0.41
32:2a:632:A:H2'	32:2a:633:G:O4'	2.20	0.41
32:2a:640:A:O2'	39:2h:115:SER:O	2.36	0.41
32:2a:1202:G:O2'	45:2n:29:ARG:HG3	2.20	0.41
41:2j:78:ASN:O	41:2j:81:THR:N	2.52	0.41
44:2m:40:ASN:HB3	44:2m:43:THR:HG23	2.03	0.41
55:2x:17:C:H2'	55:2x:17(A):U:C5	2.56	0.41
1:1A:173:C:H2'	1:1A:174:U:C6	2.55	0.41
1:1A:271:U:H1'	8:1I:50:ARG:CZ	2.51	0.41
1:1A:1550:C:H2'	1:1A:1551:C:H6	1.86	0.41
1:1A:1846:A:H8	1:1A:1846:A:OP1	2.04	0.41
1:1A:2484:G:H2'	1:1A:2487:C:H42	1.86	0.41
1:1A:2518:U:C2	1:1A:2597:U:O4	2.74	0.41
4:1E:49:LEU:N	4:1E:79:ARG:O	2.50	0.41
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	2.02	0.41
15:1T:117:ASP:OD2	15:1T:120:ARG:NE	2.36	0.41
21:1Z:120:ILE:O	21:1Z:121:HIS:ND1	2.53	0.41
32:1a:197:A:N1	32:1a:220:G:O2'	2.39	0.41
32:1a:399:G:H2'	32:1a:400:C:C6	2.55	0.41
32:1a:1179:A:H2'	32:1a:1180:A:O4'	2.21	0.41
32:1a:1202:G:O2'	45:1n:29:ARG:HG3	2.20	0.41
32:1a:1316:G:H5''	45:1n:17:LYS:HZ2	1.85	0.41
38:1g:44:TYR:HE2	40:1i:41:VAL:HG11	1.86	0.41
44:1m:9:ILE:HB	44:1m:18:ALA:HB1	2.03	0.41
1:2A:680:G:H2'	1:2A:681:G:C8	2.55	0.41
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.53	0.41
1:2A:1459:G:H2'	1:2A:1461:G:OP2	2.20	0.41
11:2P:89:ALA:O	11:2P:121:LYS:NZ	2.40	0.41
11:2P:112:LEU:HD23	11:2P:112:LEU:HA	1.86	0.41
16:2U:8:VAL:HG23	16:2U:11:ARG:NH2	2.35	0.41
29:27:26:GLY:O	29:27:30:VAL:HG23	2.21	0.41
32:2a:407:G:H5''	35:2d:115:ARG:HB3	2.03	0.41
32:2a:1052:U:O2'	32:2a:1055:A:OP2	2.20	0.41
32:2a:1095:U:N3	32:2a:1096:C:C4	2.89	0.41
32:2a:1187:G:H2'	32:2a:1188:A:C8	2.56	0.41
33:2b:68:ILE:H	33:2b:90:MET:CE	2.34	0.41
33:2b:80:ILE:HD11	33:2b:212:GLN:HA	2.02	0.41
35:2d:18:LYS:HA	35:2d:33:MET:HG3	2.02	0.41
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:26:PHE:HB2	38:2g:101:LEU:HD22	2.02	0.41
44:2m:65:LYS:O	44:2m:70:LEU:HD12	2.20	0.41
46:2o:62:GLN:NE2	46:2o:65:ARG:HD2	2.36	0.41
1:1A:759:G:C6	1:1A:760:G:C5	3.09	0.41
1:1A:878:G:O2'	11:1P:38:GLN:HB2	2.21	0.41
1:1A:1255:A:C6	1:1A:1283:A:C5	3.08	0.41
5:1F:12:LEU:HB2	5:1F:124:LEU:HD11	2.02	0.41
14:1S:49:VAL:HG22	14:1S:73:LEU:HD12	2.02	0.41
17:1V:71:LEU:HD23	17:1V:71:LEU:HA	1.90	0.41
32:1a:139:G:H2'	32:1a:140:A:H8	1.86	0.41
32:1a:601:C:H2'	32:1a:602:A:H8	1.85	0.41
34:1c:58:GLU:H	34:1c:65:ALA:HB3	1.86	0.41
34:1c:130:VAL:HG21	34:1c:157:ILE:HG23	2.03	0.41
37:1f:10:LEU:HD13	37:1f:61:LEU:HD13	2.03	0.41
37:1f:98:LEU:HA	49:1r:29:PHE:O	2.20	0.41
1:2A:768:G:C4	1:2A:769:G:C8	3.09	0.41
1:2A:799:G:C6	1:2A:800:A:C6	3.09	0.41
1:2A:851:U:OP1	25:23:49:LYS:NZ	2.44	0.41
1:2A:1639:U:O2'	1:2A:1640:C:H5'	2.20	0.41
1:2A:2685:G:P	15:2T:51:ARG:HH12	2.43	0.41
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.20	0.41
4:2E:4:ILE:HG22	4:2E:96:PHE:HE2	1.86	0.41
21:2Z:89:PHE:HE2	21:2Z:96:VAL:HG21	1.85	0.41
25:23:6:VAL:HG12	25:23:28:LEU:HD11	2.03	0.41
32:2a:129(A):G:C6	32:2a:189(H):G:H1'	2.55	0.41
32:2a:540:G:C6	32:2a:541:G:C5	3.09	0.41
32:2a:812:C:OP1	32:2a:903:G:H1'	2.21	0.41
41:2j:47:PHE:CZ	45:2n:37:PHE:HE2	2.39	0.41
42:2k:38:ASN:HA	42:2k:39:PRO:HD3	1.97	0.41
48:2q:66:SER:OG	48:2q:69:LYS:HB2	2.21	0.41
1:1A:39:C:H2'	1:1A:40:C:C6	2.55	0.41
1:1A:93:G:H2'	1:1A:94:G:O4'	2.21	0.41
1:1A:811:A:OP1	3:1D:208:LYS:NZ	2.53	0.41
1:1A:830:A:O2'	1:1A:832:G:OP1	2.33	0.41
1:1A:1121:C:H2'	1:1A:1122:C:H5'	2.02	0.41
1:1A:1143:U:O2	1:1A:1143:U:H2'	2.21	0.41
1:1A:1526:G:H1'	1:1A:1605:A:OP1	2.20	0.41
1:1A:1719:C:C2	1:1A:2594:G:H5'	2.56	0.41
1:1A:2219:U:H1'	1:1A:2220:A:C8	2.56	0.41
1:1A:2343:G:O2'	1:1A:2348:A:N1	2.50	0.41
5:1F:181:LEU:HA	5:1F:181:LEU:HD12	1.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:77:ILE:N	6:1G:82:LEU:O	2.48	0.41
8:1I:61:ARG:HD3	8:1I:61:ARG:HA	1.84	0.41
10:1O:66:LYS:HA	10:1O:79:PHE:O	2.21	0.41
11:1P:41:ARG:HH11	11:1P:41:ARG:HD3	1.72	0.41
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.91	0.41
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	2.02	0.41
21:1Z:48:PHE:CE1	21:1Z:71:VAL:HG11	2.55	0.41
21:1Z:135:GLU:HG3	21:1Z:136:PHE:H	1.85	0.41
24:12:9:GLN:HE22	24:12:56:GLN:HB3	1.86	0.41
24:12:63:VAL:O	24:12:67:LYS:HG2	2.21	0.41
27:15:49:CYS:SG	27:15:51:TYR:HB2	2.61	0.41
32:1a:115:G:H4'	32:1a:116:A:O5'	2.21	0.41
32:1a:236:G:H5''	48:1q:42:TYR:OH	2.19	0.41
32:1a:269:C:H2'	32:1a:270:A:C8	2.55	0.41
32:1a:397:A:H3'	32:1a:397:A:N3	2.35	0.41
32:1a:558:G:H8	32:1a:558:G:O5'	2.04	0.41
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.56	0.41
33:1b:70:PHE:O	33:1b:92:TYR:HA	2.21	0.41
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	2.02	0.41
33:1b:187:LEU:HA	33:1b:201:ILE:HB	2.03	0.41
34:1c:142:MET:HG3	34:1c:170:GLN:CD	2.46	0.41
35:1d:18:LYS:HE2	35:1d:31:CYS:SG	2.60	0.41
35:1d:57:ARG:HB3	35:1d:206:PHE:HB2	2.02	0.41
35:1d:110:PHE:HE1	35:1d:148:VAL:HG23	1.86	0.41
37:1f:6:VAL:HG22	37:1f:90:VAL:HG13	2.03	0.41
46:1o:48:LYS:HD2	46:1o:48:LYS:HA	1.87	0.41
48:1q:9:VAL:O	48:1q:21:VAL:HA	2.19	0.41
53:1v:16:A:H2'	53:1v:17:U:O4'	2.21	0.41
55:1x:25:C:H2'	55:1x:26:G:O4'	2.21	0.41
1:2A:127:A:H5''	1:2A:128:C:O4'	2.20	0.41
1:2A:189:G:H2'	1:2A:205:G:N2	2.36	0.41
1:2A:261:G:O2'	1:2A:610:G:O2'	2.28	0.41
1:2A:263:C:H2'	1:2A:264:C:O4'	2.21	0.41
1:2A:506:G:O3'	1:2A:507:A:H8	2.03	0.41
1:2A:948:G:H21	1:2A:985:C:P	2.44	0.41
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.69	0.41
1:2A:1263:U:C4	1:2A:1264:G:C6	3.08	0.41
1:2A:1371:G:H2'	1:2A:1372:U:C5	2.56	0.41
1:2A:1547:C:H2'	1:2A:1548:C:C6	2.56	0.41
1:2A:1721:G:H3'	1:2A:1722:A:H5''	2.02	0.41
1:2A:2138:C:H2'	1:2A:2139:C:H5''	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2160:G:H2'	1:2A:2161:C:O4'	2.20	0.41
1:2A:2543:G:H2'	1:2A:2544:G:O4'	2.21	0.41
1:2A:2576:G:OP1	62:2A:3803:HOH:O	2.22	0.41
1:2A:2689:U:H4'	1:2A:2690:C:H5'	2.03	0.41
2:2B:1:U:H2'	2:2B:2:C:C6	2.56	0.41
3:2D:233:HIS:HA	62:2D:405:HOH:O	2.19	0.41
5:2F:9:ILE:HG21	5:2F:125:LEU:HD13	2.02	0.41
5:2F:176:LEU:HD23	5:2F:176:LEU:HA	1.96	0.41
5:2F:197:ASP:O	5:2F:200:GLU:HB3	2.21	0.41
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	2.03	0.41
6:2G:41:GLN:NE2	6:2G:153:ARG:HB2	2.36	0.41
15:2T:24:PRO:HA	15:2T:49:VAL:HG23	2.02	0.41
17:2V:33:VAL:O	17:2V:58:VAL:HA	2.21	0.41
19:2X:11:PRO:HG2	19:2X:13:LEU:HD21	2.03	0.41
32:2a:243:A:H4'	32:2a:244:U:H5''	2.02	0.41
32:2a:701:C:H4'	32:2a:703:G:C8	2.55	0.41
32:2a:729:A:N1	32:2a:764:C:O2'	2.54	0.41
32:2a:757:U:O2'	32:2a:879:C:O2	2.37	0.41
32:2a:830:G:C6	32:2a:831:U:C4	3.09	0.41
32:2a:952:U:H2'	32:2a:953:G:C8	2.55	0.41
32:2a:962:C:H2'	32:2a:963:G:H8	1.85	0.41
32:2a:1434:A:H2'	32:2a:1435:G:O4'	2.21	0.41
34:2c:5:ILE:HD11	45:2n:49:HIS:CE1	2.55	0.41
34:2c:83:ARG:O	34:2c:87:LEU:HG	2.20	0.41
34:2c:110:ASN:O	34:2c:111:LEU:HD23	2.21	0.41
39:2h:49:GLU:HG3	39:2h:60:ARG:HB2	2.03	0.41
42:2k:48:ILE:H	42:2k:48:ILE:HG12	1.64	0.41
46:2o:39:LEU:O	46:2o:39:LEU:HD23	2.20	0.41
46:2o:74:ASP:OD2	46:2o:77:ARG:HB2	2.20	0.41
1:1A:806:G:OP1	62:1A:4202:HOH:O	2.22	0.41
1:1A:1335:C:H2'	1:1A:1336:C:C6	2.56	0.41
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.56	0.41
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	2.02	0.41
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.36	0.41
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.69	0.41
32:1a:404:U:O4	35:1d:2:GLY:N	2.54	0.41
32:1a:971:G:OP1	32:1a:972:C:H5''	2.21	0.41
32:1a:1176:A:H2'	32:1a:1177:G:O4'	2.20	0.41
33:1b:20:GLU:HG2	33:1b:23:ARG:HE	1.85	0.41
35:1d:176:LEU:HD12	35:1d:182:LYS:O	2.20	0.41
40:1i:18:PHE:HD2	40:1i:62:TYR:HD2	1.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1q:50:LYS:HE3	48:1q:51:TYR:CZ	2.56	0.41
49:1r:45:SER:HB3	49:1r:51:LEU:HD21	2.03	0.41
50:1s:10:PHE:HE2	50:1s:37:ARG:HG3	1.86	0.41
1:2A:77:C:H5'	24:22:59:ARG:HG2	2.03	0.41
1:2A:321:G:OP1	5:2F:135:LYS:NZ	2.51	0.41
1:2A:817:C:O2'	1:2A:839:U:OP1	2.31	0.41
1:2A:1856:G:H2'	1:2A:1857:G:O4'	2.20	0.41
1:2A:2016:U:O2'	27:25:7:PRO:O	2.37	0.41
1:2A:2198:A:O5'	8:2I:33:ARG:NH2	2.54	0.41
1:2A:2412:A:N6	1:2A:2413:G:C2	2.89	0.41
4:2E:144:ARG:HB3	4:2E:145:LYS:H	1.49	0.41
21:2Z:70:LEU:HD23	21:2Z:70:LEU:HA	1.90	0.41
33:2b:97:TRP:CZ2	33:2b:173:ALA:HA	2.56	0.41
54:2w:4:C:N4	54:2w:69:G:H1	2.18	0.41
1:1A:77:A:C2	1:1A:107:G:C2	3.09	0.40
1:1A:211:A:H5''	1:1A:448:U:OP1	2.21	0.40
1:1A:1111:U:C5	1:1A:1112:U:C4	3.09	0.40
1:1A:2225:U:O4'	3:1D:151:LYS:HE2	2.22	0.40
1:1A:2372:A:H2'	1:1A:2373:A:O4'	2.20	0.40
1:1A:2524:C:H4'	4:1E:122:PHE:CE2	2.56	0.40
1:1A:2612:A:H62	3:1D:237:GLU:HB3	1.87	0.40
1:1A:2697:G:OP2	15:1T:51:ARG:NH1	2.53	0.40
1:1A:2736:C:OP1	13:1R:3:HIS:ND1	2.34	0.40
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.50	0.40
7:1H:117:PRO:HG3	7:1H:123:PHE:CD2	2.56	0.40
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.56	0.40
12:1Q:104:PHE:HE2	12:1Q:125:LEU:HD11	1.85	0.40
15:1T:65:LYS:HG2	15:1T:66:VAL:N	2.36	0.40
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.56	0.40
32:1a:624:C:H2'	32:1a:625:G:C8	2.56	0.40
32:1a:1084:G:C5	32:1a:1085:U:C4	3.09	0.40
32:1a:1327:C:H2'	32:1a:1328:C:C6	2.56	0.40
32:1a:1349:A:OP2	40:1i:118:LYS:HE2	2.22	0.40
33:1b:188:ALA:HB1	33:1b:192:SER:OG	2.21	0.40
36:1e:92:LYS:HB3	36:1e:119:LEU:HB2	2.02	0.40
54:1w:23:A:H2'	54:1w:24:G:C8	2.56	0.40
55:1x:66:C:H2'	55:1x:67:C:O4'	2.21	0.40
1:2A:586:A:N1	1:2A:809:G:O2'	2.40	0.40
1:2A:923:C:H2'	1:2A:924:C:C6	2.56	0.40
1:2A:1003:G:N2	1:2A:1153:C:C2	2.89	0.40
1:2A:1908:C:H2'	1:2A:1909:C:H6	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:74:U:O5'	2:2B:74:U:H6	2.03	0.40
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.20	0.40
10:2O:53:LYS:N	10:2O:56:ASP:OD2	2.35	0.40
11:2P:101:VAL:HG23	11:2P:106:LEU:O	2.20	0.40
11:2P:127:ALA:HB3	11:2P:130:PHE:CE2	2.56	0.40
32:2a:18:C:H5'	36:2e:127:ASN:HD21	1.86	0.40
32:2a:921:U:O2	36:2e:19:MET:HB2	2.20	0.40
32:2a:1004:A:H62	32:2a:1037:C:H2'	1.86	0.40
32:2a:1022:G:OP1	32:2a:1022:G:H4'	2.21	0.40
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.21	0.40
32:2a:1248:A:N3	40:2i:70:LYS:HE2	2.36	0.40
41:2j:57:LYS:HE2	41:2j:60:ARG:NH2	2.37	0.40
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.21	0.40
56:2y:8:4SU:HN3	56:2y:14:A:H62	1.69	0.40
56:2y:14:A:O2'	56:2y:15:G:OP1	2.29	0.40
1:1A:121:G:H2'	1:1A:122:G:C8	2.56	0.40
1:1A:1857:G:H4'	3:1D:242:ARG:NH2	2.37	0.40
1:1A:1859:G:H4'	1:1A:1860:A:OP1	2.22	0.40
1:1A:2141:A:O2'	1:1A:2142:G:H5'	2.22	0.40
6:1G:131:TYR:HE2	6:1G:133:LEU:HD23	1.86	0.40
18:1W:7:ALA:HB2	18:1W:50:VAL:HG22	2.04	0.40
21:1Z:89:PHE:HE2	21:1Z:96:VAL:HG21	1.85	0.40
22:10:27:GLU:HB2	22:10:69:PHE:HD2	1.86	0.40
30:18:26:LYS:HB2	30:18:44:LYS:O	2.21	0.40
32:1a:198:G:C5	32:1a:220:G:C2	3.09	0.40
32:1a:271:C:H2'	32:1a:272:C:C6	2.56	0.40
32:1a:613:C:H2'	32:1a:614:A:H8	1.86	0.40
32:1a:677:U:H3	32:1a:713:G:H22	1.69	0.40
32:1a:1134:G:C2	32:1a:1141:C:C2	3.09	0.40
32:1a:1250:A:H4'	40:1i:68:GLY:N	2.36	0.40
32:1a:1503:A:H61	53:1v:12:A:H2	1.69	0.40
35:1d:61:LYS:HD2	35:1d:207:TYR:OH	2.20	0.40
44:1m:2:ALA:N	44:1m:8:GLU:OE1	2.54	0.40
47:1p:50:LYS:HD2	47:1p:50:LYS:HA	1.89	0.40
48:1q:86:GLU:O	48:1q:90:ILE:HG12	2.22	0.40
1:2A:854:G:H2'	1:2A:855:G:C8	2.55	0.40
1:2A:901:A:H2'	1:2A:902:C:C6	2.56	0.40
1:2A:1283:G:O2'	1:2A:1285:G:N7	2.48	0.40
1:2A:1314:C:OP1	62:2A:3778:HOH:O	2.22	0.40
1:2A:1579:A:C6	1:2A:1580:A:C6	3.09	0.40
11:2P:82:GLY:HA3	11:2P:115:LEU:HD11	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:93:GLY:N	11:2P:123:LEU:HD22	2.33	0.40
12:2Q:33:GLY:O	12:2Q:118:LEU:HD13	2.20	0.40
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD11	2.02	0.40
32:2a:403:C:O2'	35:2d:122:ARG:NH2	2.54	0.40
32:2a:460:G:N2	32:2a:471:G:OP2	2.50	0.40
32:2a:789:U:O2	32:2a:792:A:H8	2.04	0.40
32:2a:932:C:H5''	38:2g:4:ARG:CZ	2.51	0.40
32:2a:1053:G:N7	32:2a:1200:C:H5''	2.35	0.40
32:2a:1071:C:N4	32:2a:1104:G:H1	2.19	0.40
32:2a:1095:U:H5''	32:2a:1109:C:O2	2.21	0.40
34:2c:21:ARG:HB2	34:2c:58:GLU:HG3	2.02	0.40
35:2d:172:PRO:C	35:2d:174:LEU:H	2.29	0.40
35:2d:194:LEU:HD13	35:2d:194:LEU:HA	1.93	0.40
38:2g:29:LYS:O	38:2g:105:VAL:HG11	2.21	0.40
51:2t:92:LEU:HA	51:2t:95:ALA:HB3	2.04	0.40
1:1A:1067:A:H61	1:1A:1188:A:H61	1.69	0.40
1:1A:1201:A:OP1	16:1U:55:ARG:HD2	2.21	0.40
1:1A:1400:A:O3'	3:1D:38:LYS:HE3	2.21	0.40
1:1A:2178:G:O5'	1:1A:2178:G:H8	2.04	0.40
2:1B:12:C:H6	2:1B:12:C:O5'	2.04	0.40
2:1B:87:G:N2	2:1B:89:G:H3'	2.35	0.40
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.56	0.40
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.70	0.40
7:1H:105:LEU:HB3	7:1H:107:VAL:HG13	2.03	0.40
19:1X:47:PHE:O	19:1X:49:VAL:HG13	2.21	0.40
32:1a:45:U:H2'	32:1a:46:G:H8	1.85	0.40
32:1a:316:G:OP2	32:1a:351:G:O2'	2.38	0.40
32:1a:904:C:OP2	62:1a:3321:HOH:O	2.21	0.40
32:1a:1183:A:H3'	32:1a:1184:G:C5'	2.50	0.40
35:1d:174:LEU:HD23	35:1d:185:PHE:HA	2.03	0.40
48:1q:57:VAL:HG12	48:1q:76:LEU:HA	2.03	0.40
1:2A:49:A:H4'	1:2A:50:U:H5'	2.04	0.40
1:2A:652(A):A:H2'	1:2A:652(A):A:N3	2.35	0.40
1:2A:801:G:OP2	5:2F:55:GLY:HA2	2.21	0.40
1:2A:1354:A:H3'	1:2A:1355:G:H8	1.87	0.40
1:2A:2129:C:N3	1:2A:2159:G:N2	2.68	0.40
1:2A:2531:A:H61	1:2A:2662:A:N6	2.15	0.40
2:2B:32:C:C2	2:2B:51:G:C2	3.09	0.40
8:2I:2:LYS:NZ	8:2I:20:ASP:OD1	2.54	0.40
13:2R:63:ARG:HG2	13:2R:80:PHE:CE2	2.57	0.40
14:2S:26:LEU:HD22	14:2S:87:PHE:CD1	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:599:C:H2'	32:2a:600:C:H6	1.86	0.40
32:2a:737:A:H2'	32:2a:738:C:H6	1.86	0.40
32:2a:1003:G:C6	32:2a:1035:A:N6	2.89	0.40
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.56	0.40
40:2i:79:LEU:O	40:2i:83:ARG:HG3	2.21	0.40
56:2y:50:U:H3	56:2y:64:A:N6	2.20	0.40
1:1A:107:G:H2'	1:1A:108:G:O4'	2.21	0.40
1:1A:839:G:H5''	1:1A:840:A:H5'	2.03	0.40
1:1A:1216:G:C2	1:1A:1217:G:H1'	2.56	0.40
1:1A:1465:A:C8	1:1A:1467:G:C6	3.10	0.40
1:1A:1845:G:C6	1:1A:1846:A:C6	3.09	0.40
1:1A:2054:G:H4'	62:1A:5358:HOH:O	2.21	0.40
1:1A:2291:G:O6	22:10:14:ARG:HG3	2.21	0.40
3:1D:5:LYS:HB3	3:1D:5:LYS:HE3	1.87	0.40
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	2.04	0.40
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG13	2.03	0.40
21:1Z:105:VAL:O	21:1Z:141:VAL:HG22	2.22	0.40
27:15:8:LYS:HA	27:15:8:LYS:HD2	1.95	0.40
32:1a:526:C:OP2	43:1l:91:LYS:HE3	2.21	0.40
32:1a:666:G:H5'	32:1a:726:C:H1'	2.04	0.40
32:1a:1144:G:N2	32:1a:1146:A:H62	2.19	0.40
34:1c:189:ALA:HB3	34:1c:196:LEU:HB2	2.03	0.40
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	2.02	0.40
40:1i:85:LEU:HB3	40:1i:92:TYR:HD2	1.87	0.40
46:1o:18:PHE:CZ	46:1o:21:ASP:HB3	2.57	0.40
47:1p:18:ARG:HD3	47:1p:35:LYS:HD3	2.04	0.40
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.55	0.40
54:1w:2:C:N3	54:1w:71:G:C6	2.90	0.40
54:1w:38:A:H2'	54:1w:39:PSU:O4'	2.21	0.40
1:2A:298:G:H5''	1:2A:299:A:OP1	2.21	0.40
1:2A:1011:G:C2	1:2A:1013:C:C2	3.10	0.40
1:2A:2032:G:H1'	4:2E:145:LYS:HD3	2.02	0.40
1:2A:2070:G:H2'	1:2A:2071:A:O4'	2.22	0.40
1:2A:2466:C:OP1	31:29:4:ARG:HB2	2.21	0.40
2:2B:119:G:C6	2:2B:120:A:C6	3.10	0.40
7:2H:98:LEU:HB2	7:2H:125:VAL:HG22	2.03	0.40
10:2O:76:ALA:O	15:2T:74:ARG:HG3	2.22	0.40
32:2a:171:A:H2'	32:2a:172:A:C8	2.57	0.40
32:2a:778:G:H2'	32:2a:779:C:O4'	2.22	0.40
32:2a:827:U:C2	32:2a:874:G:N2	2.90	0.40
32:2a:1060:C:C5	34:2c:2:GLY:HA3	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1176:A:H3'	32:2a:1177:G:H8	1.85	0.40
33:2b:83:MET:HB3	33:2b:234:PRO:HG3	2.02	0.40
35:2d:158:ILE:O	35:2d:162:LEU:HB2	2.21	0.40
41:2j:6:ILE:O	41:2j:71:LEU:HD12	2.21	0.40
44:2m:82:MET:HE3	44:2m:92:HIS:HB3	2.04	0.40
45:2n:24:CYS:HB3	45:2n:29:ARG:H	1.86	0.40
46:2o:12:ILE:HG23	46:2o:27:VAL:HG11	2.04	0.40
47:2p:26:ARG:HG3	47:2p:27:LYS:N	2.37	0.40
55:2x:14:A:H8	55:2x:14:A:H5''	1.87	0.40
1:1A:747:G:O2'	1:1A:1679:A:N3	2.52	0.40
1:1A:1102:G:H21	1:1A:1149:A:H62	1.68	0.40
1:1A:2094:G:H2'	1:1A:2095:C:O4'	2.21	0.40
10:1O:70:LYS:HB3	10:1O:70:LYS:HE2	1.96	0.40
11:1P:93:GLY:H	11:1P:123:LEU:HD22	1.87	0.40
12:1Q:56:ARG:HD2	12:1Q:56:ARG:HA	1.92	0.40
15:1T:26:ASP:O	15:1T:49:VAL:HG22	2.21	0.40
15:1T:28:VAL:HG13	15:1T:86:ILE:HG23	2.04	0.40
16:1U:33:ARG:HG2	16:1U:33:ARG:H	1.57	0.40
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.56	0.40
29:17:47:ARG:HE	29:17:47:ARG:HB3	1.43	0.40
34:1c:12:LEU:HD23	34:1c:12:LEU:HA	1.95	0.40
35:1d:20:TYR:CD1	35:1d:26:CYS:HB3	2.57	0.40
37:1f:12:PRO:HG3	37:1f:57:GLN:O	2.22	0.40
38:1g:144:MET:HE3	38:1g:144:MET:HB3	1.93	0.40
39:1h:52:ASP:HA	39:1h:56:LYS:O	2.20	0.40
40:1i:85:LEU:O	40:1i:88:TYR:HB3	2.21	0.40
1:2A:176:G:O2'	1:2A:177:G:H5'	2.22	0.40
1:2A:321:G:O2'	1:2A:340:A:N3	2.50	0.40
1:2A:391:G:C2	1:2A:411:G:C5	3.09	0.40
1:2A:563:G:H21	16:2U:37:GLU:CD	2.29	0.40
1:2A:709:U:H2'	1:2A:710:G:H8	1.85	0.40
1:2A:836:G:C5	1:2A:837:C:C4	3.09	0.40
1:2A:857:C:H1'	22:20:26:TYR:CE1	2.56	0.40
1:2A:1011:G:H1'	1:2A:1013:C:O4'	2.22	0.40
1:2A:1262:A:H2	27:25:10:LYS:HD2	1.86	0.40
1:2A:1813:G:H1'	3:2D:50:THR:OG1	2.21	0.40
1:2A:1920:4OC:O2'	32:2a:1496:C:H4'	2.21	0.40
1:2A:2315:G:H2'	1:2A:2316:C:H6	1.84	0.40
1:2A:2756:U:H4'	1:2A:2757:A:OP1	2.20	0.40
2:2B:3:C:H2'	2:2B:4:C:H6	1.87	0.40
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:72:LEU:C	8:2I:74:ASN:N	2.77	0.40
14:2S:106:ARG:NE	14:2S:112:PHE:OXT	2.51	0.40
23:21:83:GLU:C	23:21:85:LEU:H	2.29	0.40
25:23:8:LEU:HD23	25:23:8:LEU:HA	1.82	0.40
32:2a:671:G:H2'	32:2a:672:U:H6	1.86	0.40
32:2a:1106:G:H2'	32:2a:1107:C:C6	2.57	0.40
32:2a:1347:G:H22	32:2a:1374:A:P	2.44	0.40
33:2b:200:ILE:HG22	33:2b:202:PRO:HD3	2.04	0.40
41:2j:13:HIS:HB3	41:2j:68:HIS:CD2	2.56	0.40
47:2p:19:ILE:N	47:2p:37:GLY:O	2.54	0.40
47:2p:28:ARG:NH1	47:2p:29:ASP:OD2	2.43	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	13 (5%)	2 (1%)	18	38
3	2D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	30	51
4	1E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	12	28
4	2E	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	12	28
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	24	46
5	2F	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	12	28
6	1G	179/182 (98%)	164 (92%)	13 (7%)	2 (1%)	11	25
6	2G	179/182 (98%)	172 (96%)	7 (4%)	0	100	100
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	42
7	2H	172/180 (96%)	162 (94%)	7 (4%)	3 (2%)	7	15
8	1I	144/148 (97%)	126 (88%)	13 (9%)	5 (4%)	3	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	2I	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	9	19
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	38
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	38
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
13	2R	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	125 (97%)	2 (2%)	2 (2%)	7	16
15	2T	129/146 (88%)	122 (95%)	6 (5%)	1 (1%)	16	34
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
17	2V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
19	2X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	11	25
20	1Y	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
21	1Z	148/206 (72%)	131 (88%)	14 (10%)	3 (2%)	6	12
21	2Z	156/206 (76%)	136 (87%)	17 (11%)	3 (2%)	6	13
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	25
23	21	95/98 (97%)	94 (99%)	0	1 (1%)	11	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	52 (78%)	11 (16%)	4 (6%)	1	1
26	24	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	203 (89%)	21 (9%)	5 (2%)	5	10
33	2b	229/256 (90%)	202 (88%)	21 (9%)	6 (3%)	4	7
34	1c	204/239 (85%)	196 (96%)	7 (3%)	1 (0%)	24	46
34	2c	204/239 (85%)	192 (94%)	11 (5%)	1 (0%)	24	46
35	1d	206/209 (99%)	196 (95%)	8 (4%)	2 (1%)	12	28
35	2d	206/209 (99%)	195 (95%)	8 (4%)	3 (2%)	8	18
36	1e	146/162 (90%)	138 (94%)	6 (4%)	2 (1%)	9	19
36	2e	146/162 (90%)	138 (94%)	6 (4%)	2 (1%)	9	19
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	9	21
38	2g	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	6	12
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
40	1i	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	7	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	2i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16	34
41	1j	95/105 (90%)	86 (90%)	8 (8%)	1 (1%)	11	25
41	2j	94/105 (90%)	81 (86%)	12 (13%)	1 (1%)	11	25
42	1k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	6	14
42	2k	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	6	14
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	10 (8%)	0	100	100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	56 (97%)	0	2 (3%)	3	4
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	21
47	2p	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	9	21
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
51	1t	94/106 (89%)	86 (92%)	7 (7%)	1 (1%)	11	25
51	2t	94/106 (89%)	86 (92%)	7 (7%)	1 (1%)	11	25
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11370/12128 (94%)	10678 (94%)	605 (5%)	87 (1%)	16	34

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
8	1I	117	GLU
21	1Z	152	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	11	3	LYS
26	14	55	ARG
33	1b	22	LYS
35	1d	168	ARG
40	1i	54	ASP
5	2F	130	ALA
8	2I	107	VAL
21	2Z	152	ALA
26	24	56	VAL
33	2b	10	LEU
33	2b	22	LYS
35	2d	168	ARG
40	2i	54	ASP
4	1E	71	GLY
26	14	65	ASP
36	1e	85	GLY
41	1j	29	ARG
42	1k	49	GLY
4	2E	71	GLY
7	2H	47	GLU
23	21	3	LYS
26	24	65	ASP
33	2b	123	ALA
35	2d	173	TRP
36	2e	85	GLY
38	2g	52	GLU
3	1D	3	VAL
8	1I	42	SER
15	1T	127	ALA
26	14	64	GLY
33	1b	10	LEU
33	1b	17	PHE
40	1i	107	ARG
47	1p	53	VAL
11	2P	29	LYS
21	2Z	2	GLU
26	24	45	GLY
26	24	64	GLY
35	2d	3	ARG
36	2e	27	ARG
42	2k	49	GLY
47	2p	53	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1D	275	LYS
4	1E	52	LEU
6	1G	51	ARG
8	1I	105	HIS
8	1I	107	VAL
33	1b	126	GLU
35	1d	5	ILE
4	2E	52	LEU
19	2X	94	GLY
33	2b	124	SER
45	2n	3	ARG
15	1T	128	GLU
21	1Z	2	GLU
26	14	57	GLU
33	1b	20	GLU
34	1c	66	VAL
38	1g	81	GLY
3	2D	3	VAL
7	2H	92	ILE
21	2Z	172	ALA
33	2b	128	GLU
34	2c	66	VAL
38	2g	54	THR
51	2t	100	ILE
6	1G	42	GLY
8	1I	73	GLU
11	1P	29	LYS
38	1g	55	GLY
5	2F	89	VAL
8	2I	85	GLU
33	2b	20	GLU
41	2j	55	LYS
7	1H	92	ILE
36	1e	69	VAL
42	1k	105	VAL
51	1t	100	ILE
38	2g	81	GLY
21	1Z	134	PRO
45	2n	14	PRO
15	2T	37	GLY
7	2H	126	PRO
42	2k	105	VAL

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%)	208 (97%)	7 (3%)	33	61
3	2D	215/218 (99%)	207 (96%)	8 (4%)	30	57
4	1E	164/166 (99%)	153 (93%)	11 (7%)	15	33
4	2E	164/166 (99%)	154 (94%)	10 (6%)	17	37
5	1F	160/166 (96%)	151 (94%)	9 (6%)	19	40
5	2F	159/166 (96%)	153 (96%)	6 (4%)	29	56
6	1G	144/156 (92%)	136 (94%)	8 (6%)	19	40
6	2G	143/156 (92%)	140 (98%)	3 (2%)	47	73
7	1H	144/148 (97%)	142 (99%)	2 (1%)	59	81
7	2H	144/148 (97%)	143 (99%)	1 (1%)	76	89
8	1I	113/124 (91%)	109 (96%)	4 (4%)	32	59
8	2I	105/124 (85%)	100 (95%)	5 (5%)	23	47
9	1N	118/119 (99%)	112 (95%)	6 (5%)	21	45
9	2N	118/119 (99%)	115 (98%)	3 (2%)	42	69
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	46
10	2O	100/100 (100%)	99 (99%)	1 (1%)	68	86
11	1P	115/116 (99%)	112 (97%)	3 (3%)	40	68
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26	51
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	24	50
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	39	67
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	20
13	2R	101/101 (100%)	96 (95%)	5 (5%)	22	46
14	1S	86/88 (98%)	84 (98%)	2 (2%)	44	71
14	2S	85/88 (97%)	85 (100%)	0	100	100
15	1T	115/127 (91%)	112 (97%)	3 (3%)	40	68
15	2T	113/127 (89%)	112 (99%)	1 (1%)	70	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	35
16	2U	93/94 (99%)	93 (100%)	0	100	100
17	1V	80/82 (98%)	74 (92%)	6 (8%)	12	28
17	2V	80/82 (98%)	78 (98%)	2 (2%)	42	69
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	40
18	2W	90/92 (98%)	88 (98%)	2 (2%)	45	72
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21	44
19	2X	77/78 (99%)	77 (100%)	0	100	100
20	1Y	85/91 (93%)	83 (98%)	2 (2%)	43	70
20	2Y	85/91 (93%)	84 (99%)	1 (1%)	63	83
21	1Z	135/179 (75%)	134 (99%)	1 (1%)	76	89
21	2Z	137/179 (76%)	135 (98%)	2 (2%)	57	80
22	10	65/67 (97%)	64 (98%)	1 (2%)	57	80
22	20	65/67 (97%)	65 (100%)	0	100	100
23	11	80/83 (96%)	76 (95%)	4 (5%)	22	46
23	21	80/83 (96%)	78 (98%)	2 (2%)	42	69
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	49 (96%)	2 (4%)	28	55
25	23	50/52 (96%)	48 (96%)	2 (4%)	28	55
26	14	59/63 (94%)	56 (95%)	3 (5%)	21	45
26	24	53/63 (84%)	52 (98%)	1 (2%)	50	75
27	15	50/52 (96%)	48 (96%)	2 (4%)	28	55
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	37
28	16	51/52 (98%)	49 (96%)	2 (4%)	28	55
28	26	50/52 (96%)	49 (98%)	1 (2%)	48	74
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	17
29	27	41/42 (98%)	39 (95%)	2 (5%)	22	47
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	40
30	28	54/55 (98%)	53 (98%)	1 (2%)	50	75
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	187 (97%)	5 (3%)	40	68
33	2b	187/220 (85%)	184 (98%)	3 (2%)	55	79
34	1c	142/188 (76%)	137 (96%)	5 (4%)	32	59
34	2c	140/188 (74%)	137 (98%)	3 (2%)	47	73
35	1d	169/181 (93%)	167 (99%)	2 (1%)	63	83
35	2d	173/181 (96%)	172 (99%)	1 (1%)	78	91
36	1e	113/123 (92%)	108 (96%)	5 (4%)	25	50
36	2e	114/123 (93%)	111 (97%)	3 (3%)	40	68
37	1f	84/90 (93%)	81 (96%)	3 (4%)	31	58
37	2f	85/90 (94%)	84 (99%)	1 (1%)	63	83
38	1g	119/127 (94%)	118 (99%)	1 (1%)	73	88
38	2g	120/127 (94%)	118 (98%)	2 (2%)	53	78
39	1h	114/119 (96%)	110 (96%)	4 (4%)	32	59
39	2h	114/119 (96%)	113 (99%)	1 (1%)	70	87
40	1i	90/99 (91%)	86 (96%)	4 (4%)	25	50
40	2i	89/99 (90%)	86 (97%)	3 (3%)	32	60
41	1j	66/92 (72%)	62 (94%)	4 (6%)	17	37
41	2j	69/92 (75%)	66 (96%)	3 (4%)	26	51
42	1k	82/99 (83%)	81 (99%)	1 (1%)	63	83
42	2k	83/99 (84%)	82 (99%)	1 (1%)	63	83
43	1l	96/108 (89%)	94 (98%)	2 (2%)	47	73
43	2l	96/108 (89%)	95 (99%)	1 (1%)	68	86
44	1m	93/101 (92%)	92 (99%)	1 (1%)	65	84
44	2m	92/101 (91%)	92 (100%)	0	100	100
45	1n	49/50 (98%)	48 (98%)	1 (2%)	48	74
45	2n	49/50 (98%)	48 (98%)	1 (2%)	48	74
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	77 (99%)	1 (1%)	61	82
47	1p	69/74 (93%)	67 (97%)	2 (3%)	37	65
47	2p	68/74 (92%)	66 (97%)	2 (3%)	37	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	93 (99%)	1 (1%)	65	84
48	2q	94/97 (97%)	94 (100%)	0	100	100
49	1r	59/77 (77%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	68 (99%)	1 (1%)	59	81
50	2s	67/80 (84%)	65 (97%)	2 (3%)	36	64
51	1t	70/82 (85%)	70 (100%)	0	100	100
51	2t	70/82 (85%)	69 (99%)	1 (1%)	59	81
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9304/10064 (92%)	9042 (97%)	262 (3%)	38	66

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	111	LEU
3	1D	142	VAL
3	1D	176	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	12	THR
4	1E	21	VAL
4	1E	33	VAL
4	1E	34	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	78	LEU
4	1E	116	VAL
4	1E	144	ARG
4	1E	175	VAL
4	1E	188	VAL
5	1F	57	VAL
5	1F	70	THR
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	5	VAL
6	1G	7	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	70	VAL
6	1G	126	ASP
6	1G	139	LEU
6	1G	175	LEU
7	1H	71	LEU
7	1H	141	VAL
8	1I	92	VAL
8	1I	107	VAL
8	1I	109	ILE
8	1I	127	VAL
9	1N	1	MET
9	1N	14	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	112	LEU
10	1O	7	TYR
10	1O	10	VAL
10	1O	24	VAL
10	1O	28	SER
10	1O	39	ILE
11	1P	95	VAL
11	1P	99	LEU
11	1P	112	LEU
12	1Q	8	LYS
12	1Q	35	VAL
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	111	GLU
13	1R	6	SER
13	1R	18	LEU
13	1R	28	LEU
13	1R	29	LEU
13	1R	36	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1R	44	LEU
13	1R	96	ARG
13	1R	111	LEU
13	1R	114	VAL
14	1S	27	SER
14	1S	49	VAL
15	1T	28	VAL
15	1T	59	THR
15	1T	89	VAL
16	1U	8	VAL
16	1U	31	SER
16	1U	52	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	78	THR
17	1V	39	LEU
17	1V	51	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	107	LEU
19	1X	35	THR
19	1X	70	LEU
19	1X	76	ARG
19	1X	95	LEU
20	1Y	72	VAL
20	1Y	85	VAL
21	1Z	155	LEU
22	10	39	ARG
23	11	4	VAL
23	11	30	VAL
23	11	59	THR
23	11	85	LEU
25	13	54	VAL
25	13	60	GLU
26	14	1	MET
26	14	49	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	56	VAL
27	15	6	VAL
27	15	58	LEU
28	16	9	LEU
28	16	48	VAL
29	17	34	ARG
29	17	43	THR
29	17	46	VAL
29	17	47	ARG
30	18	14	VAL
30	18	30	ARG
30	18	32	LEU
31	19	1	MET
31	19	17	ILE
33	1b	112	VAL
33	1b	127	ILE
33	1b	142	LEU
33	1b	221	LEU
33	1b	229	VAL
34	1c	3	ASN
34	1c	49	SER
34	1c	77	ILE
34	1c	152	ILE
34	1c	206	GLU
35	1d	83	SER
35	1d	135	LEU
36	1e	5	ASP
36	1e	20	GLN
36	1e	34	VAL
36	1e	41	VAL
36	1e	51	VAL
37	1f	40	VAL
37	1f	70	ASP
37	1f	75	LEU
38	1g	104	LEU
39	1h	51	VAL
39	1h	104	ARG
39	1h	112	LEU
39	1h	127	LEU
40	1i	50	LEU
40	1i	53	VAL
40	1i	103	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	1i	128	ARG
41	1j	38	ILE
41	1j	49	VAL
41	1j	67	THR
41	1j	92	THR
42	1k	41	THR
43	1l	83	VAL
43	1l	84	LEU
44	1m	25	ILE
45	1n	33	VAL
47	1p	20	VAL
47	1p	67	THR
48	1q	9	VAL
50	1s	78	ARG
3	2D	94	LEU
3	2D	111	LEU
3	2D	138	VAL
3	2D	173	VAL
3	2D	176	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
4	2E	21	VAL
4	2E	33	VAL
4	2E	34	VAL
4	2E	73	GLU
4	2E	75	VAL
4	2E	116	VAL
4	2E	144	ARG
4	2E	175	VAL
4	2E	181	LEU
4	2E	188	VAL
5	2F	57	VAL
5	2F	70	THR
5	2F	88	VAL
5	2F	132	VAL
5	2F	158	THR
5	2F	183	VAL
6	2G	5	VAL
6	2G	7	LEU
6	2G	175	LEU
7	2H	107	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2I	77	LEU
8	2I	92	VAL
8	2I	107	VAL
8	2I	127	VAL
8	2I	144	VAL
9	2N	14	VAL
9	2N	58	ASP
9	2N	120	LEU
10	2O	24	VAL
11	2P	45	LEU
11	2P	56	SER
11	2P	95	VAL
11	2P	106	LEU
11	2P	112	LEU
12	2Q	42	ILE
12	2Q	75	THR
12	2Q	109	VAL
13	2R	28	LEU
13	2R	29	LEU
13	2R	60	LEU
13	2R	65	LEU
13	2R	111	LEU
15	2T	28	VAL
17	2V	61	VAL
17	2V	72	VAL
18	2W	23	LEU
18	2W	107	LEU
20	2Y	72	VAL
21	2Z	56	VAL
21	2Z	146	ILE
23	21	4	VAL
23	21	85	LEU
25	23	8	LEU
25	23	54	VAL
26	24	49	PHE
27	25	6	VAL
27	25	19	ARG
27	25	29	THR
28	26	48	VAL
29	27	34	ARG
29	27	43	THR
30	28	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	112	VAL
33	2b	221	LEU
33	2b	229	VAL
34	2c	3	ASN
34	2c	70	VAL
34	2c	206	GLU
35	2d	135	LEU
36	2e	20	GLN
36	2e	41	VAL
36	2e	51	VAL
37	2f	72	VAL
38	2g	50	ILE
38	2g	75	VAL
39	2h	127	LEU
40	2i	50	LEU
40	2i	53	VAL
40	2i	128	ARG
41	2j	38	ILE
41	2j	67	THR
41	2j	74	ILE
42	2k	48	ILE
43	2l	122	THR
45	2n	33	VAL
46	2o	21	ASP
47	2p	20	VAL
47	2p	67	THR
50	2s	41	VAL
50	2s	67	VAL
51	2t	56	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
4	1E	121	ASN
5	1F	8	GLN
6	1G	41	GLN
6	1G	79	ASN
6	1G	132	ASN
9	1N	38	HIS
9	1N	94	HIS
11	1P	70	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	1Q	12	GLN
12	1Q	123	HIS
12	1Q	141	GLN
13	1R	24	GLN
13	1R	71	GLN
15	1T	58	ASN
19	1X	31	HIS
19	1X	82	GLN
21	1Z	32	HIS
21	1Z	65	GLN
21	1Z	132	ASN
21	1Z	151	HIS
22	10	3	HIS
22	10	50	ASN
25	13	32	GLN
33	1b	16	HIS
33	1b	40	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	69	HIS
34	1c	104	GLN
34	1c	123	GLN
34	1c	139	GLN
34	1c	181	ASN
35	1d	77	ASN
35	1d	161	ASN
35	1d	201	GLN
36	1e	20	GLN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	64	GLN
38	1g	86	GLN
38	1g	96	GLN
38	1g	97	GLN
38	1g	106	GLN
40	1i	31	GLN
40	1i	58	HIS
40	1i	73	GLN
40	1i	89	ASN
40	1i	117	HIS
40	1i	124	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1j	56	HIS
42	1k	116	HIS
43	1l	99	HIS
45	1n	49	HIS
46	1o	62	GLN
48	1q	26	GLN
50	1s	23	ASN
50	1s	69	HIS
50	1s	83	HIS
51	1t	75	ASN
3	2D	96	HIS
3	2D	116	GLN
3	2D	166	GLN
5	2F	75	HIS
5	2F	160	ASN
5	2F	203	GLN
7	2H	158	HIS
9	2N	56	ASN
9	2N	69	GLN
12	2Q	12	GLN
12	2Q	13	GLN
12	2Q	57	HIS
12	2Q	123	HIS
13	2R	24	GLN
13	2R	50	HIS
13	2R	71	GLN
14	2S	84	GLN
14	2S	95	HIS
15	2T	58	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	32	HIS
21	2Z	151	HIS
22	20	3	HIS
24	22	56	GLN
24	22	65	ASN
25	23	32	GLN
30	28	35	GLN
33	2b	40	HIS
33	2b	78	GLN
33	2b	95	GLN
33	2b	113	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	212	GLN
34	2c	6	HIS
34	2c	37	GLN
34	2c	102	ASN
34	2c	162	GLN
34	2c	170	GLN
35	2d	77	ASN
35	2d	201	GLN
36	2e	20	GLN
37	2f	64	GLN
37	2f	73	ASN
37	2f	100	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	73	GLN
40	2i	124	GLN
41	2j	21	GLN
41	2j	56	HIS
41	2j	84	GLN
43	2l	99	HIS
45	2n	49	HIS
46	2o	62	GLN
48	2q	26	GLN
49	2r	63	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	433 (15%)	33 (1%)
1	2A	2791/2915 (95%)	483 (17%)	26 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1497/1521 (98%)	250 (16%)	0
32	2a	1501/1521 (98%)	251 (16%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	71/76 (93%)	16 (22%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	2w	68/76 (89%)	20 (29%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	8 (10%)	0
56	1y	72/76 (94%)	22 (30%)	0
56	2y	70/76 (92%)	21 (30%)	0
All	All	9344/9620 (97%)	1555 (16%)	60 (0%)

