



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 03:17 PM EDT

PDB ID : 8FC5 / pdb_00008fc5
Title : Crystal structure of the A2058-N6-dimethylated *Thermus thermophilus* 70S ribosome in complex with protein Y, hygromycin A, and azithromycin at 2.65Å resolution
Authors : Chen, C.-W.; Syroegin, E.A.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on : 2022-12-01
Resolution : 2.65 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

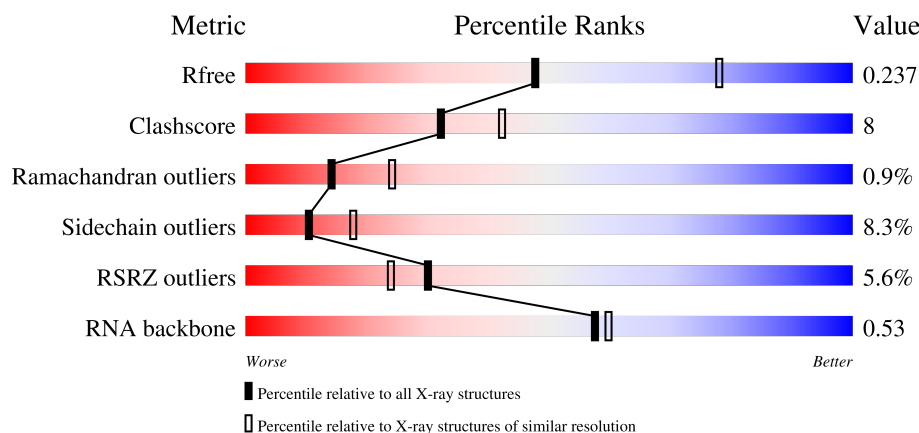
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



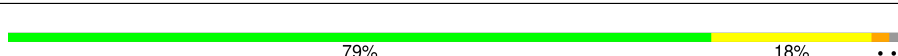
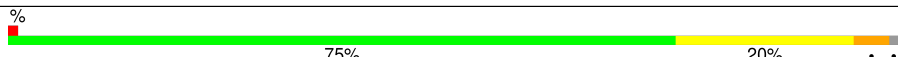
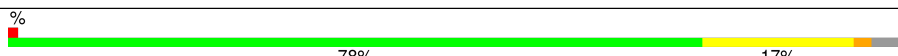
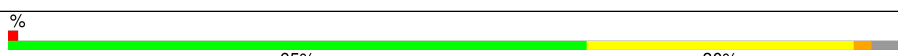
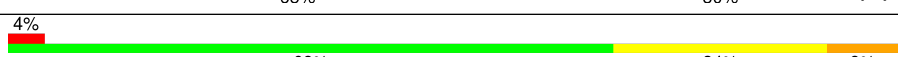
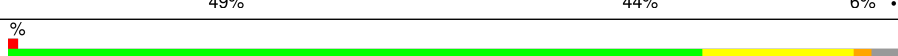
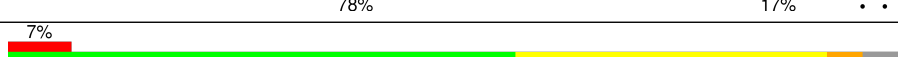
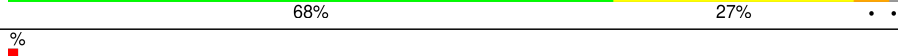
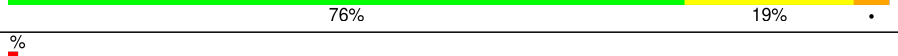
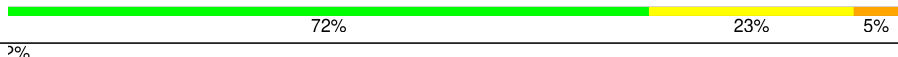
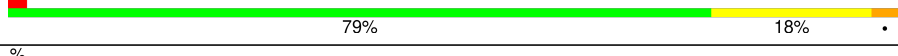
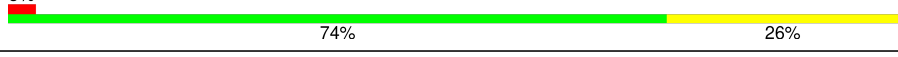
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)
RNA backbone	3983	1090 (2.90-2.42)

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% 67% 26% 6%
1	2A	2915	5% 62% 29% 7%
2	1B	121	% 69% 26% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
14	2S	112	

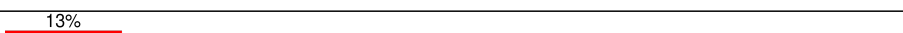
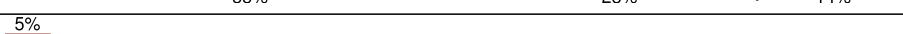
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
27	15	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
39	2h	138	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
52	1u	27	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	2u	27	
53	1y	113	
53	2y	113	

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
54	MG	1A	3601	-	-	-	X
54	MG	2A	3090	-	-	-	X
54	MG	2A	3206	-	-	-	X
54	MG	2a	3085	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 296864 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	2872	Total	C	N	O	P	0	0	0
			61871	27542	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61759	27492	11552	19850	2865			

- 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
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- 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
			2131	1346	422	360	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
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	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	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	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
			1121	722	208	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
			877	553	175	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
			775	498	141	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
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	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
			592	368	119	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
			546	346	96	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
			536	342	98	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
			459	288	90	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	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- 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
			1842	1175	330	332	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
			1558	979	305	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
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	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
			1133	716	214	199	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
			814	516	144	151	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
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	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
			1098	694	210	192	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
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- 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
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	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
			834	520	156	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	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	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
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	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
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	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 protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1031	Total	Mg	0	0
			1031	1031		
54	1B	29	Total	Mg	0	0
			29	29		
54	1D	18	Total	Mg	0	0
			18	18		
54	1E	10	Total	Mg	0	0
			10	10		
54	1F	18	Total	Mg	0	0
			18	18		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	2	Total	Mg	0	0
			2	2		
54	1N	4	Total	Mg	0	0
			4	4		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	7	Total	Mg	0	0
			7	7		
54	1Q	5	Total	Mg	0	0
			5	5		
54	1R	5	Total	Mg	0	0
			5	5		
54	1S	1	Total	Mg	0	0
			1	1		
54	1T	6	Total	Mg	0	0
			6	6		
54	1U	7	Total	Mg	0	0
			7	7		
54	1V	4	Total	Mg	0	0
			4	4		
54	1W	4	Total	Mg	0	0
			4	4		
54	1X	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1Y	1	Total	Mg	0	0
			1	1		
54	1Z	1	Total	Mg	0	0
			1	1		
54	10	6	Total	Mg	0	0
			6	6		
54	11	5	Total	Mg	0	0
			5	5		
54	13	3	Total	Mg	0	0
			3	3		
54	15	8	Total	Mg	0	0
			8	8		
54	17	7	Total	Mg	0	0
			7	7		
54	18	2	Total	Mg	0	0
			2	2		
54	19	3	Total	Mg	0	0
			3	3		
54	1a	281	Total	Mg	0	0
			281	281		
54	1b	1	Total	Mg	0	0
			1	1		
54	1d	2	Total	Mg	0	0
			2	2		
54	1e	3	Total	Mg	0	0
			3	3		
54	1f	2	Total	Mg	0	0
			2	2		
54	1g	3	Total	Mg	0	0
			3	3		
54	1h	2	Total	Mg	0	0
			2	2		
54	1i	1	Total	Mg	0	0
			1	1		
54	1l	2	Total	Mg	0	0
			2	2		
54	1m	1	Total	Mg	0	0
			1	1		
54	1n	3	Total	Mg	0	0
			3	3		
54	1o	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

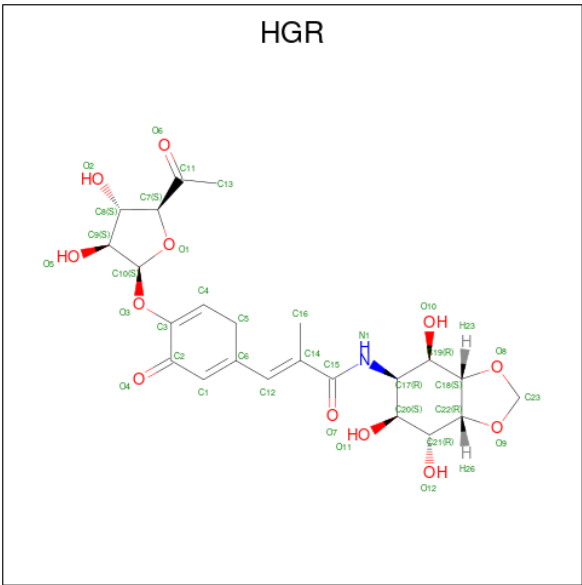
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1t	1	Total 1	Mg 1	0	0
54	1u	1	Total 1	Mg 1	0	0
54	1y	3	Total 3	Mg 3	0	0
54	2A	711	Total 711	Mg 711	0	0
54	2B	18	Total 18	Mg 18	0	0
54	2D	9	Total 9	Mg 9	0	0
54	2E	5	Total 5	Mg 5	0	0
54	2F	4	Total 4	Mg 4	0	0
54	2G	2	Total 2	Mg 2	0	0
54	2I	1	Total 1	Mg 1	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2P	1	Total 1	Mg 1	0	0
54	2Q	3	Total 3	Mg 3	0	0
54	2R	1	Total 1	Mg 1	0	0
54	2T	3	Total 3	Mg 3	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0
54	2Y	1	Total 1	Mg 1	0	0
54	20	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

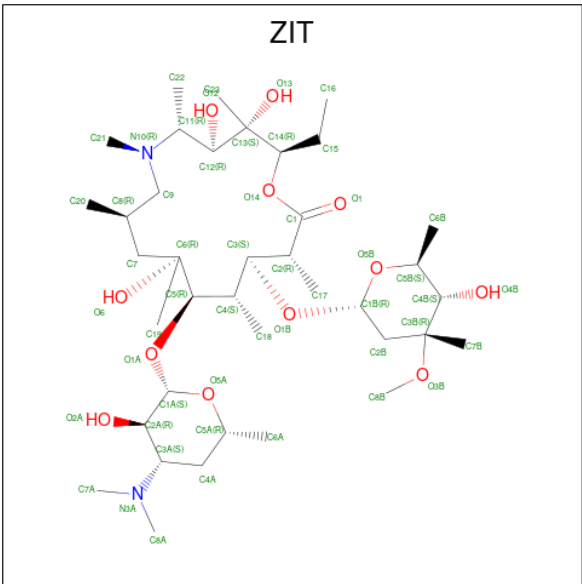
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	21	1	Total 1	Mg 1	0	0
54	23	1	Total 1	Mg 1	0	0
54	25	1	Total 1	Mg 1	0	0
54	27	1	Total 1	Mg 1	0	0
54	28	2	Total 2	Mg 2	0	0
54	2a	182	Total 182	Mg 182	0	0
54	2e	2	Total 2	Mg 2	0	0
54	2f	1	Total 1	Mg 1	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2k	1	Total 1	Mg 1	0	0
54	2l	1	Total 1	Mg 1	0	0
54	2n	1	Total 1	Mg 1	0	0
54	2t	1	Total 1	Mg 1	0	0

- Molecule 55 is Hygromycin A (CCD ID: HGR) (formula: $C_{23}H_{29}NO_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	1A	1	Total	C	N	O	0	0
			36	23	1	12		
55	2A	1	Total	C	N	O	0	0
			36	23	1	12		

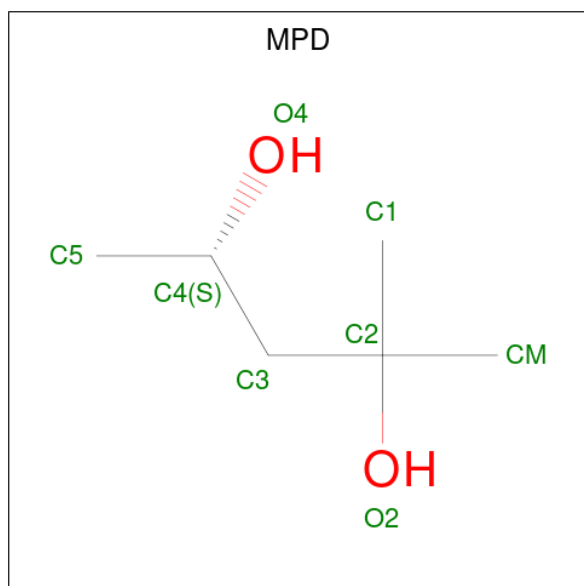
- Molecule 56 is AZITHROMYCIN (CCD ID: ZIT) (formula: $C_{38}H_{72}N_2O_{12}$) (labeled as "Ligand of Interest" by depositor).



Continued from previous page...

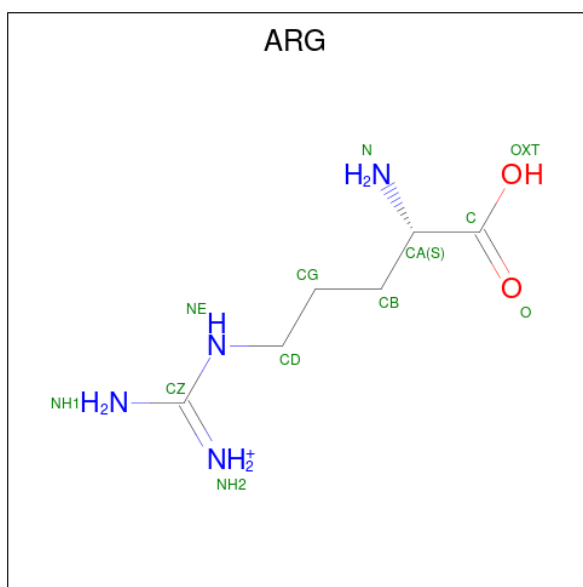
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	2A	1	Total	C	N	O	0	0
			52	38	2	12		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1A	1	Total	C	O	0	0
			8	6	2		
57	1T	1	Total	C	O	0	0
			8	6	2		
57	18	1	Total	C	O	0	0
			8	6	2		
57	1a	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 58 is ARGinine (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1B	1	Total	C	N	O	0	0
			12	6	4	2		
58	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

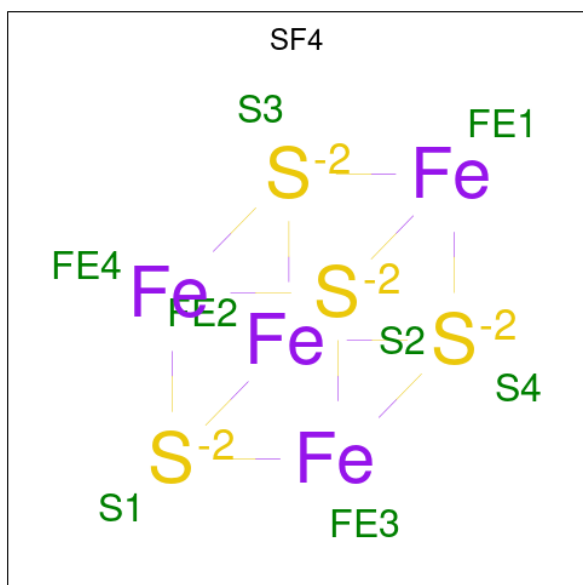
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3571	Total	O	0	0
			3571	3571		
61	1B	89	Total	O	0	0
			89	89		
61	1D	109	Total	O	0	0
			109	109		
61	1E	68	Total	O	0	0
			68	68		
61	1F	61	Total	O	0	0
			61	61		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	10	Total	O	0	0
			10	10		
61	1H	15	Total	O	0	0
			15	15		
61	1I	4	Total	O	0	0
			4	4		
61	1N	46	Total	O	0	0
			46	46		
61	1O	17	Total	O	0	0
			17	17		
61	1P	53	Total	O	0	0
			53	53		
61	1Q	30	Total	O	0	0
			30	30		
61	1R	29	Total	O	0	0
			29	29		
61	1S	7	Total	O	0	0
			7	7		
61	1T	32	Total	O	0	0
			32	32		
61	1U	38	Total	O	0	0
			38	38		
61	1V	26	Total	O	0	0
			26	26		
61	1W	28	Total	O	0	0
			28	28		
61	1X	23	Total	O	0	0
			23	23		
61	1Y	13	Total	O	0	0
			13	13		
61	1Z	9	Total	O	0	0
			9	9		
61	10	19	Total	O	0	0
			19	19		
61	11	17	Total	O	0	0
			17	17		
61	12	11	Total	O	0	0
			11	11		
61	13	20	Total	O	0	0
			20	20		
61	15	28	Total	O	0	0
			28	28		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	16	12	Total 12	O 12	0	0
61	17	12	Total 12	O 12	0	0
61	18	24	Total 24	O 24	0	0
61	19	3	Total 3	O 3	0	0
61	1a	388	Total 388	O 388	0	0
61	1d	9	Total 9	O 9	0	0
61	1f	1	Total 1	O 1	0	0
61	1h	2	Total 2	O 2	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	2	Total 2	O 2	0	0
61	1m	1	Total 1	O 1	0	0
61	1n	2	Total 2	O 2	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1y	3	Total 3	O 3	0	0
61	2A	2161	Total 2161	O 2161	0	0
61	2B	48	Total 48	O 48	0	0
61	2D	43	Total 43	O 43	0	0
61	2E	22	Total 22	O 22	0	0
61	2F	25	Total 25	O 25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2G	1	Total	O	0	0
			1	1		
61	2H	1	Total	O	0	0
			1	1		
61	2I	1	Total	O	0	0
			1	1		
61	2N	5	Total	O	0	0
			5	5		
61	2O	17	Total	O	0	0
			17	17		
61	2P	20	Total	O	0	0
			20	20		
61	2Q	19	Total	O	0	0
			19	19		
61	2R	15	Total	O	0	0
			15	15		
61	2S	4	Total	O	0	0
			4	4		
61	2T	11	Total	O	0	0
			11	11		
61	2U	15	Total	O	0	0
			15	15		
61	2V	3	Total	O	0	0
			3	3		
61	2W	16	Total	O	0	0
			16	16		
61	2X	6	Total	O	0	0
			6	6		
61	2Y	2	Total	O	0	0
			2	2		
61	2Z	6	Total	O	0	0
			6	6		
61	20	5	Total	O	0	0
			5	5		
61	21	14	Total	O	0	0
			14	14		
61	23	3	Total	O	0	0
			3	3		
61	25	8	Total	O	0	0
			8	8		
61	26	3	Total	O	0	0
			3	3		

Continued on next page...

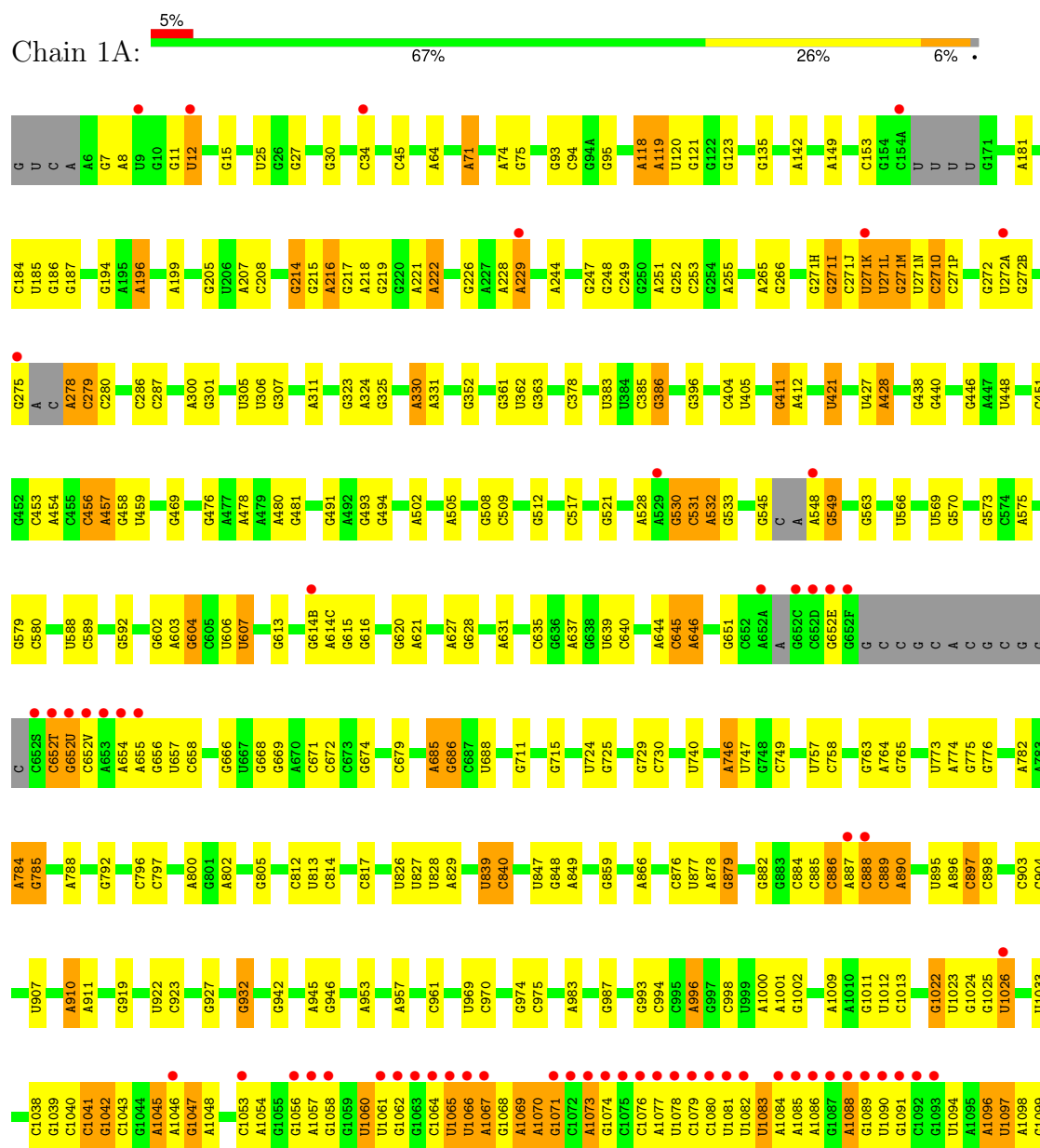
Continued from previous page...

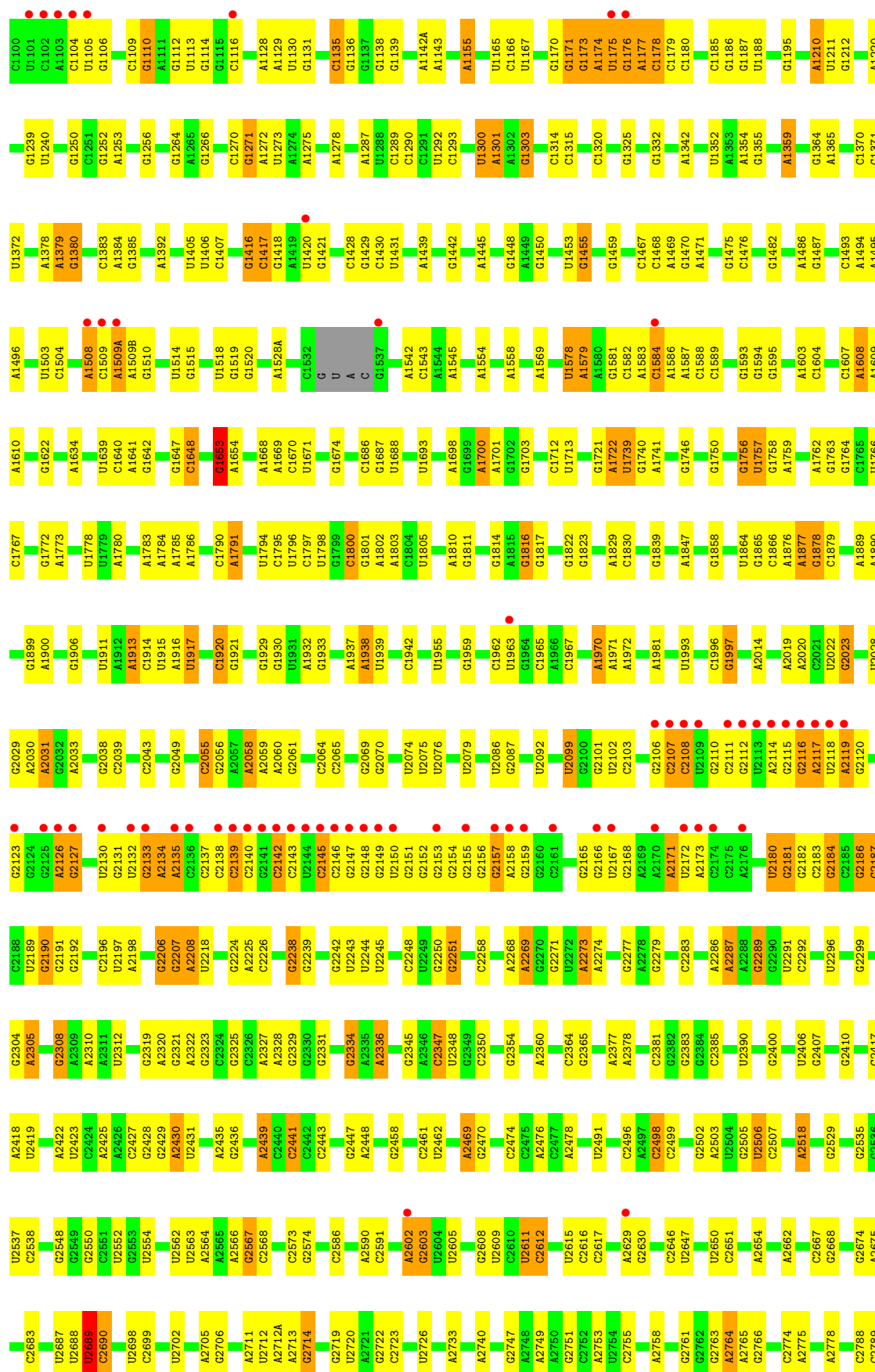
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	27	5	Total 5	O 5	0	0
61	28	8	Total 8	O 8	0	0
61	29	1	Total 1	O 1	0	0
61	2a	394	Total 394	O 394	0	0
61	2d	4	Total 4	O 4	0	0
61	2e	2	Total 2	O 2	0	0
61	2f	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	4	Total 4	O 4	0	0
61	2n	1	Total 1	O 1	0	0
61	2o	3	Total 3	O 3	0	0
61	2p	3	Total 3	O 3	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	5	Total 5	O 5	0	0
61	2t	2	Total 2	O 2	0	0
61	2y	2	Total 2	O 2	0	0

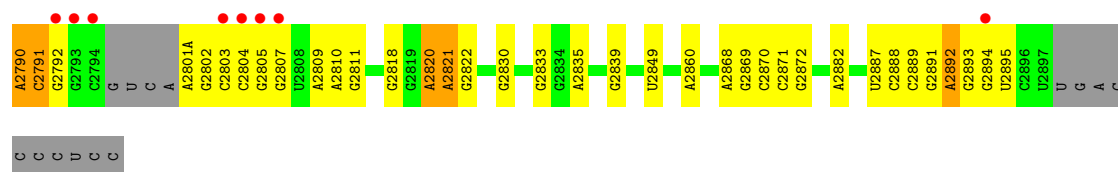
3 Residue-property plots [i](#)