All (1555) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	57	G
1	1A	63	A
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	89	U
1	1A	90	A
1	1A	92	C
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	138	G
1	1A	170	A
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	218	A
1	1A	219	U
1	1A	222	A
1	1A	237	G
1	1A	255	G
1	1A	258	U
1	1A	271	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	279	G
1	1A	288	U
1	1A	289	G
1	1A	299	G
1	1A	303	C
1	1A	305	G
1	1A	307	A
1	1A	326	C
1	1A	335	A
1	1A	348	A
1	1A	353	G
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	389	G
1	1A	399	G
1	1A	407	U
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	445	G
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	482	C
1	1A	483	A
1	1A	505	A
1	1A	507	G
1	1A	516	G
1	1A	529	U
1	1A	530	A
1	1A	534	C
1	1A	537	G
1	1A	553	A
1	1A	555	G
1	1A	556	C
1	1A	557	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	609	A
1	1A	615	G
1	1A	617	U
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	633	G
1	1A	636	G
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	697	C
1	1A	699	C
1	1A	733	G
1	1A	777	C
1	1A	787	U
1	1A	793	A
1	1A	794	U
1	1A	811	A
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	866	A
1	1A	874	U
1	1A	875	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	877	G
1	1A	906	G
1	1A	913	A
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	937	A
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	945	A
1	1A	956	A
1	1A	972	A
1	1A	977	G
1	1A	986	A
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1071	G
1	1A	1072	U
1	1A	1079	U
1	1A	1084	C
1	1A	1090	G
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1101	G
1	1A	1104	G
1	1A	1109	G
1	1A	1114	G
1	1A	1117	G
1	1A	1118	C
1	1A	1119	A
1	1A	1121	C
1	1A	1123	A
1	1A	1124	U
1	1A	1125	C
1	1A	1126	C
1	1A	1134	A
1	1A	1136	U
1	1A	1137	G
1	1A	1140	U
1	1A	1142	A
1	1A	1145	G
1	1A	1147	U
1	1A	1148	C
1	1A	1155	C
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1255	A
1	1A	1256	U
1	1A	1265	A
1	1A	1277	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1319	U
1	1A	1322	A
1	1A	1346	U
1	1A	1347	A
1	1A	1364	C
1	1A	1366	C
1	1A	1375	U
1	1A	1380	G
1	1A	1391	C
1	1A	1394	G
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1416	C
1	1A	1430	A
1	1A	1431	G
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1483	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1506	G
1	1A	1513	G
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1539	C
1	1A	1555	C
1	1A	1556	A
1	1A	1590	C
1	1A	1601	A
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1626	A
1	1A	1627	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1656	A
1	1A	1695	C
1	1A	1700	G
1	1A	1701	A
1	1A	1721	G
1	1A	1747	A
1	1A	1750	G
1	1A	1767	A
1	1A	1776	G
1	1A	1781	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1859	G
1	1A	1870	G
1	1A	1878	A
1	1A	1890	A
1	1A	1899	A
1	1A	1922	A
1	1A	1928	G
1	1A	1935	A
1	1A	1951	G
1	1A	1952	G
1	1A	1960	A
1	1A	1977	U
1	1A	1982	A
1	1A	1985	U
1	1A	1987	C
1	1A	1989	C
1	1A	1992	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1993	A
1	1A	1994	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2045	G
1	1A	2053	A
1	1A	2055	A
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2091	G
1	1A	2115	G
1	1A	2118	U
1	1A	2121	U
1	1A	2123	G
1	1A	2124	U
1	1A	2134	G
1	1A	2135	U
1	1A	2137	G
1	1A	2138	G
1	1A	2139	A
1	1A	2141	A
1	1A	2142	G
1	1A	2143	G
1	1A	2149	G
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2160	C
1	1A	2162	C
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2173	G
1	1A	2175	G
1	1A	2177	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2180	A
1	1A	2181	G
1	1A	2188	G
1	1A	2193	A
1	1A	2194	U
1	1A	2195	A
1	1A	2204	G
1	1A	2206	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2281	A
1	1A	2287	C
1	1A	2295	C
1	1A	2299	A
1	1A	2300	A
1	1A	2317	A
1	1A	2320	G
1	1A	2324	U
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2373	A
1	1A	2380	C
1	1A	2391	G
1	1A	2395	G
1	1A	2397	C
1	1A	2403	G
1	1A	2417	G
1	1A	2418	U
1	1A	2419	G
1	1A	2422	G
1	1A	2436	C
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2443	U
1	1A	2444	A
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2461	U
1	1A	2486	C
1	1A	2488	A
1	1A	2489	C
1	1A	2490	A
1	1A	2506	G
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2532	C
1	1A	2541	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2581	G
1	1A	2584	A
1	1A	2585	C
1	1A	2594	G
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2691	A
1	1A	2701	U
1	1A	2702	C
1	1A	2703	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2736	C
1	1A	2737	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2771	A
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2803	A
1	1A	2805	G
1	1A	2807	C
1	1A	2813	G
1	1A	2818	U
1	1A	2828	G
1	1A	2830	A
1	1A	2831	A
1	1A	2844	G
1	1A	2868	C
1	1A	2876	U
1	1A	2882	G
1	1A	2883	A
1	1A	2901	A
1	1A	2903	G
1	1A	2904	U
2	1B	2	C
2	1B	12	C
2	1B	35	U
2	1B	45	A
2	1B	56	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
2	1B	119	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	54	C
32	1a	61	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	99	U
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	146	G
32	1a	154	C
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	185	A
32	1a	189(A)	C
32	1a	189(B)	C
32	1a	189(J)	G
32	1a	195	A
32	1a	196	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	247	G
32	1a	251	G
32	1a	262	A
32	1a	266	G
32	1a	267	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	344	A
32	1a	349	A
32	1a	351	G
32	1a	352	C
32	1a	353	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	354	G
32	1a	355	C
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	483	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	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	619	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	630	G
32	1a	650	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	671	G
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	702	A
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	753	A
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	802	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	859	A
32	1a	870	U
32	1a	874	G
32	1a	897	C
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1016	A
32	1a	1020	U
32	1a	1021	G
32	1a	1022	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	1039	C
32	1a	1044	A
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1104	G
32	1a	1124	G
32	1a	1125	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1161	C
32	1a	1181	G
32	1a	1183	A
32	1a	1184	G
32	1a	1186	G
32	1a	1192	C
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1204	A
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1224	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1269	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1363	C
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C
32	1a	1413	A
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	1487	G
32	1a	1492	A
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1519	MA6
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	8	4SU
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1w	64	A
54	1w	70	G
54	1w	71	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	14	A
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	56	C
55	1x	59	A
55	1x	67	C
55	1x	68	C
55	1x	76	A
56	1y	3	C
56	1y	5	G
56	1y	9	A
56	1y	13	C
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	24	G
56	1y	37	MIA
56	1y	46	7MG
56	1y	47	U
56	1y	48	C
56	1y	52	G
56	1y	53	G
56	1y	54	5MU
56	1y	57	G
56	1y	59	U
56	1y	61	C
56	1y	65	G
56	1y	69	G
56	1y	70	G
56	1y	71	G
1	2A	11	G
1	2A	14	A
1	2A	15	G
1	2A	34	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	36	G
1	2A	45	C
1	2A	50	U
1	2A	51	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	98	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	150	C
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	266	G
1	2A	271(F)	C
1	2A	271(I)	G
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	271(P)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	289	A
1	2A	303	U
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	338	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(D)	G
1	2A	372	G
1	2A	380	U
1	2A	385	C
1	2A	386	G
1	2A	391	G
1	2A	396	G
1	2A	406	G
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	527	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	583	G
1	2A	586	A
1	2A	587	C
1	2A	588	U
1	2A	599	G
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	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	709	U
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	811	U
1	2A	812	C
1	2A	819	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	848	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
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	957	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	993	G
1	2A	996	A
1	2A	1006	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1039	G
1	2A	1040	C
1	2A	1043	C
1	2A	1116	C
1	2A	1126	A
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	1180	C
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1229	G
1	2A	1242	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1289	C
1	2A	1298	C
1	2A	1300	U
1	2A	1301	A
1	2A	1313	U
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	1373	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1378	A
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1392	A
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1530	C
1	2A	1531	C
1	2A	1533	G
1	2A	1537	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1582	C
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1609	A
1	2A	1610	A
1	2A	1618	A
1	2A	1648	C
1	2A	1649	G
1	2A	1653	G
1	2A	1654	A
1	2A	1674	G
1	2A	1693	U
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1714	G
1	2A	1721	G
1	2A	1722	A
1	2A	1741	A
1	2A	1743	C
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G
1	2A	1773	A
1	2A	1780	A
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1820	U
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1860	G
1	2A	1877	A
1	2A	1878	G
1	2A	1896	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
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	2092	U
1	2A	2093	G
1	2A	2099	U
1	2A	2104	G
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2113	U
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2139	C
1	2A	2142	C
1	2A	2144	U
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2152	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2160	G
1	2A	2163	C
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	2174	C
1	2A	2175	C
1	2A	2182	G
1	2A	2184	G
1	2A	2185	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2239	G
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2338	G
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2370	G
1	2A	2377	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2406	U
1	2A	2424	C
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2460	U
1	2A	2474	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2476	A
1	2A	2478	A
1	2A	2491	U
1	2A	2492	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2518	A
1	2A	2520	C
1	2A	2554	U
1	2A	2562	U
1	2A	2566	A
1	2A	2567	G
1	2A	2574	G
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2623	G
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2745	C
1	2A	2748	A
1	2A	2751	G
1	2A	2755	C
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2794	C
1	2A	2803	C
1	2A	2807	G
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2876	G
1	2A	2879	C
1	2A	2880	C
1	2A	2884	U
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	7	G
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	24	G
2	2B	33	G
2	2B	34	U
2	2B	38	C
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	57	A
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	73	A
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	89	G
2	2B	91	C
2	2B	95	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	106	G
2	2B	108	U
2	2B	110	G
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	30	U
32	2a	31	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	52	G
32	2a	58	C
32	2a	66	G
32	2a	73	G
32	2a	78	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
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	217	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	267	C
32	2a	289	G
32	2a	300	A
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	344	A
32	2a	346	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	356	A
32	2a	367	U
32	2a	372	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	411	A
32	2a	412	A
32	2a	413	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	477	A
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	508	C
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	512	U
32	2a	518	C
32	2a	528	C
32	2a	531	U
32	2a	532	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	673	G
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	819	A
32	2a	821	G
32	2a	828	A
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	859	A
32	2a	873	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	942	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	997	U
32	2a	1000	U
32	2a	1001	A
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1011	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1027	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1044	A
32	2a	1045	C
32	2a	1046	A
32	2a	1050	G
32	2a	1055	A
32	2a	1065	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1080	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1104	G
32	2a	1108	G
32	2a	1117	G
32	2a	1118	C
32	2a	1119	C
32	2a	1125	U
32	2a	1129	C
32	2a	1133	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1169	A
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1212	U
32	2a	1213	A
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1250	A
32	2a	1256	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1257	U
32	2a	1260	C
32	2a	1270	C
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1297	C
32	2a	1302	U
32	2a	1305	G
32	2a	1320	C
32	2a	1322	C
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1370	G
32	2a	1379	G
32	2a	1381	U
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1452	C
32	2a	1456	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
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1526	G
32	2a	1529	G
32	2a	1530	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	15	A
54	2w	3	C
54	2w	4	C
54	2w	8	4SU
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	26	A
54	2w	29	G
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	49	C
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	72	C
54	2w	73	A
54	2w	74	C
55	2x	9	G
55	2x	14	A
55	2x	19	G
55	2x	21	A
55	2x	47	U
55	2x	48	C
55	2x	68	C
55	2x	76	A
56	2y	2	C
56	2y	13	C
56	2y	14	A
56	2y	15	G
56	2y	19	G
56	2y	24	G
56	2y	30	G
56	2y	37	MIA
56	2y	46	7MG
56	2y	49	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	2y	52	G
56	2y	53	G
56	2y	55	PSU
56	2y	57	G
56	2y	58	A
56	2y	59	U
56	2y	60	U
56	2y	62	C
56	2y	65	G
56	2y	70	G
56	2y	73	A

All (60) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	185	A
1	1A	204	G
1	1A	509	A
1	1A	793	A
1	1A	913	A
1	1A	941	U
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1120	G
1	1A	1135	G
1	1A	1136	U
1	1A	1188	A
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1321	A
1	1A	1466	U
1	1A	1700	G
1	1A	2014	G
1	1A	2148	A
1	1A	2156	A
1	1A	2179	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2192	A
1	1A	2203	G
1	1A	2205	C
1	1A	2418	U
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	587	C
1	2A	752	A
1	2A	839	U
1	2A	856	C
1	2A	883	G
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1300	U
1	2A	1420	U
1	2A	1442	G
1	2A	1493	C
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2134	A
1	2A	2689	U
1	2A	2756	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
54	PSU	1w	39	54	18,21,22	1.32	2 (11%)	21,30,33	2.01	4 (19%)
1	5MC	1A	1984	57,1	19,22,23	1.50	3 (15%)	26,32,35	1.14	3 (11%)
1	PSU	1A	1939	1	18,21,22	1.38	2 (11%)	21,30,33	2.00	4 (19%)
32	MA6	1a	1518	32	23,26,27	1.57	5 (21%)	33,38,41	2.26	11 (33%)
56	PSU	2y	39	56	18,21,22	1.38	2 (11%)	21,30,33	1.96	3 (14%)
32	5MC	2a	1404	32	19,22,23	1.64	3 (15%)	26,32,35	1.21	3 (11%)
32	MA6	1a	1519	32	23,26,27	1.52	4 (17%)	33,38,41	2.37	12 (36%)
55	5MC	1x	32	55	19,22,23	1.65	3 (15%)	26,32,35	1.25	3 (11%)
32	MA6	2a	1519	32	23,26,27	1.63	3 (13%)	33,38,41	2.33	12 (36%)
1	5MU	1A	1961	57,1	19,22,23	1.49	6 (31%)	27,32,35	2.32	6 (22%)
56	PSU	1y	39	56	18,21,22	1.27	2 (11%)	21,30,33	2.41	4 (19%)
1	4OC	1A	1942	57,1	19,22,24	0.77	0	25,31,35	0.92	1 (4%)
32	7MG	1a	527	32	23,26,27	1.38	4 (17%)	27,39,42	2.66	7 (25%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
56	MIA	2y	37	56	21,24,32	1.63	4 (19%)	30,35,47	2.13	7 (23%)
1	5MU	2A	1939	1	19,22,23	1.46	5 (26%)	27,32,35	2.23	7 (25%)
56	4SU	1y	8	56	18,21,22	1.92	5 (27%)	25,30,33	2.32	6 (24%)
54	7MG	1w	46	54	23,26,27	1.37	3 (13%)	27,39,42	2.56	7 (25%)
1	OMG	2A	2251	1,55	23,26,27	1.25	3 (13%)	32,38,41	1.93	7 (21%)
54	PSU	1w	55	54	18,21,22	1.42	2 (11%)	21,30,33	2.02	4 (19%)
56	PSU	1y	55	56	18,21,22	1.30	2 (11%)	21,30,33	2.16	4 (19%)
56	5MU	2y	54	56	19,22,23	1.51	4 (21%)	27,32,35	2.05	7 (25%)
54	PSU	1w	32	54,57	18,21,22	1.36	2 (11%)	21,30,33	2.00	3 (14%)
55	4SU	1x	8	55	18,21,22	2.16	5 (27%)	25,30,33	1.54	4 (16%)
32	2MG	2a	1207	32,57	23,26,27	1.30	4 (17%)	33,38,41	2.01	5 (15%)
56	MIA	1y	37	56	21,24,32	1.63	4 (19%)	30,35,47	2.02	7 (23%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	2.09	5 (23%)
1	PSU	1A	2617	1	18,21,22	1.34	2 (11%)	21,30,33	1.82	3 (14%)
56	PSU	1y	32	56	18,21,22	1.40	3 (16%)	21,30,33	1.96	4 (19%)
43	0TD	2l	92	43	8,9,10	4.51	1 (12%)	6,11,13	4.75	3 (50%)
55	PSU	1x	55	55	18,21,22	1.37	2 (11%)	21,30,33	1.88	4 (19%)
32	UR3	1a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.88	5 (19%)
1	5MC	2A	1962	57,1	19,22,23	1.54	3 (15%)	26,32,35	1.23	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	2a	966	32	24,27,28	1.35	4 (16%)	33,40,43	1.91	6 (18%)
32	5MC	2a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.28	5 (19%)
55	4SU	2x	8	55	18,21,22	2.15	6 (33%)	25,30,33	1.78	7 (28%)
1	2MA	1A	2515	57,1	22,25,26	1.46	4 (18%)	32,37,40	2.63	8 (25%)
32	MA6	2a	1518	32	23,26,27	1.53	5 (21%)	33,38,41	2.26	12 (36%)
1	2MU	1A	2564	57,1	19,22,24	1.38	4 (21%)	25,31,36	1.97	6 (24%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	1.95	3 (14%)
56	7MG	1y	46	56	23,26,27	1.36	3 (13%)	27,39,42	2.71	6 (22%)
54	MIA	1w	37	54	28,31,32	2.35	6 (21%)	38,44,47	2.66	14 (36%)
54	5MU	1w	54	54	19,22,23	1.37	5 (26%)	27,32,35	2.06	7 (25%)
1	4OC	2A	1920	1	19,22,24	0.77	0	25,31,35	0.92	1 (4%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.97	4 (19%)
54	F3N	1w	76	54,1	33,36,37	1.54	5 (15%)	41,51,54	1.82	8 (19%)
32	4OC	2a	1402	32,57	20,23,24	0.79	0	25,32,35	1.17	2 (8%)
32	PSU	1a	516	32,57	18,21,22	1.35	2 (11%)	21,30,33	2.07	3 (14%)
32	5MC	1a	1407	32	19,22,23	1.67	3 (15%)	26,32,35	1.13	2 (7%)
54	PSU	2w	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.82	4 (19%)
56	PSU	2y	32	56	18,21,22	1.36	2 (11%)	21,30,33	1.91	4 (19%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.86	6 (18%)
1	5MC	1A	1964	57,1	19,22,23	1.49	3 (15%)	26,32,35	1.35	5 (19%)
32	5MC	2a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.22	2 (7%)
32	5MC	1a	1404	32	19,22,23	1.61	3 (15%)	26,32,35	1.20	2 (7%)
32	5MC	1a	967	32	19,22,23	1.76	2 (10%)	26,32,35	1.19	3 (11%)
1	OMG	1A	2263	57,1,55	23,26,27	1.23	3 (13%)	32,38,41	1.99	6 (18%)
32	UR3	2a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.71	4 (15%)
1	PSU	1A	1933	1	18,21,22	1.41	2 (11%)	21,30,33	2.11	3 (14%)
56	5MU	1y	54	56	19,22,23	1.48	5 (26%)	27,32,35	2.02	6 (22%)
56	4SU	2y	8	56	18,21,22	1.80	4 (22%)	25,30,33	2.54	7 (28%)
43	0TD	1l	92	43	8,9,10	4.76	1 (12%)	6,11,13	5.71	2 (33%)
1	PSU	2A	1917	1	18,21,22	1.43	3 (16%)	21,30,33	2.15	5 (23%)
56	PSU	2y	55	56	18,21,22	1.42	4 (22%)	21,30,33	2.02	5 (23%)
54	7MG	2w	46	54	23,26,27	1.33	3 (13%)	27,39,42	2.63	7 (25%)
1	2MU	2A	2552	57,1	19,22,24	1.24	2 (10%)	25,31,36	1.85	6 (24%)
1	5MU	2A	1915	1	19,22,23	1.43	6 (31%)	27,32,35	2.18	6 (22%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	1.92	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1937	1	19,22,23	1.39	5 (26%)	27,32,35	2.28	8 (29%)
55	5MU	2x	54	55	19,22,23	1.46	6 (31%)	27,32,35	2.04	5 (18%)
32	5MC	2a	967	32	19,22,23	1.67	3 (15%)	26,32,35	1.25	3 (11%)
54	4SU	1w	8	54	18,21,22	1.87	4 (22%)	25,30,33	1.93	4 (16%)
55	5MU	1x	54	57,55	19,22,23	1.38	5 (26%)	27,32,35	2.12	6 (22%)
32	2MG	1a	1207	32	23,26,27	1.29	2 (8%)	33,38,41	2.18	7 (21%)
1	2MA	2A	2503	57,1	22,25,26	1.47	4 (18%)	32,37,40	2.33	8 (25%)
54	4SU	2w	8	54	18,21,22	1.81	5 (27%)	25,30,33	2.15	5 (20%)
32	4OC	1a	1402	32	20,23,24	0.77	1 (5%)	25,32,35	1.00	3 (12%)
56	7MG	2y	46	56	23,26,27	1.40	4 (17%)	27,39,42	2.63	6 (22%)
55	5MC	2x	32	55	19,22,23	1.54	3 (15%)	26,32,35	1.20	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.56	3 (15%)	26,32,35	1.14	2 (7%)
54	F3N	2w	76	54,1	33,36,37	1.52	4 (12%)	41,51,54	1.65	8 (19%)
1	PSU	2A	2605	1	18,21,22	1.43	3 (16%)	21,30,33	2.12	5 (23%)
32	7MG	2a	527	32	23,26,27	1.38	4 (17%)	27,39,42	2.60	7 (25%)
32	5MC	1a	1400	32	19,22,23	1.68	3 (15%)	26,32,35	1.17	2 (7%)
54	MIA	2w	37	54	24,27,32	2.16	5 (20%)	32,39,47	2.38	11 (34%)
54	5MU	2w	54	54	19,22,23	1.44	5 (26%)	27,32,35	2.08	6 (22%)

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
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	57,1	-	2/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
1	5MU	1A	1961	57,1	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	57,1	-	1/9/27/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	7MG	1a	527	32	-	1/7/37/38	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	3/7/25/34	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	2/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	3/7/25/26	0/2/2/2
54	PSU	1w	32	54,57	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,57	-	0/9/27/28	0/3/3/3
56	MIA	1y	37	56	-	2/7/25/34	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
55	PSU	1x	55	55	-	1/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	57,1	-	1/7/25/26	0/3/3/3
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
1	2MU	1A	2564	57,1	-	0/9/27/28	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	7MG	1y	46	56	-	5/7/37/38	0/3/3/3
54	MIA	1w	37	54	-	6/15/33/34	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	2/9/27/30	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	54,1	-	0/19/37/38	0/4/4/4
32	4OC	2a	1402	32,57	-	0/9/29/30	0/2/2/2
32	PSU	1a	516	32,57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	1/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1964	57,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	57,1,55	-	0/9/27/28	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	2/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	2/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	1/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	3/7/37/38	0/3/3/3
1	2MU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	2MA	2A	2503	57,1	-	2/7/25/26	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
56	7MG	2y	46	56	-	3/7/37/38	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	54,1	-	2/19/37/38	0/4/4/4
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	1/7/37/38	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2

All (277) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-13.05	1.69	1.82
43	2l	92	0TD	CB-SB	-12.40	1.69	1.82
54	2w	37	MIA	C2-S10	-7.40	1.69	1.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C2-S10	-6.93	1.70	1.75
54	1w	37	MIA	C13-C14	6.88	1.53	1.32
32	1a	967	5MC	C5-C4	6.64	1.49	1.44
32	2a	1400	5MC	C5-C4	6.22	1.48	1.44
32	1a	1400	5MC	C5-C4	6.04	1.48	1.44
32	2a	967	5MC	C5-C4	6.01	1.48	1.44
32	2a	1404	5MC	C5-C4	5.97	1.48	1.44
32	1a	1407	5MC	C5-C4	5.97	1.48	1.44
32	2a	1407	5MC	C5-C4	5.91	1.48	1.44
55	1x	32	5MC	C5-C4	5.87	1.48	1.44
32	1a	1404	5MC	C5-C4	5.84	1.48	1.44
1	2A	1942	5MC	C5-C4	5.52	1.48	1.44
1	2A	1962	5MC	C5-C4	5.48	1.48	1.44
54	1w	76	F3N	CB-CG	-5.43	1.38	1.51
1	1A	1984	5MC	C5-C4	5.36	1.48	1.44
55	2x	32	5MC	C5-C4	5.35	1.48	1.44
1	1A	1964	5MC	C5-C4	5.18	1.48	1.44
56	1y	37	MIA	C5-C4	5.15	1.48	1.39
56	1y	8	4SU	C4-S4	-5.12	1.59	1.68
32	2a	1519	MA6	C5-C4	5.03	1.48	1.39
56	2y	37	MIA	C5-C4	5.02	1.48	1.39
54	1w	8	4SU	C4-S4	-5.02	1.59	1.68
55	1x	8	4SU	C4-N3	-5.02	1.32	1.37
54	2w	76	F3N	CB-CG	-4.94	1.39	1.51
32	2a	1518	MA6	C5-C4	4.94	1.47	1.39
55	2x	8	4SU	C4-S4	-4.91	1.60	1.68
54	2w	37	MIA	C5-C4	4.90	1.47	1.39
54	2w	8	4SU	C4-S4	-4.87	1.60	1.68
54	1w	37	MIA	C5-C4	4.87	1.47	1.39
56	2y	8	4SU	C4-S4	-4.82	1.60	1.68
32	1a	1518	MA6	C5-C4	4.76	1.47	1.39
32	1a	1519	MA6	C5-C4	4.65	1.47	1.39
55	2x	8	4SU	C4-N3	-4.49	1.33	1.37
1	2A	2503	2MA	C5-C4	4.45	1.47	1.39
55	1x	8	4SU	C4-S4	-4.44	1.60	1.68
54	1w	76	F3N	C5-N7	-4.20	1.31	1.39
1	1A	2515	2MA	C5-C4	4.02	1.46	1.39
54	1w	55	PSU	C6-C5	4.00	1.39	1.35
56	2y	39	PSU	C6-C5	4.00	1.39	1.35
54	2w	55	PSU	C6-C5	3.96	1.39	1.35
56	2y	32	PSU	C6-C5	3.94	1.39	1.35
1	1A	1933	PSU	C6-C5	3.94	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	55	PSU	C6-C5	3.83	1.39	1.35
56	1y	32	PSU	C6-C5	3.83	1.39	1.35
54	2w	76	F3N	C5-C4	-3.80	1.32	1.39
1	1A	2617	PSU	C6-C5	3.74	1.39	1.35
54	2w	76	F3N	C5-N7	-3.73	1.32	1.39
55	1x	8	4SU	C5-C4	-3.65	1.38	1.42
56	2y	46	7MG	C5-C4	3.65	1.48	1.37
54	2w	39	PSU	C6-C5	3.63	1.39	1.35
1	1A	1939	PSU	C6-C5	3.62	1.39	1.35
32	1a	516	PSU	C6-C5	3.62	1.39	1.35
56	1y	46	7MG	C5-C4	3.60	1.48	1.37
1	2A	2605	PSU	C6-C5	3.57	1.39	1.35
55	1x	55	PSU	C6-C5	3.53	1.39	1.35
54	1w	46	7MG	C4-N9	-3.53	1.33	1.37
56	1y	55	PSU	C6-C5	3.49	1.39	1.35
54	1w	32	PSU	C6-C5	3.43	1.39	1.35
55	1x	8	4SU	C2-N3	-3.42	1.32	1.38
54	1w	39	PSU	C6-C5	3.41	1.39	1.35
1	2A	1911	PSU	C6-C5	3.41	1.39	1.35
32	2a	527	7MG	C5-C4	3.40	1.48	1.37
54	2w	32	PSU	C6-C5	3.40	1.39	1.35
32	2a	1519	MA6	C5-C6	3.38	1.50	1.41
56	1y	8	4SU	C4-N3	-3.38	1.34	1.37
54	2w	46	7MG	C4-N9	-3.38	1.33	1.37
32	1a	527	7MG	C5-C4	3.35	1.47	1.37
1	2A	1917	PSU	C6-C5	3.35	1.39	1.35
55	2x	8	4SU	C5-C4	-3.34	1.38	1.42
54	2w	46	7MG	C5-C4	3.34	1.47	1.37
32	2a	516	PSU	C6-C5	3.34	1.39	1.35
54	1w	46	7MG	C5-C4	3.31	1.47	1.37
32	2a	966	M2G	C5-C4	3.31	1.47	1.38
54	1w	8	4SU	C4-N3	-3.30	1.34	1.37
56	2y	55	PSU	C6-C5	3.29	1.38	1.35
32	2a	1207	2MG	C5-C4	3.29	1.47	1.38
54	2w	8	4SU	C4-N3	-3.27	1.34	1.37
32	1a	1207	2MG	C5-C4	3.26	1.47	1.38
56	2y	54	5MU	C2-N1	3.20	1.43	1.38
32	2a	966	M2G	C2-N2	3.19	1.41	1.35
54	2w	54	5MU	C6-C5	3.18	1.39	1.34
32	1a	966	M2G	C5-C4	3.17	1.47	1.38
56	1y	39	PSU	C6-C5	3.16	1.38	1.35
1	2A	2605	PSU	C4-N3	-3.14	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2251	OMG	C5-C4	3.12	1.47	1.38
1	1A	2263	OMG	C5-C4	3.06	1.47	1.38
56	2y	8	4SU	C2-N1	3.06	1.43	1.38
32	1a	1518	MA6	C5-C6	3.06	1.49	1.41
32	1a	1407	5MC	C6-C5	3.04	1.39	1.34
1	1A	2564	2MU	C4-N3	-3.04	1.33	1.38
1	1A	1961	5MU	C4-N3	-2.98	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.97	1.33	1.38
32	2a	1407	5MC	C6-C5	2.97	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.96	1.33	1.38
56	2y	37	MIA	C5-C6	2.96	1.49	1.41
55	2x	8	4SU	C2-N1	2.95	1.43	1.38
1	2A	1917	PSU	C4-N3	-2.95	1.33	1.38
1	1A	1961	5MU	C6-C5	2.95	1.39	1.34
55	2x	32	5MC	C6-C5	2.93	1.39	1.34
56	2y	54	5MU	C6-C5	2.93	1.39	1.34
32	2a	1518	MA6	C5-C6	2.93	1.48	1.41
55	1x	32	5MC	C6-C5	2.92	1.39	1.34
32	2a	527	7MG	C4-N9	-2.91	1.34	1.37
56	1y	8	4SU	C2-N1	2.90	1.43	1.38
56	1y	54	5MU	C6-C5	2.90	1.39	1.34
54	1w	8	4SU	C5-C4	-2.89	1.39	1.42
55	2x	54	5MU	C6-C5	2.88	1.39	1.34
56	1y	37	MIA	C5-C6	2.86	1.48	1.41
54	2w	37	MIA	C5-C6	2.84	1.48	1.41
1	2A	1915	5MU	C6-C5	2.83	1.39	1.34
32	1a	967	5MC	C6-C5	2.82	1.39	1.34
54	1w	37	MIA	C5-C6	2.81	1.48	1.41
56	2y	8	4SU	C4-N3	-2.80	1.34	1.37
1	2A	1915	5MU	C4-N3	-2.80	1.33	1.38
32	1a	966	M2G	C2-N2	2.77	1.40	1.35
1	1A	1937	5MU	C4-N3	-2.76	1.33	1.38
55	2x	54	5MU	C4-N3	-2.75	1.33	1.38
32	1a	1498	UR3	C2-N1	2.74	1.42	1.38
32	1a	1519	MA6	C5-C6	2.74	1.48	1.41
54	1w	54	5MU	C6-N1	-2.72	1.33	1.38
32	2a	967	5MC	C6-C5	2.72	1.39	1.34
32	1a	527	7MG	C4-N9	-2.72	1.34	1.37
55	1x	54	5MU	C6-C5	2.71	1.39	1.34
1	2A	1939	5MU	C6-N1	-2.71	1.33	1.38
32	2a	1207	2MG	C6-N1	-2.69	1.33	1.38
32	2a	1404	5MC	C6-C5	2.69	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1961	5MU	C2-N1	2.68	1.42	1.38
56	1y	54	5MU	C4-C5	2.67	1.49	1.44
56	2y	54	5MU	C4-N3	-2.67	1.33	1.38
56	1y	54	5MU	C2-N1	2.67	1.42	1.38
55	2x	8	4SU	C2-N3	-2.65	1.33	1.38
56	2y	8	4SU	C5-C4	-2.65	1.39	1.42
54	1w	54	5MU	C4-N3	-2.65	1.33	1.38
32	1a	1207	2MG	C6-N1	-2.65	1.33	1.38
1	2A	2552	2MU	C4-N3	-2.64	1.34	1.38
1	1A	2515	2MA	C5-C6	2.63	1.48	1.41
56	2y	55	PSU	C4-N3	-2.63	1.33	1.38
55	1x	54	5MU	C4-N3	-2.63	1.33	1.38
1	1A	1961	5MU	C2-N3	-2.61	1.33	1.38
54	2w	39	PSU	C4-N3	-2.60	1.34	1.38
56	2y	46	7MG	C6-N1	-2.60	1.34	1.38
1	1A	1984	5MC	C6-N1	-2.60	1.33	1.38
32	1a	966	M2G	C6-N1	-2.60	1.34	1.38
56	1y	8	4SU	C5-C4	-2.60	1.39	1.42
1	1A	2263	OMG	C5-N7	-2.60	1.33	1.39
32	2a	516	PSU	C4-N3	-2.58	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.58	1.33	1.38
32	1a	1400	5MC	C6-C5	2.58	1.38	1.34
54	2w	8	4SU	C5-C4	-2.57	1.39	1.42
32	1a	1404	5MC	C6-C5	2.56	1.38	1.34
1	2A	1942	5MC	C6-C5	2.56	1.38	1.34
54	2w	76	F3N	C5-C6	-2.56	1.33	1.41
1	1A	1937	5MU	C4-C5	2.56	1.49	1.44
1	2A	1911	PSU	C4-N3	-2.56	1.34	1.38
1	2A	1915	5MU	C2-N1	2.55	1.42	1.38
54	1w	76	F3N	C5-C6	-2.54	1.33	1.41
1	1A	1964	5MC	C6-N1	-2.54	1.33	1.38
1	2A	1962	5MC	C6-N1	-2.54	1.33	1.38
1	1A	1939	PSU	C4-N3	-2.53	1.34	1.38
32	2a	1400	5MC	C6-C5	2.53	1.38	1.34
56	1y	32	PSU	C4-N3	-2.51	1.34	1.38
32	2a	1519	MA6	C8-N7	2.51	1.36	1.31
54	1w	32	PSU	C4-N3	-2.51	1.34	1.38
32	1a	1519	MA6	C8-N7	2.51	1.36	1.31
32	1a	527	7MG	C6-N1	-2.50	1.34	1.38
54	1w	76	F3N	C5-C4	-2.50	1.34	1.39
54	1w	76	F3N	C2'-C3'	-2.49	1.49	1.53
32	2a	527	7MG	C6-N1	-2.49	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	32	PSU	C4-N3	-2.49	1.34	1.38
55	2x	8	4SU	O2-C2	2.48	1.27	1.23
1	2A	1939	5MU	C2-N3	-2.47	1.33	1.38
32	2a	1400	5MC	C6-N1	-2.46	1.33	1.38
54	1w	39	PSU	C4-N3	-2.46	1.34	1.38
32	1a	1518	MA6	C8-N7	2.46	1.36	1.31
1	1A	2564	2MU	C5-C4	2.45	1.49	1.43
55	2x	54	5MU	C2-N1	2.45	1.42	1.38
56	1y	55	PSU	C4-N3	-2.45	1.34	1.38
54	2w	54	5MU	C4-C5	2.44	1.48	1.44
1	1A	1937	5MU	C6-C5	2.44	1.38	1.34
1	2A	1939	5MU	C6-C5	2.44	1.38	1.34
56	1y	54	5MU	C4-N3	-2.44	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.43	1.33	1.38
1	1A	2263	OMG	C6-N1	-2.43	1.34	1.38
1	2A	2503	2MA	C5-C6	2.42	1.47	1.41
56	1y	37	MIA	C8-N7	2.41	1.36	1.31
54	2w	54	5MU	C4-N3	-2.39	1.34	1.38
1	2A	1962	5MC	C6-C5	2.39	1.38	1.34
55	2x	54	5MU	C4-C5	2.39	1.48	1.44
1	2A	1917	PSU	C2-N3	-2.38	1.33	1.37
32	1a	516	PSU	C4-N3	-2.38	1.34	1.38
54	1w	55	PSU	C4-N3	-2.38	1.34	1.38
54	1w	46	7MG	C6-N1	-2.38	1.34	1.38
1	2A	1939	5MU	C4-C5	2.38	1.48	1.44
56	2y	39	PSU	C4-N3	-2.37	1.34	1.38
1	1A	2617	PSU	C4-N3	-2.37	1.34	1.38
54	2w	54	5MU	C2-N1	2.37	1.42	1.38
1	2A	1942	5MC	C6-N1	-2.37	1.34	1.38
55	2x	55	PSU	C4-N3	-2.35	1.34	1.38
54	2w	37	MIA	C5-N7	-2.35	1.34	1.39
1	1A	1984	5MC	C6-C5	2.35	1.38	1.34
32	2a	527	7MG	C8-N9	2.35	1.47	1.45
1	1A	1933	PSU	C4-N3	-2.35	1.34	1.38
1	1A	2515	2MA	C5-N7	-2.34	1.34	1.39
1	2A	1915	5MU	C4-C5	2.34	1.48	1.44
32	2a	966	M2G	C6-N1	-2.34	1.34	1.38
32	1a	1518	MA6	C5-N7	-2.33	1.34	1.39
55	1x	32	5MC	C6-N1	-2.33	1.34	1.38
54	2w	8	4SU	C2-N3	-2.33	1.33	1.38
1	2A	2552	2MU	C5-C4	2.32	1.48	1.43
1	2A	2503	2MA	C5-N7	-2.32	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1498	UR3	C2-N1	2.32	1.41	1.38
56	1y	46	7MG	C6-N1	-2.31	1.34	1.38
55	1x	54	5MU	C2-N3	-2.30	1.34	1.38
55	1x	8	4SU	O2-C2	2.30	1.27	1.23
55	1x	55	PSU	C4-N3	-2.30	1.34	1.38
54	1w	54	5MU	C6-C5	2.29	1.38	1.34
1	1A	1964	5MC	C6-C5	2.29	1.38	1.34
32	2a	966	M2G	C5-N7	-2.28	1.34	1.39
54	2w	37	MIA	C8-N7	2.28	1.36	1.31
32	2a	967	5MC	C6-N1	-2.28	1.34	1.38
1	1A	2564	2MU	C2-N3	-2.28	1.34	1.38
54	1w	37	MIA	C5-N7	-2.27	1.34	1.39
54	1w	37	MIA	C8-N7	2.27	1.36	1.31
56	2y	54	5MU	C4-C5	2.26	1.48	1.44
54	1w	8	4SU	C2-N3	-2.26	1.34	1.38
1	1A	2515	2MA	C8-N9	-2.25	1.33	1.37
56	2y	37	MIA	C8-N7	2.24	1.36	1.31
1	2A	2251	OMG	C5-N7	-2.23	1.34	1.39
1	1A	1937	5MU	C2-N1	2.23	1.42	1.38
54	2w	55	PSU	C4-N3	-2.22	1.34	1.38
1	1A	1961	5MU	C6-N1	-2.22	1.34	1.38
55	1x	54	5MU	C4-C5	2.21	1.48	1.44
32	1a	966	M2G	C5-N7	-2.21	1.34	1.39
56	2y	37	MIA	C5-N7	-2.21	1.35	1.39
55	2x	54	5MU	C2-N3	-2.20	1.34	1.38
56	1y	46	7MG	C8-N9	2.19	1.47	1.45
32	2a	1404	5MC	C6-N1	-2.19	1.34	1.38
56	1y	37	MIA	C5-N7	-2.19	1.35	1.39
56	1y	54	5MU	C6-N1	-2.18	1.34	1.38
56	2y	46	7MG	C8-N9	2.18	1.47	1.45
1	1A	2564	2MU	C2-N1	2.17	1.41	1.38
32	1a	1518	MA6	C4-N9	-2.17	1.33	1.37
32	2a	1518	MA6	C4-N9	-2.17	1.33	1.37
55	1x	54	5MU	C6-N1	-2.15	1.34	1.38
32	1a	1519	MA6	C5-N7	-2.14	1.35	1.39
32	2a	1518	MA6	C8-N7	2.13	1.35	1.31
1	2A	2605	PSU	C2-N3	-2.13	1.34	1.37
54	1w	54	5MU	C4-C5	2.13	1.48	1.44
32	2a	1207	2MG	C2-N3	2.13	1.36	1.32
56	2y	32	PSU	C4-N3	-2.13	1.34	1.38
56	1y	39	PSU	C4-N3	-2.12	1.34	1.38
1	1A	1937	5MU	C2-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	2503	2MA	C8-N7	2.10	1.35	1.31
55	2x	54	5MU	C6-N1	-2.09	1.34	1.38
54	1w	54	5MU	C2-N3	-2.09	1.34	1.38
32	1a	527	7MG	C5-N7	-2.08	1.33	1.35
54	2w	54	5MU	C6-N1	-2.08	1.34	1.38
55	2x	32	5MC	C6-N1	-2.08	1.34	1.38
32	2a	1518	MA6	C5-N7	-2.08	1.35	1.39
1	2A	1915	5MU	C2-N3	-2.07	1.34	1.38
56	2y	46	7MG	C4-N9	-2.06	1.35	1.37
32	2a	1207	2MG	C5-N7	-2.06	1.34	1.39
32	1a	1407	5MC	C6-N1	-2.06	1.34	1.38
56	2y	55	PSU	C2-N1	-2.06	1.34	1.36
56	1y	32	PSU	C4-C5	2.05	1.50	1.44
54	2w	46	7MG	C6-N1	-2.05	1.35	1.38
1	2A	1915	5MU	C6-N1	-2.04	1.34	1.38
56	1y	8	4SU	C2-N3	-2.02	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.02	1.34	1.38
32	1a	1402	4OC	C6-C5	2.01	1.39	1.35
32	1a	1498	UR3	C6-C5	2.00	1.39	1.35
56	2y	55	PSU	C2-N3	-2.00	1.34	1.37
1	1A	1961	5MU	C4-C5	2.00	1.48	1.44
54	2w	8	4SU	C2-N1	2.00	1.41	1.38