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

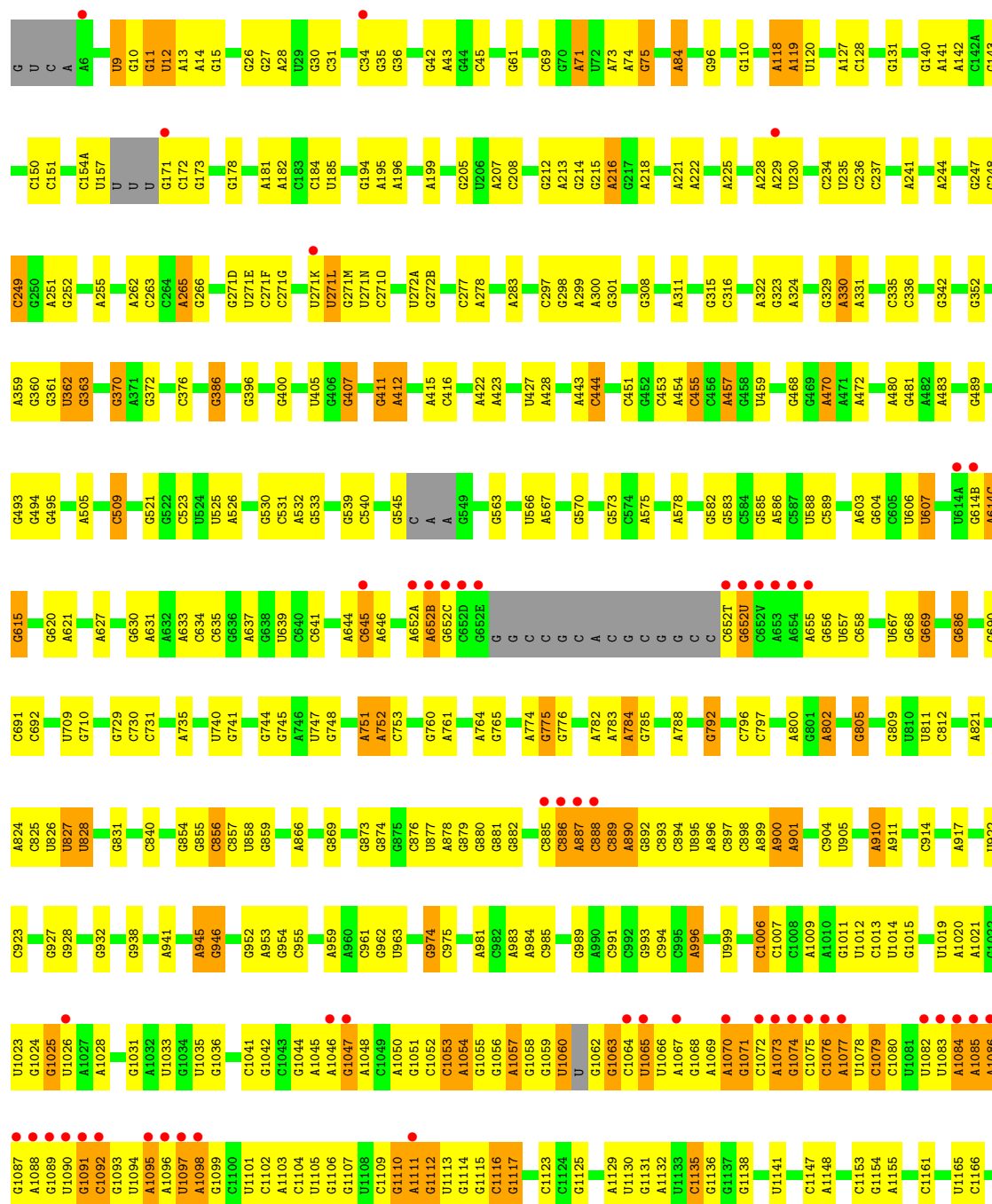
• Molecule 1: 23S Ribosomal RNA



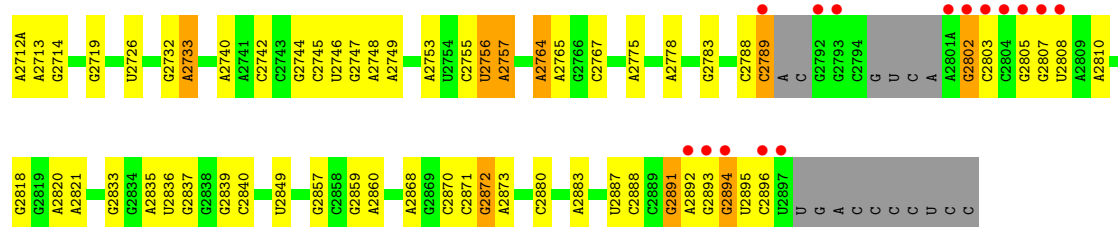




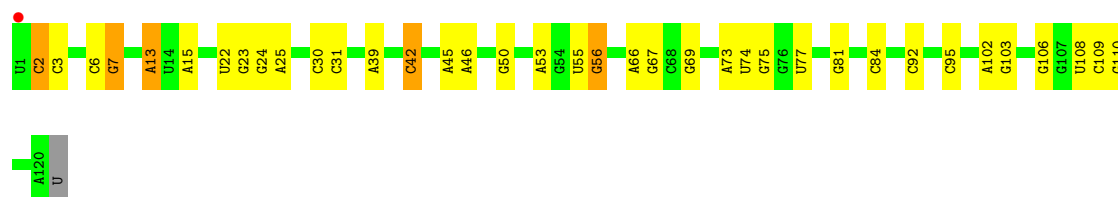
• Molecule 1: 23S Ribosomal RNA



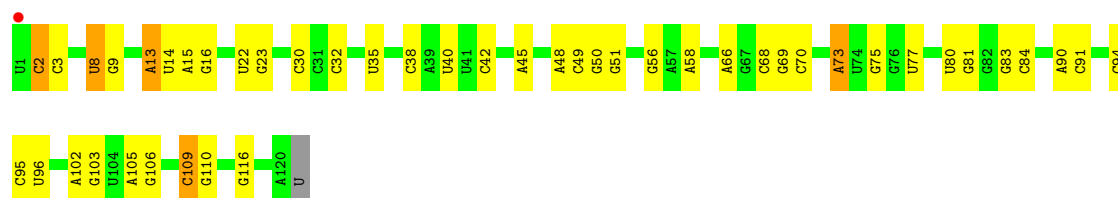




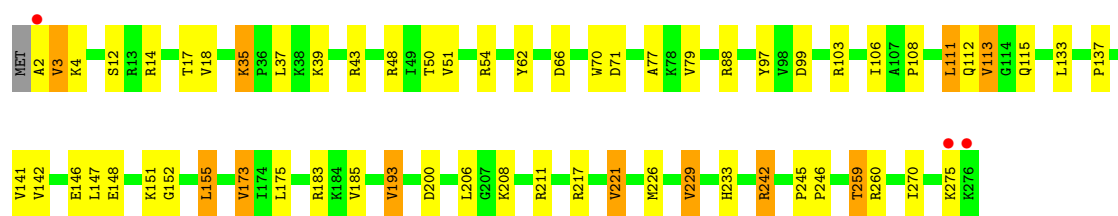
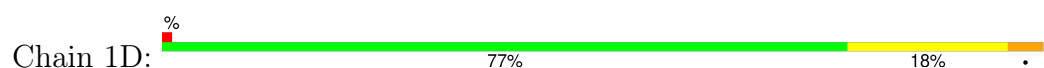
• Molecule 2: 5S Ribosomal RNA



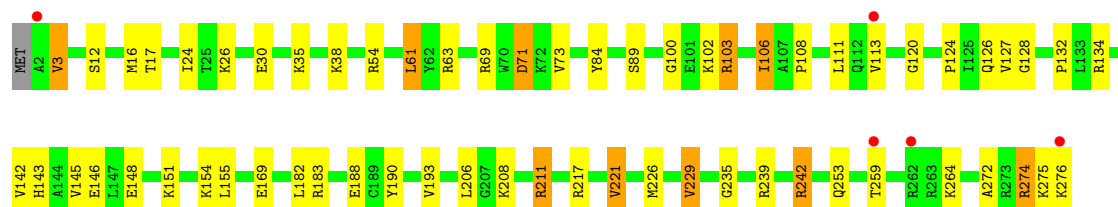
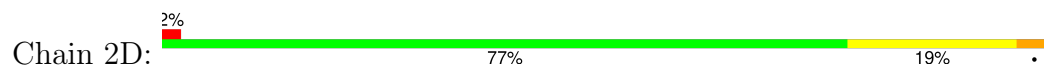
• Molecule 2: 5S Ribosomal RNA



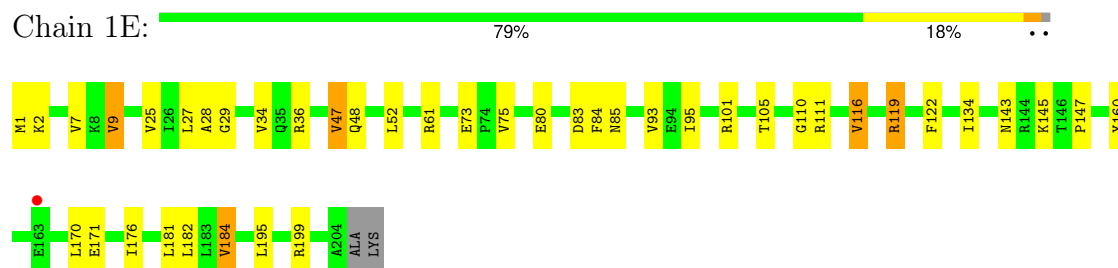
• Molecule 3: 50S ribosomal protein L2



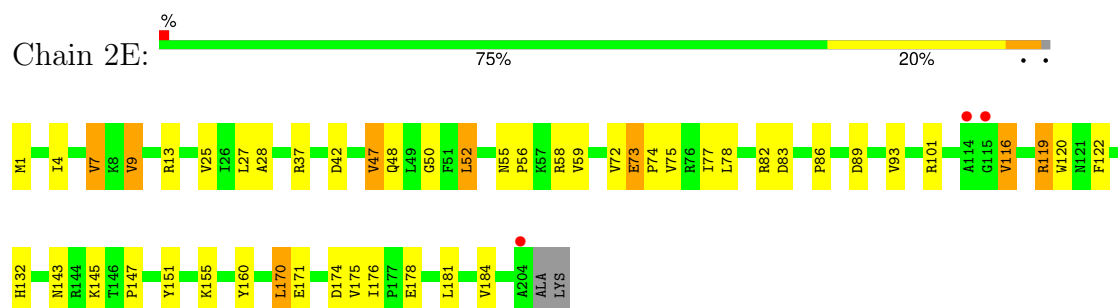
• Molecule 3: 50S ribosomal protein L2



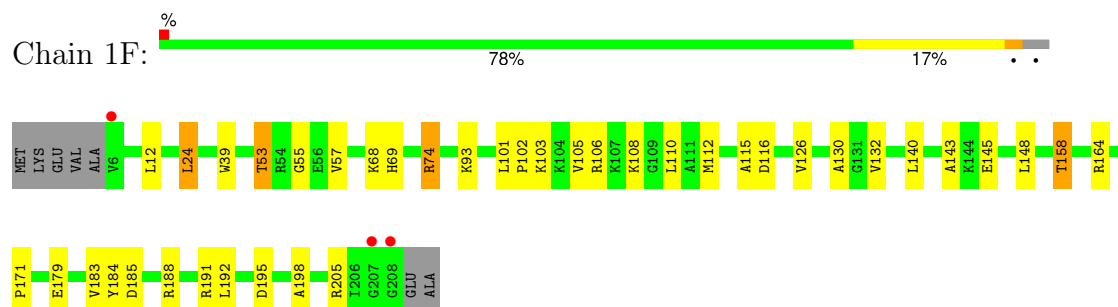
- Molecule 4: 50S ribosomal protein L3



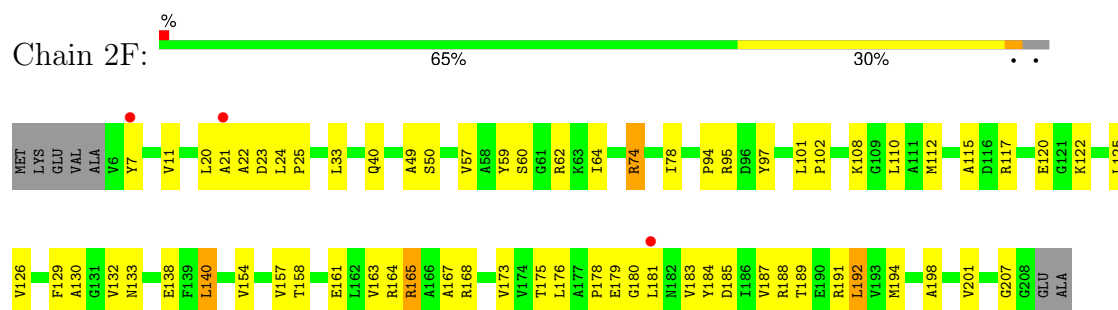
- Molecule 4: 50S ribosomal protein L3



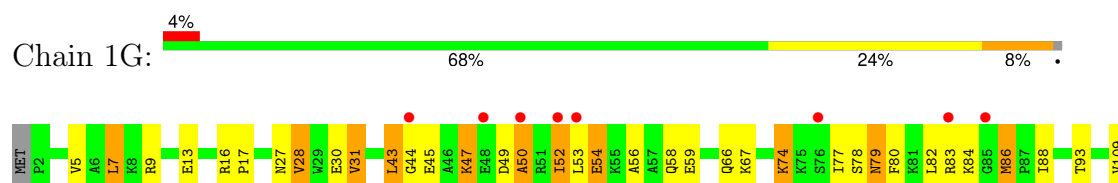
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

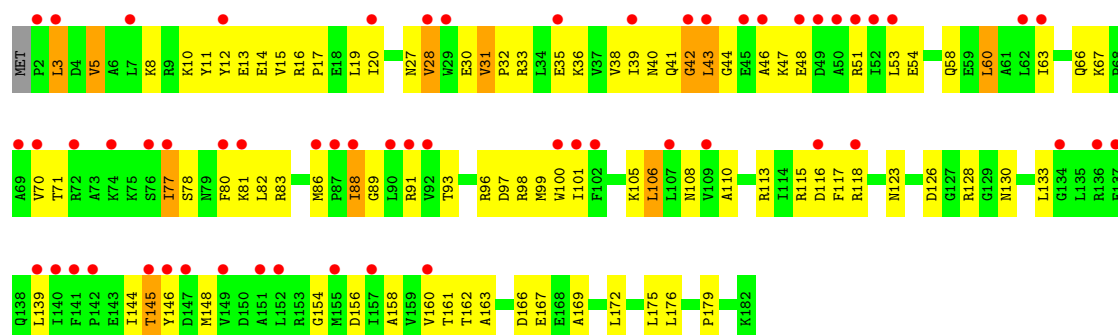


- Molecule 6: 50S ribosomal protein L5

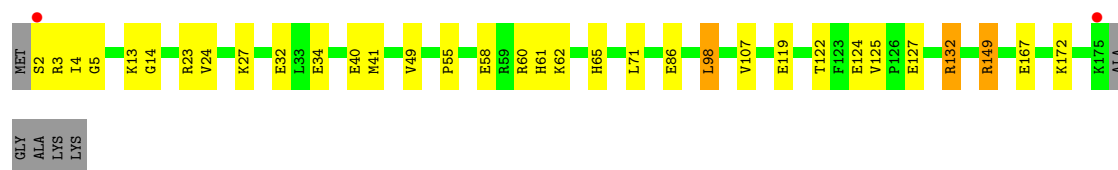
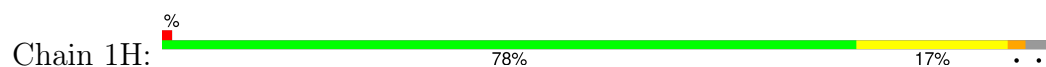




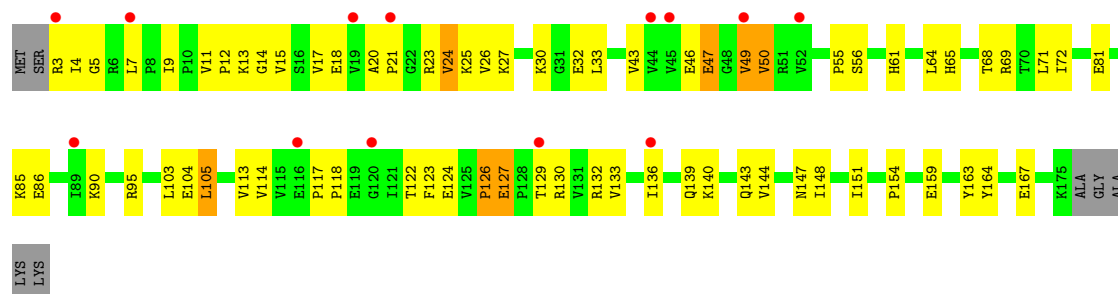
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

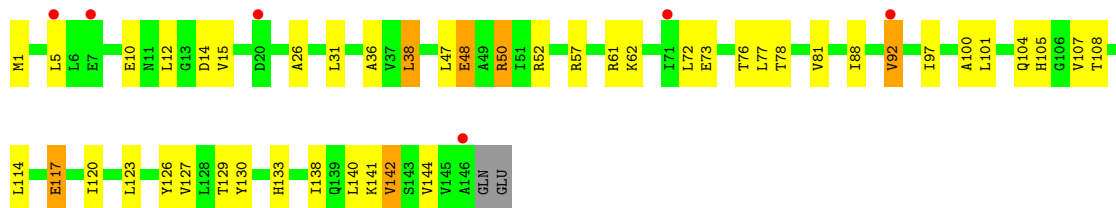


• Molecule 8: 50S ribosomal protein L9

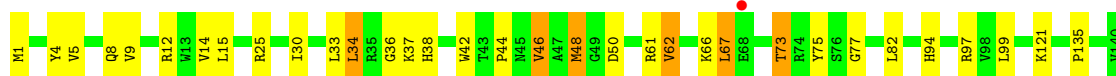
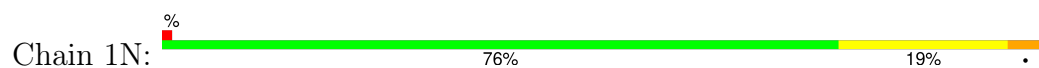




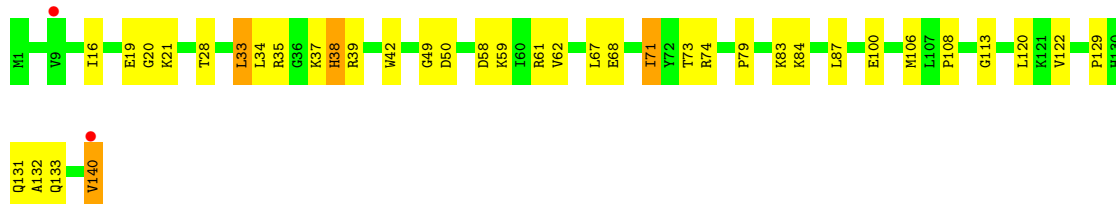
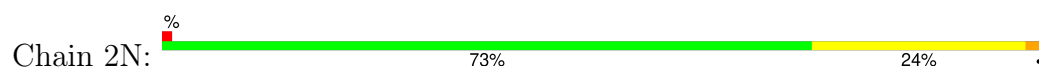
- Molecule 8: 50S ribosomal protein L9



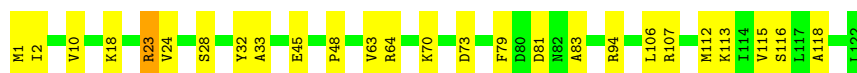
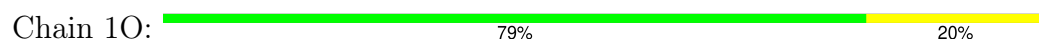
- Molecule 9: 50S ribosomal protein L13



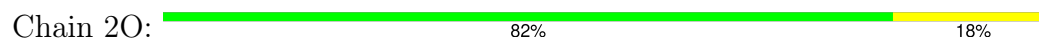
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14

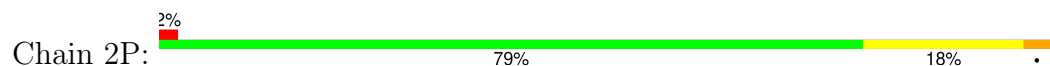


- Molecule 11: 50S ribosomal protein L15

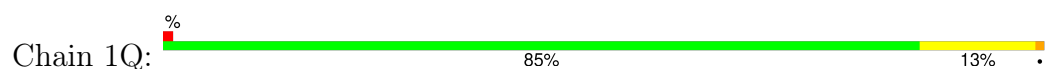




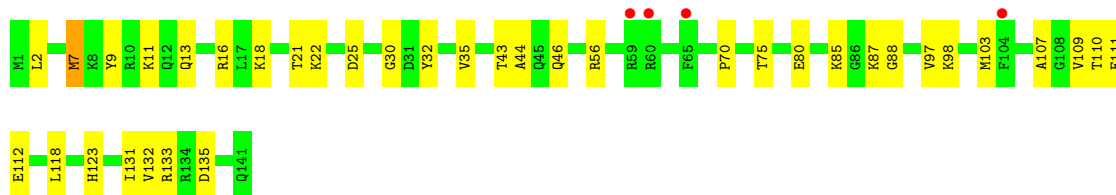
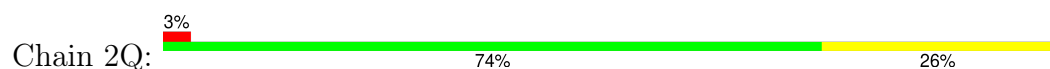
- Molecule 11: 50S ribosomal protein L15



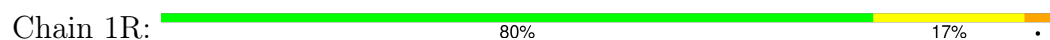
- Molecule 12: 50S ribosomal protein L16



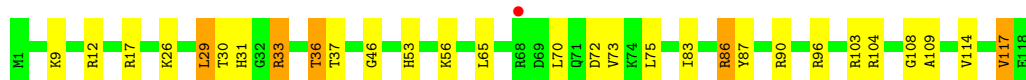
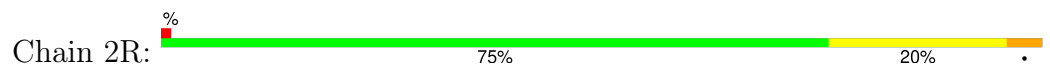
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

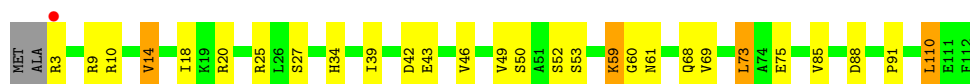


- Molecule 13: 50S ribosomal protein L17

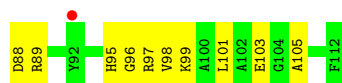


- Molecule 14: 50S ribosomal protein L18

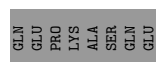
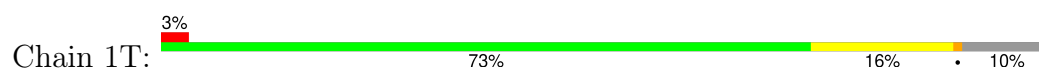




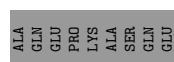
- Molecule 14: 50S ribosomal protein L18



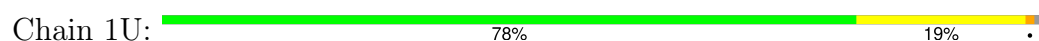
- Molecule 15: 50S ribosomal protein L19



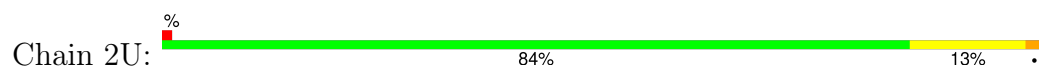
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



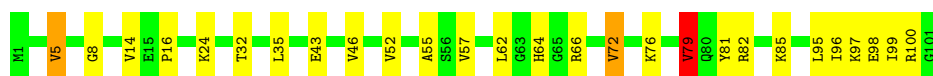
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  74% 24% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  73% 24% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  2% 78% 18% ..



- Molecule 18: 50S ribosomal protein L22

Chain 2W:  % 76% 20% ..



- Molecule 19: 50S ribosomal protein L23

Chain 1X:  3% 74% 23% ..



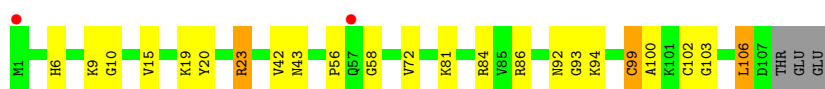
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  3% 73% 25% ..

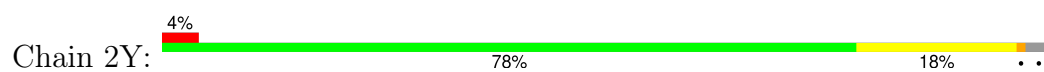


- Molecule 20: 50S ribosomal protein L24

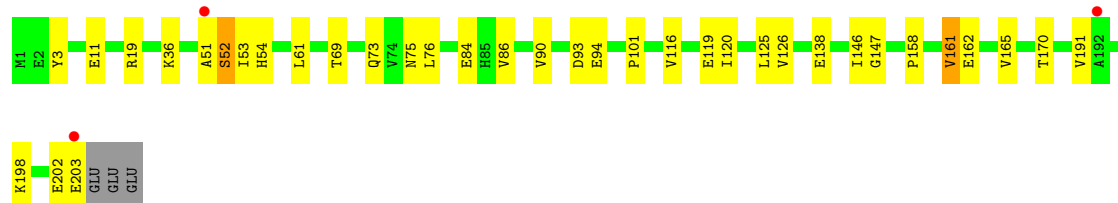
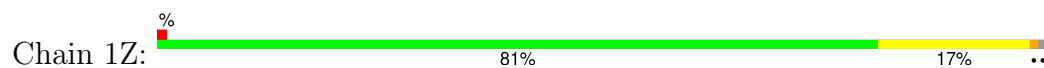
Chain 1Y:  2% 76% 18% ..



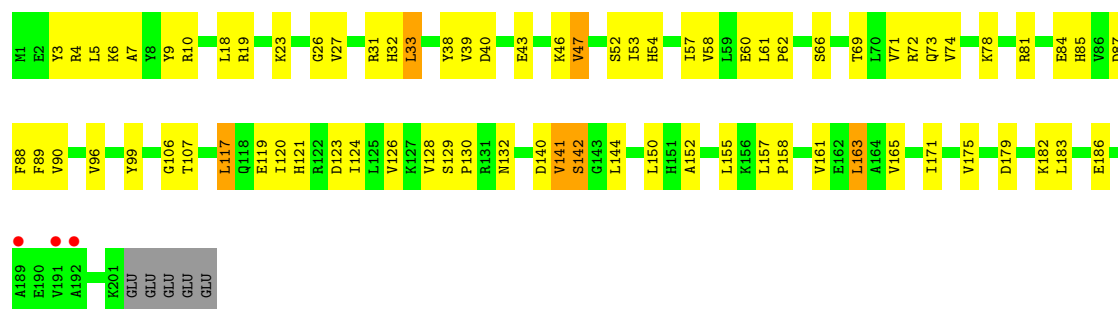
- Molecule 20: 50S ribosomal protein L24



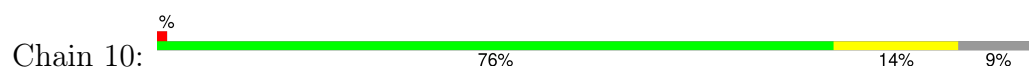
- Molecule 21: 50S ribosomal protein L25



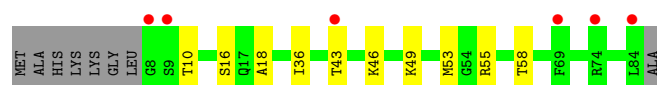
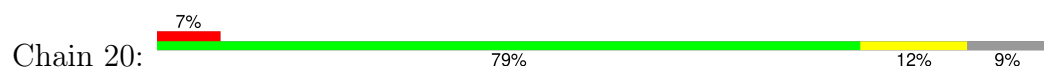
- Molecule 21: 50S ribosomal protein L25



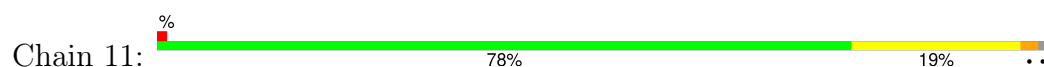
- Molecule 22: 50S ribosomal protein L27

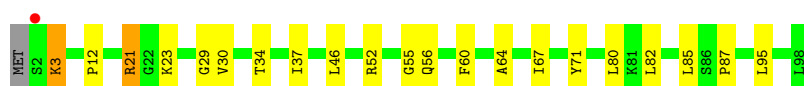


- Molecule 22: 50S ribosomal protein L27

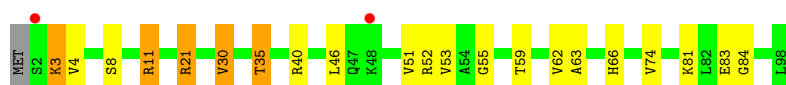
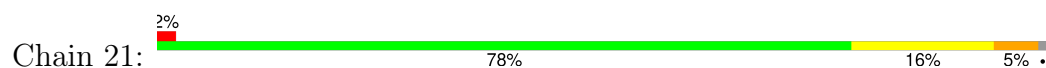


- Molecule 23: 50S ribosomal protein L28

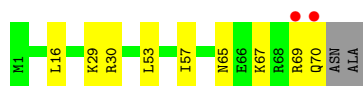
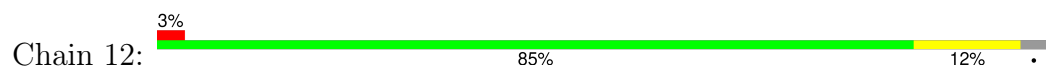




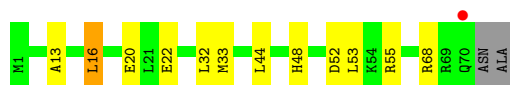
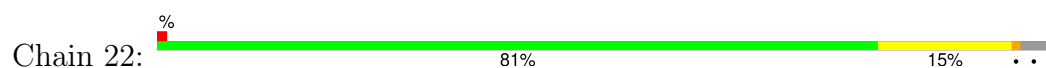
- Molecule 23: 50S ribosomal protein L28



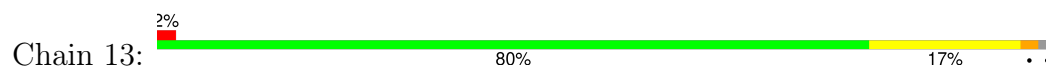
- Molecule 24: 50S ribosomal protein L29



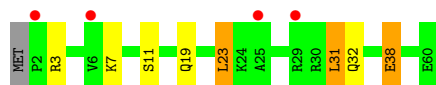
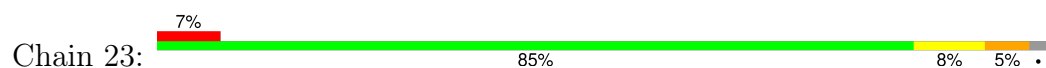
- Molecule 24: 50S ribosomal protein L29



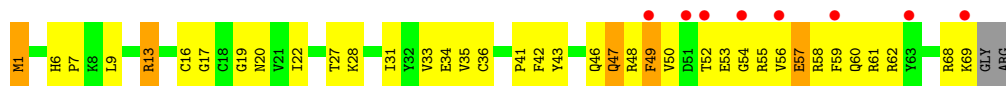
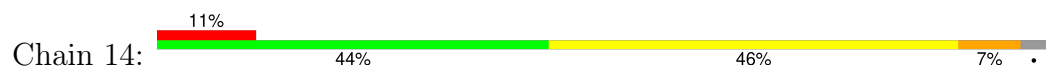
- Molecule 25: 50S ribosomal protein L30



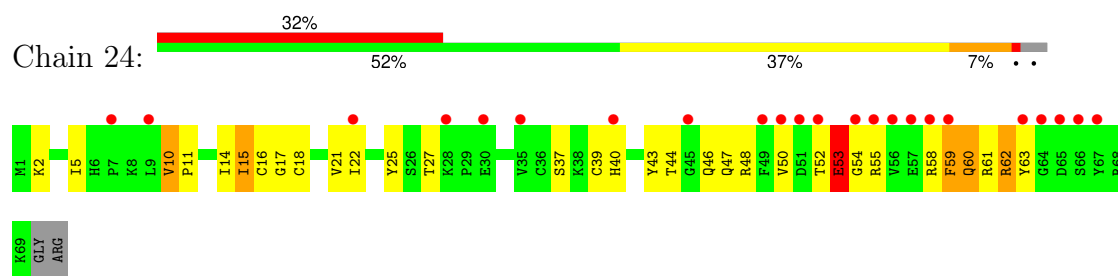
- Molecule 25: 50S ribosomal protein L30



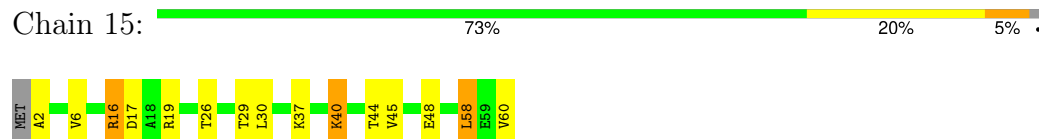
- Molecule 26: 50S ribosomal protein L31



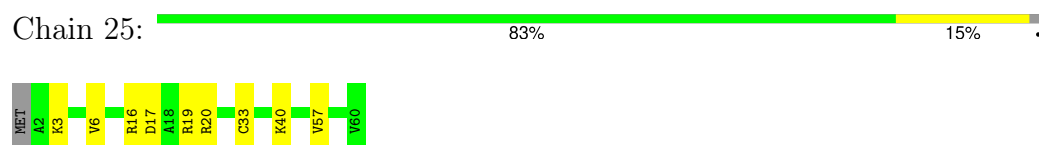
- Molecule 26: 50S ribosomal protein L31



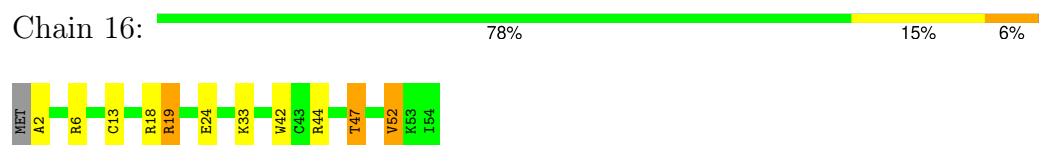
- Molecule 27: 50S ribosomal protein L32



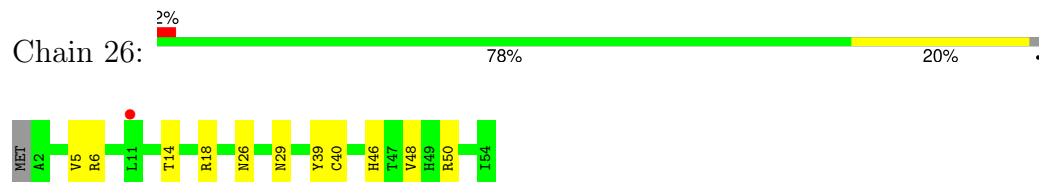
- Molecule 27: 50S ribosomal protein L32



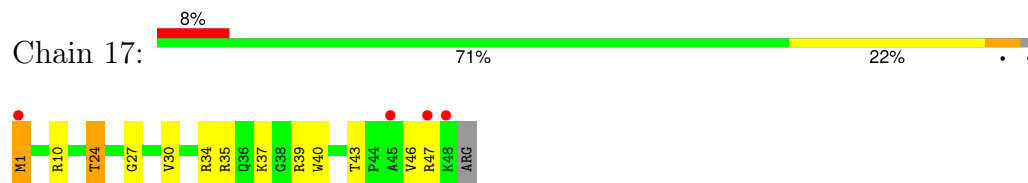
- Molecule 28: 50S ribosomal protein L33



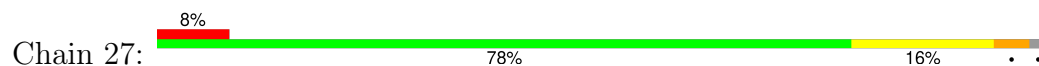
- Molecule 28: 50S ribosomal protein L33

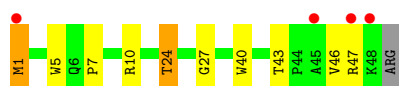


- Molecule 29: 50S ribosomal protein L34



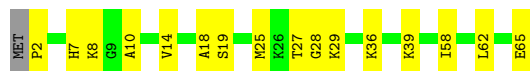
- Molecule 29: 50S ribosomal protein L34





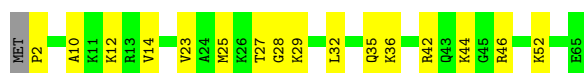
- Molecule 30: 50S ribosomal protein L35

Chain 18: 74% 25% .



- Molecule 30: 50S ribosomal protein L35

Chain 28: 74% 25% .



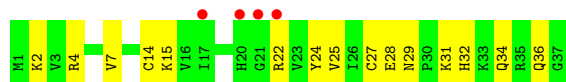
- Molecule 31: 50S ribosomal protein L36

Chain 19: 78% 19% .



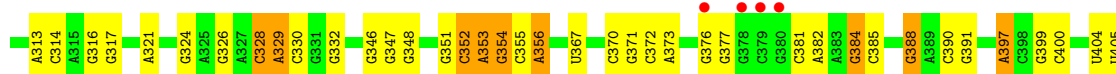
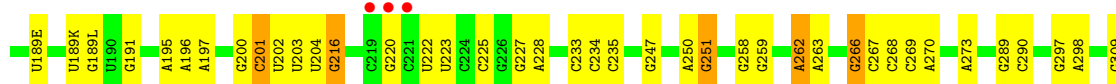
- Molecule 31: 50S ribosomal protein L36

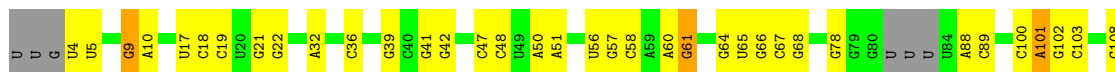
Chain 29: 11% 59% 41%



- Molecule 32: 16S Ribosomal RNA

Chain 1a: 3% 59% 33% 7% .

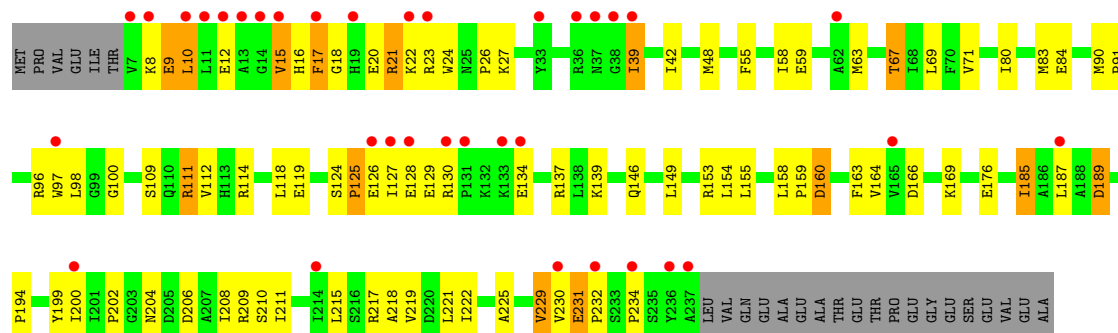




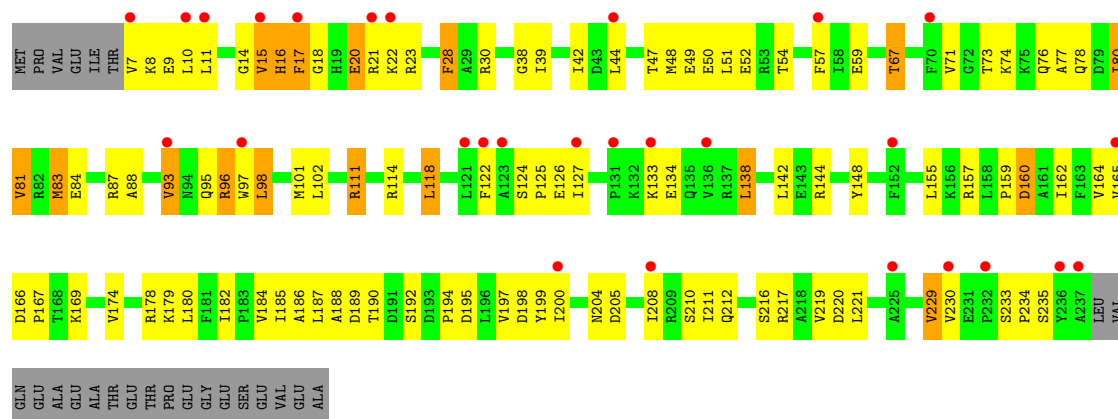
A1363	G1291	U1126	C1051	U991	C749	G644	U551	C443	U367	G227	A109
U1364	U1292	G1127	U1052	U992	G750	C645	U552	C444	U367	A228	A116
G1365	G1293	C1128	G1053	G993	A753	U646	G555	A451	C372	U229	G117
G1366	G1294	C1129	C1054	U920	G755	G649	C556	A452	A373	G230	U118
G1367	G1295	A1130	A1055	C995	C756	A653	G557	A453	G376	G231	C121
G1368	A1299	G1133	G1058	C999	U757	A653	G558	C454	G377	G247	G126
G1369	G1300	G1134	C1059	U1000	G758	C656	G559	C458	A382	G251	A130
G1370	U1301	U1135	C1060	A1001	U759	G657	U560	A461	A383	G254	C131
U1372	U1302	U1136	G1061	G1001A	A766	G657	U561	C470	G384	G255	A141
G1373	C1303	U1137	U1062	G1002	G769	G660	C564	C471	G388	U256	A151
A1374	G1304	G1138	C1063	C932	U774	G661	U565	G476	A389	G257	G156
G1375	G1305	U1139	G1064	G933	G777	G662	G566	G477	G391	G258	G157
U1376	A1306	C1140	U1065	C934	A778	A663	G664	A482	G392	C267	A161
U1377	U1307	A1146	C1066	A995	C779	G664	G665	U498	A397	A279	C163
G1378	C1226	C1147	G1068	A937	U780	U677	A573	C501	C398	C280	U164
G1379	A1227	U1150	U1070	G938	G786	A675	G576	C401	G396	A273	C165
U1380	A1238	A1151	C1071	U942	A790	U677	G577	G402	C403	A288	A172
G1381	U1239	A1152	C1072	U943	A792	G685	G584	G403	U404	G289	U173
G1382	U1240	G1153	C1073	U944	A793	U686	G587	U405	U405	U294	C174
G1383	C1244	G1154	U1077	U945	A794	G688	G596	A509	G406	U303	G175
G1384	A1245	G1155	U1078	G946	C797	G688	C600	C511	G409	U304	C176
A1385	C1246	U1156	G1079	U950	G817	U692	C601	U512	G410	C177	C177
C1386	U1247	A1157	C1080	U951	G818	U692	G610	U513	A411	C178	U179
C1387	A1248	C1158	U1081	G952	A819	A695	U605	U516	A412	C179	U180
G1388	U1251	U1159	G1082	G953	G821	A695	A611	A523	U420	G316	U182
U1391	A1252	A1170	G1084	U954	G828	G703	A614	A523	U421	C317	C187
G1392	C1255	G1171	U1085	U960	G829	G707	G615	A523	U422	C318	C189D
G1393	A1256	C1172	U1086	U961	G836	C708	G616	C528	G423	A321	U189E
G1394	U1257	G1173	U1087	G964	U839	G713	G617	C528	G424	G325	G189L
C1400	G1258	A1179	U1090	A965	U840	C719	C620	A532	G425	A326	U190
C1401	U1259	A1180	C1026	G966	U841	U723	A621	A533	G426	G327	G191
C1402	C1260	G1181	C1027	C967	C848	G724	C623	A533	U427	A329	A195
C1403	C1261	U1182	C1028	A968	C849	U728	C624	C536	U428	G328	A196
C1404	C1262	A1183	C1029	U969	U850	A729	C624	G537	U429	A329	A197
C1407	C1263	U1184	C1030	G970	G851	G730	G625	G538	A430	G332	C201
C1411	C1264	G1187	U1030A	C971	C857	G731	U626	G539	U434	G333	U202
C1412	C1265	A1188	C1030B	G972	U858	A737	G629	G540	C435	A338	U203
C1413	C1266	C1189	C1030C	G973	A860	C738	G631	C541	U437	G351	U204
C1419	C1267	G1190	G1031	A974	G888	G741	A632	C544	G438	G352	G216
G1422	G1271	A1191	G1032	A975	U889	G742	G633	C545	A439	A441	U222
G1423	A1275	C1192	G1033	A976	A901	G742	G633	G546	A442	G354	U223
C1424	G1276	G1193	C1034	A977	G902	C748					
C1431	C1277	U1194	U1035	A978							
G1432	U1278	C1195	C1036	C979							
C1434	A1279	U1196	G1037	C980							
U1435	U1280	U1197	C1038	U981							
G1436	C1282	G1202	U1040	U982							
G1437	G1283	C1203	G1042	A983							
G1438	C1284	U1204	C1043	C984							
C1439	A1285	A1204	U1044	C985							
G1442	A1286	U1205	C1045	A986							
G1442A	U1287	G1206	U1046	G902							
U1446	A1288	C1207	G1047	C989							
A1447				C990							
C1456											



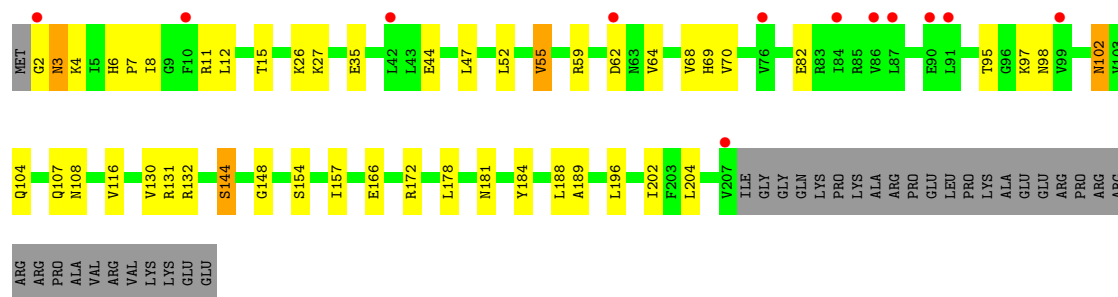
• Molecule 33: 30S ribosomal protein S2



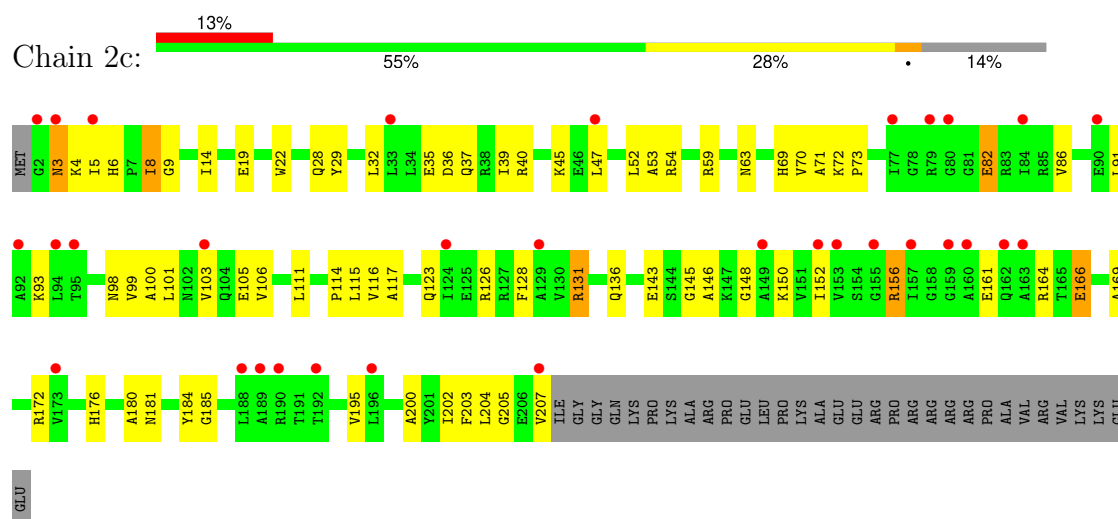
• Molecule 33: 30S ribosomal protein S2



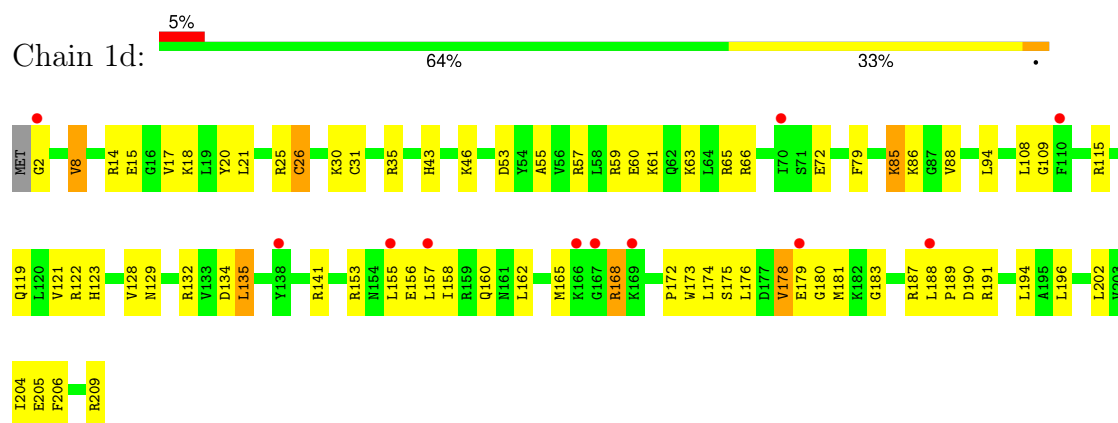
• Molecule 34: 30S ribosomal protein S3



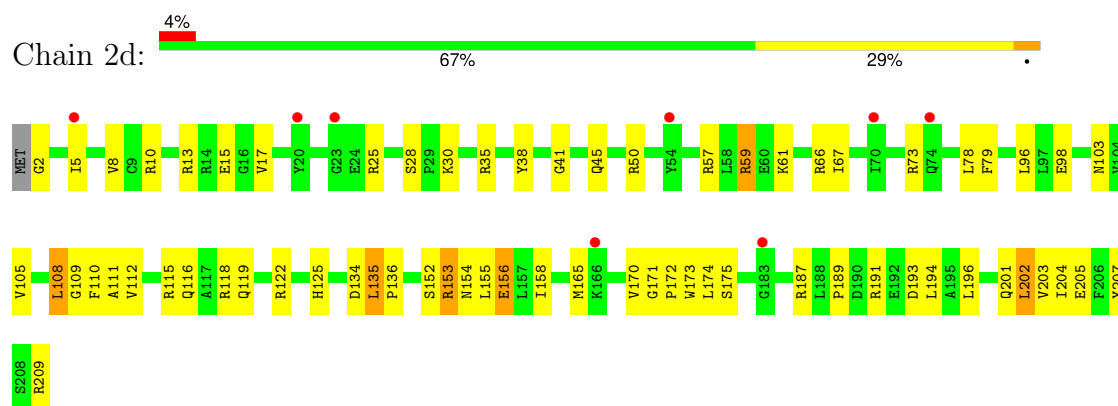
• Molecule 34: 30S ribosomal protein S3



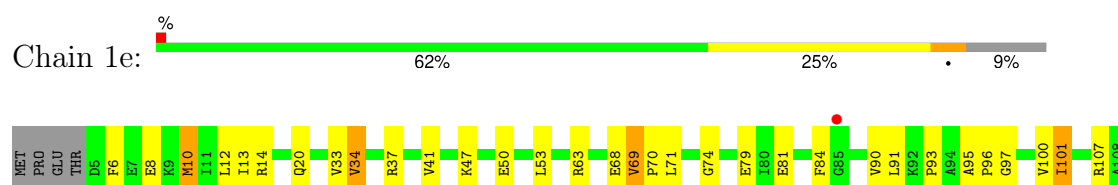
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

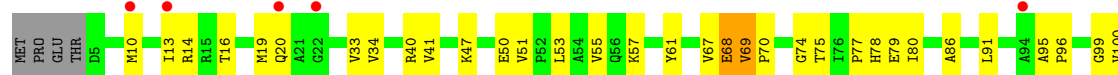


• Molecule 36: 30S ribosomal protein S5

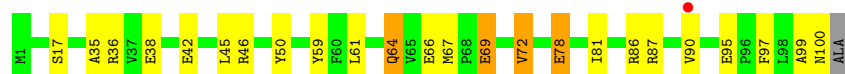
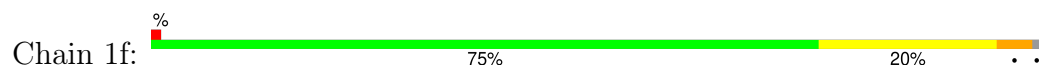




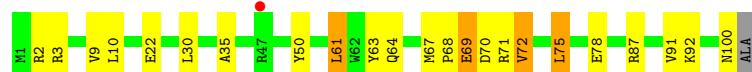
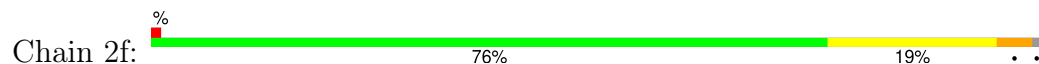
- Molecule 36: 30S ribosomal protein S5



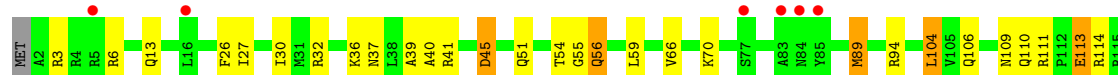
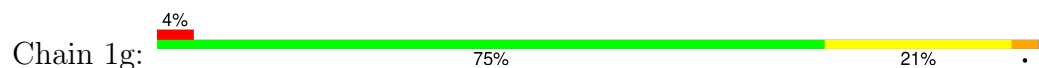
- Molecule 37: 30S ribosomal protein S6