All (450) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-13.44	78.21	102.36
43	2l	92	0TD	CSB-SB-CB	-10.79	82.97	102.36
56	1y	46	7MG	N9-C4-N3	9.64	139.59	125.46
32	1a	527	7MG	N9-C4-N3	9.43	139.28	125.46
56	2y	46	7MG	N9-C4-N3	9.37	139.19	125.46
32	2a	527	7MG	N9-C4-N3	9.09	138.78	125.46
54	2w	46	7MG	N9-C4-N3	8.88	138.47	125.46
54	1w	46	7MG	N9-C4-N3	8.73	138.26	125.46
1	1A	2515	2MA	C5-C4-N3	-8.67	118.05	127.18
54	1w	37	MIA	C12-C13-C14	-8.09	112.48	127.01
54	2w	37	MIA	C5-C4-N3	-8.06	118.69	127.18
1	2A	2503	2MA	C5-C4-N3	-7.85	118.91	127.18
54	1w	37	MIA	C5-C4-N3	-7.67	119.10	127.18
1	1A	2515	2MA	N3-C4-N9	7.51	136.52	126.99
32	1a	1207	2MG	C2-N3-C4	7.18	120.98	112.00
56	2y	8	4SU	C4-N3-C2	-7.12	120.49	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1498	UR3	C4-N3-C2	-7.08	118.88	124.58
56	1y	39	PSU	N1-C2-N3	7.03	122.59	115.17
1	2A	1917	PSU	N1-C2-N3	6.87	122.41	115.17
1	2A	2503	2MA	N3-C4-N9	6.78	135.59	126.99
1	2A	2605	PSU	N1-C2-N3	6.71	122.25	115.17
1	1A	1933	PSU	N1-C2-N3	6.63	122.16	115.17
56	1y	8	4SU	C4-N3-C2	-6.60	120.99	127.31
32	2a	1207	2MG	C2-N3-C4	6.56	120.21	112.00
32	2a	1498	UR3	C4-N3-C2	-6.50	119.35	124.58
32	2a	966	M2G	C5-C4-N3	-6.46	118.11	128.39
54	2w	8	4SU	C4-N3-C2	-6.42	121.16	127.31
32	2a	516	PSU	N1-C2-N3	6.41	121.94	115.17
54	1w	32	PSU	N1-C2-N3	6.32	121.84	115.17
1	1A	2263	OMG	C5-C4-N3	-6.30	118.36	128.39
56	1y	55	PSU	N1-C2-N3	6.24	121.75	115.17
54	2w	37	MIA	N3-C4-N9	6.23	134.89	126.99
1	2A	2251	OMG	C5-C4-N3	-6.22	118.49	128.39
32	1a	516	PSU	N1-C2-N3	6.20	121.70	115.17
54	1w	39	PSU	N1-C2-N3	6.19	121.70	115.17
54	1w	37	MIA	N3-C4-N9	6.17	134.82	126.99
54	2w	32	PSU	N1-C2-N3	6.17	121.67	115.17
54	2w	55	PSU	N1-C2-N3	6.14	121.64	115.17
56	2y	37	MIA	C5-C4-N3	-6.12	118.28	126.72
32	1a	966	M2G	C5-C4-N3	-6.11	118.67	128.39
56	1y	32	PSU	N1-C2-N3	6.10	121.60	115.17
56	1y	8	4SU	C5-C4-N3	6.09	120.42	114.75
56	1y	37	MIA	C5-C4-N3	-6.05	118.39	126.72
1	1A	1939	PSU	N1-C2-N3	6.03	121.53	115.17
56	2y	39	PSU	N1-C2-N3	6.02	121.52	115.17
55	2x	55	PSU	N1-C2-N3	5.99	121.48	115.17
1	2A	1911	PSU	N1-C2-N3	5.94	121.43	115.17
32	1a	1207	2MG	C5-C4-N3	-5.93	118.95	128.39
56	2y	55	PSU	N1-C2-N3	5.91	121.41	115.17
55	1x	55	PSU	N1-C2-N3	5.89	121.38	115.17
54	1w	55	PSU	N1-C2-N3	5.88	121.37	115.17
54	1w	76	F3N	N1-C2-N3	-5.83	119.76	128.58
32	2a	1207	2MG	C5-C4-N3	-5.82	119.12	128.39
32	1a	527	7MG	C5-C4-N3	-5.79	117.27	128.13
32	1a	1519	MA6	C5-C4-N3	-5.77	118.78	126.72
54	2w	39	PSU	N1-C2-N3	5.75	121.24	115.17
56	2y	32	PSU	N1-C2-N3	5.73	121.21	115.17
1	1A	1937	5MU	N3-C2-N1	5.70	122.31	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	8	4SU	C5-C4-N3	5.68	120.03	114.75
54	2w	8	4SU	C5-C4-N3	5.67	120.03	114.75
1	1A	2564	2MU	N3-C2-N1	5.64	122.24	114.89
1	2A	1915	5MU	N3-C2-N1	5.64	122.23	114.89
32	2a	1519	MA6	C5-C4-N3	-5.63	118.97	126.72
54	2w	46	7MG	N9-C8-N7	-5.62	95.42	103.37
1	1A	1937	5MU	C4-N3-C2	-5.59	120.01	127.34
54	1w	8	4SU	C5-C4-N3	5.59	119.95	114.75
1	2A	1939	5MU	C4-N3-C2	-5.55	120.06	127.34
1	1A	1961	5MU	N3-C2-N1	5.54	122.11	114.89
32	2a	527	7MG	C5-C4-N3	-5.53	117.74	128.13
1	1A	1961	5MU	C4-N3-C2	-5.53	120.09	127.34
56	1y	39	PSU	O2-C2-N1	-5.53	117.09	122.79
32	1a	1518	MA6	C5-C4-N3	-5.52	119.12	126.72
56	1y	46	7MG	C5-C4-N3	-5.51	117.78	128.13
54	2w	76	F3N	N1-C2-N3	-5.48	120.29	128.58
54	1w	46	7MG	N9-C8-N7	-5.46	95.64	103.37
1	2A	1915	5MU	C4-N3-C2	-5.38	120.28	127.34
55	1x	54	5MU	N3-C2-N1	5.36	121.86	114.89
56	2y	46	7MG	C5-C4-N3	-5.35	118.09	128.13
54	1w	8	4SU	C4-N3-C2	-5.33	122.20	127.31
32	2a	1518	MA6	C5-C4-N3	-5.31	119.41	126.72
1	1A	2617	PSU	N1-C2-N3	5.29	120.75	115.17
1	1A	2263	OMG	C2-N3-C4	5.18	121.23	112.30
1	2A	2552	2MU	N3-C2-N1	5.17	121.62	114.89
54	2w	54	5MU	C4-N3-C2	-5.14	120.60	127.34
1	2A	1939	5MU	N3-C2-N1	5.12	121.55	114.89
55	2x	54	5MU	N3-C2-N1	5.10	121.53	114.89
1	1A	1961	5MU	C5-C4-N3	5.08	119.74	115.32
54	2w	54	5MU	N3-C2-N1	5.08	121.51	114.89
56	2y	37	MIA	N3-C4-N9	5.06	135.77	127.17
56	1y	39	PSU	C4-N3-C2	-5.06	119.40	126.37
55	1x	54	5MU	C4-N3-C2	-5.03	120.75	127.34
32	2a	527	7MG	N9-C8-N7	-4.95	96.36	103.37
54	1w	76	F3N	C5-C4-N3	-4.93	119.93	126.72
55	2x	54	5MU	C4-N3-C2	-4.90	120.91	127.34
56	1y	46	7MG	N9-C8-N7	-4.90	96.44	103.37
54	2w	46	7MG	C5-C4-N3	-4.89	118.95	128.13
54	1w	54	5MU	C4-N3-C2	-4.87	120.95	127.34
56	1y	37	MIA	N3-C4-N9	4.86	135.44	127.17
1	2A	2251	OMG	N9-C4-N3	4.85	135.64	125.95
56	2y	46	7MG	N9-C8-N7	-4.85	96.51	103.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1y	54	5MU	C4-N3-C2	-4.84	121.00	127.34
56	2y	54	5MU	N3-C2-N1	4.83	121.18	114.89
54	1w	46	7MG	C5-C4-N3	-4.83	119.06	128.13
1	1A	2564	2MU	C4-N3-C2	-4.81	120.64	126.61
54	1w	54	5MU	N3-C2-N1	4.81	121.15	114.89
32	2a	966	M2G	N9-C4-N3	4.80	135.55	125.95
1	2A	1939	5MU	C5-C6-N1	-4.76	118.15	123.31
1	1A	2263	OMG	N9-C4-N3	4.75	135.45	125.95
32	1a	527	7MG	N9-C8-N7	-4.74	96.66	103.37
32	2a	1518	MA6	C9-N6-C6	-4.73	108.48	120.52
32	1a	966	M2G	N9-C4-N3	4.72	135.40	125.95
1	1A	1937	5MU	C5-C4-N3	4.70	119.41	115.32
32	1a	1518	MA6	C9-N6-C6	-4.69	108.59	120.52
1	2A	2251	OMG	C2-N3-C4	4.67	120.35	112.30
56	2y	8	4SU	C5-C4-S4	-4.67	118.97	124.31
32	2a	966	M2G	C2-N3-C4	4.65	121.11	112.51
32	2a	1519	MA6	C4-C5-N7	-4.65	105.27	110.58
56	2y	54	5MU	C4-N3-C2	-4.63	121.27	127.34
56	1y	46	7MG	C2-N3-C4	4.62	120.26	112.30
56	1y	54	5MU	N3-C2-N1	4.59	120.87	114.89
55	2x	8	4SU	C5-C4-N3	4.54	118.97	114.75
54	2w	76	F3N	C5-C4-N3	-4.54	120.46	126.72
1	2A	2552	2MU	C4-N3-C2	-4.50	121.02	126.61
1	2A	1915	5MU	C5-C4-N3	4.49	119.23	115.32
1	1A	1961	5MU	O4-C4-C5	-4.49	119.78	124.92
1	2A	1939	5MU	C5-C4-N3	4.49	119.22	115.32
1	1A	1933	PSU	O2-C2-N1	-4.47	118.18	122.79
56	2y	8	4SU	C1'-N1-C2	4.46	125.61	117.59
1	2A	1917	PSU	C4-N3-C2	-4.43	120.27	126.37
32	1a	1519	MA6	C9-N6-C6	-4.42	109.28	120.52
56	2y	46	7MG	C2-N3-C4	4.41	119.90	112.30
56	1y	55	PSU	C4-N3-C2	-4.39	120.32	126.37
32	1a	1519	MA6	N3-C4-N9	4.39	134.63	127.17
32	1a	1518	MA6	C4-C5-N7	-4.37	105.59	110.58
56	1y	54	5MU	C5-C4-N3	4.34	119.09	115.32
56	1y	55	PSU	O2-C2-N1	-4.29	118.37	122.79
32	1a	516	PSU	O2-C2-N1	-4.28	118.38	122.79
54	1w	39	PSU	C4-N3-C2	-4.27	120.48	126.37
56	2y	8	4SU	N3-C2-N1	4.26	120.44	114.89
32	2a	1207	2MG	N9-C4-N3	4.26	134.47	125.95
1	2A	2605	PSU	C4-N3-C2	-4.25	120.52	126.37
32	1a	527	7MG	C2-N3-C4	4.24	119.61	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1519	MA6	C2-N1-C6	4.24	122.19	111.83
32	2a	1519	MA6	C2-N1-C6	4.24	122.18	111.83
55	2x	8	4SU	C1'-N1-C2	4.24	125.20	117.59
32	2a	1518	MA6	C2-N1-C6	4.24	122.17	111.83
32	1a	1518	MA6	C2-N1-C6	4.22	122.14	111.83
56	2y	55	PSU	C4-N3-C2	-4.20	120.58	126.37
32	2a	527	7MG	C2-N3-C4	4.20	119.53	112.30
1	1A	2515	2MA	N6-C6-N1	4.19	122.69	117.03
32	1a	966	M2G	C2-N3-C4	4.18	120.25	112.51
32	2a	1519	MA6	C9-N6-C6	-4.18	109.89	120.52
54	2w	46	7MG	C2-N3-C4	4.18	119.49	112.30
54	2w	54	5MU	C5-C4-N3	4.17	118.95	115.32
56	2y	54	5MU	C5-C4-N3	4.16	118.94	115.32
32	2a	516	PSU	C4-N3-C2	-4.15	120.66	126.37
55	2x	54	5MU	C5-C4-N3	4.14	118.92	115.32
54	1w	54	5MU	O4-C4-C5	-4.12	120.20	124.92
1	1A	1939	PSU	C4-N3-C2	-4.12	120.70	126.37
32	1a	1519	MA6	C4-C5-N7	-4.08	105.91	110.58
55	1x	54	5MU	C5-C4-N3	4.07	118.86	115.32
1	2A	1911	PSU	C4-N3-C2	-4.06	120.77	126.37
55	1x	54	5MU	O4-C4-C5	-4.05	120.28	124.92
54	1w	37	MIA	C15-C14-C13	-4.04	110.52	122.66
32	2a	1519	MA6	N3-C4-N9	4.03	134.02	127.17
32	2a	1518	MA6	N3-C4-N9	4.03	134.01	127.17
54	2w	54	5MU	O4-C4-C5	-4.00	120.34	124.92
32	1a	1207	2MG	C6-C5-N7	3.97	137.52	130.29
32	1a	516	PSU	C4-N3-C2	-3.97	120.91	126.37
54	2w	32	PSU	C4-N3-C2	-3.95	120.92	126.37
1	1A	2515	2MA	C4-N9-C8	3.94	109.88	105.74
32	2a	1518	MA6	C4-C5-N7	-3.94	106.07	110.58
56	1y	8	4SU	N3-C2-N1	3.94	120.02	114.89
1	1A	1933	PSU	C4-N3-C2	-3.93	120.95	126.37
32	1a	1404	5MC	C5-C6-N1	-3.93	119.04	123.31
56	2y	39	PSU	C4-N3-C2	-3.91	120.99	126.37
32	1a	1519	MA6	C2-N3-C4	3.90	121.35	111.83
54	1w	46	7MG	C2-N3-C4	3.89	118.99	112.30
1	1A	1961	5MU	C5-C6-N1	-3.88	119.10	123.31
54	1w	32	PSU	C4-N3-C2	-3.87	121.04	126.37
54	2w	54	5MU	C5-C6-N1	-3.84	119.15	123.31
1	2A	2503	2MA	N6-C6-N1	3.84	122.20	117.03
54	1w	54	5MU	C5-C4-N3	3.83	118.66	115.32
54	1w	55	PSU	O2-C2-N1	-3.83	118.84	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1y	8	4SU	C5-C4-S4	-3.81	119.95	124.31
32	1a	1207	2MG	N9-C4-N3	3.81	133.58	125.95
55	2x	55	PSU	C4-N3-C2	-3.78	121.16	126.37
32	2a	516	PSU	O2-C2-N1	-3.78	118.89	122.79
54	2w	8	4SU	N3-C2-N1	3.77	119.79	114.89
56	1y	54	5MU	O4-C4-C5	-3.76	120.61	124.92
54	1w	32	PSU	O2-C2-N1	-3.75	118.92	122.79
55	1x	8	4SU	C6-C5-C4	-3.75	116.70	119.95
1	2A	1962	5MC	C5-C6-N1	-3.74	119.25	123.31
56	1y	32	PSU	C4-N3-C2	-3.74	121.21	126.37
56	2y	54	5MU	O4-C4-C5	-3.74	120.63	124.92
1	2A	1915	5MU	O4-C4-C5	-3.72	120.66	124.92
54	2w	55	PSU	C4-N3-C2	-3.71	121.25	126.37
32	2a	1407	5MC	C5-C6-N1	-3.71	119.29	123.31
56	2y	32	PSU	O2-C2-N1	-3.70	118.97	122.79
55	1x	32	5MC	C5-C6-N1	-3.69	119.31	123.31
55	2x	54	5MU	O4-C4-C5	-3.68	120.70	124.92
56	2y	37	MIA	C2-N3-C4	3.68	120.81	111.83
55	1x	55	PSU	C4-N3-C2	-3.66	121.32	126.37
54	2w	8	4SU	C5-C4-S4	-3.66	120.12	124.31
32	1a	1518	MA6	N3-C4-N9	3.65	133.38	127.17
32	1a	1519	MA6	N1-C2-N3	-3.65	123.06	128.58
1	2A	1942	5MC	C5-C6-N1	-3.64	119.36	123.31
56	1y	37	MIA	C2-N3-C4	3.64	120.72	111.83
54	1w	76	F3N	N9-C8-N7	-3.64	108.78	113.94
1	1A	2515	2MA	C4-C5-N7	-3.62	106.44	110.58
1	1A	2617	PSU	C4-N3-C2	-3.62	121.38	126.37
56	2y	32	PSU	C4-N3-C2	-3.62	121.39	126.37
56	2y	37	MIA	C4-C5-N7	-3.62	106.45	110.58
32	1a	1518	MA6	C2-N3-C4	3.61	120.65	111.83
32	1a	1400	5MC	C5-C6-N1	-3.60	119.40	123.31
54	2w	39	PSU	C4-N3-C2	-3.60	121.41	126.37
54	1w	55	PSU	C4-N3-C2	-3.59	121.42	126.37
56	2y	55	PSU	O2-C2-N1	-3.59	119.09	122.79
55	2x	54	5MU	C5-C6-N1	-3.58	119.43	123.31
54	1w	37	MIA	C16-C14-C13	-3.56	111.98	122.66
32	2a	1519	MA6	C2-N3-C4	3.55	120.50	111.83
1	1A	1937	5MU	O4-C4-C5	-3.53	120.88	124.92
32	2a	967	5MC	C5-C6-N1	-3.51	119.50	123.31
54	1w	76	F3N	C2-N3-C4	3.51	120.40	111.83
1	2A	1911	PSU	O2-C2-N1	-3.48	119.20	122.79
54	1w	37	MIA	C6-C5-N7	3.47	136.22	132.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	37	MIA	C4-C5-N7	-3.45	106.63	110.58
1	1A	1939	PSU	O2-C2-N1	-3.45	119.23	122.79
54	2w	55	PSU	O2-C2-N1	-3.43	119.25	122.79
54	1w	8	4SU	C5-C4-S4	-3.43	120.39	124.31
32	2a	1400	5MC	C5-C6-N1	-3.42	119.60	123.31
32	2a	1518	MA6	C2-N3-C4	3.40	120.14	111.83
56	1y	54	5MU	C5-C6-N1	-3.40	119.62	123.31
54	2w	32	PSU	O2-C2-N1	-3.38	119.30	122.79
54	2w	37	MIA	C2-N3-C4	3.38	121.14	112.29
1	2A	1939	5MU	O4-C4-C5	-3.38	121.05	124.92
55	1x	55	PSU	O2-C2-N1	-3.35	119.34	122.79
1	2A	1915	5MU	C5-C6-N1	-3.33	119.69	123.31
1	2A	2552	2MU	O2-C2-N1	-3.31	118.48	122.80
56	1y	37	MIA	C4-C5-N7	-3.31	106.80	110.58
1	2A	2503	2MA	C4-N9-C8	3.31	109.21	105.74
54	1w	76	F3N	C5-N7-C8	3.29	108.62	103.45
54	1w	37	MIA	C2-N3-C4	3.29	120.90	112.29
54	1w	37	MIA	C4-C5-N7	-3.27	106.84	110.58
56	2y	37	MIA	N3-C2-N1	-3.27	123.64	128.58
1	1A	1937	5MU	C5-C6-N1	-3.25	119.78	123.31
32	1a	1207	2MG	C4-C5-N7	-3.25	105.52	110.67
55	1x	54	5MU	C5-C6-N1	-3.25	119.79	123.31
54	1w	39	PSU	O2-C2-N1	-3.24	119.44	122.79
55	1x	32	5MC	C5-C4-N3	-3.24	118.43	121.75
43	2l	92	0TD	OD2-CG-CB	3.23	120.12	113.15
32	2a	1519	MA6	C5-N7-C8	3.23	108.52	103.45
32	2a	1207	2MG	C6-C5-N7	3.21	136.14	130.29
56	1y	37	MIA	N3-C2-N1	-3.21	123.72	128.58
55	1x	8	4SU	C1'-N1-C2	3.21	123.35	117.59
55	2x	55	PSU	O2-C2-N1	-3.20	119.49	122.79
56	1y	8	4SU	C1'-N1-C2	3.19	123.31	117.59
1	1A	1964	5MC	C5-C6-N1	-3.18	119.86	123.31
32	2a	1407	5MC	C5-C4-N3	-3.17	118.50	121.75
1	1A	2515	2MA	C5-N7-C8	3.16	108.42	103.45
1	1A	1937	5MU	O2-C2-N1	-3.14	118.71	122.80
32	1a	1407	5MC	C5-C6-N1	-3.13	119.92	123.31
55	2x	32	5MC	C5-C6-N1	-3.11	119.94	123.31
54	1w	54	5MU	C5-C6-N1	-3.11	119.94	123.31
1	1A	2617	PSU	O2-C2-N1	-3.10	119.59	122.79
32	1a	1518	MA6	N1-C2-N3	-3.10	123.89	128.58
54	2w	76	F3N	N9-C8-N7	-3.08	109.57	113.94
32	1a	1498	UR3	C5-C4-N3	3.07	119.08	115.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1404	5MC	C5-C6-N1	-3.07	119.98	123.31
54	1w	8	4SU	N3-C2-N1	3.06	118.88	114.89
55	1x	8	4SU	C5-C4-N3	3.06	117.59	114.75
54	2w	37	MIA	C6-C5-N7	3.05	135.76	132.43
55	1x	54	5MU	O2-C2-N1	-3.05	118.83	122.80
54	2w	76	F3N	C2-N3-C4	3.04	119.25	111.83
32	2a	1498	UR3	C5-C4-N3	3.03	119.03	115.04
32	2a	1519	MA6	N1-C2-N3	-3.01	124.03	128.58
54	2w	37	MIA	C11-S10-C2	-3.00	100.00	102.25
32	1a	1519	MA6	C4-N9-C8	2.99	108.88	105.74
1	2A	2503	2MA	C4-C5-N7	-2.99	107.16	110.58
32	1a	1519	MA6	C5-N7-C8	2.98	108.14	103.45
32	1a	967	5MC	C5-C4-N3	-2.98	118.70	121.75
32	1a	1518	MA6	C10-N6-C6	-2.97	112.95	120.52
55	1x	8	4SU	O2-C2-N1	2.97	126.67	122.80
56	2y	54	5MU	C5-C6-N1	-2.97	120.09	123.31
32	2a	1518	MA6	N1-C2-N3	-2.96	124.10	128.58
32	1a	1407	5MC	C5-C4-N3	-2.96	118.72	121.75
32	1a	967	5MC	C5-C6-N1	-2.95	120.11	123.31
32	1a	1498	UR3	C6-N1-C2	-2.95	119.39	121.80
54	2w	46	7MG	C5-C4-N9	-2.95	102.56	106.33
1	2A	1917	PSU	O2-C2-N1	-2.95	119.75	122.79
32	2a	1518	MA6	C10-N6-C6	-2.94	113.05	120.52
43	1l	92	0TD	OD2-CG-CB	2.93	119.48	113.15
56	2y	39	PSU	O2-C2-N1	-2.92	119.77	122.79
56	1y	46	7MG	C5-C4-N9	-2.90	102.62	106.33
1	1A	2515	2MA	N9-C8-N7	-2.89	109.83	113.94
56	2y	37	MIA	C4-N9-C8	2.89	108.77	105.74
54	1w	46	7MG	C5-C4-N9	-2.88	102.64	106.33
1	1A	1984	5MC	C5-C6-N1	-2.86	120.20	123.31
32	2a	1404	5MC	O2-C2-N3	-2.86	117.83	122.33
32	2a	1402	4OC	C6-C5-C4	2.84	120.42	117.00
56	2y	46	7MG	C5-C4-N9	-2.84	102.70	106.33
1	2A	2552	2MU	C5-C4-N3	2.81	118.74	114.80
55	2x	32	5MC	C5-C4-N3	-2.81	118.88	121.75
32	2a	1404	5MC	C5-C4-N3	-2.80	118.88	121.75
32	2a	967	5MC	O2-C2-N3	-2.80	117.91	122.33
54	1w	76	F3N	N3-C4-N9	2.80	131.93	127.17
55	2x	32	5MC	O2-C2-N3	-2.80	117.92	122.33
32	1a	966	M2G	C6-C5-N7	2.79	135.38	130.29
1	1A	1964	5MC	C1'-N1-C6	-2.79	116.56	121.15
1	2A	2605	PSU	C5-C6-N1	-2.79	118.27	122.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	966	M2G	C6-C5-N7	2.78	135.34	130.29
32	1a	1518	MA6	C5-N7-C8	2.77	107.80	103.45
1	1A	2263	OMG	C6-C5-N7	2.74	135.28	130.29
1	1A	1964	5MC	C5-C4-N3	-2.74	118.95	121.75
1	1A	2564	2MU	C2'-C1'-N1	-2.73	109.05	114.24
56	2y	37	MIA	C5-N7-C8	2.73	107.74	103.45
55	2x	8	4SU	C6-C5-C4	-2.73	117.59	119.95
55	2x	8	4SU	O2-C2-N1	2.72	126.34	122.80
1	1A	1937	5MU	C5M-C5-C4	2.72	121.68	118.78
56	1y	32	PSU	O2-C2-N1	-2.72	119.99	122.79
54	1w	37	MIA	C4-N9-C8	2.71	108.58	105.74
1	1A	2564	2MU	O2-C2-N1	-2.71	119.28	122.80
32	2a	1518	MA6	C4-N9-C8	2.70	108.57	105.74
54	1w	55	PSU	C6-C5-C4	-2.70	116.36	118.17
54	2w	54	5MU	O2-C2-N1	-2.69	119.29	122.80
32	1a	1404	5MC	C5-C4-N3	-2.69	119.00	121.75
1	1A	2564	2MU	C5-C4-N3	2.69	118.57	114.80
1	2A	2251	OMG	C6-C5-N7	2.69	135.18	130.29
32	2a	1519	MA6	C4-N9-C8	2.68	108.55	105.74
32	2a	527	7MG	C5-C6-N1	2.68	115.65	110.94
32	2a	1518	MA6	C5-N7-C8	2.68	107.66	103.45
32	1a	1400	5MC	C5-C4-N3	-2.67	119.02	121.75
54	2w	76	F3N	C5-C4-N9	2.65	108.70	105.81
1	2A	1962	5MC	C5-C4-N3	-2.64	119.05	121.75
54	2w	46	7MG	C5-C6-N1	2.64	115.59	110.94
54	1w	54	5MU	O2-C2-N1	-2.63	119.37	122.80
1	2A	1939	5MU	O2-C2-N1	-2.61	119.40	122.80
32	2a	1519	MA6	C6-C5-N7	2.59	137.57	133.43
1	2A	1920	4OC	O2-C2-N3	-2.57	118.28	122.33
32	1a	527	7MG	C5-C6-N1	2.57	115.46	110.94
32	2a	1498	UR3	C6-N1-C2	-2.56	119.71	121.80
1	2A	2552	2MU	O4-C4-C5	-2.55	120.77	125.16
1	2A	2605	PSU	O2-C2-N1	-2.54	120.17	122.79
54	1w	37	MIA	C2-N1-C6	2.54	122.36	117.54
32	1a	1498	UR3	C1'-N1-C2	2.54	121.19	117.04
1	2A	2503	2MA	C2-N1-C6	2.53	121.99	118.10
56	1y	46	7MG	C5-C6-N1	2.53	115.39	110.94
32	1a	1518	MA6	C6-C5-N7	2.51	137.45	133.43
54	2w	76	F3N	C6-C5-C4	2.51	120.61	117.18
1	2A	1915	5MU	O2-C2-N1	-2.51	119.53	122.80
32	2a	1207	2MG	C4-C5-N7	-2.50	106.71	110.67
1	2A	1917	PSU	C5-C6-N1	-2.50	118.68	122.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	54	5MU	C1'-N1-C2	2.49	122.07	117.59
54	2w	37	MIA	C5-N7-C8	2.49	107.36	103.45
56	2y	54	5MU	O2-C2-N3	-2.49	116.90	121.49
32	2a	967	5MC	C5-C4-N3	-2.48	119.21	121.75
32	2a	966	M2G	C4-C5-N7	-2.47	106.76	110.67
32	2a	1402	4OC	O2-C2-N3	-2.46	118.45	122.33
32	2a	1400	5MC	C5-C4-N3	-2.46	119.23	121.75
32	1a	1519	MA6	N9-C8-N7	-2.45	110.47	113.94
56	1y	32	PSU	C6-C5-C4	-2.44	116.53	118.17
54	1w	37	MIA	N3-C2-N1	-2.44	122.55	127.00
56	1y	37	MIA	C5-N7-C8	2.43	107.27	103.45
32	1a	1519	MA6	C6-C5-N7	2.43	137.31	133.43
43	2l	92	0TD	OD1-CG-CB	-2.43	117.36	122.44
32	1a	967	5MC	O2-C2-N3	-2.41	118.53	122.33
54	2w	37	MIA	C2-N1-C6	2.41	122.12	117.54
32	1a	966	M2G	O6-C6-C5	-2.41	120.17	126.53
1	2A	2503	2MA	C5-N7-C8	2.41	107.23	103.45
1	2A	2605	PSU	O2-C2-N3	-2.41	117.59	121.86
54	1w	37	MIA	C5-N7-C8	2.40	107.23	103.45
1	2A	1942	5MC	C5-C4-N3	-2.40	119.29	121.75
1	1A	2515	2MA	C2-N1-C6	2.40	121.79	118.10
32	2a	1519	MA6	C10-N6-C6	-2.40	114.42	120.52
54	2w	76	F3N	C5-N7-C8	2.40	107.22	103.45
32	1a	1519	MA6	C10-N6-C6	-2.40	114.42	120.52
1	2A	2552	2MU	C2'-C1'-N1	-2.40	109.69	114.24
54	2w	39	PSU	O2-C2-N1	-2.39	120.33	122.79
55	1x	32	5MC	O2-C2-N3	-2.38	118.58	122.33
1	2A	2251	OMG	O6-C6-C5	-2.36	120.30	126.53
54	1w	46	7MG	C5-C6-N1	2.35	115.08	110.94
32	2a	516	PSU	O4'-C1'-C2'	2.35	108.41	105.15
55	2x	8	4SU	O2-C2-N3	-2.34	117.17	121.49
32	2a	1519	MA6	N9-C8-N7	-2.34	110.62	113.94
56	1y	37	MIA	C4-N9-C8	2.34	108.19	105.74
1	1A	1961	5MU	O2-C2-N3	-2.34	117.18	121.49
32	1a	966	M2G	C4-C5-N7	-2.33	106.97	110.67
1	1A	1942	4OC	O2-C2-N3	-2.33	118.65	122.33
32	2a	1400	5MC	CM5-C5-C6	-2.31	119.72	122.85
54	2w	37	MIA	C12-N6-C6	-2.31	120.71	122.85
1	1A	1984	5MC	O2-C2-N3	-2.31	118.69	122.33
56	1y	39	PSU	C5-C6-N1	-2.30	118.94	122.14
54	1w	54	5MU	C5M-C5-C4	2.29	121.23	118.78
54	2w	8	4SU	C1'-N1-C2	2.29	121.70	117.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	8	4SU	C1'-N1-C6	-2.29	115.89	120.78
1	1A	2263	OMG	C4-C5-N7	-2.28	107.05	110.67
56	1y	54	5MU	C5M-C5-C4	2.28	121.22	118.78
1	1A	1937	5MU	C5M-C5-C6	-2.28	119.77	122.85
1	1A	2263	OMG	O6-C6-C5	-2.27	120.54	126.53
1	2A	1917	PSU	O2-C2-N3	-2.27	117.83	121.86
32	2a	516	PSU	C5-C6-N1	-2.26	119.01	122.14
32	1a	527	7MG	C5-C4-N9	-2.26	103.44	106.33
54	2w	37	MIA	N3-C2-N1	-2.25	122.90	127.00
32	2a	1518	MA6	C10-N6-C9	-2.24	108.97	116.18
32	1a	527	7MG	O6-C6-C5	-2.24	122.12	127.62
32	2a	527	7MG	C5-C4-N9	-2.24	103.47	106.33
1	1A	1939	PSU	C5-C6-N1	-2.22	119.06	122.14
32	2a	1400	5MC	O2-C2-N3	-2.22	118.83	122.33
56	2y	55	PSU	C5-C6-N1	-2.22	119.06	122.14
32	2a	1518	MA6	C6-C5-N7	2.22	136.97	133.43
55	2x	8	4SU	C1'-N1-C6	-2.20	116.07	120.78
54	1w	76	F3N	C4-C5-N7	-2.20	108.07	110.58
1	1A	1984	5MC	C5-C4-N3	-2.19	119.51	121.75
32	1a	1498	UR3	O2-C2-N3	-2.19	118.31	121.33
1	1A	1964	5MC	CM5-C5-C6	-2.19	119.89	122.85
32	2a	966	M2G	O6-C6-C5	-2.17	120.80	126.53
56	1y	8	4SU	O2-C2-N3	-2.17	117.49	121.49
54	2w	32	PSU	C5-C6-N1	-2.16	119.14	122.14
54	2w	37	MIA	C4-N9-C8	2.16	108.00	105.74
1	2A	1939	5MU	C5M-C5-C6	-2.15	119.94	122.85
1	2A	2503	2MA	N9-C8-N7	-2.14	110.89	113.94
54	2w	76	F3N	N3-C4-N9	2.14	130.81	127.17
54	1w	76	F3N	C5-C4-N9	2.14	108.14	105.81
54	1w	46	7MG	O6-C6-C5	-2.13	122.38	127.62
54	1w	37	MIA	C11-S10-C2	-2.12	100.66	102.25
32	1a	1207	2MG	C8-N7-C5	2.12	108.03	104.26
56	2y	46	7MG	C5-C6-N1	2.11	114.65	110.94
32	1a	1402	4OC	CM4-N4-C4	-2.10	118.34	122.45
32	1a	1402	4OC	O2-C2-N3	-2.10	119.02	122.33
56	2y	55	PSU	O4'-C1'-C2'	2.09	108.05	105.15
32	1a	1402	4OC	C6-C5-C4	2.08	119.51	117.00
32	2a	1400	5MC	C1'-N1-C6	-2.08	117.73	121.15
1	2A	2251	OMG	C4-C5-N7	-2.08	107.38	110.67
55	2x	8	4SU	C5-C4-S4	-2.08	121.94	124.31
54	1w	39	PSU	C5-C6-N1	-2.07	119.26	122.14
1	1A	2564	2MU	O4-C4-C5	-2.07	121.59	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1498	UR3	C3U-N3-C4	2.07	120.74	117.87
56	1y	55	PSU	O4-C4-C5	-2.07	118.86	124.01
32	1a	1207	2MG	N1-C2-N2	2.07	118.67	116.56
1	2A	2251	OMG	C5-C6-N1	2.07	118.52	113.25
54	2w	39	PSU	C5-C6-N1	-2.06	119.28	122.14
54	2w	46	7MG	O6-C6-C5	-2.06	122.56	127.62
55	1x	55	PSU	C5-C6-N1	-2.06	119.28	122.14
56	2y	8	4SU	C6-N1-C2	-2.05	118.50	121.00
54	1w	37	MIA	C16-C14-C15	-2.05	109.87	114.59
32	2a	527	7MG	O6-C6-C5	-2.04	122.61	127.62
32	1a	1518	MA6	C10-N6-C9	-2.04	109.62	116.18
56	2y	32	PSU	C6-C5-C4	-2.03	116.81	118.17
1	1A	1964	5MC	O2-C2-N3	-2.02	119.15	122.33
1	2A	1911	PSU	C5-C6-N1	-2.01	119.36	122.14

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C5-C6-N6-C12
54	1w	37	MIA	N1-C2-S10-C11
54	1w	37	MIA	N3-C2-S10-C11
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
54	1w	46	7MG	C4'-C5'-O5'-P
54	2w	76	F3N	C-CA-CB-CG
56	1y	37	MIA	C3'-C4'-C5'-O5'
56	1y	46	7MG	C4'-C5'-O5'-P
56	1y	54	5MU	C3'-C4'-C5'-O5'
56	1y	54	5MU	O4'-C4'-C5'-O5'
56	2y	55	PSU	C2'-C1'-C5-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
56	2y	37	MIA	C3'-C4'-C5'-O5'
56	1y	46	7MG	C3'-C4'-C5'-O5'
56	1y	37	MIA	O4'-C4'-C5'-O5'
56	2y	37	MIA	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
56	1y	46	7MG	O4'-C4'-C5'-O5'
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	2y	46	7MG	O4'-C1'-N9-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	1w	37	MIA	N1-C6-N6-C12
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C10
32	1a	1519	MA6	C3'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
56	2y	32	PSU	O4'-C4'-C5'-O5'
56	1y	46	7MG	C2'-C1'-N9-C8
56	2y	46	7MG	C2'-C1'-N9-C8
55	1x	55	PSU	O4'-C4'-C5'-O5'
54	2w	76	F3N	N-CA-CB-CG
54	2w	46	7MG	C4'-C5'-O5'-P
54	1w	46	7MG	C2'-C1'-N9-C8
56	2y	8	4SU	C2'-C1'-N1-C2
56	2y	8	4SU	C2'-C1'-N1-C6
32	1a	1519	MA6	C5-C6-N6-C9
56	2y	46	7MG	O4'-C1'-N9-C8
1	2A	1920	4OC	C3'-C2'-O2'-CM2
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
32	2a	967	5MC	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
56	1y	46	7MG	O4'-C1'-N9-C8
56	1y	8	4SU	C2'-C1'-N1-C6
54	2w	46	7MG	C2'-C1'-N9-C8
1	2A	2503	2MA	C4'-C5'-O5'-P
43	1l	92	0TD	CG-CB-SB-CSB
1	1A	1984	5MC	C2'-C1'-N1-C6
1	1A	1942	4OC	C2'-C1'-N1-C2
1	2A	1920	4OC	C2'-C1'-N1-C2
54	2w	46	7MG	C3'-C4'-C5'-O5'
56	2y	54	5MU	C2'-C1'-N1-C2
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2515	2MA	C4'-C5'-O5'-P
32	2a	527	7MG	C4'-C5'-O5'-P
56	2y	37	MIA	C4'-C5'-O5'-P
56	1y	8	4SU	C2'-C1'-N1-C2
1	1A	1984	5MC	O4'-C1'-N1-C6

There are no ring outliers.

39 monomers are involved in 60 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1w	39	PSU	1	0
32	1a	1518	MA6	2	0
32	2a	1404	5MC	1	0
32	1a	1519	MA6	3	0
32	2a	1519	MA6	2	0
1	1A	1961	5MU	1	0
56	1y	39	PSU	1	0
56	2y	37	MIA	2	0
56	1y	8	4SU	1	0
54	1w	46	7MG	2	0
56	1y	55	PSU	3	0
55	1x	8	4SU	1	0
56	1y	37	MIA	1	0
1	1A	2617	PSU	1	0
56	1y	32	PSU	1	0
32	2a	966	M2G	1	0
55	2x	8	4SU	1	0
1	1A	2515	2MA	1	0
32	2a	1518	MA6	4	0
1	1A	2564	2MU	1	0
54	1w	37	MIA	1	0
1	2A	1920	4OC	4	0
54	1w	76	F3N	2	0
32	2a	1402	4OC	2	0
56	1y	54	5MU	2	0
56	2y	8	4SU	4	0
43	1l	92	0TD	1	0
56	2y	55	PSU	5	0
54	2w	46	7MG	1	0
1	2A	2552	2MU	1	0
1	2A	1915	5MU	1	0
32	2a	967	5MC	2	0
55	1x	54	5MU	1	0
1	2A	2503	2MA	2	0
54	2w	8	4SU	1	0
32	1a	1402	4OC	2	0
56	2y	46	7MG	1	0
54	2w	76	F3N	2	0
54	2w	37	MIA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2411 ligands modelled in this entry, 2407 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
59	AQJ	2A	3677	-	37,38,38	3.29	7 (18%)	48,56,56	1.60	6 (12%)
61	SF4	2d	501	35	0,12,12	-	-	-		
59	AQJ	1A	3969	-	37,38,38	3.25	7 (18%)	48,56,56	1.63	9 (18%)
61	SF4	1d	501	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
59	AQJ	2A	3677	-	-	5/54/70/70	0/1/2/2
61	SF4	2d	501	35	-	-	0/6/5/5
59	AQJ	1A	3969	-	-	13/54/70/70	0/1/2/2
61	SF4	1d	501	35	-	-	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	3969	AQJ	CBK-CAP	-10.35	1.39	1.51
59	2A	3677	AQJ	CBK-CAP	-10.20	1.39	1.51
59	2A	3677	AQJ	CBC-CAY	-9.35	1.39	1.52
59	1A	3969	AQJ	CBA-CAW	-8.41	1.38	1.51
59	1A	3969	AQJ	CBD-CAY	-8.20	1.39	1.52
59	2A	3677	AQJ	CBC-CAX	-8.18	1.37	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	3969	AQJ	CBC-CAY	-7.73	1.42	1.52
59	2A	3677	AQJ	CBA-CAW	-7.44	1.39	1.51
59	2A	3677	AQJ	CBD-CAY	-7.35	1.40	1.52
59	1A	3969	AQJ	CBC-CAX	-5.84	1.41	1.51
59	1A	3969	AQJ	CBB-CBH	3.94	1.60	1.53
59	1A	3969	AQJ	CAO-CAP	3.24	1.39	1.32
59	2A	3677	AQJ	CAO-CAP	3.07	1.39	1.32
59	2A	3677	AQJ	OAV-CBF	2.06	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	2A	3677	AQJ	CBG-OAT-CAX	-4.88	109.67	118.20
59	1A	3969	AQJ	OAT-CAX-CBC	4.82	115.69	110.93
59	2A	3677	AQJ	OAT-CAX-CBC	4.13	115.01	110.93
59	1A	3969	AQJ	CBA-CAR-CBB	-3.97	107.98	115.09
59	1A	3969	AQJ	CBG-OAT-CAX	-3.65	111.83	118.20
59	2A	3677	AQJ	OAK-CAX-CBC	-3.60	119.99	124.65
59	2A	3677	AQJ	OAT-CBG-CAQ	3.22	113.34	107.36
59	1A	3969	AQJ	OAT-CBG-CAQ	3.13	113.18	107.36
59	1A	3969	AQJ	OAK-CAX-CBC	-3.09	120.64	124.65
59	1A	3969	AQJ	CAB-CAZ-CAS	-3.06	108.64	113.27
59	2A	3677	AQJ	CBD-CBH-CBB	-2.96	109.03	114.19
59	1A	3969	AQJ	CBF-CBE-CBI	2.32	112.86	109.15
59	1A	3969	AQJ	CAP-CAO-CAW	-2.23	117.48	122.02
59	1A	3969	AQJ	CAS-CBI-NBJ	-2.16	109.51	115.59
59	2A	3677	AQJ	CBK-CAP-CAO	-2.07	122.56	126.00

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	3969	AQJ	CAO-CAP-CBK-OAN
59	2A	3677	AQJ	CAO-CAP-CBK-OAN
59	1A	3969	AQJ	OAU-CBF-OAV-CBH
59	1A	3969	AQJ	CBA-CAR-CBB-CAD
59	2A	3677	AQJ	CAS-CBI-NBJ-CAH
59	1A	3969	AQJ	OAJ-CAW-CBA-CAC
59	1A	3969	AQJ	CAO-CAW-CBA-CAC
59	2A	3677	AQJ	CAO-CAP-CBK-CBG
59	2A	3677	AQJ	CAA-CAQ-CBG-OAT
59	1A	3969	AQJ	CBA-CAR-CBB-CBH

Continued on next page...

Continued from previous page...

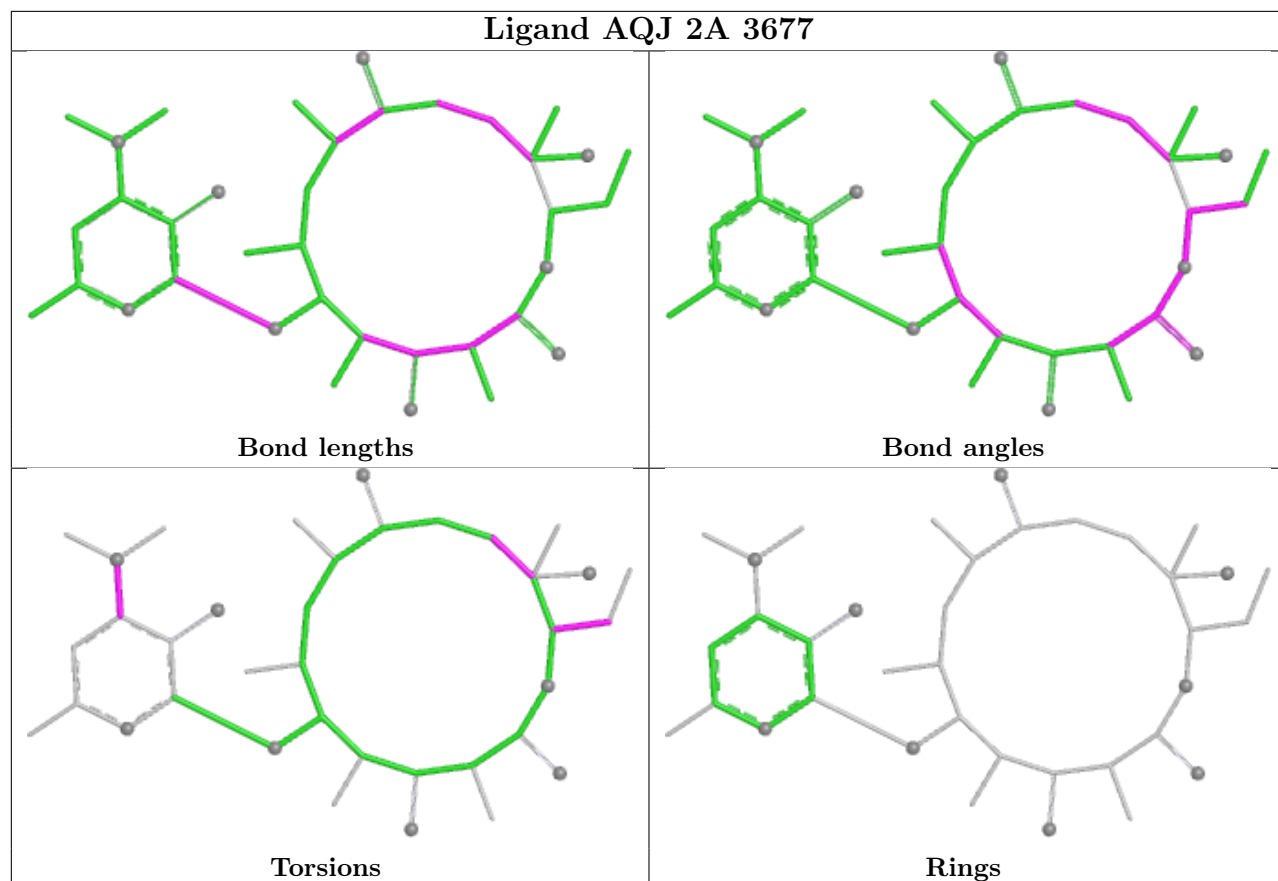
Mol	Chain	Res	Type	Atoms
59	1A	3969	AQJ	OAL-CAY-CBC-CAX
59	1A	3969	AQJ	CAS-CBI-NBJ-CAH
59	1A	3969	AQJ	CBB-CAR-CBA-CAC
59	1A	3969	AQJ	CBB-CAR-CBA-CAW
59	1A	3969	AQJ	CBE-CBF-OAV-CBH
59	2A	3677	AQJ	CAA-CAQ-CBG-CBK
59	1A	3969	AQJ	CAA-CAQ-CBG-OAT
59	1A	3969	AQJ	CAA-CAQ-CBG-CBK

There are no ring outliers.

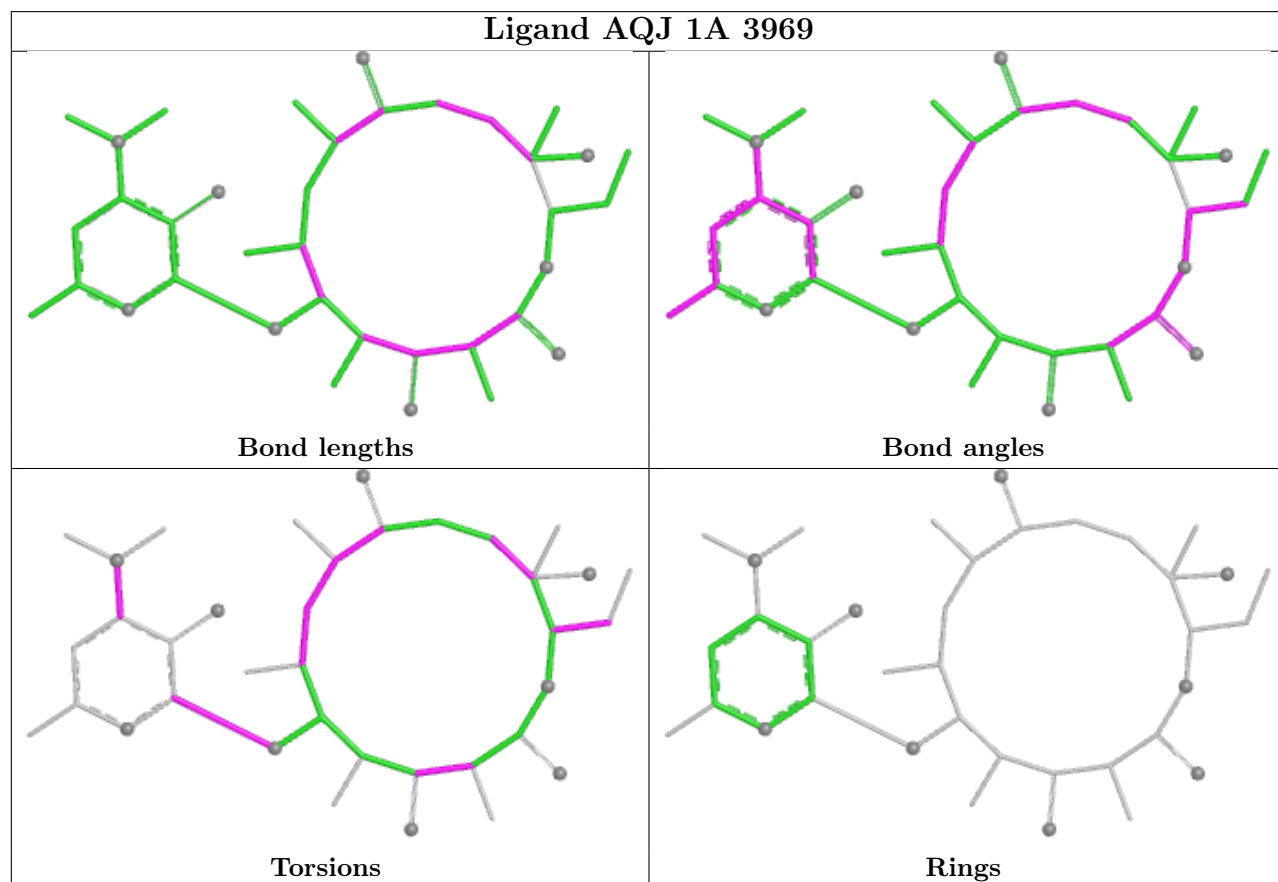
No monomer is involved in short contacts.

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

Ligand AQJ 2A 3677



Ligand AQJ 1A 3969



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.47	142 (4%) 34 28	13, 30, 84, 98	0
1	2A	2789/2915 (95%)	0.12	100 (3%) 46 40	27, 51, 81, 94	0
2	1B	120/121 (99%)	-0.40	0 100 100	21, 40, 54, 78	0
2	2B	120/121 (99%)	1.22	21 (17%) 4 3	53, 71, 81, 88	0
3	1D	275/276 (99%)	-0.03	4 (1%) 72 68	14, 34, 49, 66	0
3	2D	275/276 (99%)	0.48	5 (1%) 67 63	25, 47, 58, 76	0
4	1E	204/206 (99%)	0.02	1 (0%) 87 85	12, 37, 53, 65	0
4	2E	204/206 (99%)	0.47	2 (0%) 79 76	30, 52, 66, 79	0
5	1F	203/210 (96%)	0.07	3 (1%) 72 68	14, 38, 60, 72	0
5	2F	203/210 (96%)	0.79	11 (5%) 31 26	29, 61, 73, 80	0
6	1G	181/182 (99%)	0.54	6 (3%) 49 43	32, 50, 66, 77	0
6	2G	181/182 (99%)	1.68	55 (30%) 1 1	61, 73, 80, 85	0
7	1H	174/180 (96%)	0.39	5 (2%) 53 48	32, 48, 60, 68	0
7	2H	174/180 (96%)	1.46	35 (20%) 3 2	57, 75, 82, 87	0
8	1I	146/148 (98%)	0.98	11 (7%) 20 16	39, 64, 74, 79	0
8	2I	146/148 (98%)	1.41	31 (21%) 2 2	49, 68, 78, 85	0
9	1N	140/140 (100%)	0.03	2 (1%) 73 69	22, 35, 53, 59	0
9	2N	140/140 (100%)	0.81	5 (3%) 46 40	40, 58, 69, 73	0
10	1O	122/122 (100%)	-0.03	0 100 100	20, 37, 55, 62	0
10	2O	122/122 (100%)	0.49	0 100 100	35, 51, 62, 69	0
11	1P	149/150 (99%)	0.30	6 (4%) 42 37	12, 40, 62, 73	0
11	2P	149/150 (99%)	0.74	7 (4%) 36 30	33, 61, 74, 82	0
12	1Q	141/141 (100%)	0.03	2 (1%) 73 69	19, 36, 47, 69	0
12	2Q	141/141 (100%)	0.93	13 (9%) 14 11	37, 59, 70, 78	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%)	-0.18	0 100 100	19, 31, 46, 56	0
13	2R	118/118 (100%)	0.42	1 (0%) 82 80	35, 48, 59, 65	0
14	1S	110/112 (98%)	0.08	0 100 100	30, 43, 53, 60	0
14	2S	110/112 (98%)	1.58	32 (29%) 1 1	57, 67, 76, 79	0
15	1T	131/146 (89%)	0.30	8 (6%) 27 22	28, 41, 63, 82	0
15	2T	131/146 (89%)	0.68	8 (6%) 27 22	44, 55, 69, 79	0
16	1U	116/118 (98%)	-0.24	0 100 100	15, 26, 43, 63	0
16	2U	116/118 (98%)	0.84	4 (3%) 48 42	38, 54, 68, 75	0
17	1V	101/101 (100%)	-0.17	0 100 100	18, 36, 50, 65	0
17	2V	101/101 (100%)	0.89	6 (5%) 28 23	42, 64, 73, 77	0
18	1W	112/113 (99%)	-0.07	3 (2%) 56 50	20, 27, 46, 73	0
18	2W	112/113 (99%)	0.47	2 (1%) 67 63	34, 45, 60, 74	0
19	1X	95/96 (98%)	-0.16	0 100 100	22, 33, 53, 60	0
19	2X	95/96 (98%)	0.75	6 (6%) 26 20	44, 54, 65, 74	0
20	1Y	107/110 (97%)	0.33	3 (2%) 55 49	28, 42, 61, 72	0
20	2Y	107/110 (97%)	1.30	20 (18%) 3 2	51, 64, 74, 83	0
21	1Z	154/206 (74%)	0.95	16 (10%) 11 9	36, 54, 73, 95	0
21	2Z	160/206 (77%)	1.70	49 (30%) 1 1	61, 71, 82, 92	0
22	10	83/85 (97%)	-0.19	0 100 100	22, 31, 41, 55	0
22	20	83/85 (97%)	1.01	11 (13%) 7 5	41, 55, 65, 71	0
23	11	97/98 (98%)	0.37	3 (3%) 51 45	21, 41, 62, 71	0
23	21	97/98 (98%)	0.64	2 (2%) 63 58	35, 52, 67, 72	0
24	12	70/72 (97%)	0.29	2 (2%) 53 48	29, 43, 55, 59	0
24	22	70/72 (97%)	0.83	4 (5%) 29 24	52, 64, 70, 74	0
25	13	59/60 (98%)	-0.06	1 (1%) 69 64	22, 32, 53, 68	0
25	23	59/60 (98%)	1.07	8 (13%) 7 5	49, 59, 71, 76	0
26	14	69/71 (97%)	1.05	11 (15%) 5 4	48, 63, 79, 86	0
26	24	69/71 (97%)	2.08	35 (50%) 0 0	66, 79, 87, 88	0
27	15	59/60 (98%)	-0.05	1 (1%) 69 64	17, 28, 44, 56	0
27	25	59/60 (98%)	0.40	2 (3%) 48 42	28, 46, 61, 66	0
28	16	53/54 (98%)	-0.13	0 100 100	25, 38, 47, 57	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%)	0.68	0 100 100	45, 55, 62, 67	0
29	17	48/49 (97%)	-0.26	1 (2%) 63 58	15, 24, 52, 57	0
29	27	48/49 (97%)	0.27	2 (4%) 40 35	28, 40, 56, 63	0
30	18	64/65 (98%)	-0.14	0 100 100	23, 28, 38, 49	0
30	28	64/65 (98%)	0.62	1 (1%) 70 66	39, 50, 58, 64	0
31	19	37/37 (100%)	-0.01	0 100 100	22, 34, 50, 56	0
31	29	37/37 (100%)	0.91	0 100 100	51, 59, 69, 74	0
32	1a	1488/1521 (97%)	0.27	46 (3%) 51 45	30, 56, 80, 95	0
32	2a	1491/1521 (98%)	0.70	101 (6%) 23 19	44, 67, 83, 96	0
33	1b	231/256 (90%)	1.16	35 (15%) 5 4	52, 67, 78, 85	0
33	2b	231/256 (90%)	1.84	84 (36%) 1 0	62, 76, 84, 91	0
34	1c	206/239 (86%)	0.91	15 (7%) 21 17	50, 60, 71, 84	0
34	2c	206/239 (86%)	1.63	66 (32%) 1 1	63, 74, 80, 87	0
35	1d	208/209 (99%)	0.96	17 (8%) 17 14	47, 60, 68, 79	0
35	2d	208/209 (99%)	1.03	22 (10%) 11 9	50, 61, 70, 83	0
36	1e	148/162 (91%)	0.64	6 (4%) 41 36	44, 56, 65, 73	0
36	2e	148/162 (91%)	1.40	25 (16%) 4 3	59, 69, 77, 82	0
37	1f	100/101 (99%)	0.64	5 (5%) 34 28	44, 55, 66, 71	0
37	2f	100/101 (99%)	0.73	4 (4%) 42 37	55, 64, 72, 76	0
38	1g	155/156 (99%)	0.98	17 (10%) 10 8	49, 61, 72, 88	0
38	2g	155/156 (99%)	1.35	29 (18%) 3 2	63, 72, 80, 90	0
39	1h	137/138 (99%)	0.79	6 (4%) 39 33	49, 59, 68, 75	0
39	2h	137/138 (99%)	1.29	23 (16%) 4 3	58, 69, 76, 88	0
40	1i	127/128 (99%)	0.97	13 (10%) 12 9	40, 63, 74, 78	0
40	2i	127/128 (99%)	2.04	60 (47%) 0 0	63, 75, 81, 84	0
41	1j	97/105 (92%)	1.24	15 (15%) 5 4	46, 66, 77, 80	0
41	2j	96/105 (91%)	2.15	49 (51%) 0 0	67, 75, 82, 84	0
42	1k	114/129 (88%)	0.69	6 (5%) 32 26	35, 58, 70, 74	0
42	2k	114/129 (88%)	1.08	16 (14%) 6 5	53, 67, 74, 80	0
43	1l	121/132 (91%)	0.35	3 (2%) 58 52	39, 48, 62, 66	0
43	2l	121/132 (91%)	0.92	6 (4%) 34 28	46, 58, 67, 70	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%)	0.87	8 (6%) 25 19	43, 60, 66, 73	0
44	2m	122/126 (96%)	1.69	32 (26%) 1 1	63, 73, 80, 84	0
45	1n	60/61 (98%)	0.98	3 (5%) 34 28	49, 56, 62, 66	0
45	2n	60/61 (98%)	2.27	36 (60%) 0 0	68, 74, 80, 81	0
46	1o	88/89 (98%)	0.78	4 (4%) 38 32	42, 56, 68, 73	0
46	2o	88/89 (98%)	0.85	2 (2%) 61 55	54, 64, 72, 78	0
47	1p	82/88 (93%)	1.52	14 (17%) 4 3	53, 63, 69, 76	0
47	2p	82/88 (93%)	1.14	11 (13%) 7 5	52, 61, 68, 71	0
48	1q	99/105 (94%)	1.04	11 (11%) 10 8	48, 59, 69, 72	0
48	2q	99/105 (94%)	1.06	8 (8%) 18 14	57, 66, 72, 76	0
49	1r	68/88 (77%)	0.52	2 (2%) 53 48	46, 57, 70, 72	0
49	2r	68/88 (77%)	1.09	7 (10%) 12 9	57, 66, 74, 77	0
50	1s	83/93 (89%)	0.82	5 (6%) 27 22	48, 60, 69, 73	0
50	2s	83/93 (89%)	1.62	24 (28%) 1 1	66, 75, 81, 88	0
51	1t	96/106 (90%)	1.18	14 (14%) 6 4	54, 62, 73, 80	0
51	2t	96/106 (90%)	1.12	9 (9%) 14 11	51, 61, 73, 77	0
52	1u	23/27 (85%)	1.26	2 (8%) 16 12	51, 58, 61, 65	0
52	2u	23/27 (85%)	2.71	17 (73%) 0 0	66, 74, 80, 84	0
53	1v	13/24 (54%)	0.78	3 (23%) 2 1	37, 50, 80, 82	0
53	2v	13/24 (54%)	1.92	5 (38%) 1 0	59, 68, 88, 89	0
54	1w	66/76 (86%)	0.63	6 (9%) 15 11	24, 65, 79, 91	0
54	2w	64/76 (84%)	1.27	10 (15%) 5 4	42, 76, 83, 86	0
55	1x	72/77 (93%)	0.29	3 (4%) 40 35	22, 55, 71, 82	0
55	2x	72/77 (93%)	0.92	2 (2%) 55 49	35, 69, 79, 85	0
56	1y	67/76 (88%)	1.90	32 (47%) 0 0	43, 85, 89, 93	0
56	2y	66/76 (86%)	1.62	16 (24%) 2 1	54, 88, 91, 93	0
All	All	20873/21748 (95%)	0.49	1664 (7%) 18 14	12, 56, 79, 98	0