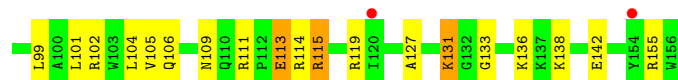
- Molecule 37: 30S ribosomal protein S6



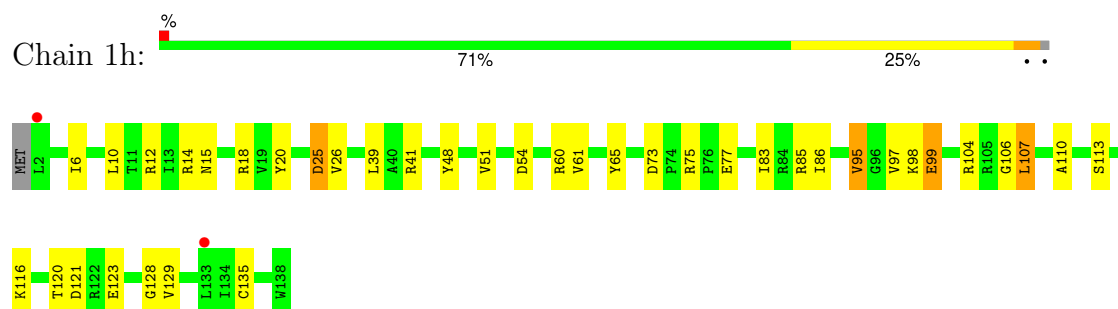
- Molecule 38: 30S ribosomal protein S7



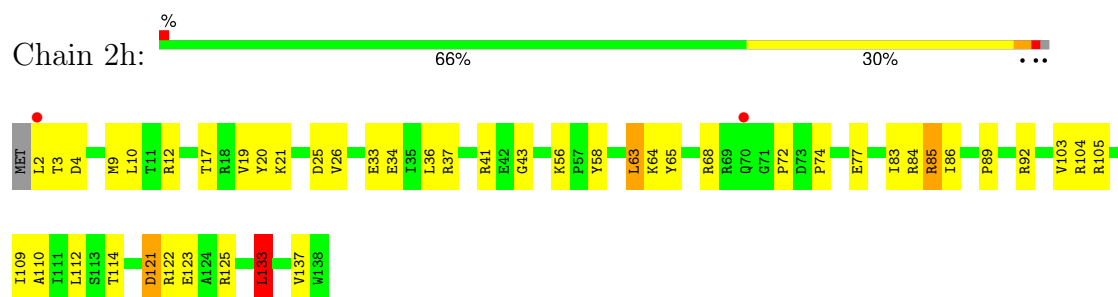
- Molecule 38: 30S ribosomal protein S7



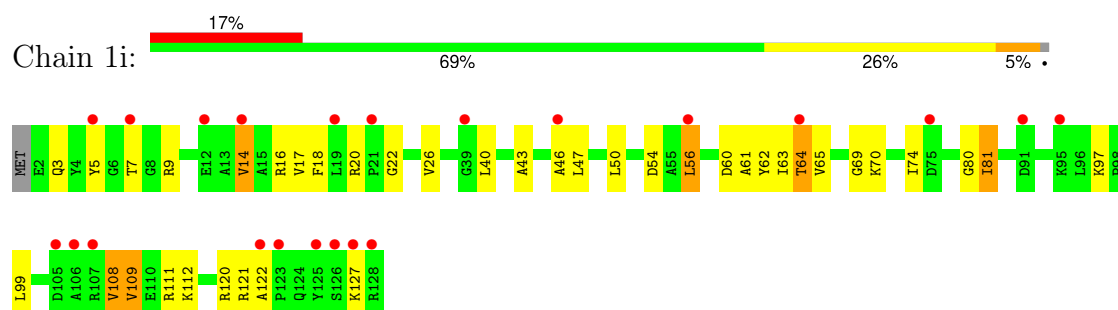
- Molecule 39: 30S ribosomal protein S8



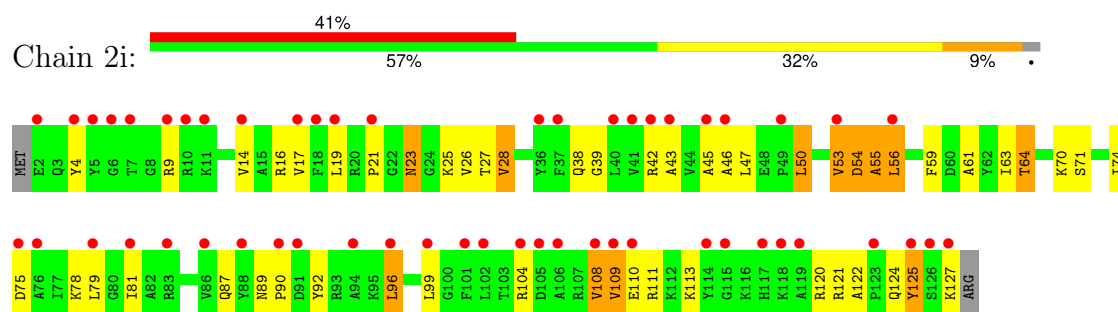
- Molecule 39: 30S ribosomal protein S8



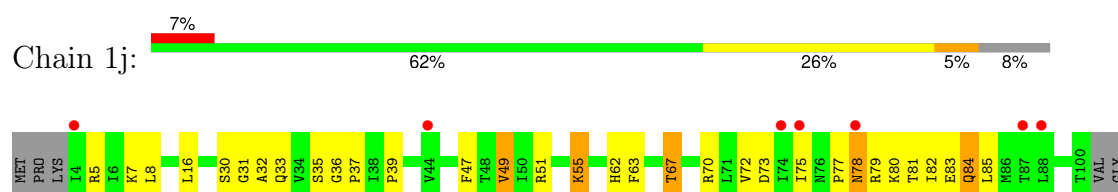
- Molecule 40: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S9

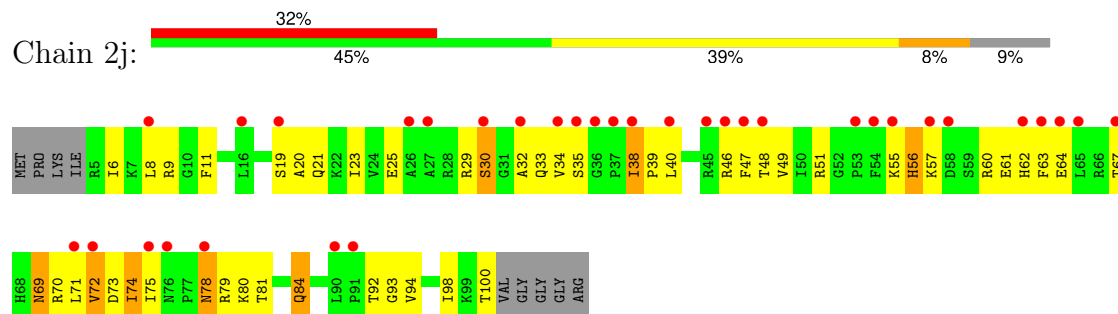


- Molecule 41: 30S ribosomal protein S10

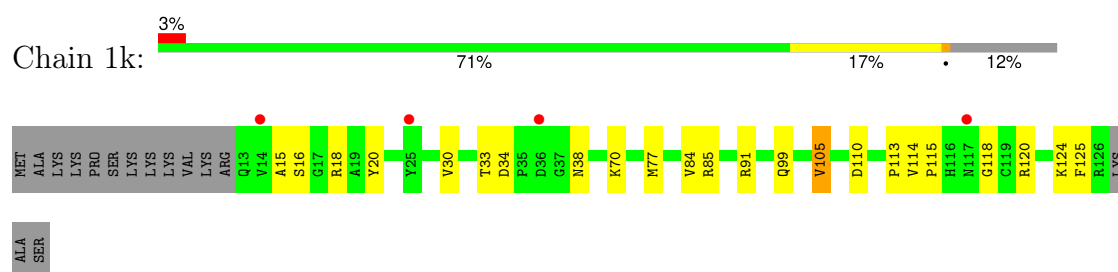


GLY
GLY
ARG

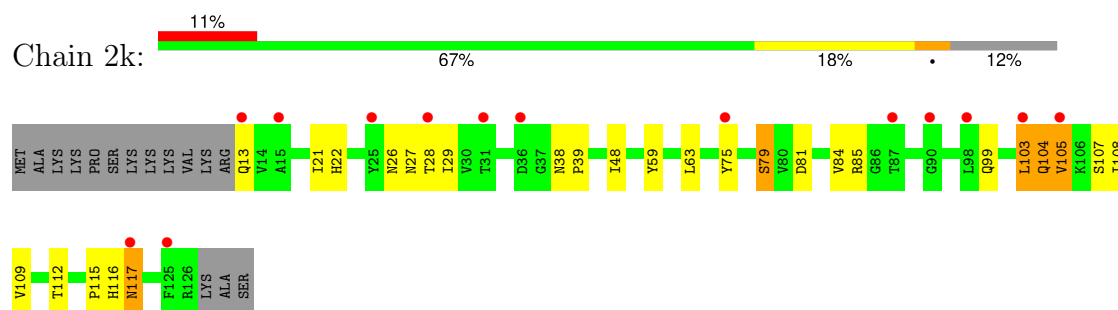
• Molecule 41: 30S ribosomal protein S10



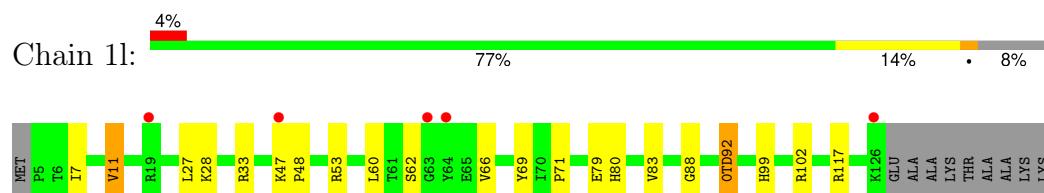
• Molecule 42: 30S ribosomal protein S11



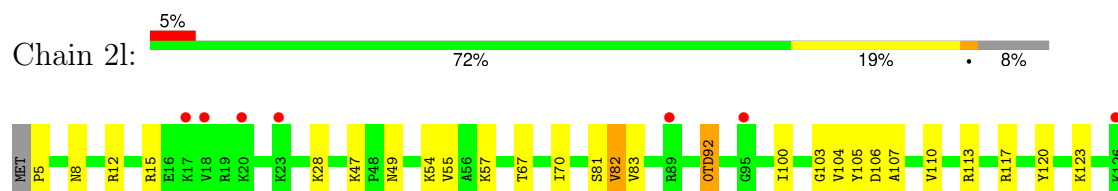
• Molecule 42: 30S ribosomal protein S11



• Molecule 43: 30S ribosomal protein S12



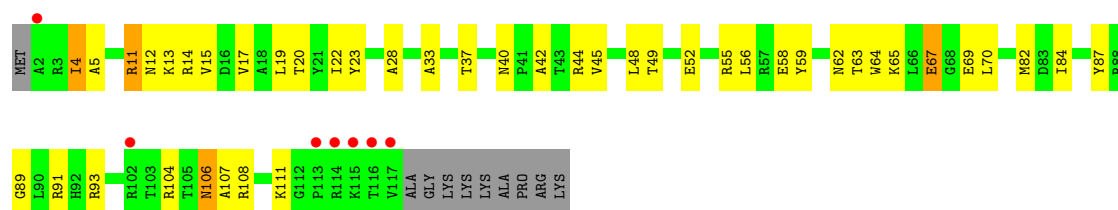
• Molecule 43: 30S ribosomal protein S12



GLU
ALA
ALA
LYS
THR
ALA
LYS
LYS

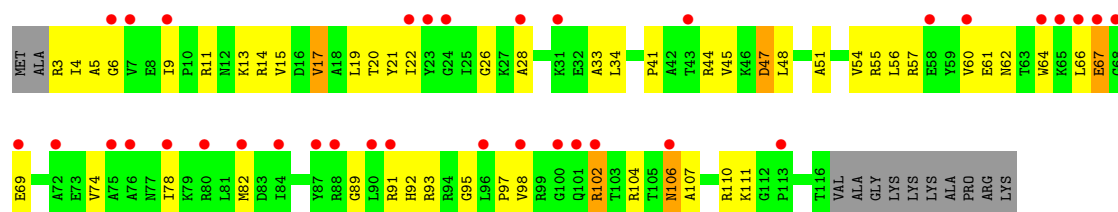
• Molecule 44: 30S ribosomal protein S13

Chain 1m: 6% 57% 32% 8%



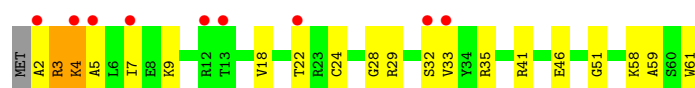
• Molecule 44: 30S ribosomal protein S13

Chain 2m: 28% 50% 37% 10%



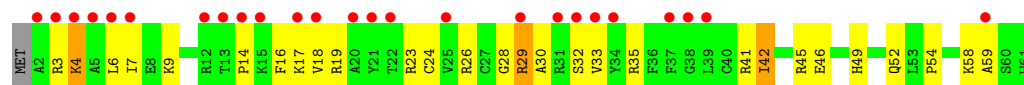
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n: 15% 66% 30% 2%



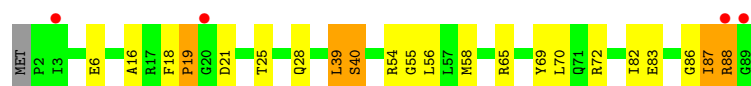
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n: 41% 52% 41% 5%



• Molecule 46: 30S ribosomal protein S15

Chain 1o: 4% 74% 19% 6%

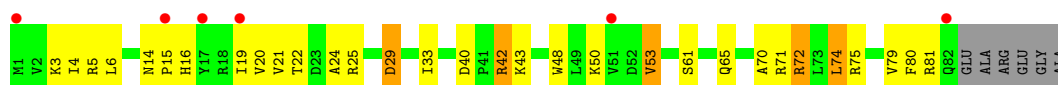


• Molecule 46: 30S ribosomal protein S15

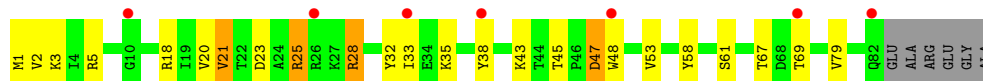
Chain 2o: 8% 66% 29% 2%



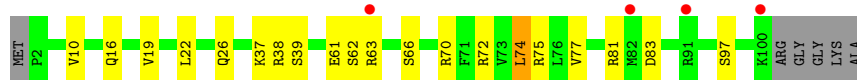
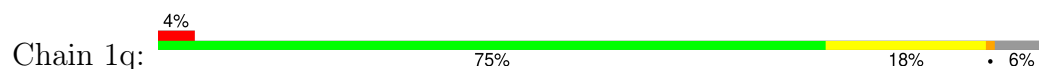
- Molecule 47: 30S ribosomal protein S16



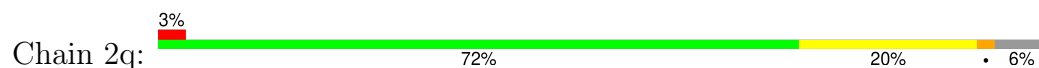
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



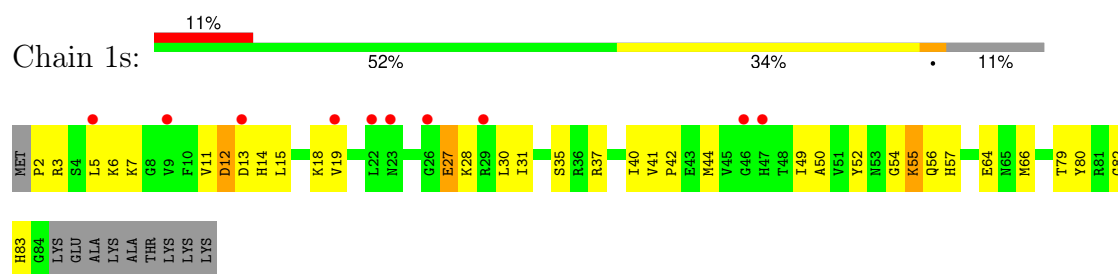
- Molecule 49: 30S ribosomal protein S18



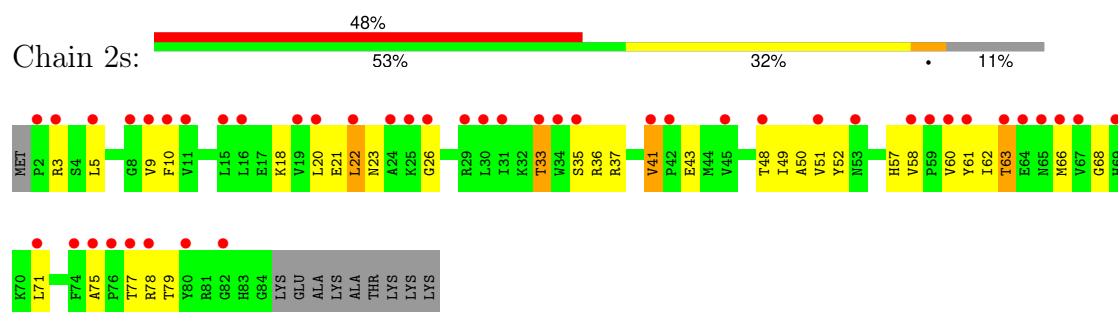
- Molecule 49: 30S ribosomal protein S18



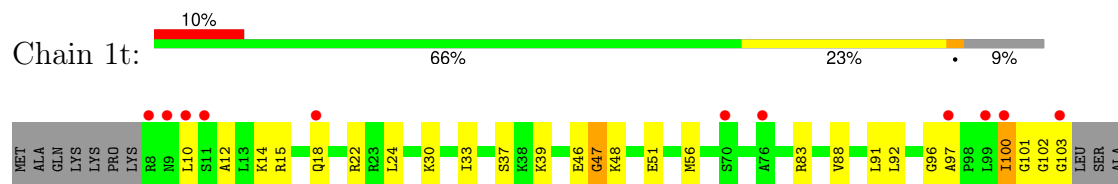
- Molecule 50: 30S ribosomal protein S19



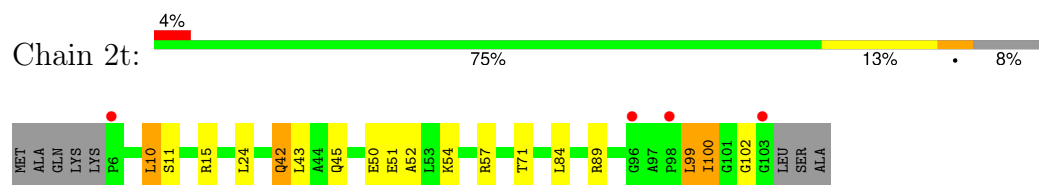
- Molecule 50: 30S ribosomal protein S19



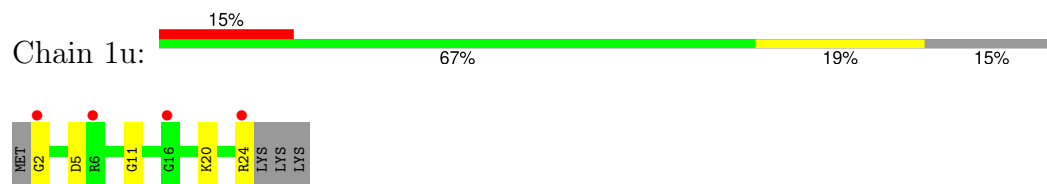
- Molecule 51: 30S ribosomal protein S20



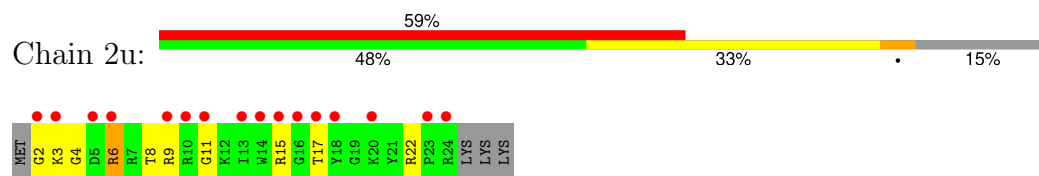
- Molecule 51: 30S ribosomal protein S20



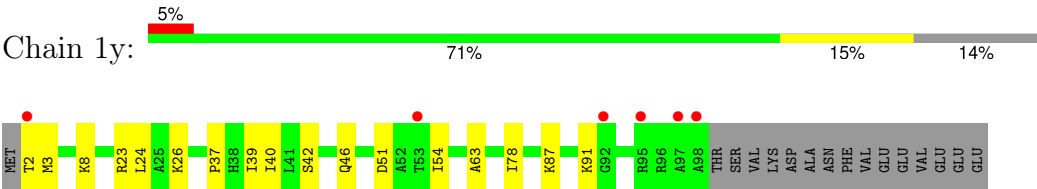
- Molecule 52: 30S ribosomal protein Thx



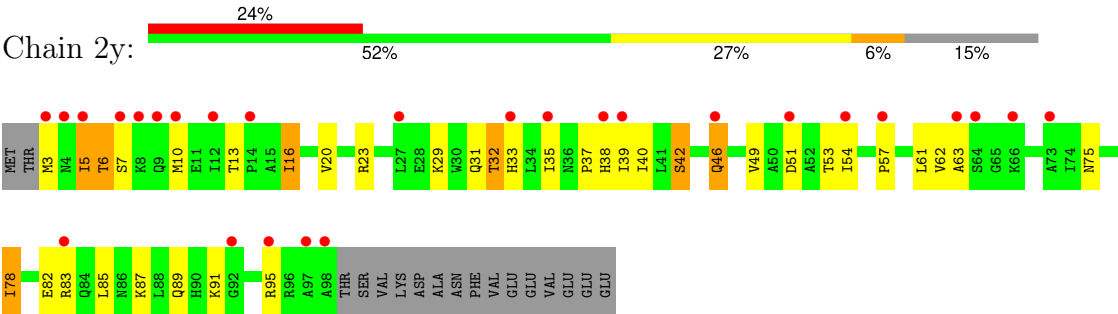
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



• Molecule 53: Ribosome-associated inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.55Å 449.77Å 619.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.31 – 2.65 153.31 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (153.31-2.65) 99.8 (153.31-2.65)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.194 , 0.236 0.197 , 0.237	Depositor DCC
R_{free} test set	83721 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	296864	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: MPD, UR3, ZIT, ZN, OMG, HGR, MG, G7M, 4OC, SF4, 2MG, OMC, 0TD, 2MA, OMU, PSU, MA6, 5MC, 5MU, M2G

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	0.30	1/69005 (0.0%)	0.48	2/107711 (0.0%)
1	2A	0.24	0/68875	0.43	1/107505 (0.0%)
2	1B	0.23	0/2876	0.42	0/4486
2	2B	0.19	0/2878	0.36	0/4490
3	1D	0.29	0/2181	0.54	2/2940 (0.1%)
3	2D	0.24	0/2186	0.49	0/2944
4	1E	0.28	0/1592	0.51	0/2149
4	2E	0.22	0/1592	0.47	0/2149
5	1F	0.27	0/1619	0.48	0/2193
5	2F	0.22	0/1615	0.47	0/2188
6	1G	0.19	0/1451	0.42	0/1961
6	2G	0.20	0/1449	0.42	0/1957
7	1H	0.23	0/1356	0.40	0/1834
7	2H	0.18	0/1350	0.40	0/1826
8	1I	0.22	0/1109	0.48	0/1512
8	2I	0.21	0/1091	0.38	0/1490
9	1N	0.26	0/1148	0.46	0/1547
9	2N	0.20	0/1144	0.43	0/1543
10	1O	0.27	0/943	0.52	0/1269
10	2O	0.23	0/943	0.48	0/1269
11	1P	0.27	0/1152	0.60	4/1533 (0.3%)
11	2P	0.23	0/1152	0.47	0/1533
12	1Q	0.27	0/1143	0.49	0/1527
12	2Q	0.20	0/1143	0.41	0/1527
13	1R	0.28	0/982	0.51	0/1312
13	2R	0.23	0/982	0.47	0/1312
14	1S	0.24	0/887	0.58	1/1180 (0.1%)
14	2S	0.22	0/880	0.46	0/1172
15	1T	0.27	0/1105	0.48	0/1477
15	2T	0.23	0/1097	0.44	0/1468
16	1U	0.29	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.40	0/1301
17	1V	0.26	0/786	0.47	0/1053
17	2V	0.19	0/782	0.42	0/1049
18	1W	0.29	0/897	0.49	0/1205
18	2W	0.23	0/897	0.42	0/1205
19	1X	0.26	0/764	0.47	0/1025
19	2X	0.20	0/764	0.44	0/1025
20	1Y	0.26	0/823	0.50	0/1099
20	2Y	0.20	0/823	0.46	0/1100
21	1Z	0.22	0/1620	0.43	0/2200
21	2Z	0.20	0/1590	0.42	0/2162
22	10	0.27	0/616	0.51	0/821
22	20	0.21	0/616	0.47	0/821
23	11	0.26	0/761	0.47	0/1013
23	21	0.25	0/766	0.43	0/1018
24	12	0.26	0/590	0.48	0/781
24	22	0.20	0/594	0.38	0/785
25	13	0.27	0/474	0.48	0/635
25	23	0.19	0/469	0.39	0/630
26	14	0.27	0/559	0.65	0/754
26	24	0.29	0/549	0.63	2/741 (0.3%)
27	15	0.29	0/473	0.55	0/639
27	25	0.29	0/469	0.48	0/635
28	16	0.28	0/460	0.46	0/613
28	26	0.22	0/456	0.44	0/608
29	17	0.31	0/426	0.53	0/561
29	27	0.25	0/426	0.48	0/561
30	18	0.28	0/525	0.49	0/691
30	28	0.22	0/525	0.40	0/691
31	19	0.28	0/310	0.51	0/407
31	29	0.22	0/310	0.48	0/407
32	1a	0.21	0/35795	0.40	1/55864 (0.0%)
32	2a	0.20	1/35890 (0.0%)	0.39	2/56012 (0.0%)
33	1b	0.21	0/1876	0.49	1/2533 (0.0%)
33	2b	0.23	0/1860	0.45	0/2518
34	1c	0.19	0/1582	0.39	0/2137
34	2c	0.22	0/1566	0.42	0/2119
35	1d	0.21	0/1695	0.44	0/2274
35	2d	0.20	0/1698	0.44	0/2277
36	1e	0.20	0/1149	0.44	0/1548
36	2e	0.20	0/1149	0.42	0/1548
37	1f	0.21	0/827	0.40	0/1120
37	2f	0.20	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1254	0.36	0/1683
38	2g	0.20	0/1248	0.40	0/1676
39	1h	0.19	0/1118	0.42	0/1506
39	2h	0.18	0/1108	0.42	0/1494
40	1i	0.20	0/1005	0.46	0/1351
40	2i	0.21	0/985	0.47	0/1329
41	1j	0.22	0/732	0.39	0/993
41	2j	0.23	0/723	0.47	0/984
42	1k	0.19	0/849	0.42	0/1150
42	2k	0.22	0/848	0.45	0/1149
43	1l	0.20	0/937	0.43	0/1260
43	2l	0.18	0/937	0.41	0/1260
44	1m	0.20	0/924	0.45	0/1242
44	2m	0.24	0/905	0.49	0/1217
45	1n	0.20	0/501	0.45	0/664
45	2n	0.21	0/501	0.41	0/664
46	1o	0.21	0/739	0.39	0/985
46	2o	0.19	0/739	0.39	0/985
47	1p	0.20	0/697	0.51	0/939
47	2p	0.19	0/693	0.45	0/935
48	1q	0.19	0/836	0.40	0/1117
48	2q	0.19	0/836	0.39	0/1117
49	1r	0.18	0/560	0.39	0/746
49	2r	0.20	0/560	0.42	0/746
50	1s	0.18	0/663	0.44	0/895
50	2s	0.20	0/660	0.38	0/893
51	1t	0.21	0/734	0.45	0/969
51	2t	0.20	0/736	0.42	0/976
52	1u	0.18	0/203	0.43	0/266
52	2u	0.18	0/203	0.46	0/266
53	1y	0.19	0/776	0.39	0/1048
53	2y	0.18	0/761	0.36	0/1030
All	All	0.24	2/309887 (0.0%)	0.44	16/463149 (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
26	14	0	1
33	1b	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	O3'-P	5.38	1.61	1.56
32	2a	527	G7M	O3'-P	5.21	1.61	1.56