All (1664) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
21	2Z	172	ALA	6.3
21	1Z	147	GLY	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1141	A	6.1
54	2w	71	G	5.8
6	2G	28	VAL	5.7
33	2b	237	ALA	5.5
38	2g	83	ALA	5.4
1	2A	885	C	5.3
21	2Z	173	ALA	5.3
40	2i	14	VAL	5.3
21	2Z	152	ALA	5.0
54	2w	70	G	5.0
38	1g	84	ASN	5.0
54	2w	3	C	5.0
33	2b	187	LEU	4.9
1	1A	1133	G	4.9
1	2A	883	G	4.8
50	2s	84	GLY	4.8
1	1A	1140	U	4.7
1	1A	1144	A	4.7
38	1g	82	GLY	4.7
1	2A	2133	G	4.7
6	2G	20	ILE	4.7
15	1T	131	ALA	4.7
1	2A	884	C	4.7
1	2A	896	A	4.7
1	1A	935	C	4.6
1	1A	1106	U	4.6
44	2m	118	ALA	4.6
32	2a	1030(B)	C	4.6
1	1A	1142	A	4.6
41	2j	32	ALA	4.6
41	2j	47	PHE	4.6
51	2t	103	GLY	4.6
45	2n	33	VAL	4.5
1	2A	1536	C	4.5
38	2g	80	VAL	4.5
40	2i	102	LEU	4.4
33	2b	122	PHE	4.4
3	2D	276	LYS	4.4
12	2Q	22	LYS	4.4
26	24	49	PHE	4.4
21	2Z	146	ILE	4.4
41	2j	43	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	2u	6	ARG	4.3
21	2Z	147	GLY	4.3
54	1w	71	G	4.3
1	2A	2146	C	4.3
38	1g	83	ALA	4.3
34	2c	2	GLY	4.3
52	2u	24	ARG	4.3
1	1A	943	C	4.3
1	1A	2139	A	4.3
32	1a	1531	A	4.3
3	2D	2	ALA	4.2
38	1g	80	VAL	4.2
54	1w	1	G	4.2
42	2k	13	GLN	4.2
1	1A	1124	U	4.2
1	1A	2211	U	4.2
1	1A	931	C	4.2
32	2a	1286	A	4.2
1	1A	1145	G	4.2
23	1l	2	SER	4.2
40	2i	126	SER	4.2
33	2b	70	PHE	4.2
44	2m	123	ALA	4.2
44	2m	121	LYS	4.2
1	1A	1110	C	4.2
1	1A	2141	A	4.2
1	2A	1509	C	4.2
33	2b	11	LEU	4.2
1	1A	1104	G	4.2
32	1a	1034	G	4.2
39	2h	72	PRO	4.1
37	1f	58	GLY	4.1
38	1g	79	ARG	4.1
45	2n	25	VAL	4.1
1	1A	2137	G	4.1
33	2b	214	ILE	4.1
26	24	45	GLY	4.0
6	2G	2	PRO	4.0
33	2b	236	TYR	4.0
47	1p	38	TYR	4.0
40	2i	105	ASP	4.0
41	2j	44	VAL	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	934	A	4.0
1	1A	932	C	4.0
49	2r	20	ALA	4.0
1	2A	2112	G	4.0
7	2H	125	VAL	4.0
32	1a	1028	C	4.0
41	2j	72	VAL	4.0
23	2l	2	SER	3.9
32	1a	1002	G	3.9
44	2m	66	LEU	3.9
6	2G	23	PHE	3.9
1	2A	886	C	3.9
40	2i	108	VAL	3.9
38	2g	82	GLY	3.9
51	1t	9	ASN	3.9
52	2u	16	GLY	3.9
1	1A	1135	G	3.9
32	1a	1003	G	3.9
52	2u	23	PRO	3.9
41	2j	46	ARG	3.9
32	2a	1001	A	3.9
53	2v	12	A	3.9
26	24	51	ASP	3.9
41	2j	66	ARG	3.8
38	2g	12	LEU	3.8
53	2v	14	A	3.8
45	2n	2	ALA	3.8
44	2m	102	ARG	3.8
1	1A	1109	G	3.8
32	1a	1257	U	3.8
40	2i	75	ASP	3.8
45	2n	34	TYR	3.8
7	2H	2	SER	3.8
51	1t	103	GLY	3.8
40	2i	10	ARG	3.8
40	2i	17	VAL	3.8
52	2u	9	ARG	3.8
1	1A	1103	A	3.8
32	2a	1034	G	3.8
38	2g	85	TYR	3.8
32	1a	1035	A	3.7
6	2G	25	TYR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	1h	2	LEU	3.7
1	1A	2134	G	3.7
32	2a	1150	U	3.7
33	2b	120	ALA	3.7
52	2u	10	ARG	3.7
33	1b	17	PHE	3.7
44	2m	124	PRO	3.7
26	24	9	LEU	3.7
33	1b	221	LEU	3.7
6	2G	140	ILE	3.7
32	1a	1030(D)	A	3.7
1	1A	2176	G	3.7
33	2b	165	VAL	3.7
42	1k	13	GLN	3.7
14	2S	32	LEU	3.7
51	2t	9	ASN	3.7
3	1D	38	LYS	3.7
24	22	51	ARG	3.7
48	1q	33	GLY	3.7
1	1A	1143	U	3.7
1	2A	2144	U	3.7
1	1A	1105	G	3.7
21	2Z	148	ASP	3.7
14	2S	7	TYR	3.7
33	2b	81	VAL	3.7
32	2a	1257	U	3.6
1	1A	2179	G	3.6
1	2A	2147	G	3.6
1	1A	1146	C	3.6
4	1E	73	GLU	3.6
8	2I	108	THR	3.6
56	1y	35	A	3.6
33	2b	21	ARG	3.6
47	2p	48	TRP	3.6
32	2a	630	G	3.6
32	2a	1036	G	3.6
44	2m	60	VAL	3.6
45	2n	18	VAL	3.6
33	2b	39	ILE	3.6
41	2j	6	ILE	3.6
1	2A	2173	A	3.6
4	2E	204	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	24	ALA	3.6
33	1b	229	VAL	3.6
1	1A	930	G	3.6
32	1a	1036	G	3.6
45	2n	5	ALA	3.6
26	24	63	TYR	3.6
35	2d	34	GLU	3.6
26	24	31	ILE	3.5
33	2b	80	ILE	3.5
32	1a	1001(A)	G	3.5
20	1Y	93	GLY	3.5
30	28	34	TRP	3.5
6	2G	31	VAL	3.5
44	2m	122	LYS	3.5
37	1f	21	LEU	3.5
21	1Z	146	ILE	3.5
41	2j	67	THR	3.5
41	2j	37	PRO	3.5
1	2A	882	G	3.5
1	2A	2131	G	3.5
45	2n	39	LEU	3.5
1	2A	229	A	3.5
33	1b	129	GLU	3.5
38	2g	156	TRP	3.5
34	2c	151	VAL	3.5
40	2i	19	LEU	3.5
1	1A	2164	C	3.5
1	2A	2159	G	3.5
56	2y	34	G	3.5
8	1I	146	ALA	3.5
6	2G	172	LEU	3.5
39	2h	2	LEU	3.5
33	1b	7	VAL	3.5
33	1b	230	VAL	3.5
21	1Z	149	SER	3.4
1	2A	34	C	3.4
32	1a	1030(B)	C	3.4
1	1A	1127	U	3.4
1	1A	2155	G	3.4
7	2H	21	PRO	3.4
33	1b	237	ALA	3.4
8	2I	68	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	69	LEU	3.4
40	2i	111	ARG	3.4
41	2j	75	ILE	3.4
40	2i	125	TYR	3.4
14	2S	33	LYS	3.4
8	1I	38	LEU	3.4
21	2Z	141	VAL	3.4
40	2i	36	TYR	3.4
41	1j	35	SER	3.4
41	2j	42	THR	3.4
37	2f	99	ALA	3.4
38	2g	7	ALA	3.4
40	2i	42	ARG	3.4
1	1A	2196	C	3.4
49	2r	86	VAL	3.4
1	2A	2113	U	3.4
32	2a	992	U	3.4
32	2a	1532	U	3.4
33	2b	97	TRP	3.4
1	1A	1139	G	3.4
1	2A	2157	G	3.4
32	1a	630	G	3.4
32	2a	1001(A)	G	3.4
32	2a	1224	G	3.4
14	2S	46	VAL	3.4
34	2c	207	VAL	3.4
1	1A	2172	U	3.3
1	1A	2807	C	3.3
1	2A	2174	C	3.3
6	1G	146	TYR	3.3
35	2d	194	LEU	3.3
45	2n	6	LEU	3.3
14	2S	34	HIS	3.3
1	2A	2110	G	3.3
1	2A	2155	G	3.3
33	1b	27	LYS	3.3
40	2i	127	LYS	3.3
1	2A	2167	U	3.3
1	1A	2186	C	3.3
1	2A	2145	C	3.3
32	1a	163	C	3.3
8	2I	48	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	66	ARG	3.3
40	2i	123	PRO	3.3
52	2u	2	GLY	3.3
50	2s	13	ASP	3.3
21	2Z	137	ILE	3.3
32	1a	1447	A	3.3
53	1v	14	A	3.3
49	2r	85	LEU	3.3
1	1A	2194	U	3.3
8	2I	65	ALA	3.3
1	1A	2162	C	3.3
41	2j	78	ASN	3.3
34	2c	8	ILE	3.3
1	1A	942	A	3.3
56	1y	64	A	3.3
52	2u	14	TRP	3.3
6	2G	128	ARG	3.3
21	2Z	155	LEU	3.3
32	1a	1026	G	3.3
33	2b	129	GLU	3.3
56	1y	15	G	3.3
41	2j	59	SER	3.3
18	1W	112	GLY	3.3
47	1p	7	ALA	3.3
54	1w	72	C	3.2
36	2e	53	LEU	3.2
25	23	51	ALA	3.2
1	1A	929	G	3.2
21	2Z	124	ILE	3.2
45	2n	3	ARG	3.2
1	1A	1555	C	3.2
41	2j	65	LEU	3.2
47	2p	82	GLN	3.2
35	2d	167	GLY	3.2
21	1Z	141	VAL	3.2
26	24	33	VAL	3.2
1	2A	881	G	3.2
45	2n	31	ARG	3.2
1	1A	944	C	3.2
21	2Z	149	SER	3.2
33	2b	227	GLY	3.2
52	2u	11	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	12	TYR	3.2
34	2c	48	TYR	3.2
1	1A	1113	A	3.2
1	1A	1134	A	3.2
54	2w	73	A	3.2
40	1i	2	GLU	3.2
1	1A	1102	G	3.2
1	1A	2143	G	3.2
33	2b	77	ALA	3.2
41	2j	82	ILE	3.2
14	2S	29	PHE	3.2
52	2u	18	TYR	3.2
53	1v	13	A	3.1
32	1a	204	U	3.1
40	2i	18	PHE	3.1
50	2s	11	VAL	3.1
1	1A	2188	G	3.1
1	2A	2166	G	3.1
40	2i	114	TYR	3.1
41	2j	60	ARG	3.1
41	2j	73	ASP	3.1
1	1A	2210	C	3.1
33	2b	10	LEU	3.1
1	1A	1132	A	3.1
41	2j	100	THR	3.1
7	2H	100	GLY	3.1
33	2b	99	GLY	3.1
7	2H	60	ARG	3.1
32	2a	982	U	3.1
33	2b	75	LYS	3.1
21	2Z	99	TYR	3.1
33	2b	25	ASN	3.1
34	2c	62	ASP	3.1
1	2A	2115	G	3.1
32	1a	1031	G	3.1
14	2S	45	GLY	3.1
38	1g	156	TRP	3.1
40	2i	81	ILE	3.1
48	1q	68	ARG	3.1
1	2A	2189	U	3.1
1	1A	1114	G	3.1
1	2A	2154	G	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2160	G	3.1
38	1g	81	GLY	3.1
1	2A	2136	C	3.1
54	2w	2	C	3.1
54	2w	4	C	3.1
1	1A	2136	A	3.0
1	1A	2192	A	3.0
42	1k	25	TYR	3.0
20	1Y	91	GLU	3.0
47	1p	65	GLN	3.0
38	2g	32	ARG	3.0
6	2G	29	TRP	3.0
1	1A	2138	G	3.0
1	2A	2143	C	3.0
32	2a	1118	C	3.0
56	1y	11	C	3.0
32	2a	996	A	3.0
14	2S	82	ILE	3.0
26	24	48	ARG	3.0
41	2j	38	ILE	3.0
52	2u	15	ARG	3.0
52	2u	17	THR	3.0
45	2n	30	ALA	3.0
21	1Z	105	VAL	3.0
26	14	56	VAL	3.0
43	1l	18	VAL	3.0
44	2m	117	VAL	3.0
21	2Z	121	HIS	3.0
1	1A	2178	G	3.0
1	1A	2181	G	3.0
11	2P	68	GLN	3.0
32	1a	1033	G	3.0
1	1A	2151	C	3.0
32	1a	92	C	3.0
32	1a	1030	C	3.0
54	2w	72	C	3.0
54	1w	73	A	3.0
26	24	44	THR	3.0
40	1i	81	ILE	3.0
41	2j	74	ILE	3.0
33	2b	161	ALA	3.0
40	2i	109	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	2d	188	LEU	3.0
40	2i	99	LEU	3.0
45	2n	8	GLU	3.0
41	2j	41	PRO	3.0
41	2j	77	PRO	3.0
33	2b	22	LYS	3.0
20	2Y	55	TYR	3.0
38	2g	151	TYR	3.0
43	2l	7	ILE	3.0
40	2i	7	THR	3.0
1	1A	2145	G	3.0
1	1A	2163	G	3.0
1	2A	2182	G	3.0
1	2A	2802	G	3.0
15	2T	131	ALA	3.0
32	2a	1003	G	3.0
32	2a	1021	G	3.0
1	2A	888	C	3.0
1	2A	2111	C	3.0
32	2a	1030	C	3.0
34	2c	137	ALA	3.0
1	1A	1130	A	3.0
1	1A	2157	A	3.0
1	2A	2158	A	3.0
39	2h	51	VAL	3.0
56	1y	23	A	3.0
11	1P	100	LEU	2.9
44	2m	67	GLU	2.9
6	2G	17	PRO	2.9
21	2Z	14	LYS	2.9
41	1j	86	MET	2.9
8	2I	109	ILE	2.9
21	1Z	171	ILE	2.9
26	24	54	GLY	2.9
34	2c	160	ALA	2.9
48	2q	44	ALA	2.9
7	2H	35	VAL	2.9
26	14	50	VAL	2.9
42	2k	14	VAL	2.9
8	1I	5	LEU	2.9
8	2I	72	LEU	2.9
21	1Z	150	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	1n	6	LEU	2.9
1	1A	2158	C	2.9
32	2a	1007	C	2.9
38	2g	8	GLU	2.9
32	2a	1250	A	2.9
34	2c	7	PRO	2.9
35	2d	91	SER	2.9
54	1w	20	U	2.9
21	2Z	106	GLY	2.9
33	2b	38	GLY	2.9
36	2e	59	GLY	2.9
40	2i	64	THR	2.9
45	2n	10	ALA	2.9
6	2G	34	LEU	2.9
33	2b	17	PHE	2.9
33	1b	40	HIS	2.9
44	2m	120	LYS	2.9
20	2Y	57	GLN	2.9
1	1A	933	C	2.9
1	1A	1126	C	2.9
1	2A	887	A	2.9
1	2A	2114	A	2.9
12	2Q	10	ARG	2.9
33	2b	36	ARG	2.9
1	1A	2187	G	2.9
1	2A	271(K)	U	2.9
18	1W	60	ASN	2.9
32	2a	1220	G	2.9
56	1y	19	G	2.9
56	2y	18	G	2.9
45	2n	7	ILE	2.9
7	2H	99	VAL	2.9
12	2Q	96	VAL	2.9
14	2S	54	LEU	2.9
33	1b	133	LYS	2.9
34	2c	175	LEU	2.9
33	2b	128	GLU	2.9
35	1d	179	GLU	2.9
26	24	11	PRO	2.9
51	2t	98	PRO	2.9
40	2i	124	GLN	2.9
41	2j	19	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2195	A	2.9
1	2A	895	U	2.9
14	2S	36	TYR	2.9
53	2v	15	A	2.9
6	2G	161	THR	2.9
1	1A	2122	G	2.9
1	1A	2132	G	2.9
8	2I	3	VAL	2.9
25	23	59	VAL	2.9
32	2a	1033	G	2.9
32	2a	1221	G	2.9
41	2j	8	LEU	2.9
42	2k	15	ALA	2.9
48	1q	74	LEU	2.9
6	2G	41	GLN	2.8
48	2q	91	ARG	2.8
33	2b	216	SER	2.8
41	2j	35	SER	2.8
14	2S	92	TYR	2.8
41	2j	10	GLY	2.8
43	1l	20	LYS	2.8
7	2H	71	LEU	2.8
8	2I	129	THR	2.8
17	2V	55	ALA	2.8
21	2Z	163	LEU	2.8
34	2c	196	LEU	2.8
36	2e	86	ALA	2.8
35	2d	112	VAL	2.8
40	2i	101	PHE	2.8
1	2A	2170	A	2.8
1	2A	2319	G	2.8
38	2g	41	ARG	2.8
21	1Z	166	SER	2.8
35	1d	77	ASN	2.8
8	1I	131	LYS	2.8
34	2c	199	LYS	2.8
21	2Z	143	GLY	2.8
26	14	63	TYR	2.8
44	2m	5	ALA	2.8
25	23	9	VAL	2.8
36	2e	67	VAL	2.8
40	1i	59	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	167	GLU	2.8
6	2G	32	PRO	2.8
32	1a	1025	U	2.8
32	2a	1358	U	2.8
1	1A	2165	C	2.8
50	1s	40	ILE	2.8
32	1a	1032	G	2.8
32	2a	1002	G	2.8
42	2k	117	ASN	2.8
6	2G	110	ALA	2.8
7	2H	123	PHE	2.8
26	24	32	TYR	2.8
44	2m	73	GLU	2.8
9	1N	61	ARG	2.8
21	1Z	167	PRO	2.8
1	1A	2152	U	2.8
1	1A	1116	A	2.8
1	1A	1119	A	2.8
32	1a	160	A	2.8
1	1A	2133	C	2.8
6	2G	19	LEU	2.8
21	2Z	144	LEU	2.8
39	2h	59	LEU	2.8
40	1i	19	LEU	2.8
45	2n	44	LEU	2.8
50	2s	16	LEU	2.8
21	1Z	148	ASP	2.8
7	2H	114	VAL	2.8
9	2N	73	THR	2.8
34	1c	65	ALA	2.8
44	2m	7	VAL	2.8
1	2A	2156	G	2.8
36	2e	60	TYR	2.8
1	1A	271	U	2.7
1	1A	1111	U	2.7
32	2a	1085	U	2.7
1	2A	899	A	2.7
32	2a	1236	A	2.7
32	2a	1251	A	2.7
32	2a	1287	A	2.7
50	2s	14	HIS	2.7
6	2G	35	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	27	VAL	2.7
21	2Z	42	VAL	2.7
26	14	57	GLU	2.7
34	2c	55	VAL	2.7
39	2h	22	GLU	2.7
45	2n	20	ALA	2.7
38	2g	155	ARG	2.7
33	2b	234	PRO	2.7
43	2l	21	LYS	2.7
45	2n	4	LYS	2.7
1	1A	1101	G	2.7
1	1A	2169	G	2.7
32	2a	1030(A)	G	2.7
56	1y	18	G	2.7
6	2G	76	SER	2.7
7	2H	56	SER	2.7
22	20	76	GLY	2.7
26	24	64	GLY	2.7
33	2b	228	GLY	2.7
52	1u	2	GLY	2.7
6	2G	33	ARG	2.7
14	2S	3	ARG	2.7
33	2b	12	GLU	2.7
20	2Y	78	ALA	2.7
26	24	65	ASP	2.7
33	2b	15	VAL	2.7
34	2c	120	VAL	2.7
39	2h	54	ASP	2.7
40	2i	83	ARG	2.7
44	2m	105	THR	2.7
45	2n	41	ARG	2.7
49	2r	42	ARG	2.7
41	2j	54	PHE	2.7
6	1G	2	PRO	2.7
26	24	46	GLN	2.7
40	2i	70	LYS	2.7
44	2m	23	TYR	2.7
45	2n	17	LYS	2.7
1	1A	1122	C	2.7
1	2A	2138	C	2.7
32	1a	1027	C	2.7
32	1a	1029	C	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	127	ILE	2.7
34	2c	39	ILE	2.7
8	2I	38	LEU	2.7
36	1e	10	MET	2.7
41	2j	36	GLY	2.7
42	2k	118	GLY	2.7
7	2H	124	GLU	2.7
24	12	69	ARG	2.7
40	2i	9	ARG	2.7
8	2I	40	THR	2.7
8	2I	107	VAL	2.7
34	2c	195	VAL	2.7
1	2A	2132	U	2.7
44	1m	122	LYS	2.7
40	1i	4	TYR	2.7
1	1A	1115	A	2.7
1	1A	1554	A	2.7
53	1v	12	A	2.7
56	2y	36	A	2.7
14	2S	18	ILE	2.7
1	1A	2197	C	2.7
22	20	84	LEU	2.7
33	2b	16	HIS	2.7
33	2b	140	HIS	2.7
6	2G	118	ARG	2.7
51	1t	102	GLY	2.7
8	2I	64	GLU	2.7
25	23	60	GLU	2.7
41	2j	61	GLU	2.7
6	2G	109	VAL	2.7
21	2Z	136	PHE	2.7
33	1b	15	VAL	2.7
41	2j	63	PHE	2.7
26	24	41	PRO	2.7
1	1A	1117	G	2.6
1	2A	2124	G	2.6
32	1a	1030(A)	G	2.6
1	2A	2122	U	2.6
47	2p	39	TYR	2.6
6	2G	144	ILE	2.6
6	2G	139	LEU	2.6
7	2H	7	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	1d	120	LEU	2.6
41	2j	40	LEU	2.6
56	2y	35	A	2.6
12	2Q	60	ARG	2.6
36	2e	27	ARG	2.6
41	1j	43	ARG	2.6
45	2n	35	ARG	2.6
8	2I	41	GLU	2.6
1	1A	2161	C	2.6
55	2x	16	C	2.6
12	2Q	121	ALA	2.6
26	14	59	PHE	2.6
26	24	10	VAL	2.6
33	1b	186	ALA	2.6
33	2b	192	SER	2.6
50	1s	9	VAL	2.6
50	2s	75	ALA	2.6
6	2G	26	GLN	2.6
38	2g	33	ASP	2.6
21	1Z	1	MET	2.6
21	2Z	57	ILE	2.6
21	2Z	171	ILE	2.6
1	1A	2182	G	2.6
1	2A	2162	G	2.6
2	2B	56	G	2.6
32	1a	1532	U	2.6
56	1y	34	G	2.6
33	2b	215	LEU	2.6
35	2d	157	LEU	2.6
26	24	40	HIS	2.6
38	2g	79	ARG	2.6
6	2G	164	GLU	2.6
26	24	38	LYS	2.6
33	1b	134	GLU	2.6
40	2i	6	GLY	2.6
48	2q	100	LYS	2.6
51	2t	30	LYS	2.6
1	2A	901	A	2.6
1	2A	2117	A	2.6
1	2A	2753	A	2.6
2	2B	53	A	2.6
32	2a	1030(D)	A	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1288	A	2.6
21	2Z	105	VAL	2.6
22	20	12	ASN	2.6
34	2c	20	SER	2.6
50	2s	45	VAL	2.6
51	1t	19	SER	2.6
1	1A	940	C	2.6
1	1A	1121	C	2.6
1	1A	2167	C	2.6
1	2A	2314	C	2.6
5	2F	7	TYR	2.6
15	2T	114	LEU	2.6
14	2S	17	ARG	2.6
15	2T	108	ARG	2.6
38	1g	4	ARG	2.6
38	2g	4	ARG	2.6
1	1A	1112	U	2.6
36	2e	83	GLU	2.6
40	2i	110	GLU	2.6
34	2c	205	GLY	2.6
1	1A	1120	G	2.6
1	1A	2175	G	2.6
1	1A	2806	G	2.6
1	2A	352	G	2.6
1	2A	2116	G	2.6
2	2B	23	G	2.6
32	1a	1024	G	2.6
32	2a	1356	G	2.6
56	2y	1	G	2.6
56	2y	15	G	2.6
7	2H	45	VAL	2.6
8	2I	19	VAL	2.6
11	2P	13	ASN	2.6
38	2g	21	VAL	2.6
40	2i	44	VAL	2.6
42	2k	115	PRO	2.6
48	2q	23	VAL	2.6
26	14	49	PHE	2.6
45	2n	16	PHE	2.6
7	2H	136	ILE	2.6
41	1j	75	ILE	2.6
47	1p	19	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2150	C	2.6
1	2A	2140	C	2.6
11	1P	15	ARG	2.6
15	1T	112	ARG	2.6
15	1T	115	ARG	2.6
26	24	67	TYR	2.6
44	1m	3	ARG	2.6
45	2n	9	LYS	2.6
45	2n	50	LYS	2.6
26	24	50	VAL	2.6
33	2b	232	PRO	2.6
41	2j	18	ALA	2.6
50	2s	9	VAL	2.6
33	2b	152	PHE	2.6
35	1d	154	ASN	2.6
36	2e	26	PHE	2.6
38	2g	84	ASN	2.6
34	2c	167	TRP	2.5
37	2f	17	SER	2.5
40	1i	126	SER	2.5
1	1A	1108	G	2.5
1	1A	2171	G	2.5
1	2A	2123	G	2.5
32	2a	1202	G	2.5
56	1y	22	G	2.5
41	2j	96	ILE	2.5
1	1A	1123	A	2.5
1	2A	2134	A	2.5
7	1H	71	LEU	2.5
32	2a	1261	A	2.5
35	1d	194	LEU	2.5
44	2m	19	LEU	2.5
51	1t	10	LEU	2.5
53	2v	13	A	2.5
9	2N	84	LYS	2.5
33	2b	53	ARG	2.5
41	2j	51	ARG	2.5
42	1k	75	TYR	2.5
44	2m	87	TYR	2.5
19	2X	94	GLY	2.5
36	1e	23	GLY	2.5
38	2g	81	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	1F	11	VAL	2.5
39	1h	93	VAL	2.5
21	1Z	136	PHE	2.5
26	24	47	GLN	2.5
40	2i	43	ALA	2.5
41	1j	33	GLN	2.5
1	1A	1128	U	2.5
1	2A	12	U	2.5
21	2Z	98	MET	2.5
56	1y	47	U	2.5
33	2b	24	TRP	2.5
7	2H	6	ARG	2.5
19	2X	66	LEU	2.5
26	24	55	ARG	2.5
34	2c	33	LEU	2.5
40	2i	56	LEU	2.5
47	1p	73	LEU	2.5
50	2s	71	LEU	2.5
34	2c	6	HIS	2.5
1	1A	928	G	2.5
1	1A	1221	G	2.5
56	1y	24	G	2.5
1	1A	2193	A	2.5
8	1I	117	GLU	2.5
32	1a	1001	A	2.5
32	2a	1285	A	2.5
32	2a	1289	A	2.5
6	2G	24	GLY	2.5
50	2s	54	GLY	2.5
36	2e	90	VAL	2.5
38	2g	9	VAL	2.5
15	1T	130	ALA	2.5
29	17	45	ALA	2.5
33	1b	120	ALA	2.5
36	2e	20	GLN	2.5
37	1f	16	GLN	2.5
44	2m	72	ALA	2.5
1	2A	645	C	2.5
20	2Y	1	MET	2.5
54	2w	13	C	2.5
21	2Z	170	THR	2.5
45	2n	22	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	1D	276	LYS	2.5
1	2A	2130	U	2.5
38	1g	155	ARG	2.5
44	2m	34	LEU	2.5
33	2b	134	GLU	2.5
42	2k	92	GLU	2.5
6	2G	146	TYR	2.5
6	2G	89	GLY	2.5
7	2H	161	GLY	2.5
20	2Y	93	GLY	2.5
21	2Z	160	GLY	2.5
2	2B	18	G	2.5
27	15	60	VAL	2.5
38	1g	105	VAL	2.5
48	2q	5	VAL	2.5
56	1y	1	G	2.5
40	1i	18	PHE	2.5
50	2s	10	PHE	2.5
51	2t	42	GLN	2.5
6	2G	145	THR	2.5
49	1r	25	THR	2.5
6	2G	16	ARG	2.5
8	2I	12	LEU	2.5
14	2S	26	LEU	2.5
35	1d	58	LEU	2.5
40	2i	74	ILE	2.5
44	2m	99	ARG	2.5
44	2m	64	TRP	2.5
45	2n	53	LEU	2.5
47	1p	61	SER	2.5
48	2q	68	ARG	2.5
32	2a	1223	C	2.5
37	1f	55	ASP	2.5
11	1P	149	GLU	2.5
22	20	68	GLU	2.5
32	2a	1000	U	2.5
14	2S	60	GLY	2.5
33	1b	236	TYR	2.5
39	2h	58	TYR	2.5
40	1i	24	GLY	2.5
40	2i	115	GLY	2.5
50	1s	84	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	158	PRO	2.5
21	2Z	159	PRO	2.5
25	23	2	PRO	2.5
33	2b	101	MET	2.5
39	2h	67	PRO	2.5
21	2Z	86	VAL	2.5
33	2b	229	VAL	2.5
44	2m	53	VAL	2.5
45	1n	25	VAL	2.5
12	2Q	104	PHE	2.5
33	2b	207	ALA	2.5
44	1m	5	ALA	2.5
42	2k	51	LYS	2.4
33	2b	67	THR	2.4
1	1A	937	A	2.4
1	1A	2191	A	2.4
20	2Y	92	ASN	2.4
32	2a	1035	A	2.4
32	2a	1180	A	2.4
40	1i	23	ASN	2.4
14	2S	39	ILE	2.4
26	24	14	ILE	2.4
1	1A	2146	G	2.4
2	2B	24	G	2.4
14	2S	31	SER	2.4
56	1y	63	G	2.4
33	2b	166	ASP	2.4
6	1G	35	GLU	2.4
41	1j	64	GLU	2.4
1	2A	2142	C	2.4
32	2a	1039	C	2.4
56	2y	62	C	2.4
1	1A	2135	U	2.4
7	2H	48	GLY	2.4
8	2I	106	GLY	2.4
12	2Q	7	MET	2.4
38	1g	73	MET	2.4
45	2n	55	GLY	2.4
56	1y	45	U	2.4
34	2c	193	TYR	2.4
3	2D	4	LYS	2.4
33	2b	136	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	66	VAL	2.4
33	2b	163	PHE	2.4
34	2c	27	LYS	2.4
46	2o	60	VAL	2.4
34	2c	163	ALA	2.4
37	2f	60	PHE	2.4
48	1q	37	LYS	2.4
6	2G	6	ALA	2.4
40	2i	15	ALA	2.4
40	2i	82	ALA	2.4
24	22	55	ARG	2.4
34	2c	95	THR	2.4
40	2i	103	THR	2.4
45	2n	13	THR	2.4
46	1o	88	ARG	2.4
33	2b	108	ILE	2.4
34	2c	152	ILE	2.4
45	2n	49	HIS	2.4
1	2A	2126	A	2.4
34	1c	18	TRP	2.4
45	2n	61	TRP	2.4
23	11	75	GLU	2.4
1	2A	652(U)	G	2.4
1	2A	2318	G	2.4
32	2a	1283	G	2.4
56	2y	19	G	2.4
7	2H	22	GLY	2.4
7	2H	39	PRO	2.4
14	2S	22	GLY	2.4
18	2W	112	GLY	2.4
38	2g	34	GLY	2.4
33	1b	8	LYS	2.4
40	2i	95	LYS	2.4
41	2j	7	LYS	2.4
1	1A	2168	C	2.4
5	2F	183	VAL	2.4
14	2S	65	VAL	2.4
34	2c	68	VAL	2.4
36	2e	69	VAL	2.4
56	1y	4	C	2.4
35	2d	49	ARG	2.4
40	2i	46	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	2p	9	PHE	2.4
56	1y	20	U	2.4
7	2H	101	ARG	2.4
45	2n	29	ARG	2.4
48	1q	75	ARG	2.4
8	2I	114	LEU	2.4
17	2V	18	LEU	2.4
23	1l	85	LEU	2.4
33	1b	200	ILE	2.4
33	2b	61	LEU	2.4
34	2c	188	LEU	2.4
36	2e	16	THR	2.4
37	2f	21	LEU	2.4
40	1i	56	LEU	2.4
44	2m	48	LEU	2.4
44	2m	109	THR	2.4
50	2s	62	ILE	2.4
8	1I	105	HIS	2.4
33	2b	124	SER	2.4
33	1b	9	GLU	2.4
33	2b	205	ASP	2.4
1	1A	2180	A	2.4
7	1H	175	LYS	2.4
7	2H	30	LYS	2.4
29	27	48	LYS	2.4
32	2a	977	A	2.4
32	2a	1183	A	2.4
32	2a	1357	A	2.4
36	2e	85	GLY	2.4
4	2E	9	VAL	2.4
21	2Z	71	VAL	2.4
33	2b	174	VAL	2.4
35	1d	140	VAL	2.4
42	2k	84	VAL	2.4
1	1A	2123	G	2.4
1	1A	2147	G	2.4
1	1A	2177	G	2.4
1	1A	2204	G	2.4
1	2A	2148	G	2.4
12	2Q	59	ARG	2.4
21	1Z	164	ALA	2.4
32	2a	1024	G	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	117	ALA	2.4
38	2g	78	ARG	2.4
38	2g	115	ARG	2.4
20	2Y	106	LEU	2.4
33	2b	223	ILE	2.4
35	1d	188	LEU	2.4
1	1A	941	U	2.4
1	1A	1138	C	2.4
1	2A	2183	C	2.4
32	2a	1040	U	2.4
32	2a	1069	C	2.4
32	2a	1249	C	2.4
6	2G	27	ASN	2.4
41	2j	76	ASN	2.4
14	2S	8	GLU	2.4
21	2Z	138	GLU	2.4
40	2i	71	SER	2.4
34	2c	17	ASP	2.4
33	2b	90	MET	2.4
6	2G	75	LYS	2.4
33	2b	169	LYS	2.4
40	2i	113	LYS	2.4
43	2l	13	LYS	2.4
17	2V	29	PRO	2.4
5	2F	208	GLY	2.4
34	2c	41	GLY	2.4
40	2i	39	GLY	2.4
41	1j	36	GLY	2.4
50	2s	82	GLY	2.4
20	2Y	45	VAL	2.4
21	2Z	174	VAL	2.4
33	2b	7	VAL	2.4
38	1g	3	ARG	2.4
40	1i	111	ARG	2.4
2	2B	58	A	2.4
32	2a	1447	A	2.4
56	1y	14	A	2.4
36	2e	146	ALA	2.4
38	2g	147	ALA	2.4
33	2b	121	LEU	2.3
34	2c	91	LEU	2.3
40	2i	5	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	88	TYR	2.3
50	2s	80	TYR	2.3
47	2p	19	ILE	2.3
52	2u	13	ILE	2.3
41	2j	62	HIS	2.3
8	1I	11	ASN	2.3
34	1c	63	ASN	2.3
41	1j	69	ASN	2.3
1	1A	2209	G	2.3
1	1A	2212	G	2.3
1	2A	879	G	2.3
2	2B	103	G	2.3
15	1T	109	GLU	2.3
32	2a	950	U	2.3
32	2a	1026	G	2.3
32	2a	1030(C)	G	2.3
32	2a	1087	G	2.3
6	1G	48	GLU	2.3
6	2G	18	GLU	2.3
35	2d	80	GLU	2.3
2	2B	12	C	2.3
6	2G	147	ASP	2.3
7	1H	2	SER	2.3
32	2a	979	C	2.3
32	2a	1028	C	2.3
32	2a	1045	C	2.3
33	1b	189	ASP	2.3
48	1q	50	LYS	2.3
51	1t	74	LYS	2.3
56	1y	13	C	2.3
20	2Y	53	PRO	2.3
34	2c	73	PRO	2.3
42	2k	119	CYS	2.3
20	2Y	80	GLY	2.3
50	1s	68	GLY	2.3
6	2G	115	ARG	2.3
15	2T	112	ARG	2.3
6	2G	15	VAL	2.3
33	2b	112	VAL	2.3
34	2c	76	VAL	2.3
41	1j	44	VAL	2.3
50	2s	19	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	1I	65	ALA	2.3
15	2T	130	ALA	2.3
21	2Z	33	LEU	2.3
26	24	25	TYR	2.3
34	2c	184	TYR	2.3
1	1A	1100	A	2.3
18	1W	111	HIS	2.3
32	2a	978	A	2.3
44	2m	63	THR	2.3
47	1p	69	THR	2.3
50	2s	79	THR	2.3
53	2v	24	A	2.3
56	2y	14	A	2.3
24	22	11	GLU	2.3
33	1b	126	GLU	2.3
33	2b	133	LYS	2.3
20	2Y	107	ASP	2.3
39	1h	4	ASP	2.3
42	1k	36	ASP	2.3
1	2A	2152	G	2.3
2	2B	61	G	2.3
11	2P	97	PRO	2.3
26	24	29	PRO	2.3
32	2a	1253	G	2.3
1	1A	2160	C	2.3
1	1A	2185	C	2.3
12	1Q	56	ARG	2.3
12	2Q	33	GLY	2.3
32	2a	1038	C	2.3
32	2a	1115	C	2.3
33	1b	21	ARG	2.3
33	2b	18	GLY	2.3
38	1g	76	ARG	2.3
40	1i	57	GLY	2.3
41	2j	93	GLY	2.3
48	1q	26	GLN	2.3
55	1x	67	C	2.3
56	1y	62	C	2.3
5	2F	89	VAL	2.3
5	2F	174	VAL	2.3
42	1k	14	VAL	2.3
35	1d	108	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	151	LEU	2.3
39	2h	31	PHE	2.3
41	1j	40	LEU	2.3
12	2Q	32	TYR	2.3
36	1e	98	THR	2.3
24	12	11	GLU	2.3
39	2h	21	LYS	2.3
52	2u	3	LYS	2.3
35	2d	154	ASN	2.3
1	2A	1508	A	2.3
2	2B	59	A	2.3
2	2B	120	A	2.3
32	2a	1004	A	2.3
7	2H	112	PRO	2.3
12	1Q	60	ARG	2.3
15	1T	111	ARG	2.3
46	1o	19	PRO	2.3
46	1o	68	ARG	2.3
47	1p	72	ARG	2.3
47	2p	41	PRO	2.3
33	2b	76	GLN	2.3
1	1A	2189	U	2.3
32	1a	90	U	2.3
32	1a	1446	U	2.3
56	2y	33	U	2.3
33	2b	93	VAL	2.3
6	2G	176	LEU	2.3
40	2i	79	LEU	2.3
50	2s	15	LEU	2.3
7	2H	20	ALA	2.3
14	2S	40	ILE	2.3
20	2Y	48	ALA	2.3
32	2a	1271	G	2.3
33	1b	39	ILE	2.3
33	2b	172	ILE	2.3
41	2j	20	ALA	2.3
43	2l	68	ALA	2.3
47	1p	70	ALA	2.3
1	1A	10	G	2.3
1	1A	938	G	2.3
1	1A	2153	G	2.3
1	1A	2184	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2200	C	2.3
1	2A	2175	C	2.3
32	1a	1021	G	2.3
32	2a	1032	G	2.3
48	1q	65	ILE	2.3
33	2b	40	HIS	2.3
56	1y	10	G	2.3
20	2Y	54	LYS	2.3
26	14	69	LYS	2.3
33	2b	103	THR	2.3
35	2d	4	TYR	2.3
6	2G	13	GLU	2.3
6	2G	30	GLU	2.3
11	1P	98	GLU	2.3
14	2S	43	GLU	2.3
33	1b	12	GLU	2.3
35	1d	24	GLU	2.3
14	2S	61	ASN	2.3
21	2Z	34	ASN	2.3
8	2I	20	ASP	2.3
20	2Y	23	ARG	2.3
21	2Z	83	PRO	2.3
22	20	82	ARG	2.3
35	2d	47	ARG	2.3
49	2r	54	ARG	2.3
7	2H	5	GLY	2.3
20	2Y	104	GLY	2.3
32	1a	1004	A	2.3
50	2s	72	GLY	2.3
56	1y	9	A	2.3
56	1y	26	A	2.3
11	1P	125	VAL	2.3
11	2P	88	LEU	2.3
12	2Q	132	VAL	2.3
34	2c	34	LEU	2.3
39	2h	63	LEU	2.3
46	2o	15	PHE	2.3
1	1A	1136	U	2.2
1	1A	2166	U	2.2
1	1A	2906	U	2.2
5	2F	26	ALA	2.2
6	2G	169	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	24	15	ILE	2.2
41	2j	23	ILE	2.2
3	2D	275	LYS	2.2
11	2P	76	LYS	2.2
3	1D	259	THR	2.2
8	2I	85	GLU	2.2
38	2g	154	TYR	2.2
1	1A	1125	C	2.2
1	2A	2128	C	2.2
2	2B	31	C	2.2
1	1A	2173	G	2.2
1	2A	2751	G	2.2
2	2B	118	G	2.2
15	2T	104	ASN	2.2
32	1a	1030(C)	G	2.2
34	2c	3	ASN	2.2
20	2Y	73	ARG	2.2
36	2e	107	ARG	2.2
40	2i	128	ARG	2.2
47	1p	42	ARG	2.2
52	1u	15	ARG	2.2
33	2b	91	PRO	2.2
36	1e	96	PRO	2.2
44	1m	124	PRO	2.2
26	24	66	SER	2.2
40	2i	38	GLN	2.2
34	2c	155	GLY	2.2
35	1d	87	GLY	2.2
40	2i	69	GLY	2.2
46	1o	89	GLY	2.2
51	1t	69	GLY	2.2
21	2Z	18	LEU	2.2
21	2Z	157	LEU	2.2
33	2b	149	LEU	2.2
35	2d	19	LEU	2.2
41	1j	16	LEU	2.2
20	2Y	89	PHE	2.2
26	24	69	LYS	2.2
32	2a	964	A	2.2
32	2a	975	A	2.2
33	2b	68	ILE	2.2
34	2c	182	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	187	ALA	2.2
34	2c	189	ALA	2.2
35	1d	158	ILE	2.2
36	2e	17	ALA	2.2
39	1h	86	ILE	2.2
41	1j	6	ILE	2.2
41	2j	57	LYS	2.2
44	2m	22	ILE	2.2
52	2u	20	LYS	2.2
32	2a	1049	U	2.2
32	2a	1062	U	2.2
56	1y	12	U	2.2
6	2G	181	ARG	2.2
7	1H	3	ARG	2.2
25	23	3	ARG	2.2
33	2b	30	ARG	2.2
45	2n	12	ARG	2.2
21	1Z	159	PRO	2.2
1	1A	2201	C	2.2
1	2A	897	C	2.2
32	1a	1037	C	2.2
32	2a	948	C	2.2
32	2a	1328	C	2.2
55	1x	69	C	2.2
33	1b	195	ASP	2.2
34	1c	17	ASP	2.2
1	2A	2807	G	2.2
32	1a	93	G	2.2
32	2a	1117	G	2.2
32	2a	1190	G	2.2
35	2d	176	LEU	2.2
56	1y	44	G	2.2
6	1G	182	LYS	2.2
7	2H	52	VAL	2.2
21	2Z	161	VAL	2.2
22	20	5	LYS	2.2
35	2d	178	VAL	2.2
47	2p	59	TRP	2.2
8	2I	4	ILE	2.2
26	24	42	PHE	2.2
40	2i	59	PHE	2.2
13	2R	101	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	123	ALA	2.2
51	1t	95	ALA	2.2
6	2G	14	GLU	2.2
9	2N	28	THR	2.2
26	14	34	GLU	2.2
26	24	24	THR	2.2
26	24	57	GLU	2.2
36	2e	111	GLU	2.2
32	2a	1531	A	2.2
7	2H	170	ARG	2.2
15	1T	129	ARG	2.2
15	2T	111	ARG	2.2
19	2X	68	ARG	2.2
25	23	29	ARG	2.2
34	2c	38	ARG	2.2
41	2j	5	ARG	2.2
56	1y	33	U	2.2
56	2y	66	U	2.2
8	2I	74	ASN	2.2
8	2I	132	PRO	2.2
33	1b	125	PRO	2.2
33	1b	202	PRO	2.2
16	2U	104	GLN	2.2
44	2m	101	GLN	2.2
8	1I	124	GLY	2.2
8	2I	47	LEU	2.2
14	2S	11	LYS	2.2
33	2b	132	LYS	2.2
34	2c	45	LYS	2.2
35	1d	86	LYS	2.2
37	1f	83	ASP	2.2
40	2i	72	GLY	2.2
45	2n	58	LYS	2.2
51	1t	72	LEU	2.2
6	2G	160	VAL	2.2
34	1c	55	VAL	2.2
34	2c	116	VAL	2.2
39	2h	9	MET	2.2
1	2A	2188	C	2.2
14	2S	35	ILE	2.2
21	2Z	88	PHE	2.2
22	20	3	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2k	125	PHE	2.2
45	2n	36	PHE	2.2
56	2y	68	C	2.2
21	2Z	17	ALA	2.2
34	2c	60	ALA	2.2
34	2c	71	ALA	2.2
34	2c	92	ALA	2.2
36	1e	94	ALA	2.2
40	2i	45	ALA	2.2
1	2A	10	G	2.2
1	2A	1533	G	2.2
1	2A	2120	G	2.2
32	2a	993	G	2.2
56	1y	65	G	2.2
56	1y	70	G	2.2
56	2y	70	G	2.2
14	2S	5	THR	2.2
34	1c	15	THR	2.2
34	2c	16	ARG	2.2
41	2j	79	ARG	2.2
44	2m	88	ARG	2.2
1	1A	2148	A	2.2
18	2W	38	TYR	2.2
19	2X	69	TYR	2.2
20	1Y	92	ASN	2.2
32	2a	983	A	2.2
32	2a	1248	A	2.2
36	2e	61	TYR	2.2
40	2i	98	PRO	2.2
1	1A	2154	U	2.2
34	2c	28	GLN	2.2
44	1m	121	LYS	2.2
19	2X	70	LEU	2.2
33	2b	142	LEU	2.2
35	1d	96	LEU	2.2
35	2d	78	LEU	2.2
33	2b	63	MET	2.2
7	2H	79	VAL	2.2
33	2b	162	ILE	2.2
35	1d	5	ILE	2.2
36	2e	32	VAL	2.2
42	2k	16	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2k	116	HIS	2.2
51	2t	100	ILE	2.2
33	2b	57	PHE	2.2
40	2i	37	PHE	2.2
3	1D	2	ALA	2.1
36	2e	21	ALA	2.1
49	2r	60	ALA	2.1
1	1A	939	C	2.1
1	2A	2108	C	2.1
14	2S	15	ARG	2.1
21	1Z	170	THR	2.1
25	13	55	ARG	2.1
27	25	29	THR	2.1
32	2a	1054	C	2.1
32	2a	1149	C	2.1
35	2d	76	ARG	2.1
38	1g	78	ARG	2.1
43	1l	89	ARG	2.1
45	2n	27	CYS	2.1
1	1A	2174	G	2.1
1	2A	2153	G	2.1
32	1a	348	G	2.1
32	2a	963	G	2.1
54	2w	44	G	2.1
56	1y	27	G	2.1
34	2c	4	LYS	2.1
36	1e	9	LYS	2.1
38	1g	85	TYR	2.1
45	2n	15	LYS	2.1
41	2j	16	LEU	2.1
1	1A	218	A	2.1
1	1A	1149	A	2.1
1	1A	1507	A	2.1
1	2A	6	A	2.1
1	2A	1507	A	2.1
2	2B	29	A	2.1
34	2c	74	GLY	2.1
50	1s	46	GLY	2.1
7	2H	17	VAL	2.1
7	2H	72	ILE	2.1
17	2V	33	VAL	2.1
32	2a	1219	U	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	222	ILE	2.1
34	2c	99	VAL	2.1
34	2c	144	SER	2.1
39	2h	134	ILE	2.1
43	2l	18	VAL	2.1
51	1t	55	ILE	2.1
48	1q	27	PHE	2.1
3	2D	19	ALA	2.1
34	1c	117	ALA	2.1
38	2g	2	ALA	2.1
49	1r	20	ALA	2.1
51	2t	78	ALA	2.1
21	2Z	168	GLU	2.1
33	2b	170	GLU	2.1
40	2i	35	GLU	2.1
11	2P	79	ARG	2.1
26	24	68	ARG	2.1
35	2d	73	ARG	2.1
38	2g	76	ARG	2.1
41	1j	46	ARG	2.1
39	2h	3	THR	2.1
41	2j	53	PRO	2.1
47	2p	50	LYS	2.1
48	1q	14	LYS	2.1
51	2t	74	LYS	2.1
1	1A	2815	C	2.1
32	2a	1119	C	2.1
34	2c	107	GLN	2.1
56	1y	56	C	2.1
5	2F	12	LEU	2.1
27	25	58	LEU	2.1
34	1c	178	LEU	2.1
39	1h	20	TYR	2.1
39	2h	112	LEU	2.1
48	1q	51	TYR	2.1
21	2Z	12	GLY	2.1
34	2c	25	GLY	2.1
22	20	80	HIS	2.1
26	14	51	ASP	2.1
26	24	35	VAL	2.1
32	2a	998	G	2.1
32	2a	1124	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1178	G	2.1
32	2a	1365	G	2.1
33	2b	200	ILE	2.1
36	2e	55	VAL	2.1
39	2h	53	VAL	2.1
47	1p	62	VAL	2.1
50	2s	41	VAL	2.1
54	1w	44	G	2.1
56	1y	5	G	2.1
16	2U	79	PHE	2.1
51	1t	11	SER	2.1
1	2A	78	A	2.1
1	2A	2176	A	2.1
2	2B	57	A	2.1
32	1a	1503	A	2.1
40	2i	76	ALA	2.1
51	1t	52	ALA	2.1
55	1x	47	U	2.1
56	2y	7	A	2.1
15	1T	108	ARG	2.1
15	2T	115	ARG	2.1
26	14	55	ARG	2.1
39	2h	37	ARG	2.1
48	2q	72	ARG	2.1
9	2N	65	LYS	2.1
8	1I	119	PRO	2.1
45	1n	14	PRO	2.1
36	2e	10	MET	2.1
38	2g	11	GLN	2.1
39	2h	70	GLN	2.1
41	2j	86	MET	2.1
7	2H	103	LEU	2.1
8	2I	101	LEU	2.1
34	2c	178	LEU	2.1
47	2p	6	LEU	2.1
38	2g	37	ASN	2.1
41	2j	69	ASN	2.1
8	2I	16	GLY	2.1
21	2Z	29	TYR	2.1
33	1b	227	GLY	2.1
38	1g	151	TYR	2.1
42	1k	50	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	1m	24	GLY	2.1
48	2q	95	TYR	2.1
1	1A	1118	C	2.1
1	2A	652(T)	C	2.1
1	2A	1118	C	2.1
1	2A	2317	C	2.1
2	2B	30	C	2.1
6	2G	149	VAL	2.1
12	2Q	66	ILE	2.1
32	1a	91	C	2.1
32	2a	1019	C	2.1
32	2a	1359	C	2.1
56	1y	68	C	2.1
8	1I	110	ASP	2.1
14	2S	42	ASP	2.1
16	2U	56	ASP	2.1
21	2Z	87	ASP	2.1
8	2I	146	ALA	2.1
20	2Y	17	SER	2.1
33	1b	23	ARG	2.1
33	1b	34	ALA	2.1
33	1b	36	ARG	2.1
34	1c	172	ARG	2.1
35	2d	149	ALA	2.1
35	2d	195	ALA	2.1
40	1i	66	ARG	2.1
1	1A	2190	G	2.1
1	1A	2203	G	2.1
1	2A	545	G	2.1
1	2A	892	G	2.1
5	2F	172	TRP	2.1
32	2a	1258	G	2.1
54	2w	69	G	2.1
56	2y	65	G	2.1
1	1A	1072	U	2.1
1	2A	614(A)	U	2.1
1	2A	1026	U	2.1
1	2A	2119	A	2.1
32	1a	162	A	2.1
32	1a	172	A	2.1
32	2a	969	A	2.1
32	2a	1196	U	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1446	U	2.1
55	2x	20	U	2.1
39	2h	5	PRO	2.1
50	2s	76	PRO	2.1
34	2c	123	GLN	2.1
6	2G	43	LEU	2.1
8	2I	77	LEU	2.1
34	1c	196	LEU	2.1
34	2c	111	LEU	2.1
38	1g	16	LEU	2.1
5	1F	208	GLY	2.1
34	1c	81	GLY	2.1
39	2h	47	GLY	2.1
40	2i	117	HIS	2.1
42	2k	25	TYR	2.1
5	1F	6	VAL	2.1
25	23	58	VAL	2.1
50	2s	58	VAL	2.1
14	2S	12	PHE	2.1
6	2G	9	ARG	2.0
11	2P	77	ARG	2.0
21	2Z	81	ARG	2.0
23	2I	26	ARG	2.0
33	2b	56	ARG	2.0
41	1j	73	ASP	2.0
47	1p	68	ASP	2.0
50	2s	12	ASP	2.0
44	1m	2	ALA	2.0
44	1m	50	GLU	2.0
52	2u	22	ARG	2.0
7	2H	38	SER	2.0
8	2I	46	ALA	2.0
21	2Z	164	ALA	2.0
1	2A	894	C	2.0
2	2B	5	C	2.0
32	1a	381	C	2.0
32	2a	934	C	2.0
32	2a	1254	C	2.0
34	2c	97	LYS	2.0
34	2c	18	TRP	2.0
6	2G	165	THR	2.0
26	14	44	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	1p	22	THR	2.0
35	2d	7	PRO	2.0
40	2i	49	PRO	2.0
1	2A	2897	U	2.0
6	2G	7	LEU	2.0
8	2I	35	LEU	2.0
11	1P	99	LEU	2.0
17	2V	95	LEU	2.0
21	2Z	125	LEU	2.0
32	1a	841	U	2.0
36	2e	71	LEU	2.0
40	2i	50	LEU	2.0
47	2p	60	LEU	2.0
1	1A	1218	G	2.0
1	2A	2165	G	2.0
1	2A	2168	G	2.0
1	2A	2207	G	2.0
2	2B	25	A	2.0
32	1a	380	G	2.0
32	2a	1031	G	2.0
32	2a	1127	G	2.0
32	2a	1355	G	2.0
56	1y	21	A	2.0
56	2y	38	A	2.0
7	2H	61	HIS	2.0
8	2I	133	HIS	2.0
34	2c	176	HIS	2.0
14	2S	90	GLY	2.0
34	2c	185	GLY	2.0
34	2c	202	ILE	2.0
35	1d	70	ILE	2.0
40	2i	63	ILE	2.0
44	2m	25	ILE	2.0
6	2G	38	VAL	2.0
7	2H	37	VAL	2.0
19	2X	52	VAL	2.0
21	2Z	139	VAL	2.0
24	22	6	VAL	2.0
26	24	56	VAL	2.0
29	27	46	VAL	2.0
34	1c	207	VAL	2.0
39	2h	103	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	34	VAL	2.0
44	2m	17	VAL	2.0
39	2h	105	ARG	2.0
47	1p	81	ARG	2.0
6	1G	147	ASP	2.0
7	2H	57	ASP	2.0
9	1N	88	GLU	2.0
34	2c	122	GLU	2.0
22	20	18	ALA	2.0
33	1b	13	ALA	2.0
33	1b	29	ALA	2.0
34	1c	92	ALA	2.0
34	2c	50	ALA	2.0
41	1j	32	ALA	2.0
49	2r	21	LYS	2.0
45	2n	32	SER	2.0
51	1t	61	SER	2.0
5	2F	175	THR	2.0
6	2G	112	PRO	2.0
8	2I	137	PRO	2.0
22	20	43	THR	2.0
33	1b	63	MET	2.0
33	2b	168	THR	2.0
34	1c	177	THR	2.0
50	2s	2	PRO	2.0
52	2u	8	THR	2.0
1	1A	696	C	2.0
2	2B	27	C	2.0
5	2F	125	LEU	2.0
6	2G	3	LEU	2.0
20	2Y	31	LEU	2.0
32	1a	1007	C	2.0
32	2a	1260	C	2.0
33	2b	146	GLN	2.0
35	1d	155	LEU	2.0
38	2g	38	LEU	2.0
39	1h	133	LEU	2.0
43	2l	60	LEU	2.0
51	1t	62	LEU	2.0
2	2B	8	U	2.0
2	2B	55	U	2.0
7	1H	174	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	96	GLY	2.0
16	2U	7	GLY	2.0
20	2Y	59	GLY	2.0
22	20	22	GLY	2.0
33	2b	127	ILE	2.0
36	2e	97	GLY	2.0
44	2m	38	GLY	2.0
51	2t	96	GLY	2.0
5	2F	132	VAL	2.0
9	2N	25	ARG	2.0
12	2Q	5	ARG	2.0
17	2V	57	VAL	2.0
21	1Z	20	ARG	2.0
32	1a	161	A	2.0
32	2a	994	A	2.0
32	2a	1151	A	2.0
32	2a	1363(A)	A	2.0
33	2b	209	ARG	2.0
34	2c	141	VAL	2.0
35	2d	140	VAL	2.0
39	2h	19	VAL	2.0
42	2k	30	VAL	2.0
42	2k	126	ARG	2.0
47	2p	53	VAL	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
56	7MG	2y	46	24/25	0.51	0.16	80,93,98,110	0
56	7MG	1y	46	24/25	0.62	0.20	78,90,96,108	0
56	MIA	2y	37	22/30	0.63	0.18	73,83,93,106	0
56	MIA	1y	37	22/30	0.65	0.16	71,81,88,101	0
54	7MG	2w	46	24/25	0.66	0.16	71,82,92,104	0
56	PSU	1y	55	20/21	0.68	0.14	80,86,94,107	0
56	PSU	2y	55	20/21	0.68	0.13	82,85,106,108	0
56	4SU	2y	8	20/21	0.69	0.14	80,89,100,105	0
54	7MG	1w	46	24/25	0.70	0.15	60,71,82,103	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	PSU	1y	32	20/21	0.70	0.15	71,77,90,107	0
56	PSU	2y	32	20/21	0.70	0.17	76,83,98,98	0
56	5MU	2y	54	21/22	0.72	0.15	81,86,90,105	0
56	PSU	2y	39	20/21	0.74	0.14	81,86,99,110	0
56	4SU	1y	8	20/21	0.77	0.13	81,88,96,101	0
56	PSU	1y	39	20/21	0.77	0.14	66,76,89,99	0
56	5MU	1y	54	21/22	0.79	0.14	76,82,87,92	0
32	2MG	2a	1207	24/25	0.86	0.14	66,73,79,82	0
54	4SU	2w	8	20/21	0.86	0.11	73,78,84,85	0
43	0TD	1l	92	10/11	0.87	0.12	37,46,49,64	0
55	4SU	2x	8	20/21	0.87	0.13	68,74,80,82	0
32	M2G	2a	966	25/26	0.88	0.18	53,62,70,75	0
55	PSU	2x	55	20/21	0.88	0.12	64,68,76,77	0
54	PSU	2w	55	20/21	0.89	0.10	55,69,77,79	0
55	5MC	2x	32	21/22	0.89	0.15	61,67,71,76	0
55	5MU	1x	54	21/22	0.89	0.13	54,59,65,70	0
55	5MU	2x	54	21/22	0.90	0.11	61,69,73,76	0
54	PSU	2w	32	20/21	0.90	0.12	63,71,87,87	0
54	5MU	2w	54	21/22	0.90	0.10	51,60,67,74	0
43	0TD	2l	92	10/11	0.90	0.14	57,63,66,75	0
1	PSU	2A	1917	20/21	0.91	0.11	46,55,61,66	0
1	4OC	2A	1920	21/23	0.91	0.11	48,53,59,63	0
32	PSU	2a	516	20/21	0.91	0.10	47,62,72,73	0
1	5MU	2A	1915	21/22	0.91	0.11	55,60,65,73	0
55	PSU	1x	55	20/21	0.91	0.10	51,56,67,68	0
32	5MC	2a	967	21/22	0.92	0.15	56,62,70,72	0
32	7MG	2a	527	24/25	0.92	0.12	50,62,71,73	0
32	4OC	2a	1402	22/23	0.92	0.12	54,61,64,66	0
54	PSU	2w	39	20/21	0.92	0.12	55,72,78,79	0
55	4SU	1x	8	20/21	0.92	0.10	44,52,59,63	0
54	MIA	2w	37	25/30	0.93	0.12	58,67,73,74	0
32	5MC	2a	1407	21/22	0.93	0.12	46,55,59,73	0
32	MA6	2a	1519	24/25	0.93	0.14	53,59,64,64	0
1	PSU	2A	1911	20/21	0.93	0.10	47,55,61,61	0
32	PSU	1a	516	20/21	0.93	0.10	48,54,59,61	0
54	PSU	1w	55	20/21	0.93	0.10	45,57,68,73	0
32	5MC	2a	1404	21/22	0.93	0.11	50,56,61,61	0
54	PSU	1w	32	20/21	0.94	0.10	54,60,65,67	0
32	MA6	2a	1518	24/25	0.94	0.12	51,58,63,63	0
1	5MU	1A	1937	21/22	0.94	0.10	38,44,52,53	0
32	2MG	1a	1207	24/25	0.94	0.09	47,54,58,64	0
54	4SU	1w	8	20/21	0.94	0.07	57,66,71,71	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	1400	21/22	0.94	0.12	56,61,65,68	0
32	UR3	2a	1498	21/22	0.95	0.11	48,54,59,61	0
32	M2G	1a	966	25/26	0.95	0.09	34,39,45,46	0
54	F3N	2w	76	33/34	0.95	0.10	31,39,44,53	0
32	5MC	1a	967	21/22	0.95	0.08	38,45,52,54	0
1	5MC	2A	1962	21/22	0.95	0.10	40,45,50,58	0
54	MIA	1w	37	29/30	0.95	0.10	39,46,53,55	0
54	5MU	1w	54	21/22	0.96	0.09	34,39,52,59	0
1	PSU	1A	1939	20/21	0.96	0.09	32,40,46,47	0
1	OMG	2A	2251	24/25	0.96	0.09	30,36,41,41	0
32	7MG	1a	527	24/25	0.96	0.08	38,45,50,57	0
54	PSU	1w	39	20/21	0.96	0.08	45,49,56,59	0
32	4OC	1a	1402	22/23	0.96	0.09	35,41,44,45	0
1	5MC	1A	1964	21/22	0.96	0.08	29,34,37,40	0
55	5MC	1x	32	21/22	0.96	0.09	38,45,48,52	0
1	5MC	2A	1942	21/22	0.96	0.09	36,51,59,60	0
1	2MA	2A	2503	23/24	0.97	0.07	26,32,35,36	0
1	2MU	2A	2552	21/23	0.97	0.08	34,41,44,47	0
32	MA6	1a	1518	24/25	0.97	0.09	32,38,40,42	0
32	MA6	1a	1519	24/25	0.97	0.09	33,38,42,45	0
1	5MU	1A	1961	21/22	0.97	0.08	19,25,31,36	0
1	PSU	1A	1933	20/21	0.97	0.08	31,41,46,47	0
1	5MC	1A	1984	21/22	0.97	0.08	25,30,35,42	0
1	PSU	1A	2617	20/21	0.97	0.07	15,21,26,26	0
32	5MC	1a	1400	21/22	0.97	0.08	29,36,43,47	0
1	5MU	2A	1939	21/22	0.97	0.08	29,36,40,42	0
1	4OC	1A	1942	21/23	0.97	0.08	32,38,40,41	0
32	5MC	1a	1404	21/22	0.97	0.08	25,35,39,42	0
32	5MC	1a	1407	21/22	0.97	0.09	29,36,42,45	0
54	F3N	1w	76	33/34	0.98	0.07	12,20,26,33	0
32	UR3	1a	1498	21/22	0.98	0.07	27,37,41,44	0
1	2MA	1A	2515	23/24	0.98	0.06	14,18,25,27	0
1	PSU	2A	2605	20/21	0.98	0.07	21,30,36,37	0
1	2MU	1A	2564	21/23	0.98	0.06	17,25,30,30	0
1	OMG	1A	2263	24/25	0.98	0.07	14,22,26,28	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
57	MG	2A	3603	1/1	0.40	0.19	77,77,77,77	0
57	MG	2a	3195	1/1	0.47	0.14	84,84,84,84	0
57	MG	2j	8002	1/1	0.56	0.16	82,82,82,82	0
57	MG	1a	3134	1/1	0.62	0.19	77,77,77,77	0
57	MG	1A	3863	1/1	0.67	0.16	60,60,60,60	0
57	MG	1Q	204	1/1	0.67	0.24	66,66,66,66	0
57	MG	1I	3001	1/1	0.68	0.21	60,60,60,60	0
57	MG	2a	3184	1/1	0.68	0.31	65,65,65,65	0
57	MG	2A	3295	1/1	0.69	0.14	66,66,66,66	0
57	MG	2a	3115	1/1	0.70	0.16	66,66,66,66	0
57	MG	1A	3662	1/1	0.70	0.14	54,54,54,54	0
57	MG	2A	3478	1/1	0.70	0.17	64,64,64,64	0
57	MG	1a	3197	1/1	0.70	0.21	78,78,78,78	0
57	MG	2x	103	1/1	0.70	0.17	73,73,73,73	0
57	MG	2A	3156	1/1	0.71	0.25	64,64,64,64	0
57	MG	1A	3782	1/1	0.71	0.14	25,25,25,25	0
57	MG	2a	3187	1/1	0.71	0.15	74,74,74,74	0
57	MG	2A	3272	1/1	0.72	0.14	53,53,53,53	0
57	MG	2Z	8001	1/1	0.72	0.18	80,80,80,80	0
57	MG	2A	3495	1/1	0.73	0.19	61,61,61,61	0
57	MG	2a	3020	1/1	0.73	0.18	65,65,65,65	0
57	MG	1A	3425	1/1	0.73	0.19	53,53,53,53	0
57	MG	2A	3647	1/1	0.73	0.15	62,62,62,62	0
57	MG	2A	3680	1/1	0.74	0.24	49,49,49,49	0
57	MG	2A	3358	1/1	0.74	0.18	54,54,54,54	0
57	MG	2A	3444	1/1	0.74	0.15	58,58,58,58	0
57	MG	2a	3036	1/1	0.74	0.19	65,65,65,65	0
57	MG	2A	3305	1/1	0.74	0.57	78,78,78,78	0
57	MG	2A	3411	1/1	0.75	0.15	40,40,40,40	0
57	MG	2a	3175	1/1	0.75	0.12	63,63,63,63	0
57	MG	2B	3015	1/1	0.75	0.21	69,69,69,69	0
57	MG	2A	3504	1/1	0.75	0.21	69,69,69,69	0
57	MG	1A	3334	1/1	0.75	0.14	47,47,47,47	0
57	MG	1A	3541	1/1	0.75	0.18	48,48,48,48	0
57	MG	2a	3052	1/1	0.75	0.26	69,69,69,69	0
57	MG	2A	3576	1/1	0.76	0.19	60,60,60,60	0
57	MG	2A	3591	1/1	0.76	0.23	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3110	1/1	0.76	0.13	57,57,57,57	0
57	MG	2A	3472	1/1	0.76	0.28	65,65,65,65	0
57	MG	2A	3482	1/1	0.76	0.17	71,71,71,71	0
57	MG	1a	3190	1/1	0.77	0.11	65,65,65,65	0
57	MG	1A	3695	1/1	0.77	0.14	52,52,52,52	0
57	MG	2B	3021	1/1	0.77	0.13	57,57,57,57	0
57	MG	1a	3210	1/1	0.77	0.13	61,61,61,61	0
57	MG	2A	3042	1/1	0.77	0.20	61,61,61,61	0
57	MG	1B	3028	1/1	0.78	0.13	53,53,53,53	0
57	MG	2a	3129	1/1	0.78	0.23	71,71,71,71	0
57	MG	1A	3447	1/1	0.78	0.17	26,26,26,26	0
57	MG	2a	3180	1/1	0.78	0.15	62,62,62,62	0
57	MG	2a	3016	1/1	0.78	0.13	78,78,78,78	0
57	MG	2A	3611	1/1	0.78	0.17	51,51,51,51	0
57	MG	2A	3496	1/1	0.78	0.18	42,42,42,42	0
57	MG	1a	3204	1/1	0.78	0.11	75,75,75,75	0
57	MG	2A	3223	1/1	0.78	0.11	48,48,48,48	0
57	MG	2A	3154	1/1	0.79	0.25	60,60,60,60	0
57	MG	2a	3022	1/1	0.79	0.13	59,59,59,59	0
57	MG	2A	3593	1/1	0.79	0.17	44,44,44,44	0
57	MG	1a	3183	1/1	0.79	0.20	52,52,52,52	0
57	MG	2A	3163	1/1	0.79	0.19	58,58,58,58	0
57	MG	2A	3214	1/1	0.79	0.11	57,57,57,57	0
57	MG	2A	3655	1/1	0.79	0.20	51,51,51,51	0
57	MG	2a	3166	1/1	0.79	0.24	62,62,62,62	0
57	MG	1A	3802	1/1	0.79	0.15	46,46,46,46	0
57	MG	2B	3011	1/1	0.79	0.27	68,68,68,68	0
57	MG	1O	207	1/1	0.79	0.12	80,80,80,80	0
57	MG	1A	3243	1/1	0.79	0.19	56,56,56,56	0
57	MG	1A	3519	1/1	0.79	0.14	38,38,38,38	0
57	MG	20	3002	1/1	0.79	0.32	64,64,64,64	0
57	MG	1a	3150	1/1	0.79	0.21	56,56,56,56	0
57	MG	2A	3594	1/1	0.80	0.14	46,46,46,46	0
57	MG	2a	3120	1/1	0.80	0.20	70,70,70,70	0
57	MG	2A	3596	1/1	0.80	0.15	46,46,46,46	0
57	MG	2a	3137	1/1	0.80	0.22	51,51,51,51	0
57	MG	2a	3162	1/1	0.80	0.12	53,53,53,53	0
57	MG	2a	3163	1/1	0.80	0.20	72,72,72,72	0
57	MG	2A	3598	1/1	0.80	0.17	52,52,52,52	0
57	MG	2a	3167	1/1	0.80	0.13	64,64,64,64	0
57	MG	2A	3399	1/1	0.80	0.19	52,52,52,52	0
57	MG	1y	3002	1/1	0.80	0.15	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
57	MG	2A	3622	1/1	0.80	0.15	61,61,61,61	0
57	MG	2A	3291	1/1	0.80	0.11	24,24,24,24	0
57	MG	2a	3190	1/1	0.80	0.18	64,64,64,64	0
57	MG	1a	3061	1/1	0.80	0.26	59,59,59,59	0
57	MG	2a	3200	1/1	0.80	0.21	69,69,69,69	0
57	MG	2A	3103	1/1	0.80	0.12	58,58,58,58	0
57	MG	1A	3692	1/1	0.80	0.15	58,58,58,58	0
57	MG	2a	3178	1/1	0.81	0.18	59,59,59,59	0
57	MG	2A	3526	1/1	0.81	0.15	59,59,59,59	0
57	MG	1A	3586	1/1	0.81	0.13	28,28,28,28	0
57	MG	2A	3258	1/1	0.81	0.12	50,50,50,50	0
57	MG	1A	3709	1/1	0.81	0.12	31,31,31,31	0
57	MG	2a	3049	1/1	0.81	0.15	52,52,52,52	0
57	MG	1G	205	1/1	0.81	0.11	61,61,61,61	0
57	MG	2A	3516	1/1	0.81	0.11	65,65,65,65	0
57	MG	2q	3002	1/1	0.81	0.11	71,71,71,71	0
57	MG	20	3003	1/1	0.81	0.18	53,53,53,53	0
57	MG	2A	3609	1/1	0.82	0.11	59,59,59,59	0
57	MG	2A	3522	1/1	0.82	0.15	68,68,68,68	0
57	MG	2A	3201	1/1	0.82	0.19	51,51,51,51	0
57	MG	2A	3542	1/1	0.82	0.15	53,53,53,53	0
57	MG	2a	3043	1/1	0.82	0.11	65,65,65,65	0
57	MG	2A	3115	1/1	0.82	0.21	62,62,62,62	0
57	MG	1A	3583	1/1	0.82	0.13	15,15,15,15	0
57	MG	2a	3185	1/1	0.82	0.18	60,60,60,60	0
57	MG	1a	3081	1/1	0.82	0.16	67,67,67,67	0
57	MG	1a	3011	1/1	0.82	0.12	50,50,50,50	0
57	MG	2A	3595	1/1	0.82	0.17	38,38,38,38	0
57	MG	2A	3189	1/1	0.82	0.13	64,64,64,64	0
57	MG	2A	3509	1/1	0.82	0.19	64,64,64,64	0
57	MG	2l	202	1/1	0.82	0.11	62,62,62,62	0
57	MG	2a	3158	1/1	0.82	0.14	65,65,65,65	0
57	MG	2r	3001	1/1	0.82	0.13	73,73,73,73	0
57	MG	2A	3469	1/1	0.82	0.26	64,64,64,64	0
57	MG	2A	3627	1/1	0.83	0.09	55,55,55,55	0
57	MG	2A	3638	1/1	0.83	0.17	57,57,57,57	0
57	MG	1A	3742	1/1	0.83	0.15	57,57,57,57	0
57	MG	2A	3334	1/1	0.83	0.21	50,50,50,50	0
57	MG	2a	3138	1/1	0.83	0.17	62,62,62,62	0
57	MG	1O	202	1/1	0.83	0.15	67,67,67,67	0
57	MG	2B	3008	1/1	0.83	0.14	53,53,53,53	0
57	MG	2A	3186	1/1	0.83	0.08	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
57	MG	2A	3556	1/1	0.83	0.12	51,51,51,51	0
57	MG	1A	3096	1/1	0.83	0.14	56,56,56,56	0
57	MG	2A	3580	1/1	0.83	0.11	41,41,41,41	0
57	MG	1A	3667	1/1	0.83	0.14	50,50,50,50	0
57	MG	1A	3830	1/1	0.83	0.16	39,39,39,39	0
57	MG	25	502	1/1	0.83	0.21	54,54,54,54	0
57	MG	2a	3004	1/1	0.83	0.15	67,67,67,67	0
57	MG	1A	3465	1/1	0.83	0.11	28,28,28,28	0
57	MG	1A	3902	1/1	0.83	0.20	44,44,44,44	0
57	MG	2A	3260	1/1	0.83	0.15	63,63,63,63	0
57	MG	2A	3262	1/1	0.83	0.16	60,60,60,60	0
57	MG	1a	3100	1/1	0.83	0.13	50,50,50,50	0
57	MG	2A	3501	1/1	0.83	0.16	57,57,57,57	0
57	MG	1A	3284	1/1	0.83	0.11	49,49,49,49	0
57	MG	2a	3064	1/1	0.83	0.17	59,59,59,59	0
57	MG	2w	101	1/1	0.83	0.14	59,59,59,59	0
57	MG	1A	3661	1/1	0.83	0.12	55,55,55,55	0
57	MG	2x	104	1/1	0.83	0.28	54,54,54,54	0
57	MG	1B	3023	1/1	0.84	0.16	51,51,51,51	0
57	MG	2A	3353	1/1	0.84	0.11	65,65,65,65	0
57	MG	2A	3121	1/1	0.84	0.15	65,65,65,65	0
57	MG	2A	3390	1/1	0.84	0.18	65,65,65,65	0
57	MG	2A	3391	1/1	0.84	0.11	26,26,26,26	0
57	MG	2a	3066	1/1	0.84	0.11	73,73,73,73	0
57	MG	2a	3098	1/1	0.84	0.14	57,57,57,57	0
57	MG	1A	3744	1/1	0.84	0.13	47,47,47,47	0
57	MG	1A	3343	1/1	0.84	0.19	49,49,49,49	0
57	MG	2A	3606	1/1	0.84	0.19	51,51,51,51	0
57	MG	2a	3121	1/1	0.84	0.10	68,68,68,68	0
57	MG	1a	3174	1/1	0.84	0.14	57,57,57,57	0
57	MG	2a	3136	1/1	0.84	0.18	67,67,67,67	0
57	MG	2A	3454	1/1	0.84	0.17	43,43,43,43	0
57	MG	2A	3619	1/1	0.84	0.14	43,43,43,43	0
57	MG	2A	3462	1/1	0.84	0.14	41,41,41,41	0
57	MG	2A	3165	1/1	0.84	0.15	53,53,53,53	0
57	MG	2A	3185	1/1	0.84	0.18	51,51,51,51	0
57	MG	1A	3396	1/1	0.84	0.09	30,30,30,30	0
57	MG	1a	3189	1/1	0.84	0.11	69,69,69,69	0
57	MG	2a	3173	1/1	0.84	0.16	68,68,68,68	0
57	MG	2a	3174	1/1	0.84	0.12	62,62,62,62	0
57	MG	2A	3661	1/1	0.84	0.12	37,37,37,37	0
57	MG	2A	3664	1/1	0.84	0.18	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
57	MG	1A	3592	1/1	0.84	0.15	37,37,37,37	0
57	MG	2A	3689	1/1	0.84	0.11	47,47,47,47	0
57	MG	1A	3834	1/1	0.84	0.18	60,60,60,60	0
57	MG	1A	3854	1/1	0.84	0.12	49,49,49,49	0
57	MG	1A	3520	1/1	0.84	0.13	45,45,45,45	0
57	MG	1a	3215	1/1	0.84	0.13	62,62,62,62	0
57	MG	1a	3025	1/1	0.84	0.18	62,62,62,62	0
57	MG	2d	503	1/1	0.84	0.22	50,50,50,50	0
57	MG	2A	3265	1/1	0.84	0.14	58,58,58,58	0
57	MG	2A	3009	1/1	0.84	0.16	59,59,59,59	0
57	MG	2A	3275	1/1	0.84	0.16	71,71,71,71	0
57	MG	1A	3449	1/1	0.84	0.10	45,45,45,45	0
57	MG	2t	3001	1/1	0.84	0.13	55,55,55,55	0
57	MG	2v	8002	1/1	0.84	0.15	66,66,66,66	0
57	MG	2A	3099	1/1	0.84	0.16	62,62,62,62	0
57	MG	1A	3949	1/1	0.84	0.15	53,53,53,53	0
57	MG	2A	3583	1/1	0.84	0.19	62,62,62,62	0
57	MG	2A	3503	1/1	0.85	0.14	45,45,45,45	0
57	MG	2a	3131	1/1	0.85	0.19	61,61,61,61	0
57	MG	1A	3874	1/1	0.85	0.15	62,62,62,62	0
57	MG	1A	3527	1/1	0.85	0.15	31,31,31,31	0
57	MG	1a	3092	1/1	0.85	0.13	60,60,60,60	0
57	MG	2a	3140	1/1	0.85	0.15	55,55,55,55	0
57	MG	2a	3146	1/1	0.85	0.16	55,55,55,55	0
57	MG	1A	3747	1/1	0.85	0.12	55,55,55,55	0
57	MG	2A	3523	1/1	0.85	0.16	68,68,68,68	0
57	MG	1B	3022	1/1	0.85	0.13	48,48,48,48	0
57	MG	2A	3536	1/1	0.85	0.10	60,60,60,60	0
57	MG	1A	3478	1/1	0.85	0.07	17,17,17,17	0
57	MG	1B	3027	1/1	0.85	0.10	53,53,53,53	0
57	MG	2A	3574	1/1	0.85	0.09	60,60,60,60	0
57	MG	1A	3488	1/1	0.85	0.10	33,33,33,33	0
57	MG	1a	3185	1/1	0.85	0.24	63,63,63,63	0
57	MG	2A	3582	1/1	0.85	0.13	52,52,52,52	0
57	MG	2A	3407	1/1	0.85	0.12	42,42,42,42	0
57	MG	1A	3812	1/1	0.85	0.10	21,21,21,21	0
57	MG	2A	3420	1/1	0.85	0.12	47,47,47,47	0
57	MG	2A	3439	1/1	0.85	0.20	46,46,46,46	0
57	MG	1A	3381	1/1	0.85	0.08	56,56,56,56	0
57	MG	1A	3469	1/1	0.85	0.16	60,60,60,60	0
57	MG	1A	3602	1/1	0.85	0.11	13,13,13,13	0
57	MG	1A	3855	1/1	0.85	0.14	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
57	MG	17	102	1/1	0.85	0.15	48,48,48,48	0
57	MG	2A	3476	1/1	0.85	0.19	65,65,65,65	0
57	MG	1a	3224	1/1	0.85	0.14	45,45,45,45	0
57	MG	2a	3099	1/1	0.85	0.25	58,58,58,58	0
57	MG	1b	3002	1/1	0.85	0.10	67,67,67,67	0
57	MG	1A	3657	1/1	0.85	0.10	50,50,50,50	0
57	MG	1A	3872	1/1	0.85	0.18	56,56,56,56	0
57	MG	1a	3040	1/1	0.85	0.22	60,60,60,60	0
59	AQJ	2A	3677	37/37	0.85	0.19	35,55,68,73	0
57	MG	1a	3086	1/1	0.86	0.20	52,52,52,52	0
57	MG	2A	3369	1/1	0.86	0.14	66,66,66,66	0
57	MG	2A	3088	1/1	0.86	0.16	48,48,48,48	0
57	MG	1A	3654	1/1	0.86	0.10	36,36,36,36	0
57	MG	2A	3589	1/1	0.86	0.23	59,59,59,59	0
57	MG	2A	3397	1/1	0.86	0.14	62,62,62,62	0
57	MG	1a	3099	1/1	0.86	0.26	48,48,48,48	0
57	MG	2A	3400	1/1	0.86	0.14	55,55,55,55	0
57	MG	1A	3490	1/1	0.86	0.10	25,25,25,25	0
57	MG	2A	3410	1/1	0.86	0.20	58,58,58,58	0
57	MG	2a	3130	1/1	0.86	0.16	51,51,51,51	0
57	MG	1a	3105	1/1	0.86	0.29	59,59,59,59	0
57	MG	1a	3111	1/1	0.86	0.19	55,55,55,55	0
57	MG	2A	3421	1/1	0.86	0.13	43,43,43,43	0
57	MG	1A	3491	1/1	0.86	0.14	29,29,29,29	0
57	MG	2A	3610	1/1	0.86	0.12	43,43,43,43	0
57	MG	2a	3145	1/1	0.86	0.12	64,64,64,64	0
57	MG	1A	3313	1/1	0.86	0.13	49,49,49,49	0
57	MG	2a	3153	1/1	0.86	0.19	59,59,59,59	0
57	MG	2a	3155	1/1	0.86	0.18	63,63,63,63	0
57	MG	1a	3169	1/1	0.86	0.20	70,70,70,70	0
57	MG	1A	3260	1/1	0.86	0.11	45,45,45,45	0
57	MG	1A	3598	1/1	0.86	0.12	38,38,38,38	0
57	MG	1A	3216	1/1	0.86	0.11	42,42,42,42	0
57	MG	1O	205	1/1	0.86	0.10	43,43,43,43	0
57	MG	1A	3605	1/1	0.86	0.10	22,22,22,22	0
57	MG	1A	3712	1/1	0.86	0.11	56,56,56,56	0
57	MG	2A	3483	1/1	0.86	0.15	60,60,60,60	0
57	MG	2A	3234	1/1	0.86	0.17	54,54,54,54	0
57	MG	1A	3620	1/1	0.86	0.09	55,55,55,55	0
57	MG	2B	3003	1/1	0.86	0.09	55,55,55,55	0
57	MG	1a	3001	1/1	0.86	0.11	50,50,50,50	0
57	MG	1A	3640	1/1	0.86	0.09	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
57	MG	1A	3920	1/1	0.86	0.17	73,73,73,73	0
57	MG	2A	3505	1/1	0.86	0.11	45,45,45,45	0
57	MG	1A	3922	1/1	0.86	0.11	52,52,52,52	0
57	MG	1y	3001	1/1	0.86	0.31	78,78,78,78	0
57	MG	2A	3288	1/1	0.86	0.08	48,48,48,48	0
57	MG	1A	3651	1/1	0.86	0.13	19,19,19,19	0
57	MG	2q	3001	1/1	0.86	0.16	42,42,42,42	0
57	MG	1B	3021	1/1	0.86	0.11	48,48,48,48	0
57	MG	2A	3017	1/1	0.86	0.16	53,53,53,53	0
57	MG	2A	3541	1/1	0.86	0.16	50,50,50,50	0
57	MG	2A	3038	1/1	0.86	0.21	52,52,52,52	0
57	MG	2a	3024	1/1	0.86	0.15	56,56,56,56	0
57	MG	2w	102	1/1	0.86	0.10	61,61,61,61	0
57	MG	2A	3551	1/1	0.86	0.25	68,68,68,68	0
57	MG	2A	3339	1/1	0.86	0.13	54,54,54,54	0
57	MG	2A	3039	1/1	0.86	0.16	58,58,58,58	0
57	MG	2a	3047	1/1	0.87	0.29	69,69,69,69	0
57	MG	1a	3045	1/1	0.87	0.21	63,63,63,63	0
57	MG	1A	3171	1/1	0.87	0.11	47,47,47,47	0
57	MG	2a	3056	1/1	0.87	0.11	66,66,66,66	0
57	MG	2a	3058	1/1	0.87	0.09	62,62,62,62	0
57	MG	2a	3059	1/1	0.87	0.19	50,50,50,50	0
57	MG	2a	3060	1/1	0.87	0.17	66,66,66,66	0
57	MG	1a	3067	1/1	0.87	0.26	56,56,56,56	0
57	MG	1A	3838	1/1	0.87	0.12	36,36,36,36	0
57	MG	2a	3087	1/1	0.87	0.12	69,69,69,69	0
57	MG	1A	3851	1/1	0.87	0.11	38,38,38,38	0
57	MG	1A	3088	1/1	0.87	0.17	40,40,40,40	0
57	MG	2a	3102	1/1	0.87	0.21	54,54,54,54	0
57	MG	1a	3098	1/1	0.87	0.23	56,56,56,56	0
57	MG	2a	3113	1/1	0.87	0.15	55,55,55,55	0
57	MG	2A	3601	1/1	0.87	0.20	55,55,55,55	0
57	MG	1A	3239	1/1	0.87	0.17	60,60,60,60	0
57	MG	1A	3642	1/1	0.87	0.09	29,29,29,29	0
57	MG	1A	3867	1/1	0.87	0.10	26,26,26,26	0
57	MG	1A	3691	1/1	0.87	0.11	48,48,48,48	0
57	MG	1a	3115	1/1	0.87	0.11	49,49,49,49	0
57	MG	2A	3500	1/1	0.87	0.13	62,62,62,62	0
57	MG	2A	3071	1/1	0.87	0.12	46,46,46,46	0
57	MG	2A	3502	1/1	0.87	0.14	49,49,49,49	0
57	MG	2A	3628	1/1	0.87	0.16	38,38,38,38	0
57	MG	1a	3133	1/1	0.87	0.13	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3313	1/1	0.87	0.16	53,53,53,53	0
57	MG	1A	3794	1/1	0.87	0.32	30,30,30,30	0
57	MG	1a	3148	1/1	0.87	0.17	56,56,56,56	0
57	MG	1A	3533	1/1	0.87	0.14	38,38,38,38	0
57	MG	2A	3668	1/1	0.87	0.12	47,47,47,47	0
57	MG	2A	3518	1/1	0.87	0.23	55,55,55,55	0
57	MG	1Y	204	1/1	0.87	0.21	52,52,52,52	0
57	MG	2A	3138	1/1	0.87	0.16	50,50,50,50	0
57	MG	2a	3172	1/1	0.87	0.17	73,73,73,73	0
57	MG	2B	3004	1/1	0.87	0.18	65,65,65,65	0
57	MG	2A	3379	1/1	0.87	0.12	48,48,48,48	0
57	MG	2A	3533	1/1	0.87	0.23	55,55,55,55	0
57	MG	2B	3014	1/1	0.87	0.21	68,68,68,68	0
57	MG	1A	3808	1/1	0.87	0.13	41,41,41,41	0
57	MG	1A	3653	1/1	0.87	0.10	18,18,18,18	0
57	MG	2F	3006	1/1	0.87	0.15	63,63,63,63	0
57	MG	2W	201	1/1	0.87	0.28	59,59,59,59	0
57	MG	2X	102	1/1	0.87	0.14	58,58,58,58	0
57	MG	2a	3191	1/1	0.87	0.19	55,55,55,55	0
57	MG	1a	3006	1/1	0.87	0.13	55,55,55,55	0
57	MG	20	3001	1/1	0.87	0.17	61,61,61,61	0
57	MG	2A	3547	1/1	0.87	0.09	37,37,37,37	0
57	MG	1a	3188	1/1	0.87	0.20	57,57,57,57	0
57	MG	2A	3171	1/1	0.87	0.11	53,53,53,53	0
57	MG	2A	3557	1/1	0.87	0.08	55,55,55,55	0
57	MG	2a	3009	1/1	0.87	0.24	66,66,66,66	0
57	MG	2A	3569	1/1	0.87	0.20	60,60,60,60	0
57	MG	1A	3826	1/1	0.87	0.15	50,50,50,50	0
57	MG	1A	3966	1/1	0.87	0.13	50,50,50,50	0
57	MG	1A	3143	1/1	0.87	0.17	34,34,34,34	0
57	MG	2a	3029	1/1	0.87	0.14	72,72,72,72	0
57	MG	2w	104	1/1	0.87	0.17	58,58,58,58	0
57	MG	2a	3035	1/1	0.87	0.20	61,61,61,61	0
57	MG	2A	3190	1/1	0.87	0.10	66,66,66,66	0
57	MG	2A	3193	1/1	0.87	0.21	50,50,50,50	0
57	MG	2A	3127	1/1	0.88	0.12	52,52,52,52	0
57	MG	2A	3132	1/1	0.88	0.10	43,43,43,43	0
57	MG	2A	3587	1/1	0.88	0.10	50,50,50,50	0
57	MG	1A	3699	1/1	0.88	0.08	29,29,29,29	0
57	MG	2A	3140	1/1	0.88	0.12	51,51,51,51	0
57	MG	1A	3173	1/1	0.88	0.23	46,46,46,46	0
57	MG	1a	3041	1/1	0.88	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
57	MG	2A	3419	1/1	0.88	0.15	54,54,54,54	0
57	MG	2a	3065	1/1	0.88	0.09	70,70,70,70	0
57	MG	1a	3044	1/1	0.88	0.26	57,57,57,57	0
57	MG	2a	3067	1/1	0.88	0.25	64,64,64,64	0
57	MG	2a	3079	1/1	0.88	0.12	63,63,63,63	0
57	MG	1A	3710	1/1	0.88	0.09	32,32,32,32	0
57	MG	2a	3089	1/1	0.88	0.11	47,47,47,47	0
57	MG	1a	3050	1/1	0.88	0.18	57,57,57,57	0
57	MG	2A	3602	1/1	0.88	0.09	44,44,44,44	0
57	MG	2a	3100	1/1	0.88	0.12	57,57,57,57	0
57	MG	2A	3178	1/1	0.88	0.27	59,59,59,59	0
57	MG	2A	3604	1/1	0.88	0.16	56,56,56,56	0
57	MG	1A	3312	1/1	0.88	0.13	30,30,30,30	0
57	MG	2A	3455	1/1	0.88	0.12	39,39,39,39	0
57	MG	2a	3116	1/1	0.88	0.15	63,63,63,63	0
57	MG	1a	3198	1/1	0.88	0.10	51,51,51,51	0
57	MG	1A	3202	1/1	0.88	0.09	49,49,49,49	0
57	MG	1a	3076	1/1	0.88	0.12	47,47,47,47	0
57	MG	2A	3474	1/1	0.88	0.19	43,43,43,43	0
57	MG	1A	3523	1/1	0.88	0.10	20,20,20,20	0
57	MG	1a	3220	1/1	0.88	0.15	63,63,63,63	0
57	MG	2A	3209	1/1	0.88	0.13	47,47,47,47	0
57	MG	1a	3222	1/1	0.88	0.12	64,64,64,64	0
57	MG	1a	3084	1/1	0.88	0.10	54,54,54,54	0
57	MG	2A	3656	1/1	0.88	0.11	36,36,36,36	0
57	MG	2A	3657	1/1	0.88	0.11	63,63,63,63	0
57	MG	2a	3152	1/1	0.88	0.23	59,59,59,59	0
57	MG	1G	204	1/1	0.88	0.10	56,56,56,56	0
57	MG	2A	3246	1/1	0.88	0.13	47,47,47,47	0
57	MG	2a	3156	1/1	0.88	0.10	44,44,44,44	0
57	MG	1r	3001	1/1	0.88	0.14	51,51,51,51	0
57	MG	1x	102	1/1	0.88	0.21	54,54,54,54	0
57	MG	1x	110	1/1	0.88	0.11	57,57,57,57	0
57	MG	1x	111	1/1	0.88	0.09	56,56,56,56	0
57	MG	1A	3406	1/1	0.88	0.11	27,27,27,27	0
57	MG	2A	3508	1/1	0.88	0.09	57,57,57,57	0
57	MG	1A	3487	1/1	0.88	0.12	23,23,23,23	0
57	MG	1A	3625	1/1	0.88	0.12	49,49,49,49	0
57	MG	1A	3680	1/1	0.88	0.12	49,49,49,49	0
57	MG	2A	3292	1/1	0.88	0.13	56,56,56,56	0
57	MG	2A	3025	1/1	0.88	0.08	40,40,40,40	0
57	MG	1A	3323	1/1	0.88	0.12	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
57	MG	2A	3532	1/1	0.88	0.11	66,66,66,66	0
57	MG	1A	3905	1/1	0.88	0.09	25,25,25,25	0
57	MG	2a	3189	1/1	0.88	0.11	49,49,49,49	0
57	MG	2A	3316	1/1	0.88	0.09	32,32,32,32	0
57	MG	1S	3003	1/1	0.88	0.11	52,52,52,52	0
57	MG	2a	3192	1/1	0.88	0.19	51,51,51,51	0
57	MG	1A	3641	1/1	0.88	0.19	64,64,64,64	0
57	MG	2a	3198	1/1	0.88	0.23	60,60,60,60	0
57	MG	1A	3825	1/1	0.88	0.22	37,37,37,37	0
57	MG	2A	3548	1/1	0.88	0.11	36,36,36,36	0
57	MG	2f	3002	1/1	0.88	0.09	71,71,71,71	0
57	MG	2g	8001	1/1	0.88	0.10	71,71,71,71	0
57	MG	2a	3006	1/1	0.88	0.14	57,57,57,57	0
57	MG	2l	201	1/1	0.88	0.12	63,63,63,63	0
57	MG	1a	3147	1/1	0.88	0.10	47,47,47,47	0
57	MG	2a	3010	1/1	0.88	0.09	47,47,47,47	0
57	MG	2A	3553	1/1	0.88	0.17	58,58,58,58	0
57	MG	2q	3003	1/1	0.88	0.09	70,70,70,70	0
57	MG	2A	3362	1/1	0.88	0.13	41,41,41,41	0
57	MG	1A	3924	1/1	0.88	0.10	34,34,34,34	0
57	MG	2A	3562	1/1	0.88	0.07	31,31,31,31	0
57	MG	2a	3025	1/1	0.88	0.29	59,59,59,59	0
57	MG	2A	3104	1/1	0.88	0.14	56,56,56,56	0
57	MG	2A	3381	1/1	0.88	0.08	51,51,51,51	0
57	MG	1A	3929	1/1	0.88	0.11	25,25,25,25	0
57	MG	2a	3038	1/1	0.88	0.22	53,53,53,53	0
57	MG	1A	3080	1/1	0.88	0.10	40,40,40,40	0
57	MG	2a	3028	1/1	0.89	0.19	56,56,56,56	0
57	MG	2A	3264	1/1	0.89	0.15	46,46,46,46	0
57	MG	2a	3030	1/1	0.89	0.25	59,59,59,59	0
57	MG	1A	3889	1/1	0.89	0.06	19,19,19,19	0
57	MG	2A	3271	1/1	0.89	0.15	53,53,53,53	0
57	MG	1A	3510	1/1	0.89	0.08	39,39,39,39	0
57	MG	1A	3749	1/1	0.89	0.10	61,61,61,61	0
57	MG	2a	3046	1/1	0.89	0.26	66,66,66,66	0
57	MG	2A	3281	1/1	0.89	0.10	39,39,39,39	0
57	MG	1a	3057	1/1	0.89	0.17	55,55,55,55	0
57	MG	1A	3916	1/1	0.89	0.12	39,39,39,39	0
57	MG	2A	3560	1/1	0.89	0.13	51,51,51,51	0
57	MG	1A	3750	1/1	0.89	0.12	18,18,18,18	0
57	MG	2A	3293	1/1	0.89	0.13	58,58,58,58	0
57	MG	1A	3753	1/1	0.89	0.14	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
57	MG	1A	3458	1/1	0.89	0.09	40,40,40,40	0
57	MG	1A	3787	1/1	0.89	0.19	47,47,47,47	0
57	MG	2A	3027	1/1	0.89	0.08	37,37,37,37	0
57	MG	1A	3945	1/1	0.89	0.14	58,58,58,58	0
57	MG	2a	3074	1/1	0.89	0.18	62,62,62,62	0
57	MG	1A	3604	1/1	0.89	0.07	17,17,17,17	0
57	MG	1a	3095	1/1	0.89	0.13	58,58,58,58	0
57	MG	2A	3055	1/1	0.89	0.12	63,63,63,63	0
57	MG	1A	3795	1/1	0.89	0.09	33,33,33,33	0
57	MG	2A	3367	1/1	0.89	0.10	42,42,42,42	0
57	MG	2A	3072	1/1	0.89	0.29	58,58,58,58	0
57	MG	2A	3079	1/1	0.89	0.16	39,39,39,39	0
57	MG	1A	3971	1/1	0.89	0.07	12,12,12,12	0
57	MG	2A	3090	1/1	0.89	0.16	52,52,52,52	0
57	MG	2A	3095	1/1	0.89	0.16	54,54,54,54	0
57	MG	1A	3797	1/1	0.89	0.12	58,58,58,58	0
57	MG	1A	3266	1/1	0.89	0.20	39,39,39,39	0
57	MG	2A	3605	1/1	0.89	0.14	49,49,49,49	0
57	MG	2a	3125	1/1	0.89	0.17	58,58,58,58	0
57	MG	1A	3468	1/1	0.89	0.14	60,60,60,60	0
57	MG	1A	3810	1/1	0.89	0.09	40,40,40,40	0
57	MG	1A	3526	1/1	0.89	0.09	18,18,18,18	0
57	MG	1A	3081	1/1	0.89	0.11	41,41,41,41	0
57	MG	1a	3137	1/1	0.89	0.08	37,37,37,37	0
57	MG	1a	3146	1/1	0.89	0.10	60,60,60,60	0
57	MG	2A	3625	1/1	0.89	0.10	68,68,68,68	0
57	MG	1A	3693	1/1	0.89	0.13	60,60,60,60	0
57	MG	2A	3144	1/1	0.89	0.23	53,53,53,53	0
57	MG	2a	3147	1/1	0.89	0.14	56,56,56,56	0
57	MG	1A	3407	1/1	0.89	0.07	20,20,20,20	0
57	MG	2A	3155	1/1	0.89	0.21	54,54,54,54	0
57	MG	2A	3653	1/1	0.89	0.12	56,56,56,56	0
57	MG	1A	3086	1/1	0.89	0.13	51,51,51,51	0
57	MG	2A	3460	1/1	0.89	0.14	35,35,35,35	0
57	MG	2A	3162	1/1	0.89	0.29	64,64,64,64	0
57	MG	1O	203	1/1	0.89	0.26	54,54,54,54	0
57	MG	1A	3836	1/1	0.89	0.14	61,61,61,61	0
57	MG	1A	3644	1/1	0.89	0.10	44,44,44,44	0
57	MG	2a	3169	1/1	0.89	0.19	48,48,48,48	0
57	MG	2a	3171	1/1	0.89	0.25	64,64,64,64	0
57	MG	2A	3670	1/1	0.89	0.16	49,49,49,49	0
57	MG	1A	3840	1/1	0.89	0.11	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
57	MG	1A	3850	1/1	0.89	0.10	33,33,33,33	0
57	MG	1A	3442	1/1	0.89	0.08	35,35,35,35	0
57	MG	2A	3187	1/1	0.89	0.19	58,58,58,58	0
57	MG	2A	3490	1/1	0.89	0.19	61,61,61,61	0
57	MG	17	101	1/1	0.89	0.22	29,29,29,29	0
57	MG	1A	3652	1/1	0.89	0.10	13,13,13,13	0
57	MG	1A	3715	1/1	0.89	0.12	60,60,60,60	0
57	MG	2B	3016	1/1	0.89	0.22	64,64,64,64	0
57	MG	2B	3017	1/1	0.89	0.08	47,47,47,47	0
57	MG	2A	3200	1/1	0.89	0.24	60,60,60,60	0
57	MG	2E	304	1/1	0.89	0.13	29,29,29,29	0
57	MG	1A	3857	1/1	0.89	0.10	40,40,40,40	0
57	MG	2P	3001	1/1	0.89	0.16	59,59,59,59	0
57	MG	2R	201	1/1	0.89	0.14	50,50,50,50	0
57	MG	1a	3007	1/1	0.89	0.13	53,53,53,53	0
57	MG	1A	3722	1/1	0.89	0.17	42,42,42,42	0
57	MG	2A	3215	1/1	0.89	0.09	38,38,38,38	0
57	MG	2A	3217	1/1	0.89	0.29	57,57,57,57	0
57	MG	1a	3216	1/1	0.89	0.13	53,53,53,53	0
57	MG	2A	3514	1/1	0.89	0.14	32,32,32,32	0
57	MG	1a	3217	1/1	0.89	0.21	56,56,56,56	0
57	MG	2A	3239	1/1	0.89	0.08	48,48,48,48	0
57	MG	1a	3014	1/1	0.89	0.07	54,54,54,54	0
57	MG	2A	3254	1/1	0.89	0.18	55,55,55,55	0
57	MG	1A	3728	1/1	0.89	0.12	45,45,45,45	0
57	MG	2A	3528	1/1	0.89	0.13	58,58,58,58	0
57	MG	1A	3020	1/1	0.89	0.08	41,41,41,41	0
57	MG	1A	3390	1/1	0.89	0.46	46,46,46,46	0
57	MG	2a	3023	1/1	0.89	0.21	66,66,66,66	0
57	MG	2x	101	1/1	0.89	0.14	57,57,57,57	0
57	MG	2A	3263	1/1	0.89	0.12	34,34,34,34	0
57	MG	2A	3539	1/1	0.89	0.09	43,43,43,43	0
59	AQJ	1A	3969	37/37	0.89	0.15	21,45,62,68	0
57	MG	2a	3026	1/1	0.89	0.09	65,65,65,65	0
57	MG	1A	3291	1/1	0.90	0.15	36,36,36,36	0
57	MG	1A	3761	1/1	0.90	0.12	31,31,31,31	0
57	MG	1A	3779	1/1	0.90	0.10	45,45,45,45	0
57	MG	2A	3597	1/1	0.90	0.20	41,41,41,41	0
57	MG	1a	3171	1/1	0.90	0.11	66,66,66,66	0
57	MG	1R	203	1/1	0.90	0.11	25,25,25,25	0
57	MG	1A	3311	1/1	0.90	0.12	31,31,31,31	0
57	MG	1A	3784	1/1	0.90	0.06	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	3071	1/1	0.90	0.20	49,49,49,49	0
57	MG	1a	3187	1/1	0.90	0.12	58,58,58,58	0
57	MG	2a	3078	1/1	0.90	0.12	61,61,61,61	0
57	MG	1A	3391	1/1	0.90	0.15	50,50,50,50	0
57	MG	2a	3082	1/1	0.90	0.17	61,61,61,61	0
57	MG	2A	3172	1/1	0.90	0.14	55,55,55,55	0
57	MG	2A	3607	1/1	0.90	0.10	50,50,50,50	0
57	MG	2A	3174	1/1	0.90	0.20	59,59,59,59	0
57	MG	2A	3435	1/1	0.90	0.13	59,59,59,59	0
57	MG	1A	3886	1/1	0.90	0.10	51,51,51,51	0
57	MG	18	101	1/1	0.90	0.07	35,35,35,35	0
57	MG	2A	3450	1/1	0.90	0.14	54,54,54,54	0
57	MG	1A	3609	1/1	0.90	0.07	25,25,25,25	0
57	MG	1a	3005	1/1	0.90	0.12	53,53,53,53	0
57	MG	1a	3201	1/1	0.90	0.08	50,50,50,50	0
57	MG	1A	3894	1/1	0.90	0.23	31,31,31,31	0
57	MG	1a	3205	1/1	0.90	0.10	55,55,55,55	0
57	MG	2A	3195	1/1	0.90	0.17	53,53,53,53	0
57	MG	1A	3393	1/1	0.90	0.10	41,41,41,41	0
57	MG	2A	3475	1/1	0.90	0.12	61,61,61,61	0
57	MG	1A	3242	1/1	0.90	0.12	40,40,40,40	0
57	MG	2A	3659	1/1	0.90	0.13	58,58,58,58	0
57	MG	2A	3205	1/1	0.90	0.08	46,46,46,46	0
57	MG	1A	3907	1/1	0.90	0.14	55,55,55,55	0
57	MG	1a	3019	1/1	0.90	0.12	47,47,47,47	0
57	MG	2a	3143	1/1	0.90	0.11	59,59,59,59	0
57	MG	1a	3024	1/1	0.90	0.25	55,55,55,55	0
57	MG	1A	3799	1/1	0.90	0.10	30,30,30,30	0
57	MG	1A	3630	1/1	0.90	0.12	33,33,33,33	0
57	MG	2A	3499	1/1	0.90	0.11	45,45,45,45	0
57	MG	2A	3226	1/1	0.90	0.09	42,42,42,42	0
57	MG	1A	3405	1/1	0.90	0.09	20,20,20,20	0
57	MG	1A	3004	1/1	0.90	0.07	17,17,17,17	0
57	MG	1A	3534	1/1	0.90	0.17	48,48,48,48	0
57	MG	1A	3940	1/1	0.90	0.10	45,45,45,45	0
57	MG	1A	3819	1/1	0.90	0.08	8,8,8,8	0
57	MG	2a	3164	1/1	0.90	0.15	45,45,45,45	0
57	MG	1A	3947	1/1	0.90	0.10	53,53,53,53	0
57	MG	1A	3537	1/1	0.90	0.10	38,38,38,38	0
57	MG	1A	3957	1/1	0.90	0.10	38,38,38,38	0
57	MG	2a	3170	1/1	0.90	0.12	46,46,46,46	0
57	MG	2F	3001	1/1	0.90	0.09	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
57	MG	1A	3539	1/1	0.90	0.18	42,42,42,42	0
57	MG	1A	3827	1/1	0.90	0.10	37,37,37,37	0
57	MG	2A	3266	1/1	0.90	0.14	53,53,53,53	0
57	MG	1B	3004	1/1	0.90	0.11	37,37,37,37	0
57	MG	2a	3176	1/1	0.90	0.14	53,53,53,53	0
57	MG	1B	3012	1/1	0.90	0.36	60,60,60,60	0
57	MG	1a	3093	1/1	0.90	0.20	59,59,59,59	0
57	MG	2A	3276	1/1	0.90	0.14	36,36,36,36	0
57	MG	2A	3279	1/1	0.90	0.13	41,41,41,41	0
57	MG	1A	3043	1/1	0.90	0.06	18,18,18,18	0
57	MG	2A	3538	1/1	0.90	0.10	62,62,62,62	0
57	MG	25	504	1/1	0.90	0.19	38,38,38,38	0
57	MG	1A	3544	1/1	0.90	0.15	50,50,50,50	0
57	MG	1A	3743	1/1	0.90	0.09	20,20,20,20	0
57	MG	1A	3414	1/1	0.90	0.08	35,35,35,35	0
57	MG	1A	3234	1/1	0.90	0.12	40,40,40,40	0
57	MG	1a	3106	1/1	0.90	0.18	47,47,47,47	0
57	MG	2A	3549	1/1	0.90	0.10	48,48,48,48	0
57	MG	2A	3302	1/1	0.90	0.16	56,56,56,56	0
57	MG	1E	307	1/1	0.90	0.09	31,31,31,31	0
57	MG	1F	301	1/1	0.90	0.10	47,47,47,47	0
57	MG	1a	3122	1/1	0.90	0.07	27,27,27,27	0
57	MG	1a	3125	1/1	0.90	0.18	68,68,68,68	0
57	MG	1A	3841	1/1	0.90	0.29	40,40,40,40	0
57	MG	2A	3346	1/1	0.90	0.08	45,45,45,45	0
57	MG	2A	3109	1/1	0.90	0.16	42,42,42,42	0
57	MG	1A	3849	1/1	0.90	0.11	50,50,50,50	0
57	MG	1A	3748	1/1	0.90	0.10	59,59,59,59	0
57	MG	2a	3037	1/1	0.90	0.18	52,52,52,52	0
57	MG	1a	3140	1/1	0.90	0.10	48,48,48,48	0
57	MG	2a	3039	1/1	0.90	0.09	57,57,57,57	0
57	MG	2A	3128	1/1	0.90	0.11	35,35,35,35	0
57	MG	2A	3373	1/1	0.90	0.09	43,43,43,43	0
57	MG	2x	102	1/1	0.90	0.18	66,66,66,66	0
57	MG	1A	3189	1/1	0.90	0.34	35,35,35,35	0
57	MG	2a	3048	1/1	0.90	0.14	57,57,57,57	0
57	MG	1A	3502	1/1	0.90	0.14	31,31,31,31	0
57	MG	2A	3389	1/1	0.90	0.13	57,57,57,57	0
57	MG	2a	3012	1/1	0.91	0.09	57,57,57,57	0
57	MG	2A	3194	1/1	0.91	0.15	56,56,56,56	0
57	MG	2a	3019	1/1	0.91	0.15	47,47,47,47	0
57	MG	1A	3492	1/1	0.91	0.09	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
57	MG	1A	3440	1/1	0.91	0.10	27,27,27,27	0
57	MG	1A	3507	1/1	0.91	0.09	49,49,49,49	0
57	MG	1A	3914	1/1	0.91	0.10	37,37,37,37	0
57	MG	1A	3265	1/1	0.91	0.12	45,45,45,45	0
57	MG	1a	3200	1/1	0.91	0.09	85,85,85,85	0
57	MG	2A	3506	1/1	0.91	0.11	43,43,43,43	0
57	MG	1A	3517	1/1	0.91	0.08	30,30,30,30	0
57	MG	1A	3702	1/1	0.91	0.09	25,25,25,25	0
57	MG	1A	3923	1/1	0.91	0.10	37,37,37,37	0
57	MG	2A	3224	1/1	0.91	0.07	39,39,39,39	0
57	MG	1a	3206	1/1	0.91	0.16	46,46,46,46	0
57	MG	1A	3613	1/1	0.91	0.11	16,16,16,16	0
57	MG	2A	3237	1/1	0.91	0.17	46,46,46,46	0
57	MG	2A	3524	1/1	0.91	0.09	51,51,51,51	0
57	MG	1a	3017	1/1	0.91	0.12	51,51,51,51	0
57	MG	2A	3242	1/1	0.91	0.09	45,45,45,45	0
57	MG	2A	3529	1/1	0.91	0.20	49,49,49,49	0
57	MG	1A	3614	1/1	0.91	0.11	23,23,23,23	0
57	MG	2A	3250	1/1	0.91	0.10	43,43,43,43	0
57	MG	2a	3053	1/1	0.91	0.18	49,49,49,49	0
57	MG	1a	3023	1/1	0.91	0.21	45,45,45,45	0
57	MG	2A	3257	1/1	0.91	0.09	51,51,51,51	0
57	MG	1A	3822	1/1	0.91	0.09	40,40,40,40	0
57	MG	1A	3943	1/1	0.91	0.09	36,36,36,36	0
57	MG	1a	3029	1/1	0.91	0.09	53,53,53,53	0
57	MG	1a	3032	1/1	0.91	0.09	55,55,55,55	0
57	MG	1a	3035	1/1	0.91	0.27	53,53,53,53	0
57	MG	1a	3037	1/1	0.91	0.19	57,57,57,57	0
57	MG	1x	108	1/1	0.91	0.12	41,41,41,41	0
57	MG	1A	3148	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	3225	1/1	0.91	0.14	45,45,45,45	0
57	MG	1A	3452	1/1	0.91	0.06	45,45,45,45	0
57	MG	1A	3951	1/1	0.91	0.15	49,49,49,49	0
57	MG	1A	3631	1/1	0.91	0.12	45,45,45,45	0
57	MG	1A	3453	1/1	0.91	0.08	26,26,26,26	0
57	MG	2a	3090	1/1	0.91	0.11	44,44,44,44	0
57	MG	1A	3158	1/1	0.91	0.17	30,30,30,30	0
57	MG	1B	3001	1/1	0.91	0.11	41,41,41,41	0
57	MG	2A	3030	1/1	0.91	0.12	51,51,51,51	0
57	MG	1a	3074	1/1	0.91	0.12	42,42,42,42	0
57	MG	1a	3075	1/1	0.91	0.23	55,55,55,55	0
57	MG	2A	3299	1/1	0.91	0.09	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
57	MG	2a	3114	1/1	0.91	0.10	57,57,57,57	0
57	MG	1A	3296	1/1	0.91	0.07	40,40,40,40	0
57	MG	2A	3049	1/1	0.91	0.14	52,52,52,52	0
57	MG	2a	3118	1/1	0.91	0.15	57,57,57,57	0
57	MG	2A	3051	1/1	0.91	0.15	60,60,60,60	0
57	MG	2A	3053	1/1	0.91	0.12	47,47,47,47	0
57	MG	2A	3317	1/1	0.91	0.10	52,52,52,52	0
57	MG	1B	3010	1/1	0.91	0.09	45,45,45,45	0
57	MG	2A	3056	1/1	0.91	0.24	57,57,57,57	0
57	MG	2A	3062	1/1	0.91	0.15	46,46,46,46	0
57	MG	1A	3839	1/1	0.91	0.23	24,24,24,24	0
57	MG	2A	3356	1/1	0.91	0.10	52,52,52,52	0
57	MG	1A	3052	1/1	0.91	0.13	45,45,45,45	0
57	MG	1A	3019	1/1	0.91	0.08	43,43,43,43	0
57	MG	2A	3364	1/1	0.91	0.14	53,53,53,53	0
57	MG	2A	3365	1/1	0.91	0.15	59,59,59,59	0
57	MG	2A	3085	1/1	0.91	0.12	57,57,57,57	0
57	MG	1A	3474	1/1	0.91	0.12	48,48,48,48	0
57	MG	2A	3370	1/1	0.91	0.20	54,54,54,54	0
57	MG	2A	3089	1/1	0.91	0.24	63,63,63,63	0
57	MG	1B	3025	1/1	0.91	0.12	54,54,54,54	0
57	MG	1A	3049	1/1	0.91	0.14	46,46,46,46	0
57	MG	1A	3751	1/1	0.91	0.10	35,35,35,35	0
57	MG	2a	3159	1/1	0.91	0.14	61,61,61,61	0
57	MG	2A	3100	1/1	0.91	0.10	52,52,52,52	0
57	MG	1A	3251	1/1	0.91	0.09	45,45,45,45	0
57	MG	2A	3392	1/1	0.91	0.07	45,45,45,45	0
57	MG	2a	3165	1/1	0.91	0.09	60,60,60,60	0
57	MG	1a	3101	1/1	0.91	0.11	50,50,50,50	0
57	MG	1E	308	1/1	0.91	0.08	48,48,48,48	0
57	MG	2A	3114	1/1	0.91	0.21	44,44,44,44	0
57	MG	1A	3552	1/1	0.91	0.14	40,40,40,40	0
57	MG	1F	306	1/1	0.91	0.15	50,50,50,50	0
57	MG	1A	3772	1/1	0.91	0.08	44,44,44,44	0
57	MG	2A	3414	1/1	0.91	0.21	58,58,58,58	0
57	MG	2A	3415	1/1	0.91	0.10	50,50,50,50	0
57	MG	2A	3418	1/1	0.91	0.14	57,57,57,57	0
57	MG	1a	3120	1/1	0.91	0.09	52,52,52,52	0
57	MG	2A	3672	1/1	0.91	0.17	36,36,36,36	0
57	MG	1A	3778	1/1	0.91	0.10	30,30,30,30	0
57	MG	1A	3572	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3426	1/1	0.91	0.12	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3430	1/1	0.91	0.15	42,42,42,42	0
57	MG	2A	3432	1/1	0.91	0.09	64,64,64,64	0
57	MG	1a	3130	1/1	0.91	0.11	45,45,45,45	0
57	MG	2A	3436	1/1	0.91	0.19	52,52,52,52	0
57	MG	2A	3143	1/1	0.91	0.10	50,50,50,50	0
57	MG	1a	3132	1/1	0.91	0.09	45,45,45,45	0
57	MG	1A	3781	1/1	0.91	0.12	58,58,58,58	0
57	MG	2B	3019	1/1	0.91	0.26	59,59,59,59	0
57	MG	1A	3331	1/1	0.91	0.19	51,51,51,51	0
57	MG	2e	3001	1/1	0.91	0.18	69,69,69,69	0
57	MG	2D	305	1/1	0.91	0.10	47,47,47,47	0
57	MG	1A	3875	1/1	0.91	0.07	34,34,34,34	0
57	MG	1A	3884	1/1	0.91	0.06	40,40,40,40	0
57	MG	1a	3143	1/1	0.91	0.09	40,40,40,40	0
57	MG	2O	8001	1/1	0.91	0.14	55,55,55,55	0
57	MG	1A	3665	1/1	0.91	0.12	52,52,52,52	0
57	MG	1A	3888	1/1	0.91	0.11	57,57,57,57	0
57	MG	2U	202	1/1	0.91	0.08	56,56,56,56	0
57	MG	1S	3001	1/1	0.91	0.19	37,37,37,37	0
57	MG	1A	3423	1/1	0.91	0.08	30,30,30,30	0
57	MG	1a	3160	1/1	0.91	0.08	51,51,51,51	0
57	MG	1X	106	1/1	0.91	0.17	33,33,33,33	0
57	MG	2A	3479	1/1	0.91	0.09	47,47,47,47	0
57	MG	2A	3481	1/1	0.91	0.10	52,52,52,52	0
57	MG	1Y	201	1/1	0.91	0.15	44,44,44,44	0
57	MG	1A	3085	1/1	0.91	0.13	40,40,40,40	0
57	MG	1Z	302	1/1	0.91	0.12	45,45,45,45	0
57	MG	2A	3491	1/1	0.91	0.14	59,59,59,59	0
57	MG	11	102	1/1	0.91	0.09	40,40,40,40	0
57	MG	14	502	1/1	0.91	0.15	54,54,54,54	0
57	MG	1A	3460	1/1	0.92	0.07	26,26,26,26	0
57	MG	2A	3378	1/1	0.92	0.06	53,53,53,53	0
57	MG	1A	3979	1/1	0.92	0.13	20,20,20,20	0
57	MG	2A	3380	1/1	0.92	0.09	46,46,46,46	0
57	MG	2A	3075	1/1	0.92	0.17	48,48,48,48	0
57	MG	2A	3388	1/1	0.92	0.12	48,48,48,48	0
57	MG	1A	3660	1/1	0.92	0.09	39,39,39,39	0
57	MG	1A	3542	1/1	0.92	0.14	41,41,41,41	0
57	MG	1B	3007	1/1	0.92	0.07	38,38,38,38	0
57	MG	1B	3009	1/1	0.92	0.12	48,48,48,48	0
57	MG	1a	3087	1/1	0.92	0.10	51,51,51,51	0
57	MG	1a	3090	1/1	0.92	0.12	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
57	MG	1A	3813	1/1	0.92	0.10	15,15,15,15	0
57	MG	2A	3403	1/1	0.92	0.18	40,40,40,40	0
57	MG	2A	3404	1/1	0.92	0.17	56,56,56,56	0
57	MG	1A	3283	1/1	0.92	0.15	38,38,38,38	0
57	MG	1B	3014	1/1	0.92	0.09	34,34,34,34	0
57	MG	1B	3015	1/1	0.92	0.07	47,47,47,47	0
57	MG	2A	3413	1/1	0.92	0.11	44,44,44,44	0
57	MG	1A	3548	1/1	0.92	0.11	37,37,37,37	0
57	MG	1A	3823	1/1	0.92	0.07	25,25,25,25	0
57	MG	1A	3551	1/1	0.92	0.09	38,38,38,38	0
57	MG	1A	3670	1/1	0.92	0.09	40,40,40,40	0
57	MG	1A	3672	1/1	0.92	0.24	24,24,24,24	0
57	MG	1A	3673	1/1	0.92	0.09	49,49,49,49	0
57	MG	1a	3113	1/1	0.92	0.16	59,59,59,59	0
57	MG	28	102	1/1	0.92	0.14	52,52,52,52	0
57	MG	2a	3002	1/1	0.92	0.08	49,49,49,49	0
57	MG	2a	3003	1/1	0.92	0.12	57,57,57,57	0
57	MG	1D	301	1/1	0.92	0.08	36,36,36,36	0
57	MG	1E	304	1/1	0.92	0.09	42,42,42,42	0
57	MG	2A	3141	1/1	0.92	0.24	40,40,40,40	0
57	MG	1A	3384	1/1	0.92	0.10	39,39,39,39	0
57	MG	1A	3687	1/1	0.92	0.10	31,31,31,31	0
57	MG	2a	3014	1/1	0.92	0.11	51,51,51,51	0
57	MG	2a	3015	1/1	0.92	0.15	46,46,46,46	0
57	MG	2A	3147	1/1	0.92	0.17	40,40,40,40	0
57	MG	2A	3150	1/1	0.92	0.15	43,43,43,43	0
57	MG	2A	3451	1/1	0.92	0.12	56,56,56,56	0
57	MG	1E	310	1/1	0.92	0.08	63,63,63,63	0
57	MG	1A	3557	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3560	1/1	0.92	0.07	35,35,35,35	0
57	MG	2A	3159	1/1	0.92	0.20	53,53,53,53	0
57	MG	2A	3465	1/1	0.92	0.13	47,47,47,47	0
57	MG	1G	203	1/1	0.92	0.07	52,52,52,52	0
57	MG	1A	3561	1/1	0.92	0.09	49,49,49,49	0
57	MG	1A	3233	1/1	0.92	0.13	23,23,23,23	0
57	MG	2A	3166	1/1	0.92	0.08	49,49,49,49	0
57	MG	2A	3167	1/1	0.92	0.17	38,38,38,38	0
57	MG	1a	3141	1/1	0.92	0.17	44,44,44,44	0
57	MG	1A	3845	1/1	0.92	0.08	39,39,39,39	0
57	MG	1O	201	1/1	0.92	0.16	41,41,41,41	0
57	MG	2a	3041	1/1	0.92	0.16	52,52,52,52	0
57	MG	1A	3847	1/1	0.92	0.12	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
57	MG	2A	3181	1/1	0.92	0.10	33,33,33,33	0
57	MG	1A	3696	1/1	0.92	0.24	27,27,27,27	0
57	MG	1A	3573	1/1	0.92	0.08	44,44,44,44	0
57	MG	1a	3154	1/1	0.92	0.12	58,58,58,58	0
57	MG	2a	3050	1/1	0.92	0.24	55,55,55,55	0
57	MG	1A	3579	1/1	0.92	0.09	35,35,35,35	0
57	MG	1A	3176	1/1	0.92	0.12	61,61,61,61	0
57	MG	2a	3055	1/1	0.92	0.22	60,60,60,60	0
57	MG	1A	3585	1/1	0.92	0.08	28,28,28,28	0
57	MG	1A	3185	1/1	0.92	0.14	49,49,49,49	0
57	MG	1a	3180	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3297	1/1	0.92	0.16	47,47,47,47	0
57	MG	2a	3061	1/1	0.92	0.20	57,57,57,57	0
57	MG	1T	8002	1/1	0.92	0.10	43,43,43,43	0
57	MG	2A	3203	1/1	0.92	0.09	43,43,43,43	0
57	MG	1V	202	1/1	0.92	0.20	42,42,42,42	0
57	MG	1A	3865	1/1	0.92	0.12	24,24,24,24	0
57	MG	2a	3068	1/1	0.92	0.06	39,39,39,39	0
57	MG	2a	3069	1/1	0.92	0.08	60,60,60,60	0
57	MG	2A	3211	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3595	1/1	0.92	0.07	14,14,14,14	0
57	MG	1A	3725	1/1	0.92	0.16	50,50,50,50	0
57	MG	2A	3216	1/1	0.92	0.19	51,51,51,51	0
57	MG	1Z	301	1/1	0.92	0.16	37,37,37,37	0
57	MG	2a	3084	1/1	0.92	0.20	58,58,58,58	0
57	MG	2A	3218	1/1	0.92	0.38	57,57,57,57	0
57	MG	2A	3222	1/1	0.92	0.10	41,41,41,41	0
57	MG	1A	3873	1/1	0.92	0.07	47,47,47,47	0
57	MG	1A	3403	1/1	0.92	0.08	16,16,16,16	0
57	MG	1A	3735	1/1	0.92	0.15	46,46,46,46	0
57	MG	2A	3530	1/1	0.92	0.12	55,55,55,55	0
57	MG	2A	3232	1/1	0.92	0.14	55,55,55,55	0
57	MG	2a	3108	1/1	0.92	0.12	64,64,64,64	0
57	MG	1A	3299	1/1	0.92	0.08	40,40,40,40	0
57	MG	2A	3535	1/1	0.92	0.15	49,49,49,49	0
57	MG	1A	3603	1/1	0.92	0.08	19,19,19,19	0
57	MG	1A	3301	1/1	0.92	0.07	51,51,51,51	0
57	MG	1a	3207	1/1	0.92	0.07	51,51,51,51	0
57	MG	2A	3540	1/1	0.92	0.16	58,58,58,58	0
57	MG	1A	3302	1/1	0.92	0.10	40,40,40,40	0
57	MG	1a	3211	1/1	0.92	0.11	62,62,62,62	0
57	MG	2A	3252	1/1	0.92	0.14	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
57	MG	2a	3127	1/1	0.92	0.12	56,56,56,56	0
57	MG	1a	3214	1/1	0.92	0.17	58,58,58,58	0
57	MG	1A	3607	1/1	0.92	0.07	17,17,17,17	0
57	MG	1A	3896	1/1	0.92	0.06	27,27,27,27	0
57	MG	2A	3259	1/1	0.92	0.10	56,56,56,56	0
57	MG	1A	3124	1/1	0.92	0.08	33,33,33,33	0
57	MG	1a	3218	1/1	0.92	0.11	36,36,36,36	0
57	MG	1A	3416	1/1	0.92	0.10	46,46,46,46	0
57	MG	1A	3198	1/1	0.92	0.09	37,37,37,37	0
57	MG	2A	3563	1/1	0.92	0.14	48,48,48,48	0
57	MG	1A	3002	1/1	0.92	0.07	40,40,40,40	0
57	MG	2A	3572	1/1	0.92	0.10	47,47,47,47	0
57	MG	1a	3227	1/1	0.92	0.18	52,52,52,52	0
57	MG	1b	3001	1/1	0.92	0.12	68,68,68,68	0
57	MG	1a	3018	1/1	0.92	0.07	44,44,44,44	0
57	MG	2A	3274	1/1	0.92	0.09	40,40,40,40	0
57	MG	2a	3157	1/1	0.92	0.10	50,50,50,50	0
57	MG	1e	3001	1/1	0.92	0.09	69,69,69,69	0
57	MG	2A	3586	1/1	0.92	0.16	35,35,35,35	0
57	MG	2a	3161	1/1	0.92	0.17	58,58,58,58	0
57	MG	1n	503	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3518	1/1	0.92	0.10	19,19,19,19	0
57	MG	2A	3590	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	3172	1/1	0.92	0.17	46,46,46,46	0
57	MG	2A	3282	1/1	0.92	0.12	38,38,38,38	0
57	MG	2A	3285	1/1	0.92	0.10	50,50,50,50	0
57	MG	2a	3168	1/1	0.92	0.18	46,46,46,46	0
57	MG	1x	104	1/1	0.92	0.12	50,50,50,50	0
57	MG	1A	3775	1/1	0.92	0.08	26,26,26,26	0
57	MG	1A	3324	1/1	0.92	0.15	59,59,59,59	0
57	MG	1A	3632	1/1	0.92	0.07	49,49,49,49	0
57	MG	1A	3446	1/1	0.92	0.09	38,38,38,38	0
57	MG	1A	3933	1/1	0.92	0.11	34,34,34,34	0
57	MG	2A	3003	1/1	0.92	0.18	46,46,46,46	0
57	MG	1A	3330	1/1	0.92	0.09	33,33,33,33	0
57	MG	2a	3177	1/1	0.92	0.12	60,60,60,60	0
57	MG	1a	3038	1/1	0.92	0.18	42,42,42,42	0
57	MG	1A	3118	1/1	0.92	0.15	34,34,34,34	0
57	MG	1A	3643	1/1	0.92	0.14	57,57,57,57	0
57	MG	2A	3319	1/1	0.92	0.06	31,31,31,31	0
57	MG	2A	3322	1/1	0.92	0.07	30,30,30,30	0
57	MG	2A	3331	1/1	0.92	0.09	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3613	1/1	0.92	0.09	55,55,55,55	0
57	MG	2A	3332	1/1	0.92	0.09	34,34,34,34	0
57	MG	2A	3029	1/1	0.92	0.12	35,35,35,35	0
57	MG	2A	3338	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3229	1/1	0.92	0.15	55,55,55,55	0
57	MG	2a	3199	1/1	0.92	0.19	45,45,45,45	0
57	MG	2A	3340	1/1	0.92	0.09	36,36,36,36	0
57	MG	2A	3632	1/1	0.92	0.14	62,62,62,62	0
57	MG	2A	3636	1/1	0.92	0.23	57,57,57,57	0
57	MG	2A	3637	1/1	0.92	0.18	63,63,63,63	0
57	MG	2A	3037	1/1	0.92	0.21	49,49,49,49	0
57	MG	2A	3643	1/1	0.92	0.15	51,51,51,51	0
57	MG	2A	3644	1/1	0.92	0.11	70,70,70,70	0
57	MG	2A	3646	1/1	0.92	0.12	57,57,57,57	0
57	MG	2A	3347	1/1	0.92	0.08	27,27,27,27	0
57	MG	2A	3349	1/1	0.92	0.13	30,30,30,30	0
57	MG	1A	3273	1/1	0.92	0.13	36,36,36,36	0
57	MG	1a	3048	1/1	0.92	0.10	40,40,40,40	0
57	MG	1a	3049	1/1	0.92	0.17	41,41,41,41	0
57	MG	1A	3455	1/1	0.92	0.07	27,27,27,27	0
57	MG	2A	3363	1/1	0.92	0.09	39,39,39,39	0
57	MG	1A	3538	1/1	0.92	0.07	30,30,30,30	0
57	MG	2w	103	1/1	0.92	0.09	61,61,61,61	0
57	MG	2A	3666	1/1	0.92	0.20	49,49,49,49	0