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1S	60	GLY	N-CA-C	9.98	119.29	110.21
1	2A	1992	G	C2'-C3'-O3'	6.63	119.45	109.50
11	1P	33	ARG	CA-C-N	-6.18	110.27	121.32
11	1P	33	ARG	C-N-CA	-6.18	110.27	121.32
32	2a	266	G	C2'-C3'-O3'	6.16	118.74	109.50
26	24	59	PHE	CA-C-N	5.89	132.30	121.70
26	24	59	PHE	C-N-CA	5.89	132.30	121.70
33	1b	23	ARG	N-CA-C	-5.77	106.85	112.97
1	1A	2689	U	C4'-C3'-O3'	5.62	117.82	109.40
11	1P	35	HIS	CA-C-N	-5.39	111.25	121.54
11	1P	35	HIS	C-N-CA	-5.39	111.25	121.54
1	1A	1653	G	C2'-C3'-O3'	5.34	117.51	109.50
3	1D	70	TRP	CA-C-N	5.33	127.69	120.38
3	1D	70	TRP	C-N-CA	5.33	127.69	120.38
32	2a	266	G	P-O3'-C3'	5.13	127.90	120.20
32	1a	1442	G	P-O3'-C3'	5.12	125.84	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	52	THR	Peptide
33	1b	231	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61871	0	31210	574	0
1	2A	61759	0	31157	664	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1B	2572	0	1305	24	0
2	2B	2573	0	1306	29	0
3	1D	2131	0	2207	45	0
3	2D	2136	0	2218	51	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	33	0
5	1F	1584	0	1625	24	0
5	2F	1580	0	1619	43	0
6	1G	1426	0	1445	35	0
6	2G	1424	0	1441	64	0
7	1H	1330	0	1407	17	0
7	2H	1324	0	1402	37	0
8	1I	1094	0	1127	19	0
8	2I	1076	0	1094	24	0
9	1N	1121	0	1195	19	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	18	0
10	2O	933	0	996	14	0
11	1P	1135	0	1212	31	0
11	2P	1135	0	1212	24	0
12	1Q	1122	0	1179	12	0
12	2Q	1122	0	1179	23	0
13	1R	968	0	1033	18	0
13	2R	968	0	1033	21	0
14	1S	877	0	938	18	0
14	2S	870	0	923	24	0
15	1T	1091	0	1151	16	0
15	2T	1083	0	1136	19	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	9	0
17	1V	775	0	841	17	0
17	2V	771	0	830	15	0
18	1W	886	0	940	14	0
18	2W	886	0	940	14	0
19	1X	750	0	814	18	0
19	2X	750	0	814	18	0
20	1Y	810	0	892	16	0
20	2Y	810	0	887	16	0
21	1Z	1587	0	1598	17	0
21	2Z	1557	0	1564	49	0
22	10	608	0	622	10	0
22	20	608	0	622	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	11	754	0	823	12	0
23	21	759	0	837	12	0
24	12	588	0	643	5	0
24	22	592	0	654	6	0
25	13	469	0	518	5	0
25	23	464	0	514	6	0
26	14	546	0	522	25	0
26	24	536	0	514	22	0
27	15	459	0	476	11	0
27	25	455	0	465	6	0
28	16	453	0	473	6	0
28	26	449	0	469	5	0
29	17	418	0	467	10	0
29	27	418	0	467	8	0
30	18	517	0	582	11	0
30	28	517	0	582	12	0
31	19	307	0	335	5	0
31	29	307	0	335	11	0
32	1a	32246	0	16293	387	0
32	2a	32331	0	16338	441	0
33	1b	1842	0	1862	55	0
33	2b	1825	0	1828	70	0
34	1c	1558	0	1557	26	0
34	2c	1542	0	1517	51	0
35	1d	1665	0	1687	50	0
35	2d	1668	0	1703	52	0
36	1e	1133	0	1191	27	0
36	2e	1133	0	1191	36	0
37	1f	814	0	808	18	0
37	2f	816	0	808	15	0
38	1g	1235	0	1249	24	0
38	2g	1229	0	1238	26	0
39	1h	1098	0	1143	27	0
39	2h	1088	0	1126	30	0
40	1i	986	0	990	31	0
40	2i	966	0	953	44	0
41	1j	719	0	672	22	0
41	2j	710	0	661	33	0
42	1k	834	0	838	13	0
42	2k	833	0	836	17	0
43	1l	932	0	981	11	0
43	2l	932	0	981	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	1m	914	0	954	33	0
44	2m	895	0	920	41	0
45	1n	492	0	529	16	0
45	2n	492	0	529	30	0
46	1o	728	0	760	12	0
46	2o	728	0	760	17	0
47	1p	681	0	697	22	0
47	2p	677	0	686	14	0
48	1q	823	0	891	13	0
48	2q	823	0	891	16	0
49	1r	555	0	618	14	0
49	2r	555	0	618	10	0
50	1s	648	0	658	25	0
50	2s	645	0	635	24	0
51	1t	732	0	809	18	0
51	2t	733	0	795	12	0
52	1u	199	0	208	3	0
52	2u	199	0	208	6	0
53	1y	764	0	786	16	0
53	2y	749	0	757	25	0
54	10	6	0	0	0	0
54	11	5	0	0	0	0
54	13	3	0	0	0	0
54	15	8	0	0	0	0
54	17	7	0	0	0	0
54	18	2	0	0	0	0
54	19	3	0	0	0	0
54	1A	1031	0	0	0	0
54	1B	29	0	0	0	0
54	1D	18	0	0	0	0
54	1E	10	0	0	0	0
54	1F	18	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	4	0	0	0	0
54	1O	1	0	0	0	0
54	1P	7	0	0	0	0
54	1Q	5	0	0	0	0
54	1R	5	0	0	0	0
54	1S	1	0	0	0	0
54	1T	6	0	0	0	0
54	1U	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1V	4	0	0	0	0
54	1W	4	0	0	0	0
54	1X	1	0	0	0	0
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	281	0	0	0	0
54	1b	1	0	0	0	0
54	1d	2	0	0	0	0
54	1e	3	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	3	0	0	0	0
54	1o	1	0	0	0	0
54	1t	1	0	0	0	0
54	1u	1	0	0	0	0
54	1y	3	0	0	0	0
54	20	1	0	0	0	0
54	21	1	0	0	0	0
54	23	1	0	0	0	0
54	25	1	0	0	0	0
54	27	1	0	0	0	0
54	28	2	0	0	0	0
54	2A	711	0	0	0	0
54	2B	18	0	0	0	0
54	2D	9	0	0	0	0
54	2E	5	0	0	0	0
54	2F	4	0	0	0	0
54	2G	2	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	2	0	0	0	0
54	2P	1	0	0	0	0
54	2Q	3	0	0	0	0
54	2R	1	0	0	0	0
54	2T	3	0	0	0	0
54	2V	3	0	0	0	0
54	2W	3	0	0	0	0
54	2X	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2Y	1	0	0	0	0
54	2a	182	0	0	0	0
54	2e	2	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2l	1	0	0	0	0
54	2n	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	36	0	29	2	0
55	2A	36	0	29	2	0
56	1A	52	0	72	6	0
56	2A	52	0	72	2	0
57	18	8	0	14	0	0
57	1A	8	0	14	1	0
57	1T	8	0	14	0	0
57	1a	8	0	12	5	0
57	2A	16	0	28	0	0
57	2B	8	0	14	0	0
58	1B	12	0	12	3	0
58	1F	12	0	12	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	1	0
60	2d	8	0	0	0	0
61	10	19	0	0	1	0
61	11	17	0	0	0	0
61	12	11	0	0	0	0
61	13	20	0	0	1	0
61	15	28	0	0	2	0
61	16	12	0	0	1	0
61	17	12	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	18	24	0	0	1	0
61	19	3	0	0	0	0
61	1A	3571	0	0	95	0
61	1B	89	0	0	8	0
61	1D	109	0	0	5	0
61	1E	68	0	0	1	0
61	1F	61	0	0	1	0
61	1G	10	0	0	0	0
61	1H	15	0	0	0	0
61	1I	4	0	0	0	0
61	1N	46	0	0	0	0
61	1O	17	0	0	0	0
61	1P	53	0	0	2	0
61	1Q	30	0	0	2	0
61	1R	29	0	0	2	0
61	1S	7	0	0	0	0
61	1T	32	0	0	0	0
61	1U	38	0	0	2	0
61	1V	26	0	0	2	0
61	1W	28	0	0	1	0
61	1X	23	0	0	2	0
61	1Y	13	0	0	1	0
61	1Z	9	0	0	1	0
61	1a	388	0	0	20	0
61	1d	9	0	0	0	0
61	1f	1	0	0	0	0
61	1h	2	0	0	0	0
61	1j	1	0	0	0	0
61	1l	2	0	0	0	0
61	1m	1	0	0	0	0
61	1n	2	0	0	0	0
61	1o	1	0	0	0	0
61	1p	3	0	0	0	0
61	1u	1	0	0	0	0
61	1y	3	0	0	0	0
61	20	5	0	0	0	0
61	21	14	0	0	1	0
61	23	3	0	0	0	0
61	25	8	0	0	0	0
61	26	3	0	0	0	0
61	27	5	0	0	0	0
61	28	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	29	1	0	0	0	0
61	2A	2161	0	0	79	0
61	2B	48	0	0	7	0
61	2D	43	0	0	3	0
61	2E	22	0	0	0	0
61	2F	25	0	0	2	0
61	2G	1	0	0	0	0
61	2H	1	0	0	0	0
61	2I	1	0	0	0	0
61	2N	5	0	0	1	0
61	2O	17	0	0	0	0
61	2P	20	0	0	1	0
61	2Q	19	0	0	0	0
61	2R	15	0	0	0	0
61	2S	4	0	0	1	0
61	2T	11	0	0	0	0
61	2U	15	0	0	0	0
61	2V	3	0	0	0	0
61	2W	16	0	0	0	0
61	2X	6	0	0	0	0
61	2Y	2	0	0	0	0
61	2Z	6	0	0	1	0
61	2a	394	0	0	20	0
61	2d	4	0	0	0	0
61	2e	2	0	0	0	0
61	2f	1	0	0	0	0
61	2j	2	0	0	1	0
61	2l	4	0	0	1	0
61	2n	1	0	0	0	0
61	2o	3	0	0	0	0
61	2p	3	0	0	0	0
61	2q	1	0	0	0	0
61	2r	5	0	0	0	0
61	2t	2	0	0	0	0
61	2y	2	0	0	0	0
All	All	296864	0	194726	3732	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (3732) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.47	1.11
1:1A:2137:C:N4	1:1A:2154:G:H1	1.54	1.05
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.19	1.03
1:2A:2139:C:N4	1:2A:2152:G:H1	1.60	0.98
1:2A:2107:C:H42	1:2A:2182:G:H1	1.06	0.97
1:2A:2122:U:H3	1:2A:2176:A:H61	1.08	0.97
1:2A:2100:G:H1	1:2A:2189:U:H3	0.97	0.96
1:1A:1082:U:O4	1:1A:1086:A:N1	2.04	0.91
1:2A:2807:G:N2	1:2A:2893:G:O6	2.02	0.91
1:2A:2099:U:H3	1:2A:2190:G:H1	1.20	0.89
1:1A:1603:A:OP1	61:1A:4102:HOH:O	1.90	0.89
1:1A:2137:C:H42	1:1A:2154:G:H1	0.88	0.88
29:17:24:THR:HG22	29:17:27:GLY:H	1.37	0.88
2:1B:95:C:N4	61:1B:301:HOH:O	2.07	0.88
1:2A:2131:G:H5''	1:2A:2132:U:H5'	1.56	0.88
1:2A:2139:C:N3	1:2A:2152:G:N2	2.20	0.88
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.56	0.88
1:2A:2122:U:H3	1:2A:2176:A:N6	1.72	0.88
1:2A:2139:C:H42	1:2A:2152:G:H1	0.92	0.87
32:1a:1003:G:H2'	32:1a:1004:A:H4'	1.56	0.87
1:1A:1970:A:OP1	61:1A:4103:HOH:O	1.92	0.87
29:27:24:THR:HG22	29:27:27:GLY:H	1.38	0.86
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.57	0.86
1:2A:2427:C:OP1	61:2A:3806:HOH:O	1.94	0.86
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.56	0.85
1:1A:2137:C:N3	1:1A:2154:G:N2	2.23	0.85
32:1a:201:C:H42	32:1a:216:G:H1	1.23	0.85
35:1d:18:LYS:NZ	35:1d:31:CYS:SG	2.49	0.84
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.43	0.84
32:1a:664:G:H22	32:1a:741:G:H1	1.26	0.84
1:2A:2602:A:H1'	1:2A:2603:G:H5''	1.60	0.83
1:2A:2128:C:H42	1:2A:2160:G:H1	1.26	0.83
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.12	0.83
32:1a:1025:U:C2	32:1a:1036:G:O6	2.31	0.82
1:1A:2143:C:N3	1:1A:2148:G:O6	2.13	0.82
1:1A:1671:U:O4	61:1A:4106:HOH:O	1.98	0.82
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.45	0.82
32:1a:612:C:O2	32:1a:629:G:N2	2.13	0.82
1:2A:2107:C:N4	1:2A:2182:G:H1	1.77	0.81
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.60	0.81
1:1A:2447:G:OP2	61:1A:4107:HOH:O	1.98	0.81
1:2A:2439:A:N1	61:2A:3827:HOH:O	2.13	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:75:THR:HG21	12:2Q:87:LYS:HE3	1.59	0.81
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.61	0.81
32:1a:992:U:H4'	32:1a:993:G:H5'	1.62	0.81
32:2a:975:A:H4'	32:2a:976:G:H5''	1.61	0.81
1:1A:2822:G:OP2	61:1A:4105:HOH:O	1.97	0.80
1:2A:585:G:OP2	61:2A:3807:HOH:O	1.98	0.80
1:1A:1604:C:OP2	61:1A:4102:HOH:O	1.99	0.80
32:1a:1086:U:H3	32:1a:1099:G:H22	1.27	0.80
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.14	0.80
1:1A:249:C:O2'	11:1P:64:LYS:NZ	2.14	0.80
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.61	0.80
32:1a:975:A:H4'	32:1a:976:G:H5''	1.64	0.80
1:2A:323:G:HO2'	1:2A:1205:U:H3	1.26	0.79
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.46	0.79
33:1b:231:GLU:HB3	33:1b:232:PRO:HD3	1.65	0.79
1:2A:1315:C:OP2	61:2A:3808:HOH:O	1.99	0.79
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.64	0.79
1:2A:2128:C:N4	1:2A:2160:G:H1	1.80	0.79
1:2A:1195:G:N7	11:2P:15:ARG:NH2	2.32	0.78
45:1n:3:ARG:HB2	45:1n:3:ARG:HH11	1.46	0.78
26:24:59:PHE:HA	26:24:61:ARG:N	1.98	0.78
51:2t:50:GLU:HG3	51:2t:100:ILE:HD11	1.66	0.78
1:2A:271(L):U:H5'	8:2I:50:ARG:HH12	1.47	0.78
32:2a:536:C:OP2	61:2a:3204:HOH:O	2.00	0.78
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.66	0.78
44:1m:37:THR:O	44:1m:55:ARG:NH1	2.17	0.77
1:1A:2821:A:OP2	61:1A:4105:HOH:O	2.02	0.77
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.67	0.77
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.66	0.77
1:1A:1271:G:OP2	61:1A:4108:HOH:O	2.01	0.77
1:2A:2499:C:OP1	61:2A:3809:HOH:O	2.03	0.76
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.66	0.76
26:14:16:CYS:SG	26:14:17:GLY:N	2.58	0.76
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.19	0.76
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.50	0.76
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.19	0.76
32:2a:1500:A:OP2	61:2a:3205:HOH:O	2.01	0.76
33:2b:111:ARG:HH11	33:2b:111:ARG:HA	1.51	0.76
19:1X:76:ARG:NH1	61:1X:201:HOH:O	2.18	0.76
1:1A:2427:C:OP1	61:1A:4109:HOH:O	2.04	0.76
32:2a:427:U:OP1	35:2d:13:ARG:NH2	2.17	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:136:ALA:HB1	21:1Z:52:SER:HB3	1.67	0.76
1:1A:1648:C:OP1	61:1A:4108:HOH:O	2.05	0.75
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.68	0.75
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.68	0.75
1:2A:2156:G:N7	1:2A:2157:G:N2	2.33	0.75
32:2a:1318:A:H5''	50:2s:3:ARG:HH22	1.50	0.75
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.52	0.75
32:1a:814:A:OP2	61:1a:1903:HOH:O	2.05	0.75
1:1A:1082:U:H3	1:1A:1086:A:H61	0.76	0.75
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.69	0.75
32:1a:235:C:H5'	48:1q:70:ARG:HG2	1.68	0.75
1:2A:826:U:OP1	61:2A:3806:HOH:O	2.04	0.74
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.19	0.74
1:1A:1669:A:OP2	61:1A:4106:HOH:O	2.04	0.74
32:1a:1441:G:H5''	32:1a:1442:G:H5'	1.68	0.74
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.03	0.74
17:1V:85:LYS:NZ	61:1V:302:HOH:O	2.20	0.73
36:1e:37:ARG:HH12	36:1e:111:GLU:HG2	1.53	0.73
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.69	0.73
6:2G:5:VAL:HG22	6:2G:8:LYS:H	1.53	0.73
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.69	0.73
1:1A:2763:G:OP2	61:1A:4112:HOH:O	2.07	0.73
1:2A:1332:G:OP1	61:2A:3808:HOH:O	2.06	0.73
1:1A:1143:A:OP1	9:1N:25:ARG:NH2	2.21	0.73
1:2A:493:G:OP2	61:2A:3810:HOH:O	2.06	0.73
1:2A:1466:G:HO2'	1:2A:1546:C:HO2'	1.33	0.73
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.70	0.73
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.52	0.73
32:1a:1025:U:O2	32:1a:1036:G:O6	2.05	0.73
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.20	0.73
33:1b:160:ASP:N	33:1b:160:ASP:OD1	2.22	0.73
1:2A:2000:G:OP2	61:2A:3811:HOH:O	2.06	0.73
8:2I:92:VAL:HG23	8:2I:120:ILE:HB	1.69	0.73
26:24:16:CYS:SG	26:24:17:GLY:N	2.61	0.73
33:2b:118:LEU:HD22	33:2b:142:LEU:HB2	1.71	0.73
1:1A:1332:G:OP1	61:1A:4110:HOH:O	2.06	0.73
1:2A:2141:G:O6	1:2A:2150:U:O2	2.06	0.73
1:1A:2116:G:OP2	1:1A:2166:G:N2	2.22	0.73
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.54	0.72
39:2h:37:ARG:HH12	39:2h:41:ARG:HH21	1.36	0.72
1:2A:2610:C:O2'	61:2A:3812:HOH:O	2.07	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1047:G:H5''	45:2n:4:LYS:HD2	1.71	0.72
1:1A:438:G:N7	61:1A:4163:HOH:O	2.22	0.72
1:2A:1065:U:H3	1:2A:1073:A:H61	1.37	0.72
35:2d:122:ARG:NH1	35:2d:134:ASP:O	2.22	0.72
38:2g:113:GLU:HG3	38:2g:119:ARG:HG2	1.70	0.72
1:1A:1195:G:N7	11:1P:15:ARG:NH2	2.37	0.72
1:2A:1041:C:H42	1:2A:1114:G:H1	1.37	0.72
44:2m:107:ALA:HB3	44:2m:111:LYS:HE3	1.72	0.72
1:1A:1068:G:O2'	1:1A:1096:A:O2'	2.08	0.72
32:1a:79:G:H1	32:1a:90:U:H3	1.36	0.72
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.72	0.72
1:1A:1772:G:O6	61:1A:4111:HOH:O	2.07	0.72
32:2a:558:G:OP1	61:2a:3206:HOH:O	2.07	0.72
32:2a:656:C:O2'	46:2o:28:GLN:NE2	2.22	0.72
33:2b:67:THR:H	33:2b:160:ASP:HB2	1.52	0.72
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB2	1.71	0.72
1:1A:1378:A:OP1	29:17:10:ARG:NH2	2.23	0.72
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.23	0.72
7:2H:11:VAL:HG12	7:2H:15:VAL:HG23	1.72	0.72
1:1A:2102:U:O2	1:1A:2187:G:O6	2.08	0.71
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.72	0.71
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.06	0.71
1:1A:1509(A):A:H2'	1:1A:1509(B):A:O4'	1.90	0.71
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.23	0.71
1:1A:1024:G:OP2	61:1A:4115:HOH:O	2.09	0.71
2:1B:92:C:OP2	61:1B:302:HOH:O	2.07	0.71
1:2A:981:A:OP1	61:2A:3813:HOH:O	2.07	0.71
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.56	0.71
21:2Z:129:SER:HB3	21:2Z:132:ASN:HD22	1.56	0.71
32:2a:1518:MA6:H93	32:2a:1519:MA6:H102	1.72	0.71
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.71	0.71
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.73	0.71
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.24	0.71
39:2h:89:PRO:HA	39:2h:92:ARG:HE	1.55	0.71
32:2a:673:G:H2'	32:2a:674:G:C8	2.25	0.70
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.24	0.70
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.72	0.70
1:1A:2242:G:OP1	61:1A:4114:HOH:O	2.09	0.70
1:2A:751:A:H5'	18:2W:90:ARG:HA	1.73	0.70
32:2a:547:A:OP1	61:2a:3207:HOH:O	2.09	0.70
1:2A:775:G:O3'	61:2A:3815:HOH:O	2.08	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:58:A:OP2	61:2B:301:HOH:O	2.09	0.70
32:2a:1016:A:HO2'	32:2a:1217:C:HO2'	1.34	0.70
23:11:52:ARG:NH2	23:11:55:GLY:O	2.24	0.70
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	1.73	0.70
1:1A:2550:G:OP1	61:1A:4106:HOH:O	2.10	0.70
1:2A:1009:A:OP2	61:2A:3814:HOH:O	2.08	0.70
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.25	0.70
1:1A:847:U:OP2	61:1A:4113:HOH:O	2.08	0.70
1:2A:2691:C:OP1	61:2A:3818:HOH:O	2.10	0.70
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	1.73	0.70
1:1A:927:G:N7	61:1A:4183:HOH:O	2.25	0.70
1:1A:2133:G:H3'	1:1A:2157:G:H21	1.57	0.70
20:1Y:23:ARG:NH1	61:1Y:301:HOH:O	2.20	0.70
32:1a:812:C:N3	61:1a:1928:HOH:O	2.25	0.70
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.25	0.70
1:1A:1138:G:OP1	61:1A:4119:HOH:O	2.10	0.70
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.24	0.70
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.74	0.70
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.72	0.69
32:1a:574:A:OP2	61:1a:1904:HOH:O	2.09	0.69
6:1G:50:ALA:HB1	6:1G:52:ILE:HG13	1.74	0.69
1:2A:1053:C:H2'	1:2A:1054:A:H8	1.56	0.69
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.73	0.69
10:2O:26:LYS:NZ	10:2O:37:ASP:OD2	2.24	0.69
11:2P:54:GLY:O	61:2P:301:HOH:O	2.10	0.69
32:2a:609:A:N7	61:2a:3222:HOH:O	2.24	0.69
1:2A:194:G:OP2	61:2A:3820:HOH:O	2.10	0.69
8:1I:68:LEU:HD21	8:1I:109:ILE:HD11	1.73	0.69
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.58	0.69
44:1m:65:LYS:HG2	44:1m:69:GLU:HG2	1.73	0.69
32:2a:617:G:OP2	61:2a:3209:HOH:O	2.11	0.69
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.25	0.69
1:1A:1173:G:O2'	1:1A:1174:A:O5'	2.10	0.69
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.74	0.69
21:2Z:10:ARG:NH1	21:2Z:26:GLY:O	2.24	0.69
1:1A:1508:A:H4'	1:1A:1509(A):A:C5	2.28	0.69
1:1A:1647:G:OP1	61:1A:4108:HOH:O	2.11	0.69
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.57	0.69
26:14:16:CYS:HB3	26:14:20:ASN:HB3	1.73	0.69
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.27	0.69
32:1a:1373:G:H5''	38:1g:36:LYS:HE2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1023:U:OP2	61:2A:3817:HOH:O	2.10	0.69
1:2A:2126:A:H4'	1:2A:2127:G:O5'	1.93	0.69
6:1G:9:ARG:NH1	6:1G:13:GLU:OE2	2.25	0.69
26:14:7:PRO:HB2	26:14:27:THR:HG21	1.75	0.69
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	1.75	0.69
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.75	0.69
32:2a:1118:C:OP1	40:2i:9:ARG:NH1	2.26	0.69
1:1A:217:G:OP2	61:1A:4117:HOH:O	2.10	0.69
1:1A:826:U:OP1	61:1A:4109:HOH:O	2.11	0.69
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.73	0.69
58:1B:230:ARG:NE	61:1B:301:HOH:O	2.22	0.68
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.27	0.68
1:1A:1634:A:OP2	61:1A:4116:HOH:O	2.10	0.68
28:16:13:CYS:SG	28:16:47:THR:HG21	2.33	0.68
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.29	0.68
1:2A:154(A):C:H42	1:2A:171:G:H1	1.41	0.68
1:2A:1356:G:OP1	61:2A:3821:HOH:O	2.10	0.68
1:1A:30:G:OP1	61:1A:4118:HOH:O	2.10	0.68
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.74	0.68
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.41	0.68
6:2G:97:ASP:HA	6:2G:100:TRP:CD1	2.29	0.68
32:2a:1004:A:H5''	32:2a:1025:U:C5	2.28	0.68
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.75	0.68
1:2A:731:C:OP1	61:2A:3823:HOH:O	2.12	0.68
1:2A:1566:A:OP1	3:2D:211:ARG:NH1	2.26	0.68
36:2e:74:GLY:HA3	36:2e:116:THR:HG22	1.73	0.68
32:1a:297:G:O2'	61:1a:1905:HOH:O	2.10	0.68
1:2A:963:U:OP2	61:2A:3824:HOH:O	2.12	0.68
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.27	0.68
1:2A:1101:U:H2'	1:2A:1102:C:H6	1.59	0.68
32:2a:1079:G:O3'	36:2e:14:ARG:NH2	2.26	0.68
6:1G:139:LEU:HD21	6:1G:149:VAL:HG11	1.75	0.68
1:2A:783:A:OP2	61:2A:3819:HOH:O	2.11	0.68
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.29	0.68
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.22	0.68
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.75	0.68
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.75	0.68
1:1A:1757:U:OP1	61:1A:4120:HOH:O	2.11	0.68
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.76	0.68
3:1D:108:PRO:HD2	3:1D:111:LEU:HG	1.75	0.68
32:1a:773:G:OP1	61:1a:1906:HOH:O	2.12	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.75	0.68
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.27	0.68
1:1A:2574:G:OP1	61:1A:4122:HOH:O	2.11	0.67
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.27	0.67
1:2A:1056:G:H4'	1:2A:1057:A:H8	1.58	0.67
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.28	0.67
32:2a:101:A:H5''	51:2t:10:LEU:HD21	1.76	0.67
32:2a:559:A:H4'	32:2a:560:U:H3'	1.76	0.67
32:2a:980:C:OP2	61:2a:3208:HOH:O	2.12	0.67
37:1f:36:ARG:NH2	37:1f:66:GLU:OE1	2.27	0.67
1:2A:1762:A:N1	61:2A:3898:HOH:O	2.27	0.67
1:2A:2448:A:OP1	61:2A:3809:HOH:O	2.11	0.67
36:2e:140:ARG:O	36:2e:143:ARG:NH2	2.27	0.67
1:1A:1364:G:N7	23:11:3:LYS:HE2	2.09	0.67
32:1a:411:A:OP2	35:1d:25:ARG:NH2	2.27	0.67
1:2A:2589:A:OP1	61:2A:3819:HOH:O	2.10	0.67
1:1A:2360:A:N1	61:1A:4192:HOH:O	2.27	0.67
40:2i:42:ARG:NH1	40:2i:71:SER:O	2.27	0.67
1:1A:1175:U:OP1	1:1A:1177:A:N6	2.27	0.67
32:1a:1256:A:H3'	34:1c:27:LYS:HZ1	1.59	0.67
1:2A:805:G:OP1	61:2A:3826:HOH:O	2.13	0.67
2:2B:116:G:N7	61:2B:309:HOH:O	2.28	0.67
53:2y:3:MET:HG3	53:2y:37:PRO:HG2	1.77	0.67
1:1A:428:A:OP1	61:1A:4123:HOH:O	2.12	0.67
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.75	0.67
1:1A:1670:C:OP2	61:1A:4106:HOH:O	2.12	0.67
7:1H:27:LYS:HG2	7:1H:32:GLU:HG2	1.77	0.67
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.30	0.67
1:2A:2102:U:O2	1:2A:2187:G:O6	2.13	0.67
1:2A:2439:A:OP1	61:2A:3825:HOH:O	2.12	0.67
1:1A:602:G:O2'	1:1A:655:A:N6	2.28	0.67
1:1A:1342:A:OP2	61:1A:4124:HOH:O	2.13	0.67
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.42	0.67
32:1a:1189:C:OP1	41:1j:51:ARG:NH2	2.28	0.67
26:24:46:GLN:O	26:24:48:ARG:N	2.27	0.67
32:1a:352:C:OP2	61:1a:1908:HOH:O	2.13	0.66
1:2A:1314:C:OP1	61:2A:3808:HOH:O	2.13	0.66
33:2b:48:MET:HA	33:2b:51:LEU:HD12	1.77	0.66
1:1A:1023:U:OP2	61:1A:4115:HOH:O	2.13	0.66
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.28	0.66
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2y:6:THR:HB	53:2y:40:ILE:HG13	1.77	0.66
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG11	1.76	0.66
32:2a:376:G:H5''	47:2p:5:ARG:HD2	1.77	0.66
34:2c:164:ARG:NH1	34:2c:166:GLU:OE2	2.28	0.66
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.28	0.66
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.78	0.66
40:1i:17:VAL:HG23	40:1i:63:ILE:HG12	1.77	0.66
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.28	0.66
32:2a:1222:G:O6	61:2a:3208:HOH:O	2.10	0.66
11:1P:141:ALA:HA	25:23:38:GLU:HG2	1.76	0.66
51:1t:46:GLU:HG3	51:1t:48:LYS:HG3	1.77	0.66
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.28	0.66
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.78	0.66
15:2T:16:ARG:NH2	15:2T:83:ILE:O	2.28	0.66
1:2A:827:U:OP1	61:2A:3828:HOH:O	2.13	0.66
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.77	0.66
1:1A:135:G:N7	61:1A:4195:HOH:O	2.27	0.66
1:1A:1508:A:H4'	1:1A:1509(A):A:C6	2.31	0.66
32:1a:73:G:H1	32:1a:96:U:H3	1.44	0.66
32:1a:1340:A:OP2	61:1a:1907:HOH:O	2.12	0.66
47:2p:43:LYS:HG2	47:2p:48:TRP:CD2	2.31	0.66
1:1A:271(M):G:H21	8:1I:50:ARG:HD3	1.61	0.66
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.30	0.66
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.21	0.66
36:2e:50:GLU:HB2	36:2e:53:LEU:HD13	1.76	0.66
2:1B:102:A:N7	61:1B:308:HOH:O	2.28	0.66
6:2G:145:THR:OG1	6:2G:146:TYR:N	2.17	0.66
40:1i:3:GLN:HE21	40:1i:20:ARG:HE	1.43	0.66
47:1p:40:ASP:HB3	47:1p:48:TRP:HB2	1.77	0.66
1:2A:1007:C:OP1	9:2N:37:LYS:NZ	2.30	0.66
1:2A:1971:A:OP1	61:2A:3830:HOH:O	2.14	0.66
32:1a:1149:C:OP2	40:1i:9:ARG:NH2	2.26	0.65
38:1g:111:ARG:NH1	38:1g:113:GLU:OE2	2.29	0.65
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.29	0.65
44:1m:58:GLU:O	44:1m:62:ASN:ND2	2.29	0.65
1:1A:1470:G:N2	1:1A:1520:G:OP2	2.22	0.65
32:1a:1131:G:OP1	40:1i:20:ARG:NH2	2.30	0.65
35:1d:108:LEU:HD21	35:1d:183:GLY:HA3	1.77	0.65
36:1e:100:VAL:O	36:1e:107:ARG:NH2	2.30	0.65
1:1A:1275:A:OP2	61:1A:4125:HOH:O	2.13	0.65
6:1G:181:ARG:HG3	6:1G:182:LYS:H	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1o:18:PHE:HB2	46:1o:19:PRO:HD2	1.78	0.65
47:1p:22:THR:HA	47:1p:33:ILE:HG13	1.78	0.65
32:2a:664:G:H22	32:2a:741:G:H1	1.41	0.65
41:2j:78:ASN:O	41:2j:80:LYS:N	2.29	0.65
1:1A:2299:G:N7	61:1A:4213:HOH:O	2.29	0.65
33:1b:9:GLU:OE1	33:1b:217:ARG:NH2	2.30	0.65
1:2A:2123:G:O6	1:2A:2175:C:N3	2.29	0.65
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.79	0.65
8:2I:1:MET:HE2	8:2I:38:LEU:HD21	1.78	0.65
32:2a:1147:C:O2	40:2i:16:ARG:NH1	2.29	0.65
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.78	0.65
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.30	0.65
41:2j:81:THR:HA	41:2j:84:GLN:HB2	1.78	0.65
2:1B:25:A:OP2	61:1B:303:HOH:O	2.14	0.65
32:1a:969:A:OP1	41:1j:55:LYS:NZ	2.30	0.65
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.32	0.65
1:2A:407:G:OP2	61:2A:3829:HOH:O	2.13	0.65
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.28	0.65
7:2H:61:HIS:HA	7:2H:64:LEU:HD12	1.77	0.65
26:24:15:ILE:HG23	26:24:21:VAL:HG22	1.79	0.65
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.78	0.65
12:2Q:11:LYS:HD3	12:2Q:87:LYS:HG2	1.78	0.65
2:1B:66:A:H61	2:1B:108:U:H2'	1.62	0.65
32:2a:1401:G:N7	53:2y:83:ARG:NH1	2.36	0.65
61:1A:4105:HOH:O	13:1R:3:HIS:NE2	2.29	0.64
32:1a:800:G:N7	61:1a:1935:HOH:O	2.28	0.64
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.61	0.64
1:1A:2258:C:OP1	61:1A:4126:HOH:O	2.14	0.64
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.78	0.64
32:1a:1103:C:OP1	33:1b:96:ARG:NH2	2.30	0.64
34:1c:47:LEU:HB2	34:1c:52:LEU:HD22	1.78	0.64
1:2A:2293:C:OP1	61:2A:3816:HOH:O	2.13	0.64
40:2i:53:VAL:O	40:2i:55:ALA:N	2.31	0.64
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.78	0.64
1:2A:962:G:OP1	61:2A:3824:HOH:O	2.14	0.64
1:2A:2134:A:O2'	1:2A:2159:G:N3	2.29	0.64
21:2Z:23:LYS:HD3	21:2Z:40:ASP:HA	1.80	0.64
41:2j:55:LYS:O	41:2j:57:LYS:N	2.30	0.64
44:2m:3:ARG:HH12	44:2m:11:ARG:HG2	1.62	0.64
1:1A:2143:C:O2	1:1A:2148:G:N1	2.18	0.64
3:2D:221:VAL:HG22	3:2D:226:MET:HE3	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1085:A:O2'	1:1A:1104:C:O2'	2.15	0.64
32:1a:1003:G:C2'	32:1a:1004:A:H4'	2.27	0.64
36:1e:8:GLU:HG2	36:1e:34:VAL:HG23	1.80	0.64
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.80	0.64
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.31	0.64
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.62	0.64
12:1Q:97:VAL:HG11	12:1Q:103:MET:HE3	1.79	0.64
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.33	0.64
40:1i:121:ARG:NH1	40:1i:122:ALA:O	2.31	0.64
1:2A:11:G:H2'	1:2A:12:U:H5''	1.78	0.64
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.31	0.64
1:2A:521:G:O6	61:2A:3822:HOH:O	2.11	0.64
32:1a:38:G:H22	32:1a:397:A:H5'	1.63	0.64
1:2A:526:A:OP1	61:2A:3833:HOH:O	2.15	0.64
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.78	0.64
35:2d:201:GLN:NE2	36:2e:116:THR:O	2.31	0.64
40:2i:28:VAL:HG13	40:2i:63:ILE:HB	1.79	0.64
51:2t:57:ARG:HH22	51:2t:100:ILE:HD12	1.62	0.64
1:1A:11:G:H2'	1:1A:12:U:H5'	1.80	0.64
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.31	0.64
50:1s:18:LYS:HD3	50:1s:31:ILE:HD12	1.80	0.64
1:2A:1714:G:H2'	1:2A:1717:G:H8	1.63	0.64
1:2A:1803:A:O2'	3:2D:259:THR:HG21	1.98	0.64
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.45	0.64
26:24:14:ILE:HB	26:24:22:ILE:HD13	1.80	0.64
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.30	0.63
1:2A:2584:U:O4	61:2A:3832:HOH:O	2.15	0.63
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.80	0.63
32:2a:1360:A:OP2	45:2n:35:ARG:NH2	2.29	0.63
1:1A:123:G:OP2	61:1A:4127:HOH:O	2.14	0.63
4:1E:181:LEU:HD21	15:1T:6:LEU:HD23	1.78	0.63
33:1b:134:GLU:HG3	33:1b:137:ARG:HH21	1.62	0.63
6:2G:46:ALA:HB2	6:2G:53:LEU:HD12	1.80	0.63
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.80	0.63
1:1A:521:G:O6	61:1A:4121:HOH:O	2.11	0.63
1:1A:2719:G:OP2	61:1A:4128:HOH:O	2.15	0.63
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.79	0.63
32:1a:1182:G:H4'	32:1a:1183:A:H5'	1.80	0.63
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.34	0.63
1:2A:2602:A:H1'	1:2A:2603:G:C5'	2.28	0.63
32:2a:17:U:H2'	32:2a:18:C:C6	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:16:2:ALA:N	61:16:601:HOH:O	2.29	0.63
1:2A:607:U:OP1	5:2F:102:PRO:HA	1.98	0.63
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.31	0.63
1:2A:2321:G:O2'	1:2A:2322:A:OP1	2.14	0.63
26:24:59:PHE:HA	26:24:60:GLN:C	2.23	0.63
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.79	0.63
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.79	0.63
1:2A:2497:A:O2'	61:2A:3834:HOH:O	2.15	0.63
32:2a:977:A:N6	32:2a:1224:G:OP1	2.29	0.63
32:1a:1124:G:N2	32:1a:1125:U:O4	2.31	0.63
1:2A:802:A:OP1	61:2A:3835:HOH:O	2.15	0.63
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.81	0.63
1:1A:2142:C:N3	1:1A:2149:G:O6	2.32	0.63
26:14:61:ARG:HH21	50:1s:42:PRO:HD3	1.63	0.63
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.78	0.63
32:2a:201:C:H42	32:2a:216:G:H1	1.47	0.63
32:1a:1183:A:H3'	32:1a:1184:G:H5''	1.80	0.63
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.32	0.63
51:1t:56:MET:HG3	51:1t:88:VAL:HG21	1.80	0.63
1:2A:2788:C:N3	1:2A:2789:C:N4	2.47	0.63
44:2m:91:ARG:NE	44:2m:97:PRO:O	2.29	0.63
1:1A:2142:C:O2	1:1A:2149:G:N1	2.31	0.62
1:1A:2319:G:N2	14:1S:3:ARG:HD3	2.03	0.62
5:1F:164:ARG:HE	58:1F:319:ARG:HH12	1.45	0.62
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.99	0.62
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.80	0.62
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.32	0.62
1:2A:641:C:O2'	1:2A:2350:C:OP1	2.10	0.62
1:1A:671:C:N4	61:1A:4244:HOH:O	2.32	0.62
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.34	0.62
18:1W:79:GLY:HA3	18:1W:100:THR:HG22	1.81	0.62
42:1k:34:ASP:OD1	42:1k:38:ASN:N	2.31	0.62
1:1A:2079:U:OP1	23:11:21:ARG:NH2	2.32	0.62
11:1P:119:GLU:HG3	25:23:3:ARG:HH21	1.65	0.62
18:1W:2:GLU:OE2	18:1W:72:LYS:NZ	2.24	0.62
30:18:28:GLY:O	30:18:36:LYS:NZ	2.31	0.62
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.81	0.62
6:1G:79:ASN:OD1	6:1G:79:ASN:N	2.32	0.62
1:1A:2058:MA6:H103	56:1A:4033:ZIT:H8A3	1.82	0.62
2:1B:81:G:N7	58:1B:230:ARG:NH2	2.43	0.62
40:1i:9:ARG:HG2	40:1i:14:VAL:HG13	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.31	0.62
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.80	0.62
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.34	0.62
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.80	0.62
34:2c:63:ASN:HB2	34:2c:98:ASN:HB2	1.82	0.62
1:1A:330:A:H2	1:1A:1210:A:HO2'	1.48	0.62
1:1A:2720:U:OP1	61:1A:4129:HOH:O	2.15	0.62
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.32	0.62
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.33	0.62
32:2a:662:G:H2'	32:2a:663:A:C8	2.34	0.62
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.81	0.62
32:2a:1239:A:O2'	38:2g:114:ARG:O	2.15	0.62
23:11:80:LEU:HB3	23:11:82:LEU:HG	1.81	0.62
41:1j:62:HIS:HB3	45:1n:59:ALA:HB3	1.82	0.62
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.27	0.62
44:2m:3:ARG:HB3	44:2m:9:ILE:H	1.64	0.62
32:1a:560:U:O2'	32:1a:561:U:OP2	2.17	0.62
1:2A:468:G:O2'	5:2F:62:ARG:NH2	2.28	0.62
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.27	0.62
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.31	0.62
35:1d:30:LYS:HA	35:1d:35:ARG:HE	1.65	0.61
40:1i:18:PHE:HB2	40:1i:62:TYR:HB3	1.82	0.61
45:1n:3:ARG:HB2	45:1n:3:ARG:NH1	2.15	0.61
32:2a:434:U:H2'	32:2a:435:C:C6	2.34	0.61
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.82	0.61
33:1b:219:VAL:HA	33:1b:222:ILE:HD12	1.82	0.61
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.82	0.61
32:2a:954:G:H21	32:2a:1227:A:H62	1.48	0.61
1:1A:773:U:OP1	61:1A:4131:HOH:O	2.16	0.61
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.28	0.61
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.82	0.61
1:1A:25:U:OP2	61:1A:4130:HOH:O	2.16	0.61
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.82	0.61
1:2A:214:G:HO2'	1:2A:216:A:HO2'	1.35	0.61
1:2A:1057:A:N6	1:2A:1086:A:N3	2.47	0.61
1:2A:1250:G:H5''	61:2A:5336:HOH:O	2.00	0.61
1:2A:2490:G:O6	61:2A:3838:HOH:O	2.16	0.61
6:1G:83:ARG:H	6:1G:86:MET:HE2	1.65	0.61
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.19	0.61
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.80	0.61
1:1A:2805:G:H2'	1:1A:2807:G:C8	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.36	0.61
36:1e:148:VAL:HG21	39:1h:107:LEU:HB3	1.83	0.61
39:1h:73:ASP:OD1	39:1h:75:ARG:NH1	2.33	0.61
40:1i:17:VAL:HG21	40:1i:81:ILE:HG22	1.82	0.61
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.19	0.61
37:2f:35:ALA:HB2	37:2f:67:MET:HE2	1.83	0.61
42:2k:117:ASN:N	42:2k:117:ASN:OD1	2.32	0.61
39:1h:14:ARG:NH1	39:1h:83:ILE:O	2.34	0.61
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.82	0.61
6:2G:38:VAL:HB	6:2G:158:ALA:HB3	1.83	0.61
38:2g:95:ARG:HE	38:2g:99:LEU:HD11	1.66	0.61
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.33	0.61
32:1a:384:G:H2'	32:1a:385:C:C6	2.36	0.61
50:1s:31:ILE:HB	50:1s:49:ILE:HG13	1.81	0.61
33:2b:95:GLN:HG3	33:2b:96:ARG:H	1.65	0.61
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.32	0.61
26:14:61:ARG:HG3	26:14:62:ARG:H	1.64	0.61
1:2A:668:G:H5'	1:2A:669:G:OP2	2.01	0.61
1:2A:1084:A:H3'	1:2A:1085:A:H4'	1.81	0.61
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.19	0.61
1:2A:1839:G:O6	61:2A:3831:HOH:O	2.15	0.61
1:2A:2016:U:OP2	61:2A:3839:HOH:O	2.16	0.61
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.64	0.61
26:14:57:GLU:HB2	26:14:58:ARG:HA	1.81	0.61
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.01	0.60
1:1A:1300:U:H4'	1:1A:1301:A:C5'	2.30	0.60
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.82	0.60
19:1X:60:ARG:NH1	29:17:47:ARG:HH22	1.99	0.60
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.01	0.60
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.36	0.60
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.34	0.60
47:2p:21:VAL:HG22	47:2p:33:ILE:HB	1.83	0.60
4:1E:2:LYS:HB2	4:1E:95:ILE:HD12	1.83	0.60
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.82	0.60
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.83	0.60
5:2F:122:LYS:HD2	5:2F:191:ARG:HD2	1.82	0.60
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.82	0.60
32:2a:649:G:O6	61:2a:3210:HOH:O	2.14	0.60
32:2a:1096:C:H2'	32:2a:1097:C:H6	1.65	0.60
35:1d:59:ARG:HH12	35:1d:66:ARG:HH12	1.49	0.60
26:24:10:VAL:HG22	26:24:11:PRO:HD2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:64:G:H4'	32:2a:65:U:H3'	1.83	0.60
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.34	0.60
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.33	0.60
1:2A:2504:U:OP2	61:2A:3837:HOH:O	2.16	0.60
1:1A:2130:U:O2'	1:1A:2133:G:O2'	2.19	0.60
13:1R:78:LYS:NZ	61:1R:301:HOH:O	2.34	0.60
39:1h:116:LYS:HD2	39:1h:129:VAL:HG11	1.83	0.60
47:1p:53:VAL:HG12	47:1p:79:VAL:HG12	1.83	0.60
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.36	0.60
1:2A:2206:G:H5''	1:2A:2207:G:C8	2.36	0.60
2:2B:23:G:O6	61:2B:302:HOH:O	2.15	0.60
8:2I:126:TYR:HB2	8:2I:142:VAL:HG23	1.81	0.60
33:2b:174:VAL:O	33:2b:178:ARG:HG2	2.02	0.60
32:1a:1069:C:OP2	61:1a:1909:HOH:O	2.15	0.60
1:2A:1062:G:C5	1:2A:1070:A:H1'	2.37	0.60
32:2a:662:G:H2'	32:2a:663:A:H8	1.66	0.60
1:1A:2683:C:OP1	15:1T:53:ARG:NH2	2.34	0.60
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.29	0.60
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.83	0.60
1:2A:110:G:N7	61:2A:3926:HOH:O	2.31	0.60
1:2A:323:G:O2'	1:2A:1205:U:N3	2.26	0.60
1:2A:588:U:OP2	61:2A:3836:HOH:O	2.16	0.60
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.34	0.60
1:1A:1762:A:H2'	61:1A:7279:HOH:O	2.02	0.60
1:2A:400:G:N7	61:2A:3918:HOH:O	2.31	0.60
1:2A:2107:C:N3	1:2A:2182:G:N2	2.45	0.60
1:2A:2127:G:O6	1:2A:2161:C:N3	2.35	0.60
50:2s:41:VAL:HG13	50:2s:43:GLU:H	1.67	0.60
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.84	0.60
32:1a:673:G:H2'	32:1a:674:G:C8	2.37	0.60
32:1a:920:U:H2'	32:1a:921:U:C6	2.37	0.60
40:1i:43:ALA:HA	40:1i:74:ILE:HD13	1.83	0.60
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.84	0.60
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.66	0.60
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.83	0.60
1:1A:1359:A:H61	1:1A:1372:U:H3	1.49	0.60
1:1A:2155:G:H2'	1:1A:2156:G:O4'	2.02	0.60
32:1a:636:U:H2'	32:1a:637:G:H8	1.67	0.60
42:1k:99:GLN:HG3	42:1k:105:VAL:HG21	1.83	0.60
43:1l:27:LEU:HD23	43:1l:33:ARG:HB2	1.84	0.60
1:1A:1174:A:H1'	1:1A:1175:U:H5'	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:77:ILE:HB	6:1G:82:LEU:HB2	1.84	0.59
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.37	0.59
1:2A:1098:A:H3'	1:2A:1099:G:H8	1.67	0.59
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.25	0.59
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.08	0.59
32:1a:636:U:H2'	32:1a:637:G:C8	2.36	0.59
1:2A:1064:C:H3'	1:2A:1065:U:C5'	2.32	0.59
1:1A:1026:U:OP1	61:1A:4115:HOH:O	2.16	0.59
1:1A:1094:U:H1'	1:1A:1097:U:H5	1.66	0.59
1:1A:1920:OMC:HM22	1:1A:1921:G:H5'	1.84	0.59
5:1F:195:ASP:HB2	5:1F:198:ALA:H	1.67	0.59
32:1a:317:G:OP2	61:1a:1910:HOH:O	2.16	0.59
32:1a:1070:U:H2'	32:1a:1071:C:H6	1.68	0.59
33:1b:208:ILE:H	33:1b:208:ILE:HD12	1.67	0.59
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.85	0.59
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.84	0.59
32:2a:674:G:H2'	32:2a:675:A:H8	1.67	0.59
1:1A:1315:C:OP2	61:1A:4110:HOH:O	2.16	0.59
32:1a:96:U:H2'	32:1a:97:G:C8	2.38	0.59
32:1a:330:C:OP2	61:1a:1911:HOH:O	2.17	0.59
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.19	0.59
34:2c:37:GLN:HE22	45:2n:52:GLN:HB3	1.67	0.59
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.84	0.59
1:1A:226:G:H21	1:1A:228:A:H62	1.49	0.59
32:1a:407:G:H5''	35:1d:115:ARG:HB3	1.83	0.59
1:2A:1056:G:H4'	1:2A:1057:A:C8	2.36	0.59
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.19	0.59
32:2a:937:A:OP2	61:2a:3211:HOH:O	2.15	0.59
32:1a:946:A:H2'	32:1a:947:G:C8	2.38	0.59
31:29:2:LYS:NZ	31:29:31:LYS:O	2.29	0.59
32:2a:1503:A:H5'	32:2a:1531:A:H1'	1.84	0.59
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.35	0.59
1:1A:2107:C:N3	1:1A:2182:G:O6	2.36	0.59
1:1A:2114:A:H3'	1:1A:2115:G:H8	1.66	0.59
35:1d:155:LEU:HB3	35:1d:158:ILE:HG12	1.84	0.59
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.35	0.59
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.38	0.59
7:2H:24:VAL:HG11	7:2H:72:ILE:HD11	1.85	0.59
34:2c:73:PRO:HB3	34:2c:103:VAL:HG11	1.84	0.59
45:2n:6:LEU:HD23	45:2n:9:LYS:HD2	1.85	0.59
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1062:G:O2'	1:2A:1063:G:H8	1.86	0.59
1:2A:2155:G:C2	1:2A:2156:G:H1'	2.37	0.59
1:2A:2507:C:OP1	61:2A:3840:HOH:O	2.17	0.59
1:1A:1468:C:OP1	61:1A:4133:HOH:O	2.17	0.59
33:1b:21:ARG:HA	33:1b:39:ILE:HA	1.84	0.59
1:2A:752:A:H3'	29:27:1:MET:HE1	1.85	0.59
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.85	0.59
1:1A:942:G:O6	61:1A:4132:HOH:O	2.16	0.59
15:1T:127:ALA:O	15:1T:128:GLU:HB3	2.02	0.59
1:2A:1891:G:N7	61:2A:3935:HOH:O	2.32	0.59
1:2A:2117:A:H5'	1:2A:2147:G:O2'	2.03	0.59
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.38	0.59
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.68	0.59
1:2A:2602:A:H4'	1:2A:2603:G:OP1	2.02	0.58
1:1A:2602:A:H4'	1:1A:2603:G:OP1	2.02	0.58
32:1a:642:A:N3	39:1h:113:SER:OG	2.27	0.58
1:2A:1508:A:H4'	1:2A:1509(A):A:C6	2.39	0.58
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.85	0.58
19:2X:54:VAL:HG22	19:2X:81:VAL:HG12	1.85	0.58
25:23:7:LYS:HE3	25:23:32:GLN:HE21	1.68	0.58
32:2a:117:G:OP2	61:2a:3213:HOH:O	2.16	0.58
41:2j:6:ILE:HB	41:2j:72:VAL:HG22	1.85	0.58
19:1X:63:LYS:O	19:1X:64:LYS:HD3	2.03	0.58
32:1a:79:G:N2	32:1a:90:U:O2	2.37	0.58
9:2N:21:LYS:HE3	9:2N:140:VAL:HG23	1.86	0.58
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.27	0.58
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.34	0.58
42:2k:115:PRO:C	42:2k:117:ASN:HA	2.28	0.58
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.03	0.58
32:1a:100:C:H2'	32:1a:101:A:C8	2.37	0.58
32:1a:222:U:H2'	32:1a:223:U:C6	2.39	0.58
32:1a:1260:C:H5'	32:1a:1284:C:H4'	1.85	0.58
1:1A:184:C:H2'	1:1A:185:U:C6	2.38	0.58
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.38	0.58
14:1S:34:HIS:ND1	14:1S:53:SER:OG	2.37	0.58
21:2Z:152:ALA:HA	21:2Z:155:LEU:HD13	1.85	0.58
32:2a:1172:C:H2'	32:2a:1173:G:H8	1.69	0.58
2:1B:6:C:H2'	2:1B:7:G:H5''	1.85	0.58
1:2A:1064:C:H3'	1:2A:1065:U:H5'	1.84	0.58