57	MG	1a	3060	1/1	0.92	0.23	45,45,45,45	0
57	MG	1A	3963	1/1	0.92	0.11	33,33,33,33	0
57	MG	1a	3064	1/1	0.92	0.11	58,58,58,58	0
57	MG	1A	3348	1/1	0.92	0.08	38,38,38,38	0
57	MG	2x	105	1/1	0.92	0.08	45,45,45,45	0
58	K	2A	3676	1/1	0.92	0.08	50,50,50,50	0
57	MG	2A	3371	1/1	0.92	0.17	46,46,46,46	0
57	MG	2B	3001	1/1	0.92	0.15	54,54,54,54	0
57	MG	1A	3060	1/1	0.93	0.18	41,41,41,41	0
57	MG	2A	3383	1/1	0.93	0.07	38,38,38,38	0
57	MG	2B	3009	1/1	0.93	0.15	48,48,48,48	0
57	MG	2A	3386	1/1	0.93	0.08	46,46,46,46	0
57	MG	2B	3012	1/1	0.93	0.08	68,68,68,68	0
57	MG	2B	3013	1/1	0.93	0.07	61,61,61,61	0
57	MG	1A	3554	1/1	0.93	0.10	38,38,38,38	0
57	MG	2A	3096	1/1	0.93	0.06	54,54,54,54	0
57	MG	1a	3088	1/1	0.93	0.08	59,59,59,59	0
57	MG	1a	3089	1/1	0.93	0.34	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3255	1/1	0.93	0.07	50,50,50,50	0
57	MG	2B	3020	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3820	1/1	0.93	0.10	45,45,45,45	0
57	MG	1A	3559	1/1	0.93	0.09	52,52,52,52	0
57	MG	2A	3113	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3256	1/1	0.93	0.22	55,55,55,55	0
57	MG	2F	3004	1/1	0.93	0.22	36,36,36,36	0
57	MG	1B	3019	1/1	0.93	0.08	44,44,44,44	0
57	MG	2G	3001	1/1	0.93	0.11	64,64,64,64	0
57	MG	2A	3116	1/1	0.93	0.14	43,43,43,43	0
57	MG	2A	3120	1/1	0.93	0.10	59,59,59,59	0
57	MG	2Q	3001	1/1	0.93	0.09	63,63,63,63	0
57	MG	2Q	3002	1/1	0.93	0.14	44,44,44,44	0
57	MG	1A	3690	1/1	0.93	0.08	52,52,52,52	0
57	MG	2A	3122	1/1	0.93	0.23	43,43,43,43	0
57	MG	1A	3257	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3566	1/1	0.93	0.08	19,19,19,19	0
57	MG	2A	3417	1/1	0.93	0.18	45,45,45,45	0
57	MG	2A	3129	1/1	0.93	0.08	50,50,50,50	0
57	MG	2A	3131	1/1	0.93	0.18	46,46,46,46	0
57	MG	1A	3259	1/1	0.93	0.07	45,45,45,45	0
57	MG	1A	3374	1/1	0.93	0.09	39,39,39,39	0
57	MG	1A	3005	1/1	0.93	0.13	46,46,46,46	0
57	MG	1A	3382	1/1	0.93	0.07	38,38,38,38	0
57	MG	2a	3001	1/1	0.93	0.10	45,45,45,45	0
57	MG	1A	3190	1/1	0.93	0.08	40,40,40,40	0
57	MG	1a	3117	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3146	1/1	0.93	0.23	61,61,61,61	0
57	MG	1A	3705	1/1	0.93	0.09	29,29,29,29	0
57	MG	2a	3007	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3475	1/1	0.93	0.07	23,23,23,23	0
57	MG	1a	3123	1/1	0.93	0.06	35,35,35,35	0
57	MG	1A	3385	1/1	0.93	0.09	44,44,44,44	0
57	MG	2a	3013	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3453	1/1	0.93	0.20	58,58,58,58	0
57	MG	1a	3129	1/1	0.93	0.11	50,50,50,50	0
57	MG	1A	3482	1/1	0.93	0.07	44,44,44,44	0
57	MG	2A	3160	1/1	0.93	0.09	40,40,40,40	0
57	MG	1A	3713	1/1	0.93	0.11	49,49,49,49	0
57	MG	1F	309	1/1	0.93	0.13	39,39,39,39	0
57	MG	1A	3486	1/1	0.93	0.09	35,35,35,35	0
57	MG	1A	3717	1/1	0.93	0.18	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
57	MG	2A	3473	1/1	0.93	0.17	47,47,47,47	0
57	MG	1A	3192	1/1	0.93	0.18	32,32,32,32	0
57	MG	2a	3027	1/1	0.93	0.13	60,60,60,60	0
57	MG	1A	3724	1/1	0.93	0.06	40,40,40,40	0
57	MG	1N	3004	1/1	0.93	0.12	54,54,54,54	0
57	MG	1a	3144	1/1	0.93	0.12	40,40,40,40	0
57	MG	2A	3176	1/1	0.93	0.07	44,44,44,44	0
57	MG	2A	3480	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3177	1/1	0.93	0.19	44,44,44,44	0
57	MG	1A	3196	1/1	0.93	0.10	26,26,26,26	0
57	MG	1A	3858	1/1	0.93	0.16	26,26,26,26	0
57	MG	1A	3859	1/1	0.93	0.22	33,33,33,33	0
57	MG	1A	3860	1/1	0.93	0.06	27,27,27,27	0
57	MG	2A	3493	1/1	0.93	0.09	55,55,55,55	0
57	MG	2A	3494	1/1	0.93	0.08	34,34,34,34	0
57	MG	1A	3131	1/1	0.93	0.08	37,37,37,37	0
57	MG	2A	3188	1/1	0.93	0.09	43,43,43,43	0
57	MG	1a	3155	1/1	0.93	0.22	40,40,40,40	0
57	MG	1a	3159	1/1	0.93	0.12	67,67,67,67	0
57	MG	1A	3729	1/1	0.93	0.06	30,30,30,30	0
57	MG	1a	3166	1/1	0.93	0.15	42,42,42,42	0
57	MG	1Q	206	1/1	0.93	0.05	45,45,45,45	0
57	MG	2a	3057	1/1	0.93	0.18	73,73,73,73	0
57	MG	1a	3170	1/1	0.93	0.09	52,52,52,52	0
57	MG	1R	202	1/1	0.93	0.09	39,39,39,39	0
57	MG	2A	3202	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	3141	1/1	0.93	0.09	44,44,44,44	0
57	MG	2a	3062	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	3868	1/1	0.93	0.09	24,24,24,24	0
57	MG	2A	3207	1/1	0.93	0.14	52,52,52,52	0
57	MG	1A	3870	1/1	0.93	0.07	51,51,51,51	0
57	MG	1a	3184	1/1	0.93	0.13	38,38,38,38	0
57	MG	2A	3212	1/1	0.93	0.16	39,39,39,39	0
57	MG	2A	3213	1/1	0.93	0.09	58,58,58,58	0
57	MG	1T	8001	1/1	0.93	0.09	40,40,40,40	0
57	MG	2a	3072	1/1	0.93	0.14	62,62,62,62	0
57	MG	1a	3186	1/1	0.93	0.10	55,55,55,55	0
57	MG	1A	3739	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3741	1/1	0.93	0.12	47,47,47,47	0
57	MG	1W	203	1/1	0.93	0.24	47,47,47,47	0
57	MG	1A	3399	1/1	0.93	0.16	44,44,44,44	0
57	MG	1a	3191	1/1	0.93	0.10	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
57	MG	1A	3400	1/1	0.93	0.07	20,20,20,20	0
57	MG	1A	3877	1/1	0.93	0.08	24,24,24,24	0
57	MG	2a	3092	1/1	0.93	0.11	59,59,59,59	0
57	MG	2A	3537	1/1	0.93	0.11	25,25,25,25	0
57	MG	1A	3879	1/1	0.93	0.16	23,23,23,23	0
57	MG	1A	3883	1/1	0.93	0.10	35,35,35,35	0
57	MG	10	102	1/1	0.93	0.14	44,44,44,44	0
57	MG	2a	3106	1/1	0.93	0.14	62,62,62,62	0
57	MG	1A	3204	1/1	0.93	0.10	32,32,32,32	0
57	MG	2A	3241	1/1	0.93	0.06	42,42,42,42	0
57	MG	2A	3543	1/1	0.93	0.10	58,58,58,58	0
57	MG	2A	3546	1/1	0.93	0.08	45,45,45,45	0
57	MG	13	101	1/1	0.93	0.15	36,36,36,36	0
57	MG	1A	3508	1/1	0.93	0.08	51,51,51,51	0
57	MG	2a	3117	1/1	0.93	0.10	48,48,48,48	0
57	MG	15	103	1/1	0.93	0.09	37,37,37,37	0
57	MG	16	502	1/1	0.93	0.06	34,34,34,34	0
57	MG	1A	3404	1/1	0.93	0.05	33,33,33,33	0
57	MG	2a	3124	1/1	0.93	0.24	61,61,61,61	0
57	MG	2A	3554	1/1	0.93	0.17	56,56,56,56	0
57	MG	1A	3295	1/1	0.93	0.16	32,32,32,32	0
57	MG	1A	3890	1/1	0.93	0.10	40,40,40,40	0
57	MG	2A	3558	1/1	0.93	0.08	38,38,38,38	0
57	MG	1A	3626	1/1	0.93	0.16	61,61,61,61	0
57	MG	2a	3132	1/1	0.93	0.19	61,61,61,61	0
57	MG	2a	3135	1/1	0.93	0.10	56,56,56,56	0
57	MG	1A	3142	1/1	0.93	0.22	24,24,24,24	0
57	MG	1A	3220	1/1	0.93	0.08	41,41,41,41	0
57	MG	2A	3564	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3568	1/1	0.93	0.10	45,45,45,45	0
57	MG	2a	3142	1/1	0.93	0.14	54,54,54,54	0
57	MG	1a	3221	1/1	0.93	0.13	57,57,57,57	0
57	MG	2a	3144	1/1	0.93	0.10	70,70,70,70	0
57	MG	2A	3570	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3754	1/1	0.93	0.08	31,31,31,31	0
57	MG	2A	3573	1/1	0.93	0.08	71,71,71,71	0
57	MG	2a	3148	1/1	0.93	0.10	64,64,64,64	0
57	MG	1A	3760	1/1	0.93	0.07	51,51,51,51	0
57	MG	1A	3908	1/1	0.93	0.07	15,15,15,15	0
57	MG	2A	3577	1/1	0.93	0.06	43,43,43,43	0
57	MG	2A	3578	1/1	0.93	0.07	56,56,56,56	0
57	MG	1A	3910	1/1	0.93	0.08	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3912	1/1	0.93	0.07	51,51,51,51	0
57	MG	1A	3411	1/1	0.93	0.09	39,39,39,39	0
57	MG	2a	3160	1/1	0.93	0.18	51,51,51,51	0
57	MG	1a	3020	1/1	0.93	0.12	39,39,39,39	0
57	MG	1a	3022	1/1	0.93	0.08	47,47,47,47	0
57	MG	1t	3001	1/1	0.93	0.11	46,46,46,46	0
57	MG	1A	3763	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3919	1/1	0.93	0.25	36,36,36,36	0
57	MG	2A	3283	1/1	0.93	0.13	51,51,51,51	0
57	MG	1x	106	1/1	0.93	0.18	43,43,43,43	0
57	MG	2A	3287	1/1	0.93	0.09	38,38,38,38	0
57	MG	1A	3766	1/1	0.93	0.11	41,41,41,41	0
57	MG	2A	3290	1/1	0.93	0.11	48,48,48,48	0
57	MG	1a	3026	1/1	0.93	0.16	43,43,43,43	0
57	MG	1A	3767	1/1	0.93	0.06	19,19,19,19	0
57	MG	1A	3768	1/1	0.93	0.10	42,42,42,42	0
57	MG	1A	3006	1/1	0.93	0.17	53,53,53,53	0
57	MG	2A	3001	1/1	0.93	0.13	43,43,43,43	0
57	MG	1A	3525	1/1	0.93	0.06	26,26,26,26	0
57	MG	2A	3004	1/1	0.93	0.21	58,58,58,58	0
57	MG	1A	3014	1/1	0.93	0.09	26,26,26,26	0
57	MG	2A	3314	1/1	0.93	0.12	52,52,52,52	0
57	MG	1A	3232	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3016	1/1	0.93	0.10	33,33,33,33	0
57	MG	1A	3431	1/1	0.93	0.11	61,61,61,61	0
57	MG	1A	3433	1/1	0.93	0.06	10,10,10,10	0
57	MG	2A	3326	1/1	0.93	0.08	21,21,21,21	0
57	MG	1A	3948	1/1	0.93	0.15	44,44,44,44	0
57	MG	2A	3031	1/1	0.93	0.09	35,35,35,35	0
57	MG	2a	3193	1/1	0.93	0.15	55,55,55,55	0
57	MG	2a	3194	1/1	0.93	0.09	44,44,44,44	0
57	MG	1A	3786	1/1	0.93	0.11	21,21,21,21	0
57	MG	2a	3197	1/1	0.93	0.24	52,52,52,52	0
57	MG	2A	3629	1/1	0.93	0.15	59,59,59,59	0
57	MG	2A	3630	1/1	0.93	0.20	47,47,47,47	0
57	MG	1A	3439	1/1	0.93	0.08	49,49,49,49	0
57	MG	1a	3051	1/1	0.93	0.21	48,48,48,48	0
57	MG	1A	3956	1/1	0.93	0.11	58,58,58,58	0
57	MG	2A	3342	1/1	0.93	0.09	31,31,31,31	0
57	MG	2A	3043	1/1	0.93	0.24	55,55,55,55	0
57	MG	2h	8001	1/1	0.93	0.09	41,41,41,41	0
57	MG	1A	3018	1/1	0.93	0.12	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3057	1/1	0.93	0.10	57,57,57,57	0
57	MG	2A	3350	1/1	0.93	0.08	32,32,32,32	0
57	MG	2A	3651	1/1	0.93	0.10	47,47,47,47	0
57	MG	2A	3052	1/1	0.93	0.09	61,61,61,61	0
57	MG	2A	3654	1/1	0.93	0.15	46,46,46,46	0
57	MG	1A	3445	1/1	0.93	0.06	30,30,30,30	0
57	MG	1a	3065	1/1	0.93	0.27	64,64,64,64	0
57	MG	2v	8001	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3543	1/1	0.93	0.07	44,44,44,44	0
57	MG	2A	3060	1/1	0.93	0.08	47,47,47,47	0
57	MG	1a	3070	1/1	0.93	0.17	50,50,50,50	0
57	MG	2A	3068	1/1	0.93	0.07	49,49,49,49	0
57	MG	1A	3972	1/1	0.93	0.18	23,23,23,23	0
57	MG	1A	3319	1/1	0.93	0.06	42,42,42,42	0
57	MG	1A	3986	1/1	0.93	0.18	27,27,27,27	0
57	MG	2A	3671	1/1	0.93	0.23	46,46,46,46	0
57	MG	1a	3080	1/1	0.93	0.34	45,45,45,45	0
57	MG	2A	3082	1/1	0.93	0.24	56,56,56,56	0
57	MG	1A	3099	1/1	0.93	0.12	58,58,58,58	0
57	MG	1a	3083	1/1	0.93	0.06	34,34,34,34	0
57	MG	1A	3101	1/1	0.93	0.18	25,25,25,25	0
57	MG	2A	3018	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3667	1/1	0.94	0.07	34,34,34,34	0
57	MG	1A	3927	1/1	0.94	0.08	31,31,31,31	0
57	MG	2A	3335	1/1	0.94	0.10	24,24,24,24	0
57	MG	1A	3513	1/1	0.94	0.06	28,28,28,28	0
57	MG	2A	3028	1/1	0.94	0.06	36,36,36,36	0
57	MG	2A	3673	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3675	1/1	0.94	0.09	49,49,49,49	0
57	MG	1a	3039	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3688	1/1	0.94	0.10	57,57,57,57	0
57	MG	1A	3208	1/1	0.94	0.09	38,38,38,38	0
57	MG	2A	3345	1/1	0.94	0.08	28,28,28,28	0
57	MG	2B	3002	1/1	0.94	0.12	66,66,66,66	0
57	MG	1A	3774	1/1	0.94	0.06	25,25,25,25	0
57	MG	1a	3043	1/1	0.94	0.19	44,44,44,44	0
57	MG	2B	3005	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3288	1/1	0.94	0.06	36,36,36,36	0
57	MG	1A	3944	1/1	0.94	0.07	20,20,20,20	0
57	MG	2A	3351	1/1	0.94	0.17	60,60,60,60	0
57	MG	1A	3776	1/1	0.94	0.06	34,34,34,34	0
57	MG	2A	3354	1/1	0.94	0.10	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
57	MG	2A	3355	1/1	0.94	0.10	47,47,47,47	0
57	MG	1A	3633	1/1	0.94	0.11	28,28,28,28	0
57	MG	2A	3357	1/1	0.94	0.09	41,41,41,41	0
57	MG	2A	3046	1/1	0.94	0.12	55,55,55,55	0
57	MG	2A	3361	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3634	1/1	0.94	0.11	54,54,54,54	0
57	MG	1A	3636	1/1	0.94	0.08	32,32,32,32	0
57	MG	2D	301	1/1	0.94	0.10	62,62,62,62	0
57	MG	2D	302	1/1	0.94	0.09	48,48,48,48	0
57	MG	1a	3053	1/1	0.94	0.11	41,41,41,41	0
57	MG	1a	3055	1/1	0.94	0.14	38,38,38,38	0
57	MG	1a	3056	1/1	0.94	0.09	44,44,44,44	0
57	MG	2F	3002	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3214	1/1	0.94	0.18	43,43,43,43	0
57	MG	2A	3057	1/1	0.94	0.07	54,54,54,54	0
57	MG	2A	3059	1/1	0.94	0.11	42,42,42,42	0
57	MG	1a	3059	1/1	0.94	0.30	50,50,50,50	0
57	MG	1A	3079	1/1	0.94	0.24	41,41,41,41	0
57	MG	1A	3522	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3070	1/1	0.94	0.08	41,41,41,41	0
57	MG	1A	3008	1/1	0.94	0.13	43,43,43,43	0
57	MG	2U	201	1/1	0.94	0.10	29,29,29,29	0
57	MG	1A	3790	1/1	0.94	0.17	24,24,24,24	0
57	MG	2A	3074	1/1	0.94	0.14	48,48,48,48	0
57	MG	1A	3792	1/1	0.94	0.26	39,39,39,39	0
57	MG	2Y	502	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3011	1/1	0.94	0.14	42,42,42,42	0
57	MG	1A	3228	1/1	0.94	0.20	31,31,31,31	0
57	MG	1A	3796	1/1	0.94	0.16	20,20,20,20	0
57	MG	2A	3086	1/1	0.94	0.09	35,35,35,35	0
57	MG	2A	3393	1/1	0.94	0.08	50,50,50,50	0
57	MG	1A	3989	1/1	0.94	0.10	37,37,37,37	0
57	MG	1a	3079	1/1	0.94	0.12	42,42,42,42	0
57	MG	1A	3991	1/1	0.94	0.16	30,30,30,30	0
57	MG	2A	3401	1/1	0.94	0.19	50,50,50,50	0
57	MG	2A	3091	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	4002	1/1	0.94	0.09	35,35,35,35	0
57	MG	2a	3005	1/1	0.94	0.22	53,53,53,53	0
57	MG	1A	3050	1/1	0.94	0.11	32,32,32,32	0
57	MG	2A	3409	1/1	0.94	0.15	51,51,51,51	0
57	MG	2a	3008	1/1	0.94	0.17	41,41,41,41	0
57	MG	2A	3098	1/1	0.94	0.07	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3529	1/1	0.94	0.06	29,29,29,29	0
57	MG	1A	3417	1/1	0.94	0.07	23,23,23,23	0
57	MG	1A	3803	1/1	0.94	0.06	20,20,20,20	0
57	MG	1A	3656	1/1	0.94	0.05	18,18,18,18	0
57	MG	1A	3149	1/1	0.94	0.14	28,28,28,28	0
57	MG	2A	3112	1/1	0.94	0.12	59,59,59,59	0
57	MG	1A	3536	1/1	0.94	0.11	23,23,23,23	0
57	MG	1A	3303	1/1	0.94	0.07	29,29,29,29	0
57	MG	2a	3021	1/1	0.94	0.08	37,37,37,37	0
57	MG	1A	3308	1/1	0.94	0.13	36,36,36,36	0
57	MG	2A	3425	1/1	0.94	0.14	41,41,41,41	0
57	MG	1A	3051	1/1	0.94	0.07	32,32,32,32	0
57	MG	2A	3428	1/1	0.94	0.08	31,31,31,31	0
57	MG	2A	3118	1/1	0.94	0.15	50,50,50,50	0
57	MG	1a	3096	1/1	0.94	0.14	54,54,54,54	0
57	MG	1A	3170	1/1	0.94	0.07	24,24,24,24	0
57	MG	1A	3017	1/1	0.94	0.05	37,37,37,37	0
57	MG	2A	3124	1/1	0.94	0.06	61,61,61,61	0
57	MG	2a	3033	1/1	0.94	0.11	53,53,53,53	0
57	MG	1B	3024	1/1	0.94	0.06	37,37,37,37	0
57	MG	1A	3318	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3094	1/1	0.94	0.06	31,31,31,31	0
57	MG	1A	3674	1/1	0.94	0.10	49,49,49,49	0
57	MG	1a	3107	1/1	0.94	0.16	39,39,39,39	0
57	MG	2a	3040	1/1	0.94	0.11	44,44,44,44	0
57	MG	2A	3137	1/1	0.94	0.12	34,34,34,34	0
57	MG	1a	3108	1/1	0.94	0.17	38,38,38,38	0
57	MG	1A	3675	1/1	0.94	0.12	31,31,31,31	0
57	MG	1E	302	1/1	0.94	0.15	52,52,52,52	0
57	MG	2A	3466	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3468	1/1	0.94	0.07	38,38,38,38	0
57	MG	1A	3831	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3320	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3835	1/1	0.94	0.09	43,43,43,43	0
57	MG	1A	3681	1/1	0.94	0.08	42,42,42,42	0
57	MG	1A	3322	1/1	0.94	0.13	40,40,40,40	0
57	MG	2A	3152	1/1	0.94	0.15	40,40,40,40	0
57	MG	1a	3124	1/1	0.94	0.15	56,56,56,56	0
57	MG	1A	3095	1/1	0.94	0.07	35,35,35,35	0
57	MG	1a	3126	1/1	0.94	0.17	48,48,48,48	0
57	MG	2A	3157	1/1	0.94	0.10	35,35,35,35	0
57	MG	1A	3553	1/1	0.94	0.10	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
57	MG	1A	3245	1/1	0.94	0.14	24,24,24,24	0
57	MG	2A	3487	1/1	0.94	0.17	50,50,50,50	0
57	MG	1a	3131	1/1	0.94	0.18	46,46,46,46	0
57	MG	1A	3844	1/1	0.94	0.05	30,30,30,30	0
57	MG	1A	3246	1/1	0.94	0.12	40,40,40,40	0
57	MG	1A	3248	1/1	0.94	0.10	44,44,44,44	0
57	MG	1a	3135	1/1	0.94	0.11	34,34,34,34	0
57	MG	2A	3168	1/1	0.94	0.20	38,38,38,38	0
57	MG	2a	3073	1/1	0.94	0.17	51,51,51,51	0
57	MG	2A	3170	1/1	0.94	0.07	43,43,43,43	0
57	MG	2a	3075	1/1	0.94	0.11	38,38,38,38	0
57	MG	1N	3002	1/1	0.94	0.05	38,38,38,38	0
57	MG	1A	3456	1/1	0.94	0.07	18,18,18,18	0
57	MG	1A	3250	1/1	0.94	0.13	26,26,26,26	0
57	MG	1a	3142	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3700	1/1	0.94	0.07	20,20,20,20	0
57	MG	1A	3852	1/1	0.94	0.06	22,22,22,22	0
57	MG	2A	3180	1/1	0.94	0.17	47,47,47,47	0
57	MG	1a	3145	1/1	0.94	0.07	45,45,45,45	0
57	MG	2a	3096	1/1	0.94	0.13	53,53,53,53	0
57	MG	1A	3562	1/1	0.94	0.10	37,37,37,37	0
57	MG	1A	3563	1/1	0.94	0.07	25,25,25,25	0
57	MG	1Q	203	1/1	0.94	0.14	37,37,37,37	0
57	MG	2a	3101	1/1	0.94	0.20	60,60,60,60	0
57	MG	1A	3856	1/1	0.94	0.14	45,45,45,45	0
57	MG	2a	3104	1/1	0.94	0.14	56,56,56,56	0
57	MG	1A	3708	1/1	0.94	0.15	31,31,31,31	0
57	MG	1A	3565	1/1	0.94	0.10	45,45,45,45	0
57	MG	2a	3109	1/1	0.94	0.10	47,47,47,47	0
57	MG	1A	3459	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	3339	1/1	0.94	0.09	23,23,23,23	0
57	MG	2A	3527	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3054	1/1	0.94	0.14	44,44,44,44	0
57	MG	2A	3197	1/1	0.94	0.10	48,48,48,48	0
57	MG	2A	3199	1/1	0.94	0.13	41,41,41,41	0
57	MG	1a	3167	1/1	0.94	0.13	36,36,36,36	0
57	MG	2a	3119	1/1	0.94	0.09	64,64,64,64	0
57	MG	1A	3574	1/1	0.94	0.06	34,34,34,34	0
57	MG	2A	3534	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	3577	1/1	0.94	0.07	47,47,47,47	0
57	MG	1A	3719	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3204	1/1	0.94	0.20	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
57	MG	1a	3172	1/1	0.94	0.13	32,32,32,32	0
57	MG	1V	203	1/1	0.94	0.07	50,50,50,50	0
57	MG	2A	3208	1/1	0.94	0.07	42,42,42,42	0
57	MG	1a	3175	1/1	0.94	0.10	36,36,36,36	0
57	MG	2a	3133	1/1	0.94	0.12	33,33,33,33	0
57	MG	1a	3178	1/1	0.94	0.10	47,47,47,47	0
57	MG	1A	3721	1/1	0.94	0.06	24,24,24,24	0
57	MG	1W	204	1/1	0.94	0.14	32,32,32,32	0
57	MG	1X	103	1/1	0.94	0.11	46,46,46,46	0
57	MG	2a	3139	1/1	0.94	0.17	51,51,51,51	0
57	MG	1A	3056	1/1	0.94	0.05	19,19,19,19	0
57	MG	1A	3370	1/1	0.94	0.06	21,21,21,21	0
57	MG	1A	3471	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3726	1/1	0.94	0.06	35,35,35,35	0
57	MG	1A	3727	1/1	0.94	0.08	46,46,46,46	0
57	MG	1Z	303	1/1	0.94	0.14	51,51,51,51	0
57	MG	1A	3025	1/1	0.94	0.13	51,51,51,51	0
57	MG	1a	3194	1/1	0.94	0.12	49,49,49,49	0
57	MG	2A	3227	1/1	0.94	0.09	51,51,51,51	0
57	MG	1a	3196	1/1	0.94	0.14	58,58,58,58	0
57	MG	2a	3154	1/1	0.94	0.14	47,47,47,47	0
57	MG	10	104	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3881	1/1	0.94	0.06	30,30,30,30	0
57	MG	2A	3566	1/1	0.94	0.06	34,34,34,34	0
57	MG	11	103	1/1	0.94	0.08	52,52,52,52	0
57	MG	1A	3376	1/1	0.94	0.11	43,43,43,43	0
57	MG	1A	3113	1/1	0.94	0.07	36,36,36,36	0
57	MG	2A	3243	1/1	0.94	0.14	45,45,45,45	0
57	MG	2A	3245	1/1	0.94	0.07	45,45,45,45	0
57	MG	1A	3597	1/1	0.94	0.14	37,37,37,37	0
57	MG	2A	3247	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3248	1/1	0.94	0.12	47,47,47,47	0
57	MG	15	105	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	3887	1/1	0.94	0.07	32,32,32,32	0
57	MG	1a	3209	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3258	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	3191	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	3027	1/1	0.94	0.12	30,30,30,30	0
57	MG	18	102	1/1	0.94	0.21	43,43,43,43	0
57	MG	2A	3261	1/1	0.94	0.17	54,54,54,54	0
57	MG	18	103	1/1	0.94	0.07	35,35,35,35	0
57	MG	19	502	1/1	0.94	0.06	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3387	1/1	0.94	0.09	23,23,23,23	0
57	MG	1a	3002	1/1	0.94	0.17	38,38,38,38	0
57	MG	1a	3004	1/1	0.94	0.12	55,55,55,55	0
57	MG	2A	3269	1/1	0.94	0.06	26,26,26,26	0
57	MG	2a	3183	1/1	0.94	0.11	34,34,34,34	0
57	MG	1A	3263	1/1	0.94	0.14	35,35,35,35	0
57	MG	1A	3900	1/1	0.94	0.07	39,39,39,39	0
57	MG	1A	3901	1/1	0.94	0.12	40,40,40,40	0
57	MG	1a	3228	1/1	0.94	0.15	38,38,38,38	0
57	MG	1a	3008	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3277	1/1	0.94	0.12	47,47,47,47	0
57	MG	1A	3074	1/1	0.94	0.28	26,26,26,26	0
57	MG	1a	3012	1/1	0.94	0.10	29,29,29,29	0
57	MG	1l	202	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3125	1/1	0.94	0.07	31,31,31,31	0
57	MG	1a	3015	1/1	0.94	0.12	46,46,46,46	0
57	MG	1a	3016	1/1	0.94	0.20	45,45,45,45	0
57	MG	2A	3614	1/1	0.94	0.16	38,38,38,38	0
57	MG	1w	3001	1/1	0.94	0.18	52,52,52,52	0
57	MG	2A	3621	1/1	0.94	0.10	48,48,48,48	0
57	MG	1w	3004	1/1	0.94	0.07	51,51,51,51	0
57	MG	1A	3610	1/1	0.94	0.05	25,25,25,25	0
57	MG	1A	3611	1/1	0.94	0.06	20,20,20,20	0
57	MG	1x	105	1/1	0.94	0.24	56,56,56,56	0
57	MG	2A	3294	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3497	1/1	0.94	0.07	8,8,8,8	0
57	MG	1A	3394	1/1	0.94	0.12	43,43,43,43	0
57	MG	2A	3301	1/1	0.94	0.19	54,54,54,54	0
57	MG	1A	3759	1/1	0.94	0.07	43,43,43,43	0
57	MG	2A	3303	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3915	1/1	0.94	0.07	35,35,35,35	0
57	MG	2A	3306	1/1	0.94	0.07	46,46,46,46	0
57	MG	2A	3310	1/1	0.94	0.11	56,56,56,56	0
57	MG	2A	3311	1/1	0.94	0.07	45,45,45,45	0
57	MG	2A	3648	1/1	0.94	0.09	52,52,52,52	0
57	MG	2A	3649	1/1	0.94	0.15	56,56,56,56	0
57	MG	1A	3618	1/1	0.94	0.10	31,31,31,31	0
57	MG	1A	3126	1/1	0.94	0.08	62,62,62,62	0
57	MG	1A	3762	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3622	1/1	0.94	0.08	27,27,27,27	0
57	MG	1A	3277	1/1	0.94	0.09	29,29,29,29	0
57	MG	2A	3007	1/1	0.94	0.10	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
57	MG	2A	3325	1/1	0.94	0.10	43,43,43,43	0
57	MG	1a	3034	1/1	0.94	0.19	42,42,42,42	0
57	MG	2A	3663	1/1	0.94	0.11	31,31,31,31	0
57	MG	1A	3078	1/1	0.94	0.14	18,18,18,18	0
57	MG	1A	3892	1/1	0.95	0.10	52,52,52,52	0
57	MG	1a	3168	1/1	0.95	0.13	46,46,46,46	0
57	MG	1A	3893	1/1	0.95	0.06	40,40,40,40	0
57	MG	1A	3413	1/1	0.95	0.09	8,8,8,8	0
57	MG	2B	3018	1/1	0.95	0.12	58,58,58,58	0
57	MG	2A	3158	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3203	1/1	0.95	0.06	24,24,24,24	0
57	MG	2A	3412	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3639	1/1	0.95	0.05	29,29,29,29	0
57	MG	1A	3117	1/1	0.95	0.09	51,51,51,51	0
57	MG	2D	303	1/1	0.95	0.15	46,46,46,46	0
57	MG	1A	3531	1/1	0.95	0.08	13,13,13,13	0
57	MG	2D	306	1/1	0.95	0.08	29,29,29,29	0
57	MG	2E	301	1/1	0.95	0.06	34,34,34,34	0
57	MG	2E	302	1/1	0.95	0.12	44,44,44,44	0
57	MG	1a	3176	1/1	0.95	0.15	34,34,34,34	0
57	MG	1A	3206	1/1	0.95	0.08	33,33,33,33	0
57	MG	1A	3168	1/1	0.95	0.05	10,10,10,10	0
57	MG	15	104	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3321	1/1	0.95	0.07	47,47,47,47	0
57	MG	2A	3423	1/1	0.95	0.11	54,54,54,54	0
57	MG	2A	3424	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3770	1/1	0.95	0.06	28,28,28,28	0
57	MG	1A	3771	1/1	0.95	0.08	28,28,28,28	0
57	MG	2A	3427	1/1	0.95	0.06	38,38,38,38	0
57	MG	1A	3645	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3428	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3431	1/1	0.95	0.09	42,42,42,42	0
57	MG	2V	202	1/1	0.95	0.07	38,38,38,38	0
57	MG	1A	3061	1/1	0.95	0.06	22,22,22,22	0
57	MG	2A	3433	1/1	0.95	0.09	30,30,30,30	0
57	MG	1A	3918	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3070	1/1	0.95	0.06	32,32,32,32	0
57	MG	1a	3192	1/1	0.95	0.11	51,51,51,51	0
57	MG	2A	3443	1/1	0.95	0.09	31,31,31,31	0
57	MG	2A	3182	1/1	0.95	0.09	43,43,43,43	0
57	MG	23	3001	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3448	1/1	0.95	0.13	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3184	1/1	0.95	0.22	40,40,40,40	0
57	MG	1A	3777	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3437	1/1	0.95	0.06	26,26,26,26	0
57	MG	1a	3003	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3655	1/1	0.95	0.11	26,26,26,26	0
57	MG	2A	3456	1/1	0.95	0.06	38,38,38,38	0
57	MG	2A	3458	1/1	0.95	0.09	30,30,30,30	0
57	MG	1A	3261	1/1	0.95	0.08	34,34,34,34	0
57	MG	1A	3262	1/1	0.95	0.07	30,30,30,30	0
57	MG	2A	3191	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	3658	1/1	0.95	0.08	21,21,21,21	0
57	MG	1A	3015	1/1	0.95	0.07	45,45,45,45	0
57	MG	1a	3009	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3547	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3221	1/1	0.95	0.05	28,28,28,28	0
57	MG	1A	3663	1/1	0.95	0.06	24,24,24,24	0
57	MG	1A	3338	1/1	0.95	0.11	35,35,35,35	0
57	MG	1A	3097	1/1	0.95	0.18	42,42,42,42	0
57	MG	1A	3226	1/1	0.95	0.15	40,40,40,40	0
57	MG	1A	3344	1/1	0.95	0.10	29,29,29,29	0
57	MG	1A	3950	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3274	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3952	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3352	1/1	0.95	0.12	37,37,37,37	0
57	MG	2A	3485	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3362	1/1	0.95	0.13	19,19,19,19	0
57	MG	2A	3489	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3364	1/1	0.95	0.09	50,50,50,50	0
57	MG	1a	3226	1/1	0.95	0.12	41,41,41,41	0
57	MG	1A	3366	1/1	0.95	0.04	19,19,19,19	0
57	MG	1A	3967	1/1	0.95	0.16	45,45,45,45	0
57	MG	1a	3231	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3685	1/1	0.95	0.08	42,42,42,42	0
57	MG	1a	3033	1/1	0.95	0.23	50,50,50,50	0
57	MG	2A	3219	1/1	0.95	0.13	45,45,45,45	0
57	MG	2A	3221	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3367	1/1	0.95	0.09	27,27,27,27	0
57	MG	2a	3042	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3976	1/1	0.95	0.12	25,25,25,25	0
57	MG	2a	3045	1/1	0.95	0.08	44,44,44,44	0
57	MG	1n	502	1/1	0.95	0.21	33,33,33,33	0
57	MG	2A	3225	1/1	0.95	0.21	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
57	MG	1A	3814	1/1	0.95	0.07	38,38,38,38	0
57	MG	1A	3980	1/1	0.95	0.27	35,35,35,35	0
57	MG	2A	3228	1/1	0.95	0.13	35,35,35,35	0
57	MG	2A	3511	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3230	1/1	0.95	0.12	48,48,48,48	0
57	MG	2a	3054	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3515	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3981	1/1	0.95	0.17	29,29,29,29	0
57	MG	1A	3818	1/1	0.95	0.06	28,28,28,28	0
57	MG	1A	3988	1/1	0.95	0.07	22,22,22,22	0
57	MG	1a	3042	1/1	0.95	0.13	44,44,44,44	0
57	MG	2A	3240	1/1	0.95	0.21	44,44,44,44	0
57	MG	1A	3462	1/1	0.95	0.07	27,27,27,27	0
57	MG	1A	3368	1/1	0.95	0.10	35,35,35,35	0
57	MG	1A	3994	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3998	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3821	1/1	0.95	0.06	40,40,40,40	0
57	MG	1A	3369	1/1	0.95	0.08	37,37,37,37	0
57	MG	1B	3002	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3175	1/1	0.95	0.15	37,37,37,37	0
57	MG	1A	3001	1/1	0.95	0.07	24,24,24,24	0
57	MG	1A	3375	1/1	0.95	0.05	32,32,32,32	0
57	MG	2A	3256	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3578	1/1	0.95	0.08	53,53,53,53	0
57	MG	2A	3006	1/1	0.95	0.23	52,52,52,52	0
57	MG	2a	3077	1/1	0.95	0.16	55,55,55,55	0
57	MG	1A	3828	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3180	1/1	0.95	0.12	33,33,33,33	0
57	MG	2A	3011	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3377	1/1	0.95	0.07	31,31,31,31	0
57	MG	2A	3544	1/1	0.95	0.07	41,41,41,41	0
57	MG	1A	3832	1/1	0.95	0.08	37,37,37,37	0
57	MG	2A	3019	1/1	0.95	0.44	54,54,54,54	0
57	MG	2A	3024	1/1	0.95	0.18	49,49,49,49	0
57	MG	2a	3094	1/1	0.95	0.09	62,62,62,62	0
57	MG	2a	3095	1/1	0.95	0.20	46,46,46,46	0
57	MG	1A	3380	1/1	0.95	0.24	30,30,30,30	0
57	MG	2A	3550	1/1	0.95	0.09	42,42,42,42	0
57	MG	1A	3706	1/1	0.95	0.15	60,60,60,60	0
57	MG	1a	3068	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3483	1/1	0.95	0.09	30,30,30,30	0
57	MG	1a	3073	1/1	0.95	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
57	MG	1A	3587	1/1	0.95	0.09	29,29,29,29	0
57	MG	2A	3034	1/1	0.95	0.08	31,31,31,31	0
57	MG	2A	3035	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3278	1/1	0.95	0.12	59,59,59,59	0
57	MG	1A	3589	1/1	0.95	0.17	33,33,33,33	0
57	MG	1B	3026	1/1	0.95	0.10	42,42,42,42	0
57	MG	1a	3077	1/1	0.95	0.12	39,39,39,39	0
57	MG	2A	3040	1/1	0.95	0.15	53,53,53,53	0
57	MG	1A	3485	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3286	1/1	0.95	0.23	31,31,31,31	0
57	MG	1B	3029	1/1	0.95	0.08	54,54,54,54	0
57	MG	2A	3289	1/1	0.95	0.10	23,23,23,23	0
57	MG	1A	3842	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3050	1/1	0.95	0.07	49,49,49,49	0
57	MG	1D	309	1/1	0.95	0.08	38,38,38,38	0
57	MG	1D	311	1/1	0.95	0.07	49,49,49,49	0
57	MG	2a	3126	1/1	0.95	0.08	63,63,63,63	0
57	MG	2A	3579	1/1	0.95	0.07	39,39,39,39	0
57	MG	2a	3128	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3843	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3054	1/1	0.95	0.06	47,47,47,47	0
57	MG	2A	3298	1/1	0.95	0.10	45,45,45,45	0
57	MG	1A	3287	1/1	0.95	0.08	53,53,53,53	0
57	MG	1E	306	1/1	0.95	0.06	23,23,23,23	0
57	MG	2a	3134	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3588	1/1	0.95	0.10	45,45,45,45	0
57	MG	1A	3184	1/1	0.95	0.07	28,28,28,28	0
57	MG	1a	3091	1/1	0.95	0.14	39,39,39,39	0
57	MG	1A	3290	1/1	0.95	0.10	40,40,40,40	0
57	MG	1A	3720	1/1	0.95	0.07	23,23,23,23	0
57	MG	2A	3309	1/1	0.95	0.17	51,51,51,51	0
57	MG	2A	3064	1/1	0.95	0.06	44,44,44,44	0
57	MG	2A	3066	1/1	0.95	0.10	33,33,33,33	0
57	MG	2A	3312	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3067	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3138	1/1	0.95	0.36	26,26,26,26	0
57	MG	1F	302	1/1	0.95	0.08	22,22,22,22	0
57	MG	1A	3029	1/1	0.95	0.12	18,18,18,18	0
57	MG	2a	3149	1/1	0.95	0.13	53,53,53,53	0
57	MG	1A	3723	1/1	0.95	0.08	36,36,36,36	0
57	MG	1A	3853	1/1	0.95	0.12	49,49,49,49	0
57	MG	2A	3323	1/1	0.95	0.05	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
57	MG	1A	3104	1/1	0.95	0.09	33,33,33,33	0
57	MG	2A	3077	1/1	0.95	0.08	45,45,45,45	0
57	MG	2A	3328	1/1	0.95	0.16	37,37,37,37	0
57	MG	2A	3329	1/1	0.95	0.08	50,50,50,50	0
57	MG	1A	3499	1/1	0.95	0.07	21,21,21,21	0
57	MG	1A	3608	1/1	0.95	0.06	15,15,15,15	0
57	MG	2A	3616	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3617	1/1	0.95	0.07	30,30,30,30	0
57	MG	2A	3618	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3500	1/1	0.95	0.10	21,21,21,21	0
57	MG	2A	3620	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3392	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3337	1/1	0.95	0.11	56,56,56,56	0
57	MG	2A	3623	1/1	0.95	0.11	50,50,50,50	0
57	MG	2A	3087	1/1	0.95	0.08	40,40,40,40	0
57	MG	1a	3110	1/1	0.95	0.18	45,45,45,45	0
57	MG	1N	3005	1/1	0.95	0.06	27,27,27,27	0
57	MG	1N	3007	1/1	0.95	0.20	25,25,25,25	0
57	MG	1A	3109	1/1	0.95	0.09	23,23,23,23	0
57	MG	2A	3631	1/1	0.95	0.16	55,55,55,55	0
57	MG	2A	3094	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3731	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3348	1/1	0.95	0.07	45,45,45,45	0
57	MG	1a	3118	1/1	0.95	0.18	38,38,38,38	0
57	MG	2A	3641	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3612	1/1	0.95	0.08	26,26,26,26	0
57	MG	1a	3121	1/1	0.95	0.13	36,36,36,36	0
57	MG	2A	3645	1/1	0.95	0.08	50,50,50,50	0
57	MG	1A	3864	1/1	0.95	0.06	32,32,32,32	0
57	MG	1A	3737	1/1	0.95	0.08	37,37,37,37	0
57	MG	1P	203	1/1	0.95	0.21	34,34,34,34	0
57	MG	1P	204	1/1	0.95	0.07	34,34,34,34	0
57	MG	2A	3650	1/1	0.95	0.16	30,30,30,30	0
57	MG	1Q	201	1/1	0.95	0.13	28,28,28,28	0
57	MG	1a	3128	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3738	1/1	0.95	0.09	38,38,38,38	0
57	MG	2a	3196	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3298	1/1	0.95	0.17	30,30,30,30	0
57	MG	1Q	205	1/1	0.95	0.16	30,30,30,30	0
57	MG	1A	3869	1/1	0.95	0.09	35,35,35,35	0
57	MG	1A	3740	1/1	0.95	0.08	47,47,47,47	0
57	MG	2a	3201	1/1	0.95	0.10	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2d	502	1/1	0.95	0.12	63,63,63,63	0
57	MG	1A	3244	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3111	1/1	0.95	0.09	31,31,31,31	0
57	MG	1A	3515	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3090	1/1	0.95	0.13	45,45,45,45	0
57	MG	1A	3745	1/1	0.95	0.13	34,34,34,34	0
57	MG	2j	8001	1/1	0.95	0.07	61,61,61,61	0
57	MG	2A	3377	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3746	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	3623	1/1	0.95	0.05	22,22,22,22	0
57	MG	1A	3155	1/1	0.95	0.12	33,33,33,33	0
57	MG	2A	3134	1/1	0.95	0.05	34,34,34,34	0
57	MG	2A	3382	1/1	0.95	0.17	31,31,31,31	0
57	MG	2A	3678	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	3305	1/1	0.95	0.04	38,38,38,38	0
57	MG	2A	3686	1/1	0.95	0.11	48,48,48,48	0
57	MG	1W	205	1/1	0.95	0.15	31,31,31,31	0
57	MG	2A	3387	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3139	1/1	0.95	0.24	50,50,50,50	0
57	MG	1X	101	1/1	0.95	0.08	34,34,34,34	0
57	MG	1A	3201	1/1	0.95	0.07	38,38,38,38	0
57	MG	1A	3310	1/1	0.95	0.06	32,32,32,32	0
57	MG	1A	3157	1/1	0.95	0.07	27,27,27,27	0
57	MG	1Y	203	1/1	0.95	0.11	39,39,39,39	0
57	MG	1A	3253	1/1	0.95	0.10	36,36,36,36	0
57	MG	2B	3010	1/1	0.95	0.08	48,48,48,48	0
57	MG	2A	3148	1/1	0.95	0.13	28,28,28,28	0
57	MG	1Y	205	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3758	1/1	0.95	0.07	33,33,33,33	0
60	ZN	2Y	501	1/1	0.95	0.07	92,92,92,92	0
60	ZN	24	501	1/1	0.95	0.09	115,115,115,115	0
57	MG	1A	3990	1/1	0.96	0.17	38,38,38,38	0
57	MG	2A	3336	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3194	1/1	0.96	0.12	29,29,29,29	0
57	MG	1a	3062	1/1	0.96	0.08	39,39,39,39	0
57	MG	2A	3058	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3133	1/1	0.96	0.06	23,23,23,23	0
57	MG	2A	3665	1/1	0.96	0.14	43,43,43,43	0
57	MG	1A	3995	1/1	0.96	0.12	30,30,30,30	0
57	MG	2A	3343	1/1	0.96	0.12	47,47,47,47	0
57	MG	1a	3066	1/1	0.96	0.07	34,34,34,34	0
57	MG	2A	3063	1/1	0.96	0.15	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3996	1/1	0.96	0.19	31,31,31,31	0
57	MG	1A	3997	1/1	0.96	0.12	27,27,27,27	0
57	MG	1A	3811	1/1	0.96	0.04	20,20,20,20	0
57	MG	1a	3071	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3134	1/1	0.96	0.06	25,25,25,25	0
57	MG	2A	3352	1/1	0.96	0.08	35,35,35,35	0
57	MG	2A	3681	1/1	0.96	0.09	38,38,38,38	0
57	MG	2A	3685	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3137	1/1	0.96	0.06	32,32,32,32	0
57	MG	2A	3687	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3420	1/1	0.96	0.06	22,22,22,22	0
57	MG	2A	3073	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3024	1/1	0.96	0.13	48,48,48,48	0
57	MG	1B	3005	1/1	0.96	0.18	46,46,46,46	0
57	MG	2A	3076	1/1	0.96	0.21	40,40,40,40	0
57	MG	2A	3360	1/1	0.96	0.06	29,29,29,29	0
57	MG	1a	3078	1/1	0.96	0.16	37,37,37,37	0
57	MG	2B	3006	1/1	0.96	0.16	61,61,61,61	0
57	MG	2B	3007	1/1	0.96	0.14	61,61,61,61	0
57	MG	1B	3006	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3080	1/1	0.96	0.21	47,47,47,47	0
57	MG	2A	3081	1/1	0.96	0.18	44,44,44,44	0
57	MG	1A	3328	1/1	0.96	0.08	33,33,33,33	0
57	MG	1A	3427	1/1	0.96	0.09	36,36,36,36	0
57	MG	1a	3082	1/1	0.96	0.11	53,53,53,53	0
57	MG	1A	3063	1/1	0.96	0.07	22,22,22,22	0
57	MG	1B	3011	1/1	0.96	0.11	37,37,37,37	0
57	MG	1a	3085	1/1	0.96	0.13	41,41,41,41	0
57	MG	1A	3429	1/1	0.96	0.04	26,26,26,26	0
57	MG	1A	3430	1/1	0.96	0.07	27,27,27,27	0
57	MG	2A	3092	1/1	0.96	0.09	43,43,43,43	0
57	MG	2A	3093	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3824	1/1	0.96	0.08	34,34,34,34	0
57	MG	1A	3546	1/1	0.96	0.06	39,39,39,39	0
57	MG	1A	3064	1/1	0.96	0.09	22,22,22,22	0
57	MG	1A	3683	1/1	0.96	0.05	52,52,52,52	0
57	MG	2D	304	1/1	0.96	0.06	49,49,49,49	0
57	MG	1A	3010	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3549	1/1	0.96	0.07	55,55,55,55	0
57	MG	2D	308	1/1	0.96	0.12	51,51,51,51	0
57	MG	2A	3101	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3689	1/1	0.96	0.09	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3435	1/1	0.96	0.07	19,19,19,19	0
57	MG	2E	305	1/1	0.96	0.06	48,48,48,48	0
57	MG	2A	3105	1/1	0.96	0.06	46,46,46,46	0
57	MG	1a	3097	1/1	0.96	0.11	43,43,43,43	0
57	MG	2A	3394	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3207	1/1	0.96	0.06	42,42,42,42	0
57	MG	2A	3398	1/1	0.96	0.05	46,46,46,46	0
57	MG	1A	3072	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3210	1/1	0.96	0.04	27,27,27,27	0
57	MG	1A	3269	1/1	0.96	0.13	25,25,25,25	0
57	MG	1a	3102	1/1	0.96	0.17	43,43,43,43	0
57	MG	1a	3103	1/1	0.96	0.09	34,34,34,34	0
57	MG	2A	3406	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3119	1/1	0.96	0.10	37,37,37,37	0
57	MG	1a	3104	1/1	0.96	0.15	49,49,49,49	0
57	MG	1D	305	1/1	0.96	0.07	28,28,28,28	0
57	MG	2X	101	1/1	0.96	0.08	52,52,52,52	0
57	MG	1A	3444	1/1	0.96	0.13	31,31,31,31	0
57	MG	2A	3123	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3345	1/1	0.96	0.08	53,53,53,53	0
57	MG	1D	312	1/1	0.96	0.10	29,29,29,29	0
57	MG	1a	3109	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3416	1/1	0.96	0.10	37,37,37,37	0
57	MG	1E	301	1/1	0.96	0.06	33,33,33,33	0
57	MG	2A	3130	1/1	0.96	0.10	38,38,38,38	0
57	MG	25	503	1/1	0.96	0.14	51,51,51,51	0
57	MG	1A	3026	1/1	0.96	0.14	21,21,21,21	0
57	MG	28	101	1/1	0.96	0.09	43,43,43,43	0
57	MG	1E	303	1/1	0.96	0.11	22,22,22,22	0
57	MG	1A	3350	1/1	0.96	0.06	26,26,26,26	0
57	MG	2A	3136	1/1	0.96	0.12	35,35,35,35	0
57	MG	1A	3704	1/1	0.96	0.07	31,31,31,31	0
57	MG	1A	3152	1/1	0.96	0.06	24,24,24,24	0
57	MG	1a	3119	1/1	0.96	0.09	51,51,51,51	0
57	MG	1A	3450	1/1	0.96	0.12	54,54,54,54	0
57	MG	1A	3846	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3355	1/1	0.96	0.12	19,19,19,19	0
57	MG	1A	3571	1/1	0.96	0.04	37,37,37,37	0
57	MG	1A	3356	1/1	0.96	0.09	19,19,19,19	0
57	MG	1F	307	1/1	0.96	0.12	40,40,40,40	0
57	MG	1F	308	1/1	0.96	0.15	34,34,34,34	0
57	MG	2A	3149	1/1	0.96	0.14	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
57	MG	2A	3437	1/1	0.96	0.13	31,31,31,31	0
57	MG	2A	3438	1/1	0.96	0.06	23,23,23,23	0
57	MG	2a	3018	1/1	0.96	0.16	43,43,43,43	0
57	MG	1A	3711	1/1	0.96	0.08	39,39,39,39	0
57	MG	2A	3440	1/1	0.96	0.12	43,43,43,43	0
57	MG	2A	3441	1/1	0.96	0.07	49,49,49,49	0