2:1B:23:G:O6	61:1B:305:HOH:O	2.17	0.58
32:1a:160:A:H2'	32:1a:161:A:O4'	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:262:A:H2'	32:1a:263:A:C8	2.39	0.58
53:1y:26:LYS:HD3	53:1y:78:ILE:HG21	1.86	0.58
1:2A:2469:A:H4'	12:2Q:56:ARG:HG2	1.84	0.58
34:2c:70:VAL:HG22	34:2c:72:LYS:H	1.69	0.58
5:1F:108:LYS:HD2	5:1F:112:MET:HE3	1.85	0.58
32:1a:1456:G:N1	51:1t:51:GLU:OE2	2.33	0.58
17:2V:97:LYS:HE2	17:2V:97:LYS:HA	1.85	0.58
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.39	0.58
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.86	0.58
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.04	0.58
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.69	0.58
34:2c:6:HIS:HD2	45:2n:49:HIS:HB3	1.69	0.58
1:1A:456:C:H4'	61:1A:5191:HOH:O	2.03	0.58
32:1a:840:C:H4'	32:1a:841:U:OP2	2.03	0.58
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.86	0.58
15:2T:127:ALA:C	15:2T:129:ARG:H	2.10	0.58
19:2X:35:THR:HG22	19:2X:37:THR:H	1.67	0.58
32:2a:1003:G:H3'	32:2a:1003:G:N3	2.18	0.58
37:2f:68:PRO:HG2	37:2f:71:ARG:HH11	1.68	0.58
1:1A:1064:C:H3'	1:1A:1065:U:H5''	1.86	0.57
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.67	0.57
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.69	0.57
34:2c:6:HIS:CD2	45:2n:49:HIS:HB3	2.39	0.57
44:2m:102:ARG:NE	44:2m:102:ARG:HA	2.18	0.57
1:1A:1300:U:H4'	1:1A:1301:A:H5'	1.85	0.57
1:1A:1359:A:N6	1:1A:1372:U:H3	2.01	0.57
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.86	0.57
47:2p:47:ASP:OD1	47:2p:47:ASP:N	2.36	0.57
1:1A:2142:C:C2	1:1A:2149:G:N1	2.72	0.57
32:1a:1347:G:N2	32:1a:1373:G:H2'	2.19	0.57
3:2D:127:VAL:HA	3:2D:193:VAL:HG23	1.86	0.57
6:2G:41:GLN:NE2	6:2G:154:GLY:O	2.34	0.57
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	1.86	0.57
20:1Y:92:ASN:H	20:1Y:93:GLY:HA2	1.69	0.57
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.36	0.57
17:2V:14:VAL:HB	17:2V:96:ILE:HG13	1.85	0.57
32:2a:737:A:H2'	32:2a:738:C:C6	2.39	0.57
1:1A:2751:G:C2	7:1H:2:SER:HB3	2.40	0.57
6:1G:53:LEU:O	6:1G:56:ALA:N	2.32	0.57
32:1a:965:A:OP2	53:1y:8:LYS:NZ	2.37	0.57
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.21	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:1p:43:LYS:HG2	47:1p:48:TRP:CE2	2.40	0.57
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.37	0.57
1:2A:1814:G:OP1	61:2A:3842:HOH:O	2.17	0.57
5:2F:50:SER:HB2	5:2F:94:PRO:HD3	1.87	0.57
32:2a:1003:G:C5	32:2a:1004:A:H1'	2.39	0.57
32:2a:1054:C:N4	53:2y:46:GLN:OE1	2.26	0.57
32:2a:1323:G:HO2'	32:2a:1362:C:HO2'	1.52	0.57
1:1A:746:A:C2	56:1A:4033:ZIT:H161	2.40	0.57
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.05	0.57
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.33	0.57
51:1t:33:ILE:O	51:1t:37:SER:OG	2.18	0.57
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.20	0.57
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.20	0.57
1:2A:2218:U:O4'	23:21:52:ARG:NH2	2.37	0.57
10:2O:64:ARG:HB2	10:2O:79:PHE:CD2	2.40	0.57
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	1.87	0.57
17:1V:21:ARG:NH1	17:1V:93:GLU:OE2	2.38	0.57
1:2A:2119:A:H61	1:2A:2168:G:H21	1.51	0.57
32:2a:888:G:O6	61:2a:3212:HOH:O	2.16	0.57
32:2a:1256:A:H61	32:2a:1278:U:H1'	1.70	0.57
1:1A:286:C:H2'	1:1A:287:C:C6	2.39	0.57
33:1b:231:GLU:HB3	33:1b:232:PRO:CD	2.34	0.57
37:1f:95:GLU:O	49:1r:32:ARG:NH1	2.37	0.57
7:2H:46:GLU:HB2	7:2H:49:VAL:HG12	1.86	0.57
34:2c:181:ASN:N	34:2c:205:GLY:O	2.34	0.57
1:2A:1798:U:OP2	3:2D:274:ARG:NH2	2.37	0.57
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.05	0.57
26:24:61:ARG:O	26:24:61:ARG:NH1	2.32	0.57
33:2b:78:GLN:NE2	33:2b:95:GLN:OE1	2.38	0.57
34:2c:22:TRP:HA	41:2j:93:GLY:HA2	1.87	0.57
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	1.87	0.57
9:1N:12:ARG:NH1	9:1N:50:ASP:OD2	2.38	0.57
4:2E:176:ILE:HB	4:2E:181:LEU:HB2	1.86	0.57
32:2a:617:G:N7	61:2a:3248:HOH:O	2.33	0.57
32:2a:992:U:H4'	32:2a:993:G:O5'	2.05	0.57
32:2a:1030(C):G:H2'	32:2a:1030(D):A:C8	2.39	0.57
3:1D:66:ASP:OD2	61:1D:401:HOH:O	2.18	0.56
1:2A:1024:G:OP2	61:2A:3817:HOH:O	2.17	0.56
32:2a:545:C:OP1	35:2d:61:LYS:NZ	2.37	0.56
32:2a:1005:A:H1'	32:2a:1025:U:C2	2.39	0.56
1:1A:998:C:OP1	61:1A:4137:HOH:O	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.35	0.56
37:1f:78:GLU:O	37:1f:81:ILE:HG22	2.05	0.56
1:2A:1104:C:H2'	1:2A:1105:U:C6	2.40	0.56
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.05	0.56
1:2A:2115:G:H22	1:2A:2119:A:H5'	1.70	0.56
32:2a:632:A:H5'	32:2a:633:G:OP2	2.05	0.56
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.20	0.56
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.38	0.56
1:1A:1094:U:H2'	1:1A:1096:A:OP2	2.06	0.56
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.53	0.56
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.86	0.56
32:1a:677:U:H3	32:1a:713:G:H22	1.52	0.56
32:1a:1003:G:C2	32:1a:1004:A:H1'	2.40	0.56
32:1a:1010:G:N2	32:1a:1020:U:H1'	2.20	0.56
1:2A:1920:OMC:HM22	1:2A:1921:G:H5'	1.87	0.56
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.23	0.56
2:2B:49:C:OP1	61:2B:303:HOH:O	2.17	0.56
2:2B:50:G:OP1	14:2S:63:THR:OG1	2.24	0.56
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.37	0.56
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.20	0.56
32:2a:1070:U:H2'	32:2a:1071:C:H6	1.71	0.56
35:2d:187:ARG:NH2	35:2d:193:ASP:OD2	2.38	0.56
44:2m:19:LEU:HD21	44:2m:56:LEU:HD21	1.87	0.56
2:1B:55:U:OP2	61:1B:304:HOH:O	2.17	0.56
35:1d:18:LYS:NZ	60:1d:303:SF4:S1	2.78	0.56
1:2A:495:G:N3	18:2W:61:ASN:ND2	2.51	0.56
1:2A:922:U:H2'	1:2A:923:C:C6	2.40	0.56
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.05	0.56
1:1A:1069:A:H4'	1:1A:1070:A:H5''	1.86	0.56
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.39	0.56
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.38	0.56
1:1A:1890:A:OP2	61:1A:4135:HOH:O	2.17	0.56
6:1G:43:LEU:HD11	6:1G:153:ARG:HD3	1.88	0.56
32:1a:737:A:H2'	32:1a:738:C:C6	2.40	0.56
41:1j:16:LEU:HD21	41:1j:70:ARG:HG2	1.88	0.56
41:1j:37:PRO:HA	41:1j:72:VAL:HG12	1.88	0.56
6:2G:36:LYS:HG2	6:2G:160:VAL:HB	1.87	0.56
21:2Z:96:VAL:N	21:2Z:128:VAL:O	2.24	0.56
32:2a:392:G:H2'	32:2a:393:A:H8	1.70	0.56
32:2a:975:A:N1	41:2j:48:THR:HB	2.20	0.56
32:2a:1318:A:H5''	50:2s:3:ARG:NH2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:286:C:H2'	1:1A:287:C:H6	1.71	0.56
8:1I:133:HIS:ND1	8:1I:134:PRO:O	2.37	0.56
32:1a:1003:G:N2	32:1a:1004:A:H1'	2.20	0.56
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.20	0.56
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.20	0.56
37:1f:35:ALA:HA	37:1f:67:MET:HB2	1.87	0.56
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.70	0.56
32:2a:677:U:H3	32:2a:713:G:H22	1.53	0.56
1:1A:715:G:H21	46:1o:40:SER:HB2	1.71	0.56
32:1a:7:G:H5'	32:1a:298:A:O4'	2.06	0.56
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.33	0.56
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.87	0.56
1:2A:370:G:OP2	1:2A:370:G:H8	1.88	0.56
1:2A:1101:U:H2'	1:2A:1102:C:C6	2.40	0.56
1:2A:1987:G:OP2	61:2A:3843:HOH:O	2.18	0.56
13:2R:104:ARG:HD2	13:2R:109:ALA:HB3	1.87	0.56
32:2a:1030(A):G:H21	32:2a:1030(C):G:H3'	1.69	0.56
41:2j:8:LEU:HB2	41:2j:70:ARG:HB2	1.87	0.56
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.39	0.56
1:1A:987:G:O2'	1:1A:1000:A:N3	2.33	0.56
21:1Z:3:TYR:CE2	21:1Z:51:ALA:HB2	2.41	0.56
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.41	0.56
40:1i:16:ARG:HD3	40:1i:64:THR:HG21	1.88	0.56
1:2A:2127:G:N1	1:2A:2161:C:O2	2.39	0.56
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.39	0.56
26:24:48:ARG:HG3	26:24:52:THR:HG23	1.87	0.56
32:2a:528:C:N4	43:2l:49:ASN:OD1	2.39	0.56
38:2g:109:ASN:HA	38:2g:119:ARG:HE	1.70	0.56
50:2s:20:LEU:HA	50:2s:23:ASN:HB2	1.86	0.56
1:1A:2791:C:OP2	1:1A:2791:C:H6	1.89	0.56
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.88	0.56
32:1a:620:C:OP1	61:1a:1912:HOH:O	2.17	0.56
1:2A:1062:G:O2'	1:2A:1063:G:H5'	2.06	0.56
1:2A:1378:A:OP1	29:27:10:ARG:NH2	2.39	0.56
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.88	0.56
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.88	0.56
1:1A:620:G:N3	1:1A:620:G:H5'	2.21	0.56
1:1A:1009:A:OP2	61:1A:4139:HOH:O	2.18	0.56
1:1A:1721:G:H8	1:1A:1741:A:H62	1.54	0.56
12:1Q:108:GLY:HA3	21:1Z:116:VAL:HG13	1.88	0.56
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.05	0.56
1:2A:2058:MA6:H93	56:2A:3713:ZIT:H8A3	1.88	0.56
11:2P:125:VAL:HG11	11:2P:138:LEU:HD21	1.86	0.56
32:2a:1278:U:H5''	32:2a:1279:A:H5'	1.87	0.56
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.36	0.55
6:1G:114:ILE:HG12	6:1G:140:ILE:HG12	1.87	0.55
11:1P:68:GLN:HG3	61:1P:315:HOH:O	2.04	0.55
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.87	0.55
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.88	0.55
42:1k:91:ARG:NH1	42:1k:110:ASP:OD2	2.40	0.55
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.69	0.55
32:2a:164:U:H2'	32:2a:165:C:C6	2.41	0.55
32:2a:757:U:H2'	32:2a:758:G:O4'	2.05	0.55
32:2a:1366:C:O2'	41:2j:60:ARG:NH2	2.38	0.55
36:2e:40:ARG:NH2	36:2e:68:GLU:OE2	2.39	0.55
6:1G:59:GLU:OE2	6:1G:153:ARG:NH2	2.40	0.55
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.21	0.55
32:1a:176:C:H2'	32:1a:177:C:C6	2.40	0.55
36:1e:143:ARG:NH1	39:1h:77:GLU:OE2	2.39	0.55
1:2A:75:G:H4'	24:22:55:ARG:NH1	2.21	0.55
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.42	0.55
1:2A:1011:G:OP1	16:2U:77:SER:OG	2.24	0.55
8:2I:26:ALA:HB1	8:2I:31:LEU:HD13	1.89	0.55
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	1.88	0.55
32:1a:130:A:H5'	48:1q:63:ARG:HE	1.72	0.55
1:2A:362:U:O2'	1:2A:363:G:H5'	2.05	0.55
1:2A:2128:C:N3	1:2A:2160:G:N2	2.50	0.55
6:2G:36:LYS:HE2	6:2G:160:VAL:HG21	1.88	0.55
32:2a:625:G:H2'	32:2a:626:U:H6	1.72	0.55
1:1A:2206:G:OP2	1:1A:2206:G:H4'	2.06	0.55
12:1Q:26:TYR:OH	61:1Q:301:HOH:O	2.17	0.55
32:1a:1030(C):G:H2'	32:1a:1030(D):A:H8	1.70	0.55
44:1m:15:VAL:HG11	44:1m:48:LEU:HD21	1.87	0.55
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.24	0.55
53:2y:5:ILE:HG23	53:2y:39:ILE:HB	1.88	0.55
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.06	0.55
1:1A:2114:A:H3'	1:1A:2115:G:C8	2.42	0.55
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.42	0.55
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	1.87	0.55
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.06	0.55
1:2A:588:U:H2'	1:2A:589:C:C6	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1106:G:H2'	1:2A:1107:G:H8	1.72	0.55
1:2A:2112:G:H2'	1:2A:2113:U:C6	2.41	0.55
32:2a:402:G:O2'	32:2a:620:C:N3	2.37	0.55
32:2a:1203:C:H2'	32:2a:1204:A:C8	2.42	0.55
1:1A:187:G:OP2	61:1A:4136:HOH:O	2.18	0.55
7:1H:40:GLU:OE2	7:1H:60:ARG:NH1	2.40	0.55
32:1a:1177:G:OP2	40:1i:97:LYS:NZ	2.32	0.55
26:24:18:CYS:SG	26:24:39:CYS:HB3	2.46	0.55
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.40	0.55
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.20	0.55
41:2j:8:LEU:HD12	41:2j:20:ALA:HB2	1.89	0.55
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.42	0.55
1:1A:588:U:H2'	1:1A:589:C:C6	2.41	0.55
1:1A:1959:G:O2'	61:1A:4138:HOH:O	2.18	0.55
1:1A:2049:G:H5''	61:1A:5631:HOH:O	2.05	0.55
16:1U:36:ARG:NH2	61:1U:302:HOH:O	2.40	0.55
37:1f:100:ASN:ND2	49:1r:23:LYS:HE2	2.22	0.55
1:2A:1020:A:N1	1:2A:1141:U:O2'	2.38	0.55
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.21	0.55
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.42	0.55
2:2B:13:A:N1	2:2B:69:G:O2'	2.39	0.55
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.88	0.55
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.42	0.55
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.89	0.55
1:1A:2790:A:H2'	1:1A:2790:A:N3	2.22	0.55
1:2A:774:A:H2'	1:2A:774:A:N3	2.22	0.55
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.21	0.55
13:2R:33:ARG:NH2	27:25:57:VAL:O	2.33	0.55
32:2a:67:C:H2'	32:2a:68:G:C8	2.41	0.55
41:2j:63:PHE:HE1	45:2n:58:LYS:HG2	1.71	0.55
1:2A:881:G:H1	1:2A:895:U:H3	1.55	0.55
1:2A:1621:U:OP1	61:2A:3846:HOH:O	2.18	0.55
6:2G:12:TYR:HA	6:2G:16:ARG:HG3	1.89	0.55
7:2H:7:LEU:HB3	7:2H:69:ARG:HH21	1.72	0.55
32:2a:1035:A:H2'	32:2a:1037:C:H41	1.72	0.55
33:2b:77:ALA:HB2	33:2b:211:ILE:HD13	1.88	0.55
50:2s:61:TYR:HE2	50:2s:63:THR:HG23	1.72	0.55
1:1A:2563:U:H4'	10:1O:28:SER:HA	1.88	0.55
4:1E:29:GLY:HA3	61:1E:7809:HOH:O	2.05	0.55
27:15:40:LYS:NZ	27:15:44:THR:O	2.40	0.55
36:1e:10:MET:HE3	36:1e:13:ILE:HD11	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.41	0.55
9:2N:71:ILE:HG21	9:2N:84:LYS:HD3	1.89	0.55
32:2a:979:C:H2'	32:2a:980:C:H5'	1.89	0.55
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.42	0.55
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.41	0.54
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.39	0.54
6:1G:44:GLY:HA2	6:1G:88:ILE:HG22	1.88	0.54
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.89	0.54
34:1c:69:HIS:CD2	34:1c:104:GLN:HG2	2.42	0.54
44:1m:11:ARG:C	44:1m:13:LYS:H	2.15	0.54
1:2A:451:C:H5'	61:2A:3876:HOH:O	2.05	0.54
1:2A:2111:C:H42	1:2A:2147:G:H22	1.54	0.54
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	1.88	0.54
32:2a:1291:G:O2'	40:2i:38:GLN:OE1	2.25	0.54
1:1A:749:C:OP2	61:1A:4140:HOH:O	2.18	0.54
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.42	0.54
47:1p:4:ILE:HG22	47:1p:19:ILE:HD11	1.88	0.54
1:2A:1815:A:OP2	61:2A:3841:HOH:O	2.17	0.54
1:2A:2128:C:H3'	1:2A:2129:C:H5''	1.89	0.54
36:2e:95:ALA:HB1	36:2e:96:PRO:HD2	1.89	0.54
1:1A:548:A:N6	17:1V:19:LYS:H	2.04	0.54
1:1A:802:A:OP1	61:1A:4142:HOH:O	2.18	0.54
32:1a:60:A:H4'	32:1a:61:G:H5'	1.88	0.54
38:1g:27:ILE:HD13	38:1g:40:ALA:HA	1.88	0.54
1:2A:1105:U:H2'	1:2A:1106:G:C8	2.42	0.54
8:2I:123:LEU:HD23	8:2I:144:VAL:HG12	1.88	0.54
32:2a:273:A:H1'	48:2q:16:GLN:NE2	2.23	0.54
32:2a:1005:A:O3'	32:2a:1037:C:O2'	2.24	0.54
1:1A:2296:U:OP2	14:1S:9:ARG:NH2	2.40	0.54
6:2G:145:THR:HG22	6:2G:148:MET:HE3	1.88	0.54
9:2N:120:LEU:HG	9:2N:122:VAL:HG23	1.89	0.54
26:24:58:ARG:HH21	50:2s:68:GLY:H	1.54	0.54
32:2a:434:U:H2'	32:2a:435:C:H6	1.68	0.54
32:2a:1133:G:H2'	32:2a:1134:G:C8	2.42	0.54
42:2k:79:SER:HB2	42:2k:104:GLN:HB3	1.88	0.54
1:1A:2111:C:OP2	1:1A:2145:C:N4	2.34	0.54
10:1O:64:ARG:HB2	10:1O:79:PHE:CD2	2.43	0.54
25:13:26:LEU:O	25:13:35:ARG:NE	2.30	0.54
32:1a:269:C:H2'	32:1a:270:A:C8	2.43	0.54
44:1m:19:LEU:HD11	44:1m:56:LEU:HD21	1.89	0.54
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2171:A:H4'	1:2A:2172:U:OP1	2.06	0.54
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.42	0.54
41:2j:63:PHE:CE1	45:2n:58:LYS:HG2	2.43	0.54
1:1A:774:A:N3	1:1A:774:A:H2'	2.22	0.54
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.43	0.54
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.43	0.54
1:1A:2805:G:H2'	1:1A:2807:G:H8	1.71	0.54
2:1B:22:U:O4	61:1B:306:HOH:O	2.18	0.54
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.20	0.54
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.41	0.54
35:1d:109:GLY:HA3	35:1d:165:MET:HG3	1.90	0.54
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.08	0.54
1:2A:2134:A:H5''	1:2A:2156:G:H22	1.71	0.54
21:2Z:117:LEU:HD23	21:2Z:119:GLU:HG2	1.90	0.54
32:2a:1030(A):G:H1'	32:2a:1030(C):G:N7	2.23	0.54
39:2h:19:VAL:HG23	39:2h:21:LYS:HD3	1.90	0.54
1:1A:884:C:H2'	1:1A:885:C:O4'	2.08	0.54
18:1W:18:ARG:NH1	18:1W:76:VAL:O	2.41	0.54
32:1a:1305:G:OP1	52:1u:2:GLY:N	2.41	0.54
46:1o:82:ILE:O	46:1o:86:GLY:N	2.37	0.54
18:2W:80:PRO:O	18:2W:100:THR:HB	2.07	0.54
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HB	1.89	0.54
32:2a:266:G:N3	32:2a:266:G:H5''	2.22	0.54
32:2a:1004:A:H5''	32:2a:1025:U:C4	2.43	0.54
34:2c:6:HIS:CD2	34:2c:9:GLY:H	2.25	0.54
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.89	0.54
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.32	0.54
32:1a:1289:A:N1	32:1a:1371:G:O2'	2.41	0.54
36:1e:101:ILE:HG13	36:1e:119:LEU:HD23	1.89	0.54
40:1i:18:PHE:N	40:1i:62:TYR:O	2.33	0.54
45:1n:4:LYS:HA	45:1n:7:ILE:HD12	1.90	0.54
1:2A:2306:C:N4	6:2G:42:GLY:O	2.41	0.54
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.90	0.54
8:2I:77:LEU:HD21	8:2I:100:ALA:HB3	1.90	0.54
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.08	0.54
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.39	0.54
1:1A:796:C:H2'	1:1A:797:C:C6	2.43	0.54
1:1A:897:C:H2'	1:1A:898:C:C6	2.43	0.54
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.08	0.54
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.42	0.54
32:1a:355:C:O2'	32:1a:388:G:N3	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.43	0.54
3:2D:12:SER:HB3	3:2D:208:LYS:HB3	1.89	0.54
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.88	0.54
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.43	0.54
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.90	0.54
32:1a:266:G:H5''	32:1a:268:C:H41	1.71	0.54
32:1a:1226:C:O3'	44:1m:111:LYS:NZ	2.40	0.54
53:1y:40:ILE:HB	53:1y:51:ASP:HB2	1.90	0.54
1:2A:2179:C:C4	1:2A:2180:U:C4	2.96	0.54
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.43	0.54
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.42	0.54
32:2a:1015:A:H2'	32:2a:1016:A:C8	2.42	0.54
32:2a:1207:2MG:H2'	32:2a:1208:C:H6	1.73	0.54
34:2c:6:HIS:CE1	34:2c:8:ILE:HB	2.43	0.54
38:2g:114:ARG:H	38:2g:115:ARG:NH2	2.06	0.54
40:2i:23:ASN:N	40:2i:23:ASN:OD1	2.41	0.54
1:1A:2099:U:H3	1:1A:2190:G:H1	1.56	0.53
1:1A:2791:C:H5'	1:1A:2893:G:N2	2.23	0.53
25:13:39:ASP:OD2	25:13:44:ARG:NH2	2.34	0.53
32:1a:142:G:H2'	32:1a:143:A:C8	2.43	0.53
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.91	0.53
1:2A:2313:C:H4'	6:2G:91:ARG:HD3	1.90	0.53
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.33	0.53
6:2G:71:THR:N	6:2G:89:GLY:O	2.40	0.53
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.41	0.53
1:1A:1155:A:OP1	16:1U:55:ARG:HD3	2.09	0.53
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.43	0.53
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.90	0.53
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.32	0.53
41:1j:5:ARG:HE	41:1j:73:ASP:CG	2.16	0.53
44:1m:11:ARG:O	44:1m:13:LYS:N	2.40	0.53
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.07	0.53
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.43	0.53
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.73	0.53
9:2N:50:ASP:OD1	61:2N:301:HOH:O	2.19	0.53
21:2Z:140:ASP:OD1	21:2Z:142:SER:OG	2.25	0.53
32:2a:222:U:H2'	32:2a:223:U:C6	2.43	0.53
38:2g:15:ASP:OD1	38:2g:20:ASP:N	2.41	0.53
50:2s:62:ILE:HG23	50:2s:66:MET:HG3	1.90	0.53
1:1A:2092:U:OP1	61:1A:4143:HOH:O	2.18	0.53
12:1Q:98:LYS:NZ	61:1Q:302:HOH:O	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1W:37:ARG:HD3	18:1W:38:TYR:CE2	2.43	0.53
32:1a:600:C:H2'	32:1a:601:C:H6	1.73	0.53
33:1b:96:ARG:HG2	33:1b:98:LEU:HD23	1.89	0.53
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.40	0.53
5:2F:187:VAL:HG12	11:2P:3:LEU:HD12	1.91	0.53
32:2a:1025:U:O2'	32:2a:1026:G:N7	2.42	0.53
44:2m:15:VAL:HG12	44:2m:45:VAL:HG22	1.91	0.53
1:1A:2305:A:H5''	6:1G:134:GLY:HA3	1.90	0.53
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.43	0.53
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.26	0.53
18:1W:12:ILE:HD13	18:1W:17:VAL:HG13	1.91	0.53
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.80	0.53
32:1a:461:A:O2'	32:1a:470:C:H5'	2.09	0.53
33:1b:71:VAL:HB	33:1b:164:VAL:HG22	1.90	0.53
37:1f:46:ARG:HH21	49:1r:37:VAL:HG11	1.72	0.53
38:1g:26:PHE:O	38:1g:30:ILE:HG13	2.08	0.53
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.08	0.53
32:2a:993:G:H1	32:2a:1045:C:H42	1.55	0.53
1:1A:635:C:O2'	1:1A:639:U:OP1	2.24	0.53
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.43	0.53
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.43	0.53
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.41	0.53
32:1a:524:G:H2'	32:1a:525:C:C6	2.43	0.53
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.44	0.53
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.89	0.53