57	MG	2A	3442	1/1	0.96	0.12	45,45,45,45	0
57	MG	1G	202	1/1	0.96	0.19	46,46,46,46	0
57	MG	2A	3153	1/1	0.96	0.04	37,37,37,37	0
57	MG	2A	3446	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	3454	1/1	0.96	0.08	24,24,24,24	0
57	MG	1A	3357	1/1	0.96	0.23	42,42,42,42	0
57	MG	1A	3714	1/1	0.96	0.09	30,30,30,30	0
57	MG	2A	3452	1/1	0.96	0.06	24,24,24,24	0
57	MG	1A	3575	1/1	0.96	0.06	29,29,29,29	0
57	MG	2a	3032	1/1	0.96	0.06	48,48,48,48	0
57	MG	1N	3001	1/1	0.96	0.13	28,28,28,28	0
57	MG	1A	3358	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3718	1/1	0.96	0.09	26,26,26,26	0
57	MG	1A	3361	1/1	0.96	0.08	39,39,39,39	0
57	MG	2A	3459	1/1	0.96	0.14	38,38,38,38	0
57	MG	1A	3102	1/1	0.96	0.09	22,22,22,22	0
57	MG	1A	3582	1/1	0.96	0.09	20,20,20,20	0
57	MG	2A	3463	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3363	1/1	0.96	0.07	21,21,21,21	0
57	MG	1A	3278	1/1	0.96	0.08	35,35,35,35	0
57	MG	2a	3044	1/1	0.96	0.08	64,64,64,64	0
57	MG	2A	3467	1/1	0.96	0.15	38,38,38,38	0
57	MG	1O	204	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3463	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3866	1/1	0.96	0.11	50,50,50,50	0
57	MG	1P	201	1/1	0.96	0.16	24,24,24,24	0
57	MG	1A	3280	1/1	0.96	0.35	37,37,37,37	0
57	MG	2a	3051	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3175	1/1	0.96	0.13	49,49,49,49	0
57	MG	1a	3152	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3588	1/1	0.96	0.06	28,28,28,28	0
57	MG	1A	3281	1/1	0.96	0.22	17,17,17,17	0
57	MG	1a	3156	1/1	0.96	0.06	42,42,42,42	0
57	MG	1a	3157	1/1	0.96	0.06	50,50,50,50	0
57	MG	1a	3158	1/1	0.96	0.14	41,41,41,41	0
57	MG	2A	3183	1/1	0.96	0.14	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
57	MG	2A	3484	1/1	0.96	0.16	39,39,39,39	0
57	MG	1A	3282	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3103	1/1	0.96	0.20	31,31,31,31	0
57	MG	1A	3730	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3596	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3021	1/1	0.96	0.09	19,19,19,19	0
57	MG	1A	3736	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3372	1/1	0.96	0.13	25,25,25,25	0
57	MG	1A	3476	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3477	1/1	0.96	0.06	19,19,19,19	0
57	MG	1A	3107	1/1	0.96	0.14	17,17,17,17	0
57	MG	1U	202	1/1	0.96	0.14	24,24,24,24	0
57	MG	1U	204	1/1	0.96	0.13	28,28,28,28	0
57	MG	1A	3885	1/1	0.96	0.06	58,58,58,58	0
57	MG	1A	3479	1/1	0.96	0.10	25,25,25,25	0
57	MG	1a	3181	1/1	0.96	0.06	42,42,42,42	0
57	MG	1a	3182	1/1	0.96	0.14	48,48,48,48	0
57	MG	2a	3080	1/1	0.96	0.22	45,45,45,45	0
57	MG	2a	3081	1/1	0.96	0.11	55,55,55,55	0
57	MG	1W	202	1/1	0.96	0.07	34,34,34,34	0
57	MG	2a	3083	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3169	1/1	0.96	0.05	22,22,22,22	0
57	MG	2a	3085	1/1	0.96	0.14	50,50,50,50	0
57	MG	1A	3108	1/1	0.96	0.06	30,30,30,30	0
57	MG	2A	3206	1/1	0.96	0.07	59,59,59,59	0
57	MG	2A	3512	1/1	0.96	0.07	55,55,55,55	0
57	MG	2A	3513	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3484	1/1	0.96	0.17	35,35,35,35	0
57	MG	1W	206	1/1	0.96	0.08	26,26,26,26	0
57	MG	1A	3289	1/1	0.96	0.05	30,30,30,30	0
57	MG	1A	3231	1/1	0.96	0.08	23,23,23,23	0
57	MG	2A	3519	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3520	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3028	1/1	0.96	0.06	14,14,14,14	0
57	MG	1X	107	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3022	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3895	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3055	1/1	0.96	0.11	30,30,30,30	0
57	MG	1A	3898	1/1	0.96	0.07	23,23,23,23	0
57	MG	1A	3899	1/1	0.96	0.08	40,40,40,40	0
57	MG	1a	3199	1/1	0.96	0.13	52,52,52,52	0
57	MG	2A	3531	1/1	0.96	0.06	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
57	MG	2A	3220	1/1	0.96	0.14	45,45,45,45	0
57	MG	1A	3615	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3616	1/1	0.96	0.06	14,14,14,14	0
57	MG	1a	3203	1/1	0.96	0.11	67,67,67,67	0
57	MG	1A	3617	1/1	0.96	0.07	14,14,14,14	0
57	MG	10	103	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3903	1/1	0.96	0.08	57,57,57,57	0
57	MG	2a	3122	1/1	0.96	0.09	50,50,50,50	0
57	MG	2a	3123	1/1	0.96	0.09	47,47,47,47	0
57	MG	10	105	1/1	0.96	0.07	55,55,55,55	0
57	MG	11	101	1/1	0.96	0.08	35,35,35,35	0
57	MG	2A	3229	1/1	0.96	0.12	42,42,42,42	0
57	MG	1A	3116	1/1	0.96	0.05	21,21,21,21	0
57	MG	1A	3906	1/1	0.96	0.09	36,36,36,36	0
57	MG	1a	3212	1/1	0.96	0.13	58,58,58,58	0
57	MG	1a	3213	1/1	0.96	0.10	58,58,58,58	0
57	MG	2A	3238	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3756	1/1	0.96	0.09	26,26,26,26	0
57	MG	1A	3619	1/1	0.96	0.05	27,27,27,27	0
57	MG	15	102	1/1	0.96	0.16	36,36,36,36	0
57	MG	1A	3240	1/1	0.96	0.05	33,33,33,33	0
57	MG	2A	3552	1/1	0.96	0.15	37,37,37,37	0
57	MG	1A	3495	1/1	0.96	0.09	16,16,16,16	0
57	MG	1A	3388	1/1	0.96	0.21	32,32,32,32	0
57	MG	1A	3389	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3241	1/1	0.96	0.12	28,28,28,28	0
57	MG	2a	3141	1/1	0.96	0.10	70,70,70,70	0
57	MG	1A	3765	1/1	0.96	0.05	44,44,44,44	0
57	MG	1A	3627	1/1	0.96	0.06	16,16,16,16	0
57	MG	1A	3628	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3083	1/1	0.96	0.08	54,54,54,54	0
57	MG	2A	3255	1/1	0.96	0.07	48,48,48,48	0
57	MG	2A	3565	1/1	0.96	0.07	25,25,25,25	0
57	MG	1a	3229	1/1	0.96	0.14	51,51,51,51	0
57	MG	2A	3567	1/1	0.96	0.08	34,34,34,34	0
57	MG	2a	3151	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3503	1/1	0.96	0.11	20,20,20,20	0
57	MG	1A	3505	1/1	0.96	0.11	52,52,52,52	0
57	MG	1A	3925	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3084	1/1	0.96	0.07	15,15,15,15	0
57	MG	1A	3036	1/1	0.96	0.11	38,38,38,38	0
57	MG	1A	3931	1/1	0.96	0.14	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
57	MG	1A	3635	1/1	0.96	0.04	30,30,30,30	0
57	MG	1q	3001	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3934	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3936	1/1	0.96	0.12	38,38,38,38	0
57	MG	2A	3267	1/1	0.96	0.08	32,32,32,32	0
57	MG	2A	3268	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3938	1/1	0.96	0.12	22,22,22,22	0
57	MG	1A	3039	1/1	0.96	0.19	23,23,23,23	0
57	MG	1A	3637	1/1	0.96	0.05	43,43,43,43	0
57	MG	2A	3273	1/1	0.96	0.10	49,49,49,49	0
57	MG	1A	3511	1/1	0.96	0.05	45,45,45,45	0
57	MG	1A	3512	1/1	0.96	0.08	21,21,21,21	0
57	MG	1A	3307	1/1	0.96	0.11	29,29,29,29	0
57	MG	2A	3592	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3398	1/1	0.96	0.05	29,29,29,29	0
57	MG	1A	3783	1/1	0.96	0.08	27,27,27,27	0
57	MG	1A	3187	1/1	0.96	0.18	20,20,20,20	0
57	MG	2A	3280	1/1	0.96	0.06	49,49,49,49	0
57	MG	1A	3247	1/1	0.96	0.09	49,49,49,49	0
57	MG	1a	3021	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3599	1/1	0.96	0.06	46,46,46,46	0
57	MG	2a	3179	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3401	1/1	0.96	0.07	48,48,48,48	0
57	MG	2a	3181	1/1	0.96	0.13	72,72,72,72	0
57	MG	2a	3182	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3284	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3953	1/1	0.96	0.10	53,53,53,53	0
57	MG	2A	3286	1/1	0.96	0.06	33,33,33,33	0
57	MG	2a	3186	1/1	0.96	0.07	56,56,56,56	0
57	MG	1A	3954	1/1	0.96	0.08	22,22,22,22	0
57	MG	1A	3955	1/1	0.96	0.09	34,34,34,34	0
57	MG	1A	3789	1/1	0.96	0.20	29,29,29,29	0
57	MG	2A	3608	1/1	0.96	0.10	61,61,61,61	0
57	MG	1a	3027	1/1	0.96	0.07	39,39,39,39	0
57	MG	2A	3010	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3646	1/1	0.96	0.07	37,37,37,37	0
57	MG	2A	3014	1/1	0.96	0.07	37,37,37,37	0
57	MG	1a	3030	1/1	0.96	0.16	48,48,48,48	0
57	MG	1A	3960	1/1	0.96	0.24	29,29,29,29	0
57	MG	1A	3961	1/1	0.96	0.11	28,28,28,28	0
57	MG	1A	3402	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	3964	1/1	0.96	0.10	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
57	MG	1A	3965	1/1	0.96	0.05	29,29,29,29	0
57	MG	1A	3058	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3129	1/1	0.96	0.06	29,29,29,29	0
57	MG	1A	3130	1/1	0.96	0.09	34,34,34,34	0
57	MG	2A	3624	1/1	0.96	0.06	44,44,44,44	0
57	MG	2A	3307	1/1	0.96	0.08	47,47,47,47	0
57	MG	2A	3626	1/1	0.96	0.05	44,44,44,44	0
57	MG	2A	3308	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3317	1/1	0.96	0.15	48,48,48,48	0
57	MG	1A	3974	1/1	0.96	0.10	29,29,29,29	0
57	MG	1A	3975	1/1	0.96	0.08	29,29,29,29	0
57	MG	2A	3036	1/1	0.96	0.12	52,52,52,52	0
57	MG	1A	3798	1/1	0.96	0.12	36,36,36,36	0
57	MG	2A	3634	1/1	0.96	0.07	41,41,41,41	0
57	MG	2A	3635	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3977	1/1	0.96	0.11	30,30,30,30	0
57	MG	2A	3315	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3978	1/1	0.96	0.14	28,28,28,28	0
57	MG	2A	3640	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3252	1/1	0.96	0.17	31,31,31,31	0
57	MG	1A	3800	1/1	0.96	0.11	47,47,47,47	0
57	MG	2A	3320	1/1	0.96	0.05	45,45,45,45	0
57	MG	1A	3041	1/1	0.96	0.16	26,26,26,26	0
57	MG	2A	3044	1/1	0.96	0.19	47,47,47,47	0
57	MG	1a	3052	1/1	0.96	0.27	52,52,52,52	0
57	MG	1A	3985	1/1	0.96	0.20	27,27,27,27	0
57	MG	1A	3530	1/1	0.96	0.06	16,16,16,16	0
57	MG	1A	3987	1/1	0.96	0.12	29,29,29,29	0
57	MG	2A	3330	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3806	1/1	0.96	0.07	35,35,35,35	0
57	MG	1a	3058	1/1	0.96	0.18	50,50,50,50	0
57	MG	1A	3807	1/1	0.96	0.05	20,20,20,20	0
57	MG	1A	3093	1/1	0.97	0.10	41,41,41,41	0
57	MG	1A	3983	1/1	0.97	0.12	31,31,31,31	0
57	MG	1A	3540	1/1	0.97	0.07	41,41,41,41	0
57	MG	2D	307	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3677	1/1	0.97	0.04	43,43,43,43	0
57	MG	1A	3679	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3314	1/1	0.97	0.17	42,42,42,42	0
57	MG	1A	3315	1/1	0.97	0.09	31,31,31,31	0
57	MG	1a	3219	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3316	1/1	0.97	0.06	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	3028	1/1	0.97	0.23	41,41,41,41	0
57	MG	2F	3003	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3418	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3545	1/1	0.97	0.05	9,9,9,9	0
57	MG	1a	3031	1/1	0.97	0.04	39,39,39,39	0
57	MG	1A	3688	1/1	0.97	0.05	46,46,46,46	0
57	MG	1A	3419	1/1	0.97	0.04	23,23,23,23	0
57	MG	1A	3119	1/1	0.97	0.06	25,25,25,25	0
57	MG	1A	3422	1/1	0.97	0.06	18,18,18,18	0
57	MG	2Q	3003	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3999	1/1	0.97	0.14	32,32,32,32	0
57	MG	2R	202	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	4001	1/1	0.97	0.12	29,29,29,29	0
57	MG	1A	3833	1/1	0.97	0.04	46,46,46,46	0
57	MG	2V	201	1/1	0.97	0.21	53,53,53,53	0
57	MG	1f	3001	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	4003	1/1	0.97	0.06	19,19,19,19	0
57	MG	1A	3120	1/1	0.97	0.09	35,35,35,35	0
57	MG	1A	3424	1/1	0.97	0.09	38,38,38,38	0
57	MG	1B	3003	1/1	0.97	0.09	24,24,24,24	0
57	MG	2A	3471	1/1	0.97	0.05	29,29,29,29	0
57	MG	1A	3694	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3121	1/1	0.97	0.09	19,19,19,19	0
57	MG	1a	3046	1/1	0.97	0.11	37,37,37,37	0
57	MG	1w	3002	1/1	0.97	0.14	34,34,34,34	0
57	MG	1w	3003	1/1	0.97	0.04	27,27,27,27	0
57	MG	2A	3477	1/1	0.97	0.04	46,46,46,46	0
57	MG	1A	3426	1/1	0.97	0.05	23,23,23,23	0
57	MG	1x	101	1/1	0.97	0.15	35,35,35,35	0
57	MG	1A	3697	1/1	0.97	0.08	41,41,41,41	0
57	MG	1x	103	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3698	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3122	1/1	0.97	0.17	31,31,31,31	0
57	MG	1A	3556	1/1	0.97	0.06	31,31,31,31	0
57	MG	1x	107	1/1	0.97	0.12	54,54,54,54	0
57	MG	2A	3486	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3231	1/1	0.97	0.06	39,39,39,39	0
57	MG	2A	3488	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3701	1/1	0.97	0.07	25,25,25,25	0
57	MG	2A	3233	1/1	0.97	0.05	35,35,35,35	0
57	MG	2a	3011	1/1	0.97	0.08	35,35,35,35	0
57	MG	1B	3013	1/1	0.97	0.09	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3235	1/1	0.97	0.09	30,30,30,30	0
57	MG	1A	3123	1/1	0.97	0.15	27,27,27,27	0
57	MG	1A	3077	1/1	0.97	0.17	24,24,24,24	0
57	MG	1B	3018	1/1	0.97	0.05	26,26,26,26	0
57	MG	2a	3017	1/1	0.97	0.08	44,44,44,44	0
57	MG	2A	3497	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3178	1/1	0.97	0.08	39,39,39,39	0
57	MG	1A	3179	1/1	0.97	0.20	26,26,26,26	0
57	MG	1A	3033	1/1	0.97	0.10	23,23,23,23	0
57	MG	1A	3182	1/1	0.97	0.08	22,22,22,22	0
57	MG	2A	3244	1/1	0.97	0.06	34,34,34,34	0
57	MG	1a	3063	1/1	0.97	0.21	44,44,44,44	0
57	MG	1A	3436	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3009	1/1	0.97	0.04	18,18,18,18	0
57	MG	2A	3507	1/1	0.97	0.15	46,46,46,46	0
57	MG	1A	3568	1/1	0.97	0.03	13,13,13,13	0
57	MG	2A	3249	1/1	0.97	0.12	48,48,48,48	0
57	MG	2A	3013	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3333	1/1	0.97	0.05	36,36,36,36	0
57	MG	2A	3253	1/1	0.97	0.07	47,47,47,47	0
57	MG	2a	3034	1/1	0.97	0.09	53,53,53,53	0
57	MG	2A	3016	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3127	1/1	0.97	0.06	28,28,28,28	0
57	MG	1a	3069	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3335	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3021	1/1	0.97	0.13	39,39,39,39	0
57	MG	2A	3023	1/1	0.97	0.12	34,34,34,34	0
57	MG	1B	3031	1/1	0.97	0.11	26,26,26,26	0
57	MG	1a	3072	1/1	0.97	0.13	41,41,41,41	0
57	MG	1A	3336	1/1	0.97	0.05	22,22,22,22	0
57	MG	2A	3525	1/1	0.97	0.04	37,37,37,37	0
57	MG	1D	302	1/1	0.97	0.10	31,31,31,31	0
57	MG	1D	303	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3337	1/1	0.97	0.10	36,36,36,36	0
57	MG	1D	307	1/1	0.97	0.19	32,32,32,32	0
57	MG	2A	3033	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3186	1/1	0.97	0.14	20,20,20,20	0
57	MG	1A	3254	1/1	0.97	0.05	28,28,28,28	0
57	MG	2A	3270	1/1	0.97	0.05	66,66,66,66	0
57	MG	1A	3340	1/1	0.97	0.07	19,19,19,19	0
57	MG	1A	3580	1/1	0.97	0.07	14,14,14,14	0
57	MG	1A	3341	1/1	0.97	0.14	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
57	MG	1A	3342	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3128	1/1	0.97	0.03	20,20,20,20	0
57	MG	1A	3031	1/1	0.97	0.13	24,24,24,24	0
57	MG	1A	3098	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3871	1/1	0.97	0.05	41,41,41,41	0
57	MG	1E	309	1/1	0.97	0.20	39,39,39,39	0
57	MG	2A	3047	1/1	0.97	0.07	28,28,28,28	0
57	MG	2a	3063	1/1	0.97	0.12	60,60,60,60	0
57	MG	2A	3048	1/1	0.97	0.07	25,25,25,25	0
57	MG	1A	3346	1/1	0.97	0.04	30,30,30,30	0
57	MG	1A	3347	1/1	0.97	0.06	27,27,27,27	0
57	MG	1A	3065	1/1	0.97	0.07	10,10,10,10	0
57	MG	1A	3100	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3876	1/1	0.97	0.11	24,24,24,24	0
57	MG	1A	3732	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3878	1/1	0.97	0.05	36,36,36,36	0
57	MG	1G	201	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3733	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	3880	1/1	0.97	0.11	37,37,37,37	0
57	MG	2a	3076	1/1	0.97	0.05	29,29,29,29	0
57	MG	1A	3351	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3082	1/1	0.97	0.09	25,25,25,25	0
57	MG	2A	3559	1/1	0.97	0.09	28,28,28,28	0
57	MG	2A	3061	1/1	0.97	0.07	50,50,50,50	0
57	MG	2A	3561	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3195	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3135	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3066	1/1	0.97	0.05	24,24,24,24	0
57	MG	2A	3300	1/1	0.97	0.04	21,21,21,21	0
57	MG	2a	3086	1/1	0.97	0.16	38,38,38,38	0
57	MG	2A	3065	1/1	0.97	0.14	50,50,50,50	0
57	MG	2a	3088	1/1	0.97	0.09	46,46,46,46	0
57	MG	1N	3003	1/1	0.97	0.04	32,32,32,32	0
57	MG	1A	3199	1/1	0.97	0.13	16,16,16,16	0
57	MG	2a	3091	1/1	0.97	0.06	49,49,49,49	0
57	MG	2A	3304	1/1	0.97	0.11	31,31,31,31	0
57	MG	1A	3359	1/1	0.97	0.15	35,35,35,35	0
57	MG	2A	3069	1/1	0.97	0.08	32,32,32,32	0
57	MG	1A	3067	1/1	0.97	0.10	22,22,22,22	0
57	MG	1A	3267	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3891	1/1	0.97	0.06	10,10,10,10	0
57	MG	1A	3268	1/1	0.97	0.25	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	3112	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3140	1/1	0.97	0.11	35,35,35,35	0
57	MG	1a	3114	1/1	0.97	0.12	42,42,42,42	0
57	MG	2A	3581	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3365	1/1	0.97	0.04	19,19,19,19	0
57	MG	2A	3078	1/1	0.97	0.07	25,25,25,25	0
57	MG	2A	3584	1/1	0.97	0.05	35,35,35,35	0
57	MG	2a	3111	1/1	0.97	0.07	35,35,35,35	0
57	MG	2a	3112	1/1	0.97	0.14	43,43,43,43	0
57	MG	1O	206	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3480	1/1	0.97	0.06	16,16,16,16	0
57	MG	1A	3271	1/1	0.97	0.09	35,35,35,35	0
57	MG	1A	3272	1/1	0.97	0.08	36,36,36,36	0
57	MG	2A	3321	1/1	0.97	0.09	60,60,60,60	0
57	MG	1A	3069	1/1	0.97	0.05	20,20,20,20	0
57	MG	1A	3106	1/1	0.97	0.22	26,26,26,26	0
57	MG	2A	3324	1/1	0.97	0.04	35,35,35,35	0
57	MG	1A	3276	1/1	0.97	0.18	21,21,21,21	0
57	MG	1A	3371	1/1	0.97	0.05	24,24,24,24	0
57	MG	1A	3040	1/1	0.97	0.13	27,27,27,27	0
57	MG	1A	3904	1/1	0.97	0.11	38,38,38,38	0
57	MG	1A	3373	1/1	0.97	0.08	9,9,9,9	0
57	MG	1A	3145	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	3279	1/1	0.97	0.04	16,16,16,16	0
57	MG	1A	3624	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3909	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3494	1/1	0.97	0.08	13,13,13,13	0
57	MG	2A	3097	1/1	0.97	0.08	35,35,35,35	0
57	MG	1A	3087	1/1	0.97	0.16	32,32,32,32	0
57	MG	1U	203	1/1	0.97	0.29	27,27,27,27	0
57	MG	1A	3913	1/1	0.97	0.15	23,23,23,23	0
57	MG	1A	3032	1/1	0.97	0.05	27,27,27,27	0
57	MG	2A	3102	1/1	0.97	0.12	28,28,28,28	0
57	MG	2A	3344	1/1	0.97	0.07	35,35,35,35	0
57	MG	2A	3612	1/1	0.97	0.06	42,42,42,42	0
57	MG	1A	3211	1/1	0.97	0.05	24,24,24,24	0
57	MG	1A	3212	1/1	0.97	0.06	28,28,28,28	0
57	MG	1A	3917	1/1	0.97	0.10	35,35,35,35	0
57	MG	2A	3106	1/1	0.97	0.10	51,51,51,51	0
57	MG	2A	3108	1/1	0.97	0.14	43,43,43,43	0
57	MG	1A	3213	1/1	0.97	0.04	21,21,21,21	0
57	MG	2A	3110	1/1	0.97	0.11	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
57	MG	1A	3383	1/1	0.97	0.20	28,28,28,28	0
57	MG	1A	3504	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3921	1/1	0.97	0.08	27,27,27,27	0
57	MG	1A	3151	1/1	0.97	0.11	19,19,19,19	0
57	MG	2a	3150	1/1	0.97	0.07	69,69,69,69	0
57	MG	1a	3149	1/1	0.97	0.13	35,35,35,35	0
57	MG	1A	3506	1/1	0.97	0.05	24,24,24,24	0
57	MG	1a	3151	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3089	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3217	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3926	1/1	0.97	0.04	32,32,32,32	0
57	MG	1A	3638	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3509	1/1	0.97	0.07	15,15,15,15	0
57	MG	2A	3633	1/1	0.97	0.06	46,46,46,46	0
57	MG	2A	3125	1/1	0.97	0.05	51,51,51,51	0
57	MG	2A	3126	1/1	0.97	0.09	39,39,39,39	0
57	MG	1A	3930	1/1	0.97	0.04	25,25,25,25	0
57	MG	1A	3218	1/1	0.97	0.12	33,33,33,33	0
57	MG	1A	3154	1/1	0.97	0.09	41,41,41,41	0
57	MG	2A	3639	1/1	0.97	0.09	41,41,41,41	0
57	MG	1a	3161	1/1	0.97	0.04	52,52,52,52	0
57	MG	2A	3375	1/1	0.97	0.10	47,47,47,47	0
57	MG	2A	3642	1/1	0.97	0.13	46,46,46,46	0
57	MG	2A	3376	1/1	0.97	0.12	37,37,37,37	0
57	MG	1a	3163	1/1	0.97	0.05	43,43,43,43	0
57	MG	1a	3164	1/1	0.97	0.13	55,55,55,55	0
57	MG	2A	3133	1/1	0.97	0.09	45,45,45,45	0
57	MG	1a	3165	1/1	0.97	0.11	48,48,48,48	0
57	MG	1A	3112	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3935	1/1	0.97	0.12	44,44,44,44	0
57	MG	1A	3292	1/1	0.97	0.15	21,21,21,21	0
57	MG	1A	3222	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3516	1/1	0.97	0.09	18,18,18,18	0
57	MG	1A	3223	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3142	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3788	1/1	0.97	0.06	36,36,36,36	0
57	MG	1a	3173	1/1	0.97	0.08	47,47,47,47	0
57	MG	12	3001	1/1	0.97	0.04	30,30,30,30	0
57	MG	1A	3649	1/1	0.97	0.10	19,19,19,19	0
57	MG	2A	3662	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3224	1/1	0.97	0.18	25,25,25,25	0
57	MG	2A	3396	1/1	0.97	0.17	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
57	MG	1a	3177	1/1	0.97	0.17	49,49,49,49	0
57	MG	1A	3791	1/1	0.97	0.20	28,28,28,28	0
57	MG	2A	3151	1/1	0.97	0.14	32,32,32,32	0
57	MG	1a	3179	1/1	0.97	0.04	41,41,41,41	0
57	MG	2A	3669	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3395	1/1	0.97	0.09	21,21,21,21	0
57	MG	1A	3793	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3156	1/1	0.97	0.15	29,29,29,29	0
57	MG	2A	3405	1/1	0.97	0.14	45,45,45,45	0
57	MG	1A	3053	1/1	0.97	0.08	27,27,27,27	0
57	MG	1A	3227	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3679	1/1	0.97	0.09	29,29,29,29	0
57	MG	2A	3408	1/1	0.97	0.04	25,25,25,25	0
57	MG	1A	3091	1/1	0.97	0.09	38,38,38,38	0
57	MG	2A	3684	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3159	1/1	0.97	0.12	37,37,37,37	0
57	MG	2f	3001	1/1	0.97	0.10	43,43,43,43	0
57	MG	1A	3161	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3659	1/1	0.97	0.10	21,21,21,21	0
57	MG	1A	3959	1/1	0.97	0.04	31,31,31,31	0
57	MG	2A	3164	1/1	0.97	0.11	31,31,31,31	0
57	MG	1A	3801	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3165	1/1	0.97	0.12	23,23,23,23	0
57	MG	1A	3962	1/1	0.97	0.07	10,10,10,10	0
57	MG	1a	3193	1/1	0.97	0.11	43,43,43,43	0
57	MG	1A	3167	1/1	0.97	0.10	28,28,28,28	0
57	MG	1A	3804	1/1	0.97	0.04	16,16,16,16	0
57	MG	1A	3309	1/1	0.97	0.04	24,24,24,24	0
57	MG	2A	3422	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3092	1/1	0.97	0.09	17,17,17,17	0
57	MG	1A	3236	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3535	1/1	0.97	0.13	44,44,44,44	0
57	MG	1a	3010	1/1	0.97	0.06	47,47,47,47	0
57	MG	1a	3202	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3668	1/1	0.97	0.05	22,22,22,22	0
57	MG	2A	3429	1/1	0.97	0.06	42,42,42,42	0
57	MG	1A	3669	1/1	0.97	0.10	37,37,37,37	0
57	MG	1A	3410	1/1	0.97	0.04	18,18,18,18	0
57	MG	1A	3238	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3815	1/1	0.97	0.09	40,40,40,40	0
57	MG	2A	3434	1/1	0.97	0.05	34,34,34,34	0
57	MG	1a	3208	1/1	0.97	0.11	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
57	MG	1A	3816	1/1	0.97	0.05	13,13,13,13	0
57	MG	1A	3817	1/1	0.97	0.05	20,20,20,20	0
57	MG	1A	3412	1/1	0.97	0.06	30,30,30,30	0
57	MG	2A	3366	1/1	0.98	0.06	18,18,18,18	0
57	MG	2A	3015	1/1	0.98	0.10	20,20,20,20	0
57	MG	2A	3368	1/1	0.98	0.14	44,44,44,44	0
57	MG	1A	3769	1/1	0.98	0.11	49,49,49,49	0
57	MG	1A	3576	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3235	1/1	0.98	0.21	26,26,26,26	0
57	MG	2A	3372	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3105	1/1	0.98	0.04	18,18,18,18	0
57	MG	2A	3374	1/1	0.98	0.06	38,38,38,38	0
57	MG	2A	3575	1/1	0.98	0.06	36,36,36,36	0
57	MG	2A	3020	1/1	0.98	0.12	41,41,41,41	0
57	MG	2a	3031	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3237	1/1	0.98	0.05	35,35,35,35	0
57	MG	2A	3022	1/1	0.98	0.05	29,29,29,29	0
57	MG	12	3002	1/1	0.98	0.16	29,29,29,29	0
57	MG	1A	3501	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3196	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3003	1/1	0.98	0.04	19,19,19,19	0
57	MG	2A	3198	1/1	0.98	0.04	31,31,31,31	0
57	MG	2A	3026	1/1	0.98	0.04	46,46,46,46	0
57	MG	2A	3585	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3200	1/1	0.98	0.12	20,20,20,20	0
57	MG	1A	3678	1/1	0.98	0.05	18,18,18,18	0
57	MG	1A	3584	1/1	0.98	0.13	51,51,51,51	0
57	MG	1A	3044	1/1	0.98	0.08	34,34,34,34	0
57	MG	1A	3325	1/1	0.98	0.04	25,25,25,25	0
57	MG	2A	3032	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3682	1/1	0.98	0.16	43,43,43,43	0
57	MG	1B	3008	1/1	0.98	0.13	46,46,46,46	0
57	MG	1a	3136	1/1	0.98	0.03	22,22,22,22	0
57	MG	2A	3395	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3045	1/1	0.98	0.05	10,10,10,10	0
57	MG	2A	3210	1/1	0.98	0.10	35,35,35,35	0
57	MG	1a	3139	1/1	0.98	0.13	38,38,38,38	0
57	MG	1A	3785	1/1	0.98	0.21	24,24,24,24	0
57	MG	2A	3600	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3684	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3434	1/1	0.98	0.03	13,13,13,13	0
57	MG	2A	3402	1/1	0.98	0.08	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3041	1/1	0.98	0.09	44,44,44,44	0
57	MG	1A	3686	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3379	1/1	0.98	0.06	33,33,33,33	0
57	MG	1A	3590	1/1	0.98	0.05	48,48,48,48	0
57	MG	2A	3045	1/1	0.98	0.06	34,34,34,34	0
57	MG	1B	3017	1/1	0.98	0.09	39,39,39,39	0
57	MG	1A	3591	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3329	1/1	0.98	0.05	29,29,29,29	0
57	MG	1B	3020	1/1	0.98	0.05	18,18,18,18	0
57	MG	1A	3593	1/1	0.98	0.06	29,29,29,29	0
57	MG	1A	3037	1/1	0.98	0.05	24,24,24,24	0
57	MG	2a	3070	1/1	0.98	0.18	39,39,39,39	0
57	MG	1A	3144	1/1	0.98	0.06	19,19,19,19	0
57	MG	1a	3153	1/1	0.98	0.04	47,47,47,47	0
57	MG	1A	3332	1/1	0.98	0.03	39,39,39,39	0
57	MG	1A	3441	1/1	0.98	0.06	25,25,25,25	0
57	MG	1a	3013	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3599	1/1	0.98	0.07	8,8,8,8	0
57	MG	1A	3600	1/1	0.98	0.12	34,34,34,34	0
57	MG	1A	3601	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3514	1/1	0.98	0.06	22,22,22,22	0
57	MG	1A	3205	1/1	0.98	0.19	25,25,25,25	0
57	MG	2A	3236	1/1	0.98	0.07	40,40,40,40	0
57	MG	1a	3162	1/1	0.98	0.10	32,32,32,32	0
57	MG	1A	3443	1/1	0.98	0.03	9,9,9,9	0
57	MG	1A	3911	1/1	0.98	0.06	35,35,35,35	0
57	MG	1A	3110	1/1	0.98	0.09	30,30,30,30	0
57	MG	1D	304	1/1	0.98	0.06	15,15,15,15	0
57	MG	1A	3386	1/1	0.98	0.11	36,36,36,36	0
57	MG	1A	3146	1/1	0.98	0.07	26,26,26,26	0
57	MG	1D	308	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3174	1/1	0.98	0.04	26,26,26,26	0
57	MG	1D	310	1/1	0.98	0.09	10,10,10,10	0
57	MG	1A	3809	1/1	0.98	0.05	32,32,32,32	0
57	MG	2a	3093	1/1	0.98	0.08	40,40,40,40	0
57	MG	1A	3521	1/1	0.98	0.04	20,20,20,20	0
57	MG	1A	3448	1/1	0.98	0.08	11,11,11,11	0
57	MG	1A	3147	1/1	0.98	0.09	27,27,27,27	0
57	MG	2A	3251	1/1	0.98	0.08	58,58,58,58	0
57	MG	1A	3524	1/1	0.98	0.08	28,28,28,28	0
57	MG	1A	3249	1/1	0.98	0.07	21,21,21,21	0
57	MG	1E	305	1/1	0.98	0.04	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3071	1/1	0.98	0.11	20,20,20,20	0
57	MG	2a	3103	1/1	0.98	0.05	51,51,51,51	0
57	MG	1a	3036	1/1	0.98	0.09	38,38,38,38	0
57	MG	2a	3105	1/1	0.98	0.11	37,37,37,37	0
57	MG	1A	3177	1/1	0.98	0.03	20,20,20,20	0
57	MG	2a	3107	1/1	0.98	0.06	52,52,52,52	0
57	MG	2A	3447	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	3528	1/1	0.98	0.10	20,20,20,20	0
57	MG	2A	3449	1/1	0.98	0.06	34,34,34,34	0
57	MG	2A	3083	1/1	0.98	0.14	39,39,39,39	0
57	MG	2A	3084	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3716	1/1	0.98	0.09	26,26,26,26	0
57	MG	1A	3293	1/1	0.98	0.10	39,39,39,39	0
57	MG	1A	3294	1/1	0.98	0.09	20,20,20,20	0
57	MG	1A	3038	1/1	0.98	0.17	28,28,28,28	0
57	MG	2A	3658	1/1	0.98	0.09	35,35,35,35	0
57	MG	1F	303	1/1	0.98	0.06	22,22,22,22	0
57	MG	2A	3660	1/1	0.98	0.04	56,56,56,56	0
57	MG	2A	3457	1/1	0.98	0.06	32,32,32,32	0
57	MG	1F	305	1/1	0.98	0.17	26,26,26,26	0
57	MG	1A	3457	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	3150	1/1	0.98	0.04	39,39,39,39	0
57	MG	2A	3461	1/1	0.98	0.08	41,41,41,41	0
57	MG	1a	3047	1/1	0.98	0.09	23,23,23,23	0
57	MG	1A	3932	1/1	0.98	0.11	42,42,42,42	0
57	MG	2A	3464	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3397	1/1	0.98	0.07	22,22,22,22	0
57	MG	1A	3007	1/1	0.98	0.07	19,19,19,19	0
57	MG	1a	3195	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3181	1/1	0.98	0.16	28,28,28,28	0
57	MG	1A	3114	1/1	0.98	0.09	36,36,36,36	0
57	MG	2A	3674	1/1	0.98	0.06	40,40,40,40	0
57	MG	2A	3470	1/1	0.98	0.06	44,44,44,44	0
57	MG	1A	3937	1/1	0.98	0.13	16,16,16,16	0
57	MG	1a	3054	1/1	0.98	0.13	38,38,38,38	0
57	MG	1A	3464	1/1	0.98	0.06	49,49,49,49	0
57	MG	1A	3629	1/1	0.98	0.05	35,35,35,35	0
57	MG	2A	3682	1/1	0.98	0.08	33,33,33,33	0
57	MG	2A	3683	1/1	0.98	0.05	52,52,52,52	0
57	MG	1A	3942	1/1	0.98	0.04	16,16,16,16	0
57	MG	1A	3300	1/1	0.98	0.11	31,31,31,31	0
57	MG	1A	3466	1/1	0.98	0.09	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
57	MG	2A	3107	1/1	0.98	0.25	52,52,52,52	0
57	MG	1A	3467	1/1	0.98	0.09	17,17,17,17	0
57	MG	1A	3349	1/1	0.98	0.12	23,23,23,23	0
57	MG	1N	3006	1/1	0.98	0.08	31,31,31,31	0
57	MG	2A	3111	1/1	0.98	0.12	42,42,42,42	0
57	MG	1A	3219	1/1	0.98	0.16	33,33,33,33	0
57	MG	1A	3470	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3837	1/1	0.98	0.04	35,35,35,35	0
57	MG	1A	3734	1/1	0.98	0.05	58,58,58,58	0
57	MG	1A	3183	1/1	0.98	0.19	26,26,26,26	0
57	MG	1A	3472	1/1	0.98	0.09	20,20,20,20	0
57	MG	1A	3153	1/1	0.98	0.09	22,22,22,22	0
57	MG	1A	3353	1/1	0.98	0.08	24,24,24,24	0
57	MG	2A	3297	1/1	0.98	0.05	40,40,40,40	0
57	MG	2A	3492	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3304	1/1	0.98	0.12	35,35,35,35	0
57	MG	1A	3408	1/1	0.98	0.08	35,35,35,35	0
57	MG	1A	3958	1/1	0.98	0.19	31,31,31,31	0
57	MG	1A	3409	1/1	0.98	0.06	35,35,35,35	0
57	MG	1Q	202	1/1	0.98	0.08	17,17,17,17	0
57	MG	2A	3498	1/1	0.98	0.09	46,46,46,46	0
57	MG	1A	3075	1/1	0.98	0.08	39,39,39,39	0
57	MG	1A	3555	1/1	0.98	0.09	13,13,13,13	0
57	MG	1a	3223	1/1	0.98	0.15	37,37,37,37	0
57	MG	1A	3132	1/1	0.98	0.23	30,30,30,30	0
57	MG	1a	3225	1/1	0.98	0.11	35,35,35,35	0
57	MG	1A	3481	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3648	1/1	0.98	0.05	17,17,17,17	0
57	MG	1A	3062	1/1	0.98	0.06	21,21,21,21	0
57	MG	1A	3650	1/1	0.98	0.04	23,23,23,23	0
57	MG	1a	3230	1/1	0.98	0.09	33,33,33,33	0
57	MG	1S	3002	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3510	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3013	1/1	0.98	0.07	16,16,16,16	0
57	MG	2E	303	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3970	1/1	0.98	0.08	24,24,24,24	0
57	MG	1A	3264	1/1	0.98	0.07	21,21,21,21	0
57	MG	2E	306	1/1	0.98	0.09	40,40,40,40	0
57	MG	1U	201	1/1	0.98	0.08	26,26,26,26	0
57	MG	1l	201	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	3035	1/1	0.98	0.15	25,25,25,25	0
57	MG	2A	3517	1/1	0.98	0.06	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
57	MG	2F	3005	1/1	0.98	0.15	39,39,39,39	0
57	MG	1A	3973	1/1	0.98	0.15	25,25,25,25	0
57	MG	2a	3188	1/1	0.98	0.04	47,47,47,47	0
57	MG	2A	3145	1/1	0.98	0.08	37,37,37,37	0
57	MG	1A	3752	1/1	0.98	0.05	18,18,18,18	0
57	MG	2A	3521	1/1	0.98	0.05	36,36,36,36	0
57	MG	1V	201	1/1	0.98	0.17	24,24,24,24	0
57	MG	1A	3136	1/1	0.98	0.10	9,9,9,9	0
57	MG	1A	3564	1/1	0.98	0.08	44,44,44,44	0
57	MG	2A	3327	1/1	0.98	0.07	30,30,30,30	0
57	MG	1a	3094	1/1	0.98	0.07	48,48,48,48	0
57	MG	1W	201	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3755	1/1	0.98	0.18	21,21,21,21	0
57	MG	1A	3861	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3862	1/1	0.98	0.03	22,22,22,22	0
57	MG	2A	3333	1/1	0.98	0.10	32,32,32,32	0
57	MG	1A	3160	1/1	0.98	0.06	10,10,10,10	0
57	MG	1A	3757	1/1	0.98	0.08	34,34,34,34	0
57	MG	1A	3982	1/1	0.98	0.13	18,18,18,18	0
57	MG	1X	102	1/1	0.98	0.04	22,22,22,22	0
57	MG	1A	3193	1/1	0.98	0.09	32,32,32,32	0
57	MG	1X	104	1/1	0.98	0.09	33,33,33,33	0
57	MG	2A	3161	1/1	0.98	0.07	33,33,33,33	0
57	MG	2A	3341	1/1	0.98	0.09	46,46,46,46	0
57	MG	1X	105	1/1	0.98	0.07	33,33,33,33	0
57	MG	1x	109	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3984	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3567	1/1	0.98	0.07	17,17,17,17	0
57	MG	1A	3042	1/1	0.98	0.16	27,27,27,27	0
57	MG	1A	3569	1/1	0.98	0.08	25,25,25,25	0
57	MG	1A	3570	1/1	0.98	0.04	31,31,31,31	0
57	MG	2A	3169	1/1	0.98	0.05	23,23,23,23	0
57	MG	2A	3002	1/1	0.98	0.15	23,23,23,23	0
57	MG	1A	3421	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3764	1/1	0.98	0.06	35,35,35,35	0
57	MG	2A	3173	1/1	0.98	0.09	37,37,37,37	0
57	MG	2A	3005	1/1	0.98	0.09	37,37,37,37	0
57	MG	1A	3163	1/1	0.98	0.04	37,37,37,37	0
57	MG	2A	3555	1/1	0.98	0.06	44,44,44,44	0
57	MG	1A	3992	1/1	0.98	0.05	25,25,25,25	0
57	MG	2A	3008	1/1	0.98	0.08	37,37,37,37	0
57	MG	10	101	1/1	0.98	0.14	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
57	MG	2A	3179	1/1	0.98	0.12	35,35,35,35	0
58	K	1A	3968	1/1	0.98	0.05	31,31,31,31	0
57	MG	1a	3116	1/1	0.98	0.10	37,37,37,37	0
57	MG	1A	3493	1/1	0.98	0.02	24,24,24,24	0
57	MG	2A	3012	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3164	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3197	1/1	0.98	0.04	26,26,26,26	0
60	ZN	29	501	1/1	0.98	0.04	64,64,64,64	0
60	ZN	2n	501	1/1	0.98	0.05	91,91,91,91	0
61	SF4	1d	501	8/8	0.98	0.05	46,53,55,72	0
61	SF4	2d	501	8/8	0.98	0.04	52,59,68,73	0
57	MG	1A	3076	1/1	0.99	0.12	26,26,26,26	0
57	MG	1A	3928	1/1	0.99	0.11	28,28,28,28	0
57	MG	1A	3166	1/1	0.99	0.13	24,24,24,24	0
57	MG	1A	3354	1/1	0.99	0.12	15,15,15,15	0
57	MG	1A	3993	1/1	0.99	0.15	22,22,22,22	0
57	MG	1A	3438	1/1	0.99	0.03	8,8,8,8	0
57	MG	1A	3671	1/1	0.99	0.03	16,16,16,16	0
57	MG	1F	304	1/1	0.99	0.11	15,15,15,15	0
57	MG	1A	3306	1/1	0.99	0.03	33,33,33,33	0
57	MG	1A	3285	1/1	0.99	0.14	34,34,34,34	0
57	MG	1A	3473	1/1	0.99	0.02	21,21,21,21	0
57	MG	2A	3135	1/1	0.99	0.03	34,34,34,34	0
57	MG	1A	3773	1/1	0.99	0.05	53,53,53,53	0
57	MG	1A	4000	1/1	0.99	0.08	27,27,27,27	0
57	MG	2A	3359	1/1	0.99	0.10	35,35,35,35	0
57	MG	1A	3047	1/1	0.99	0.03	23,23,23,23	0
57	MG	1A	3676	1/1	0.99	0.03	28,28,28,28	0
57	MG	1A	3939	1/1	0.99	0.04	31,31,31,31	0
57	MG	1A	3882	1/1	0.99	0.03	38,38,38,38	0
57	MG	1A	3941	1/1	0.99	0.10	10,10,10,10	0
57	MG	1A	3230	1/1	0.99	0.21	21,21,21,21	0
57	MG	1A	3829	1/1	0.99	0.03	25,25,25,25	0
57	MG	2A	3445	1/1	0.99	0.05	25,25,25,25	0
57	MG	1A	3068	1/1	0.99	0.05	17,17,17,17	0
57	MG	2a	3097	1/1	0.99	0.06	25,25,25,25	0
57	MG	1A	3550	1/1	0.99	0.04	25,25,25,25	0
57	MG	1A	3360	1/1	0.99	0.07	21,21,21,21	0
57	MG	1A	3780	1/1	0.99	0.03	28,28,28,28	0
57	MG	1A	3415	1/1	0.99	0.05	17,17,17,17	0
57	MG	2A	3296	1/1	0.99	0.07	29,29,29,29	0
57	MG	1a	3127	1/1	0.99	0.05	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
57	MG	1A	3048	1/1	0.99	0.13	24,24,24,24	0
57	MG	1A	3594	1/1	0.99	0.04	15,15,15,15	0
57	MG	1A	3215	1/1	0.99	0.12	22,22,22,22	0
57	MG	1A	3270	1/1	0.99	0.11	22,22,22,22	0
57	MG	2A	3615	1/1	0.99	0.04	42,42,42,42	0
57	MG	1A	3034	1/1	0.99	0.12	16,16,16,16	0
57	MG	1A	3030	1/1	0.99	0.17	18,18,18,18	0
57	MG	1B	3016	1/1	0.99	0.06	21,21,21,21	0
57	MG	1A	3558	1/1	0.99	0.04	20,20,20,20	0
57	MG	18	104	1/1	0.99	0.08	26,26,26,26	0
57	MG	1A	3897	1/1	0.99	0.03	18,18,18,18	0
57	MG	2A	3384	1/1	0.99	0.04	31,31,31,31	0
57	MG	1a	3138	1/1	0.99	0.04	29,29,29,29	0
57	MG	1P	202	1/1	0.99	0.21	22,22,22,22	0
57	MG	1A	3451	1/1	0.99	0.10	26,26,26,26	0
57	MG	2A	3545	1/1	0.99	0.07	32,32,32,32	0
57	MG	1A	3012	1/1	0.99	0.04	17,17,17,17	0
57	MG	1A	3073	1/1	0.99	0.04	25,25,25,25	0
57	MG	1A	3275	1/1	0.99	0.03	27,27,27,27	0
57	MG	1A	3188	1/1	0.99	0.10	19,19,19,19	0
57	MG	1A	3647	1/1	0.99	0.04	14,14,14,14	0
57	MG	1A	3848	1/1	0.99	0.06	28,28,28,28	0
57	MG	1A	3489	1/1	0.99	0.04	14,14,14,14	0
57	MG	2A	3318	1/1	0.99	0.04	39,39,39,39	0
57	MG	1R	201	1/1	0.99	0.03	26,26,26,26	0
57	MG	1A	3606	1/1	0.99	0.04	31,31,31,31	0
57	MG	1A	3046	1/1	0.99	0.06	15,15,15,15	0
57	MG	1A	3115	1/1	0.99	0.06	24,24,24,24	0
57	MG	1B	3030	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3162	1/1	0.99	0.08	18,18,18,18	0
57	MG	1A	3059	1/1	0.99	0.03	16,16,16,16	0
57	MG	1A	3139	1/1	0.99	0.12	20,20,20,20	0
57	MG	1A	3461	1/1	0.99	0.05	19,19,19,19	0
57	MG	1A	3703	1/1	0.99	0.05	17,17,17,17	0
57	MG	1A	3532	1/1	0.99	0.04	8,8,8,8	0
57	MG	1D	306	1/1	0.99	0.09	27,27,27,27	0
57	MG	1A	3805	1/1	0.99	0.03	22,22,22,22	0
57	MG	1A	3496	1/1	0.99	0.04	14,14,14,14	0
57	MG	1A	3209	1/1	0.99	0.06	25,25,25,25	0
57	MG	1A	3707	1/1	0.99	0.03	25,25,25,25	0
57	MG	1A	3498	1/1	0.99	0.05	17,17,17,17	0
57	MG	2A	3652	1/1	0.99	0.03	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
57	MG	2A	3571	1/1	0.99	0.08	35,35,35,35	0
57	MG	1A	3326	1/1	0.99	0.03	26,26,26,26	0
57	MG	2A	3117	1/1	0.99	0.06	35,35,35,35	0
57	MG	1A	3432	1/1	0.99	0.03	25,25,25,25	0
60	ZN	1Y	202	1/1	0.99	0.03	61,61,61,61	0
60	ZN	14	501	1/1	0.99	0.04	68,68,68,68	0
60	ZN	15	101	1/1	0.99	0.04	35,35,35,35	0
60	ZN	19	501	1/1	0.99	0.03	40,40,40,40	0
60	ZN	1n	501	1/1	0.99	0.06	55,55,55,55	0
57	MG	1A	3327	1/1	0.99	0.03	24,24,24,24	0
57	MG	2A	3192	1/1	0.99	0.10	26,26,26,26	0
60	ZN	25	501	1/1	0.99	0.04	48,48,48,48	0
60	ZN	26	501	1/1	0.99	0.05	56,56,56,56	0
57	MG	1A	3378	1/1	0.99	0.06	9,9,9,9	0
57	MG	1A	3664	1/1	0.99	0.04	16,16,16,16	0
57	MG	1A	3621	1/1	0.99	0.03	38,38,38,38	0
57	MG	1A	3666	1/1	0.99	0.03	16,16,16,16	0
57	MG	1A	3023	1/1	1.00	0.01	14,14,14,14	0
57	MG	1A	3581	1/1	1.00	0.10	20,20,20,20	0
57	MG	1A	3946	1/1	1.00	0.03	19,19,19,19	0
57	MG	2A	3385	1/1	1.00	0.06	34,34,34,34	0
60	ZN	16	501	1/1	1.00	0.02	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.