1:2A:212:G:H2'	1:2A:213:A:O4'	2.08	0.53
1:2A:2321:G:HO2'	1:2A:2322:A:P	2.28	0.53
21:2Z:72:ARG:HG2	21:2Z:89:PHE:HB2	1.89	0.53
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.43	0.53
34:2c:35:GLU:OE2	34:2c:59:ARG:NH2	2.42	0.53
35:2d:78:LEU:HD22	35:2d:96:LEU:HB3	1.91	0.53
1:1A:763:G:OP1	61:1A:4144:HOH:O	2.18	0.53
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.08	0.53
32:1a:536:C:OP2	61:1a:1914:HOH:O	2.19	0.53
41:1j:8:LEU:HB2	41:1j:70:ARG:HB2	1.90	0.53
1:2A:686:G:N2	1:2A:788:A:H61	2.07	0.53
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.44	0.53
1:2A:2162:G:H4'	1:2A:2172:U:O2'	2.08	0.53
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.44	0.53
7:2H:9:ILE:HB	7:2H:50:VAL:HG23	1.90	0.53
8:2I:48:GLU:OE2	8:2I:52:ARG:NH1	2.33	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.34	0.53
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.91	0.53
32:2a:1014:A:C2	32:2a:1219:U:H1'	2.44	0.53
36:2e:102:ALA:HB1	36:2e:106:PRO:HG2	1.91	0.53
44:2m:13:LYS:NZ	44:2m:21:TYR:OH	2.42	0.53
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.44	0.53
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.09	0.53
1:1A:2507:C:OP2	61:1A:4146:HOH:O	2.19	0.53
3:1D:106:ILE:HG12	61:1D:456:HOH:O	2.08	0.53
32:1a:828:A:H2'	32:1a:829:G:O4'	2.08	0.53
35:1d:128:VAL:HG12	35:1d:129:ASN:HD22	1.74	0.53
51:1t:92:LEU:O	51:1t:96:GLY:N	2.33	0.53
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.44	0.53
32:2a:437:U:O2'	35:2d:125:HIS:HE1	1.92	0.53
33:2b:21:ARG:O	33:2b:23:ARG:N	2.39	0.53
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.91	0.53
36:1e:79:GLU:HG3	36:1e:93:PRO:HD2	1.91	0.53
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.91	0.53
1:2A:241:A:H5''	61:2A:5548:HOH:O	2.09	0.53
1:2A:494:G:H3'	61:2A:3917:HOH:O	2.08	0.53
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.09	0.53
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.91	0.53
1:2A:652(A):A:O2'	1:2A:652(B):A:H5'	2.09	0.53
1:2A:989:G:O2'	61:2A:3847:HOH:O	2.19	0.53
3:2D:61:LEU:O	3:2D:63:ARG:NH1	2.42	0.53
21:2Z:179:ASP:O	21:2Z:182:LYS:HG2	2.09	0.53
31:29:22:ARG:HB3	31:29:24:TYR:CE2	2.44	0.53
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.91	0.53
1:1A:2110:G:H5''	1:1A:2111:C:H5	1.74	0.53
1:1A:2207:G:O2'	1:1A:2208:A:OP1	2.27	0.53
1:1A:2304:G:H22	1:1A:2312:U:H3	1.57	0.53
1:1A:2562:U:H1'	10:1O:23:ARG:HD3	1.91	0.53
7:1H:41:MET:HE2	7:1H:65:HIS:HA	1.91	0.53
32:1a:1030(C):G:H2'	32:1a:1030(D):A:C8	2.43	0.53
32:1a:1034:G:H3'	32:1a:1035:A:H8	1.73	0.53
1:2A:251:A:C5	1:2A:252:G:H1'	2.44	0.53
2:2B:38:C:OP2	61:2B:304:HOH:O	2.18	0.53
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.42	0.53
40:2i:54:ASP:O	40:2i:56:LEU:N	2.42	0.53
41:2j:38:ILE:HG12	41:2j:71:LEU:HB3	1.90	0.53
24:12:16:LEU:O	24:12:67:LYS:NZ	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:955:U:O2'	50:1s:83:HIS:HD2	1.92	0.52
43:1l:28:LYS:HD3	43:1l:62:SER:HB2	1.92	0.52
6:2G:27:ASN:HB3	6:2G:30:GLU:HG3	1.91	0.52
32:2a:1133:G:H2'	32:2a:1134:G:H8	1.73	0.52
33:2b:80:ILE:HD13	33:2b:211:ILE:HG22	1.91	0.52
43:2l:54:LYS:NZ	61:2l:301:HOH:O	2.31	0.52
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.42	0.52
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.42	0.52
6:1G:179:PRO:HB2	26:14:42:PHE:HE2	1.74	0.52
41:1j:81:THR:C	41:1j:83:GLU:H	2.17	0.52
1:2A:271(L):U:H5'	8:2I:50:ARG:NH1	2.22	0.52
1:2A:898:C:H2'	1:2A:899:A:O4'	2.10	0.52
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.43	0.52
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.39	0.52
5:2F:74:ARG:HD2	61:2F:414:HOH:O	2.09	0.52
32:2a:17:U:O2'	32:2a:1079:G:N3	2.43	0.52
33:2b:212:GLN:NE2	33:2b:235:SER:OG	2.42	0.52
45:2n:26:ARG:NH1	45:2n:46:GLU:OE1	2.38	0.52
1:1A:1823:G:OP1	3:1D:54:ARG:NH1	2.42	0.52
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.45	0.52
32:1a:123:C:O2'	32:1a:290:C:O2	2.27	0.52
33:2b:197:VAL:HG12	33:2b:200:ILE:HG13	1.90	0.52
41:2j:62:HIS:HB3	45:2n:59:ALA:HB3	1.91	0.52
1:1A:2126:A:H4'	1:1A:2127:G:O5'	2.07	0.52
1:1A:2689:U:H4'	1:1A:2690:C:H5'	1.91	0.52
26:14:28:LYS:HB2	26:14:31:ILE:HD11	1.92	0.52
35:1d:168:ARG:N	35:1d:168:ARG:HH11	2.08	0.52
44:1m:89:GLY:O	44:1m:93:ARG:HG3	2.08	0.52
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.10	0.52
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.43	0.52
17:2V:24:LYS:HG3	17:2V:64:HIS:HD2	1.75	0.52
21:2Z:32:HIS:NE2	61:2Z:302:HOH:O	2.33	0.52
32:2a:920:U:H2'	32:2a:921:U:C6	2.43	0.52
37:2f:61:LEU:HB3	37:2f:63:TYR:CE2	2.44	0.52
1:1A:566:U:H5''	11:1P:29:LYS:HE3	1.92	0.52
1:1A:1082:U:C4	1:1A:1086:A:N1	2.77	0.52
1:1A:2139:C:H2'	1:1A:2140:C:H6	1.74	0.52
32:1a:434:U:H2'	32:1a:435:C:C6	2.44	0.52
32:1a:656:C:O2'	46:1o:28:GLN:NE2	2.29	0.52
32:1a:926:G:O6	53:1y:87:LYS:HE2	2.10	0.52
36:1e:147:ASP:OD1	36:1e:147:ASP:N	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:84:VAL:HG11	42:1k:91:ARG:HD2	1.92	0.52
53:1y:2:THR:OG1	53:1y:3:MET:N	2.43	0.52
1:2A:984:A:H5''	1:2A:985:C:H5	1.74	0.52
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.28	0.52
6:2G:108:ASN:HA	26:24:37:SER:HB3	1.91	0.52
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.92	0.52
32:2a:1291:G:OP1	38:2g:37:ASN:ND2	2.43	0.52
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.45	0.52
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.43	0.52
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.92	0.52
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.10	0.52
32:1a:38:G:N2	32:1a:397:A:H5'	2.25	0.52
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.74	0.52
1:2A:796:C:H2'	1:2A:797:C:C6	2.44	0.52
2:2B:102:A:OP2	61:2B:305:HOH:O	2.19	0.52
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.92	0.52
11:2P:59:LEU:HD21	30:28:10:ALA:HA	1.91	0.52
32:2a:944:G:N1	32:2a:1338:G:OP2	2.38	0.52
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.93	0.52
33:2b:87:ARG:CZ	33:2b:233:SER:HB3	2.40	0.52
41:2j:74:ILE:O	61:2j:302:HOH:O	2.19	0.52
1:1A:1175:U:O3'	1:1A:1176:G:H4'	2.08	0.52
1:1A:2115:G:H2'	1:1A:2117:A:N6	2.25	0.52
3:1D:71:ASP:OD2	3:1D:103:ARG:NH2	2.43	0.52
32:1a:731:G:H5'	32:1a:766:A:H4'	1.91	0.52
32:1a:735:C:H2'	32:1a:736:C:H6	1.75	0.52
32:1a:838:G:H2'	32:1a:839:U:H2'	1.92	0.52
32:1a:1338:G:H2'	32:1a:1339:A:C8	2.44	0.52
1:2A:1053:C:H2'	1:2A:1054:A:C8	2.41	0.52
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.45	0.52
3:2D:145:VAL:HG12	3:2D:146:GLU:O	2.10	0.52
32:2a:1004:A:N7	32:2a:1037:C:H2'	2.24	0.52
32:2a:1030(A):G:H2'	32:2a:1030(B):C:H5''	1.91	0.52
32:2a:1338:G:H2'	32:2a:1339:A:C8	2.44	0.52
37:2f:68:PRO:HG2	37:2f:71:ARG:NH1	2.25	0.52
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.91	0.52
1:1A:247:G:H4'	1:1A:386:G:C5	2.44	0.52
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.44	0.52
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.10	0.52
4:1E:176:ILE:HB	4:1E:181:LEU:HB2	1.92	0.52
32:1a:143:A:H5'	32:1a:144:G:H5'	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:667:U:O2	30:28:2:PRO:HD2	2.09	0.52
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.45	0.52
1:2A:1833:U:OP1	61:2A:3848:HOH:O	2.19	0.52
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.45	0.52
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.25	0.52
11:2P:35:HIS:O	11:2P:36:LYS:HB2	2.09	0.52
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.92	0.52
36:2e:152:ARG:HB3	39:2h:43:GLY:HA3	1.92	0.52
1:1A:1070:A:C8	1:1A:1097:U:H4'	2.44	0.52
32:1a:1151:A:O2'	32:1a:1152:A:H8	1.93	0.52
32:1a:1256:A:OP2	34:1c:26:LYS:NZ	2.39	0.52
32:1a:1400:5MC:C2	53:1y:63:ALA:HA	2.45	0.52
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.17	0.52
1:2A:2110:G:H5''	1:2A:2118:U:O2	2.10	0.52
1:2A:2149:G:C2	1:2A:2150:U:H1'	2.45	0.52
7:2H:103:LEU:HB2	7:2H:123:PHE:CD2	2.44	0.52
33:2b:57:PHE:HE2	33:2b:185:ILE:HD11	1.75	0.52
46:2o:55:GLY:HA2	46:2o:58:MET:HE3	1.91	0.52
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.75	0.52
1:1A:1830:C:OP2	61:1A:4141:HOH:O	2.18	0.52
3:1D:4:LYS:HB3	3:1D:18:VAL:HG23	1.90	0.52
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.92	0.52
39:2h:10:LEU:HD23	39:2h:83:ILE:HG12	1.92	0.52
1:1A:1653:G:H3'	13:1R:2:ARG:HD3	1.92	0.51
32:1a:840:C:H5''	32:1a:841:U:C4	2.45	0.51
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.44	0.51
44:1m:82:MET:HE3	44:1m:93:ARG:HG2	1.91	0.51
1:2A:885:C:H2'	1:2A:886:C:O4'	2.10	0.51
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.37	0.51
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.10	0.51
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.45	0.51
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.45	0.51
32:2a:1182:G:H4'	32:2a:1183:A:H3'	1.91	0.51
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.75	0.51
34:2c:82:GLU:O	34:2c:86:VAL:N	2.43	0.51
35:2d:201:GLN:NE2	36:2e:99:GLY:HA2	2.25	0.51
40:2i:26:VAL:HA	40:2i:61:ALA:O	2.10	0.51
42:2k:116:HIS:N	42:2k:117:ASN:HA	2.24	0.51
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.26	0.51
1:1A:2336:A:H61	22:10:43:THR:CG2	2.24	0.51
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1119:C:H2'	32:1a:1120:G:H8	1.75	0.51
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.10	0.51
34:1c:12:LEU:HD11	45:1n:51:GLY:HA2	1.93	0.51
4:2E:178:GLU:CD	4:2E:178:GLU:H	2.18	0.51
8:2I:5:LEU:HD23	8:2I:36:ALA:HB2	1.93	0.51
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.43	0.51
53:2y:38:HIS:CD2	53:2y:40:ILE:HD11	2.45	0.51
35:1d:20:TYR:HA	35:1d:26:CYS:SG	2.51	0.51
39:1h:14:ARG:O	39:1h:18:ARG:HG2	2.09	0.51
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.42	0.51
1:2A:2450:A:OP2	61:2A:3844:HOH:O	2.18	0.51
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.91	0.51
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.92	0.51
7:2H:103:LEU:O	7:2H:114:VAL:HA	2.10	0.51
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.43	0.51
32:2a:406:G:N2	35:2d:119:GLN:OE1	2.36	0.51
32:2a:979:C:O2	45:2n:19:ARG:NE	2.43	0.51
32:2a:1154:G:H2'	32:2a:1155:G:H8	1.75	0.51
44:2m:82:MET:HE3	44:2m:93:ARG:HD3	1.91	0.51
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.10	0.51
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.46	0.51
35:1d:15:GLU:OE2	35:1d:66:ARG:NH1	2.43	0.51
35:1d:88:VAL:HG13	36:1e:97:GLY:HA2	1.91	0.51
1:2A:615:G:OP1	5:2F:40:GLN:NE2	2.42	0.51
1:2A:1014:U:H2'	1:2A:1015:G:H8	1.76	0.51
1:2A:2134:A:H8	1:2A:2156:G:H21	1.58	0.51
19:2X:35:THR:HG22	19:2X:37:THR:N	2.26	0.51
32:2a:1239:A:H62	32:2a:1299:A:H62	1.58	0.51
32:2a:1500:A:OP1	61:2a:3215:HOH:O	2.19	0.51
50:2s:20:LEU:HD21	50:2s:43:GLU:HG2	1.92	0.51
50:2s:51:VAL:O	50:2s:57:HIS:HA	2.10	0.51
1:1A:2058:MA6:H103	56:1A:4033:ZIT:O2A	2.10	0.51
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.92	0.51
33:1b:229:VAL:HG12	33:1b:230:VAL:H	1.75	0.51
40:1i:40:LEU:HD11	40:1i:70:LYS:HG2	1.92	0.51
1:2A:234:C:H2'	1:2A:235:U:H6	1.76	0.51
1:2A:493:G:H2'	1:2A:494:G:O4'	2.11	0.51
1:2A:858:U:O2	1:2A:2268:A:H2'	2.09	0.51
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.27	0.51
3:2D:71:ASP:HB3	3:2D:103:ARG:HH22	1.76	0.51
6:2G:28:VAL:O	6:2G:31:VAL:HG13	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2R:87:TYR:HE1	13:2R:117:VAL:HG12	1.76	0.51
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.92	0.51
5:1F:191:ARG:NH2	61:1F:406:HOH:O	2.43	0.51
11:1P:119:GLU:HG3	25:23:3:ARG:NH2	2.25	0.51
32:1a:1123:A:H4'	41:1j:36:GLY:HA3	1.91	0.51
39:1h:86:ILE:HG12	39:1h:135:CYS:HA	1.91	0.51
1:2A:888:C:H2'	1:2A:889:C:C4	2.46	0.51
32:2a:280:C:N3	48:2q:39:SER:OG	2.39	0.51
32:2a:565:U:OP2	32:2a:566:G:O2'	2.27	0.51
32:2a:1108:G:H5'	34:2c:176:HIS:HD2	1.75	0.51
32:2a:1256:A:H61	32:2a:1278:U:C1'	2.24	0.51
1:1A:548:A:H61	17:1V:19:LYS:H	1.58	0.51
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.40	0.51
32:1a:166:G:H2'	32:1a:167:G:H8	1.75	0.51
1:2A:411:G:C5	11:2P:72:PRO:HB3	2.46	0.51
1:2A:470:A:OP1	5:2F:59:TYR:HE1	1.94	0.51
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.18	0.51
1:2A:2810:A:N6	1:2A:2891:G:O2'	2.43	0.51
9:2N:20:GLY:HA2	9:2N:61:ARG:HG3	1.92	0.51
32:2a:41:G:H2'	32:2a:42:G:C8	2.45	0.51
32:2a:560:U:H4'	32:2a:561:U:O5'	2.11	0.51
34:2c:116:VAL:HG21	34:2c:202:ILE:HD11	1.93	0.51
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.10	0.51
35:2d:189:PRO:HB2	35:2d:194:LEU:HD11	1.92	0.51
50:2s:77:THR:HG23	50:2s:78:ARG:HG2	1.93	0.51
1:1A:1078:U:C4	1:1A:1088:A:H5''	2.46	0.51
8:1I:40:THR:HG22	8:1I:42:SER:H	1.74	0.51
10:1O:118:ALA:O	57:1a:1882:MPD:H12	2.11	0.51
18:1W:15:ARG:NH1	61:1W:302:HOH:O	2.40	0.51
32:1a:353:A:H5'	32:1a:353:A:H8	1.76	0.51
51:1t:47:GLY:HA2	51:1t:48:LYS:HB2	1.92	0.51
1:2A:335:C:H4'	20:2Y:73:ARG:HD2	1.93	0.51
1:2A:999:U:OP2	61:2A:3850:HOH:O	2.19	0.51
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.76	0.51
5:2F:7:TYR:O	5:2F:22:ALA:N	2.42	0.51
11:2P:125:VAL:CG1	11:2P:138:LEU:HD21	2.41	0.51
21:2Z:128:VAL:HG13	21:2Z:161:VAL:HG12	1.91	0.51
32:2a:1329:A:P	44:2m:28:ALA:HB3	2.51	0.51
33:2b:93:VAL:HG21	33:2b:97:TRP:HD1	1.75	0.51
35:2d:111:ALA:HB1	35:2d:116:GLN:HE21	1.76	0.51
1:1A:279:C:H42	1:1A:361:G:H1	1.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1865:G:OP1	61:1A:4150:HOH:O	2.19	0.51
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.09	0.51
45:1n:24:CYS:HB3	45:1n:28:GLY:H	1.75	0.51
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.46	0.51
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.92	0.51
21:2Z:18:LEU:HD21	21:2Z:38:TYR:HB3	1.93	0.51
21:2Z:23:LYS:NZ	21:2Z:40:ASP:OD1	2.43	0.51
32:2a:1295:G:O2'	32:2a:1302:U:O4	2.25	0.51
32:2a:1456:G:O6	51:2t:54:LYS:NZ	2.42	0.51
1:1A:7:G:H2'	1:1A:8:A:O4'	2.11	0.51
1:1A:1040:C:H2'	1:1A:1041:C:O4'	2.11	0.51
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.46	0.51
21:1Z:125:LEU:HB3	21:1Z:165:VAL:HG13	1.91	0.51
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.44	0.51
48:1q:37:LYS:O	48:1q:38:ARG:NH2	2.44	0.51
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.92	0.51
1:2A:2117:A:N6	1:2A:2172:U:O4	2.44	0.51
1:2A:2122:U:H2'	1:2A:2123:G:H5''	1.91	0.51
2:2B:16:G:H1	2:2B:68:C:H42	1.58	0.51
6:2G:96:ARG:H	6:2G:99:MET:HE2	1.76	0.51
42:2k:81:ASP:OD1	42:2k:107:SER:HB3	2.11	0.51
50:2s:22:LEU:O	50:2s:26:GLY:N	2.44	0.51
1:1A:330:A:H2	1:1A:1210:A:O2'	1.93	0.50
1:1A:889:C:O2'	1:1A:890:A:OP2	2.24	0.50
1:1A:2548:G:O6	61:1A:4147:HOH:O	2.19	0.50
31:19:2:LYS:NZ	31:19:31:LYS:O	2.37	0.50
32:1a:352:C:O2'	32:1a:354:G:OP1	2.28	0.50
32:1a:1518:MA6:C9	32:1a:1519:MA6:H92	2.41	0.50
33:1b:83:MET:HG2	33:1b:234:PRO:HB2	1.92	0.50
39:1h:110:ALA:HB3	39:1h:121:ASP:HB3	1.92	0.50
1:2A:1115:G:H2'	1:2A:1116:C:C6	2.46	0.50
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.46	0.50
1:2A:2134:A:H5''	1:2A:2156:G:N2	2.27	0.50
1:2A:2206:G:H8	1:2A:2207:G:N7	2.09	0.50
6:2G:19:LEU:HD13	6:2G:32:PRO:HD2	1.92	0.50
14:2S:74:ALA:HB2	14:2S:105:ALA:HA	1.92	0.50
44:2m:3:ARG:HG2	44:2m:4:ILE:HG12	1.93	0.50
45:2n:41:ARG:HG3	45:2n:42:ILE:HG13	1.93	0.50
1:1A:2138:C:H2'	1:1A:2139:C:C5	2.46	0.50
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.46	0.50
3:1D:113:VAL:HG12	61:1D:438:HOH:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:47:VAL:HG22	4:1E:84:PHE:O	2.11	0.50
19:1X:5:TYR:CZ	24:12:30:ARG:HB2	2.46	0.50
32:1a:186:C:H2'	32:1a:187:C:C6	2.47	0.50
32:1a:347:G:C8	57:1a:1882:MPD:H53	2.46	0.50
32:1a:457:C:H2'	32:1a:458:C:H6	1.77	0.50
32:2a:1090:U:H2'	32:2a:1091:U:C6	2.47	0.50
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.44	0.50
1:1A:2390:U:OP2	61:1A:4149:HOH:O	2.19	0.50
39:1h:104:ARG:C	39:1h:106:GLY:H	2.19	0.50
44:1m:40:ASN:HD21	44:1m:42:ALA:HB3	1.76	0.50
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.26	0.50
7:2H:90:LYS:HD3	7:2H:159:GLU:HG2	1.92	0.50
1:1A:469:G:O6	29:17:37:LYS:HE2	2.12	0.50
1:1A:652(T):C:H2'	1:1A:652(U):G:O4'	2.11	0.50
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.11	0.50
32:1a:346:G:H5''	57:1a:1882:MPD:H4	1.92	0.50
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.44	0.50
35:1d:8:VAL:HG22	35:1d:21:LEU:HD13	1.92	0.50
1:2A:1064:C:H42	1:2A:1074:G:H1	1.58	0.50
1:2A:1064:C:H1'	1:2A:1076:C:C5	2.46	0.50
1:2A:1071:G:H1'	1:2A:1089:G:N7	2.26	0.50
1:2A:1358:G:O2'	1:2A:1359:A:H5''	2.12	0.50
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.94	0.50
7:2H:12:PRO:O	7:2H:15:VAL:HG22	2.12	0.50
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.11	0.50
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.12	0.50
34:2c:54:ARG:HB2	34:2c:69:HIS:HB2	1.93	0.50
35:2d:57:ARG:NH2	35:2d:205:GLU:OE1	2.41	0.50
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.27	0.50
1:1A:1607:C:N4	1:1A:1622:G:OP2	2.33	0.50
1:1A:1877:A:H5'	1:1A:1878:G:OP2	2.12	0.50
1:1A:2788:C:HO2'	1:1A:2809:A:HO2'	1.57	0.50
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.45	0.50
1:2A:171:G:H2'	1:2A:172:C:C6	2.46	0.50
1:2A:1057:A:H62	1:2A:1086:A:H2'	1.75	0.50
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.46	0.50
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.11	0.50
30:28:29:LYS:HG2	30:28:44:LYS:HB3	1.94	0.50
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.26	0.50
32:2a:1329:A:H5''	44:2m:26:GLY:H	1.76	0.50
40:2i:92:TYR:O	40:2i:96:LEU:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:2l:103:GLY:N	43:2l:107:ALA:O	2.43	0.50
1:1A:207:A:H2'	1:1A:208:C:O4'	2.10	0.50
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.46	0.50
1:1A:2443:C:OP1	5:1F:68:LYS:HD3	2.12	0.50
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.26	0.50
27:15:16:ARG:HG3	27:15:17:ASP:N	2.25	0.50
32:1a:176:C:H2'	32:1a:177:C:H6	1.76	0.50
32:1a:1315:U:H2'	32:1a:1316:G:O4'	2.12	0.50
34:1c:62:ASP:O	34:1c:97:LYS:HB2	2.11	0.50
35:1d:156:GLU:O	35:1d:160:GLN:HG2	2.10	0.50
1:2A:247:G:H4'	1:2A:386:G:C5	2.46	0.50
1:2A:644:A:H4'	1:2A:645:C:C5	2.46	0.50
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.77	0.50
4:2E:48:GLN:NE2	4:2E:78:LEU:HD13	2.26	0.50
12:2Q:32:TYR:CE1	12:2Q:133:ARG:HB3	2.47	0.50
32:2a:542:G:OP1	35:2d:10:ARG:NH1	2.35	0.50
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.93	0.50
1:1A:2365:G:O6	30:18:39:LYS:HE3	2.12	0.50
33:1b:112:VAL:HG12	33:1b:149:LEU:HD13	1.94	0.50
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.12	0.50
1:2A:1815:A:OP2	3:2D:54:ARG:NH2	2.45	0.50
3:2D:134:ARG:NH1	3:2D:188:GLU:OE2	2.34	0.50
12:2Q:97:VAL:HG11	12:2Q:103:MET:HE3	1.93	0.50
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.94	0.50
32:2a:255:G:OP1	48:2q:69:LYS:NZ	2.35	0.50
32:2a:560:U:H5'	32:2a:566:G:N2	2.27	0.50
32:2a:625:G:H2'	32:2a:626:U:C6	2.47	0.50
32:2a:1086:U:H3	32:2a:1099:G:H22	1.58	0.50
44:2m:13:LYS:HA	44:2m:44:ARG:NH1	2.26	0.50
1:1A:1179:C:H2'	1:1A:1180:C:C6	2.47	0.50
6:1G:50:ALA:C	6:1G:52:ILE:H	2.20	0.50
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.93	0.50
32:1a:1298:C:P	38:1g:114:ARG:HH22	2.34	0.50
32:1a:1343:G:O2'	40:1i:121:ARG:HD2	2.11	0.50
33:1b:189:ASP:OD1	33:1b:189:ASP:N	2.44	0.50
39:1h:51:VAL:HG21	39:1h:60:ARG:HH11	1.76	0.50
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.44	0.50
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.46	0.50
19:2X:60:ARG:NH1	29:27:47:ARG:HH22	2.09	0.50
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.27	0.50
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.76	0.50
33:2b:15:VAL:O	33:2b:17:PHE:N	2.43	0.50
34:2c:6:HIS:NE2	34:2c:8:ILE:HB	2.27	0.50
39:2h:12:ARG:HD2	39:2h:26:VAL:HG12	1.94	0.50
41:2j:11:PHE:HE1	41:2j:67:THR:HG22	1.76	0.50
1:1A:639:U:H2'	1:1A:640:C:C6	2.47	0.50
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.44	0.50
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.43	0.50
1:1A:1578:U:H2'	1:1A:1579:A:H5'	1.94	0.50
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.26	0.50
11:1P:95:VAL:HG22	11:1P:125:VAL:HB	1.94	0.50
13:1R:24:GLN:NE2	61:1R:304:HOH:O	2.43	0.50
32:1a:964:A:OP1	61:1a:1913:HOH:O	2.18	0.50
32:1a:1360:A:H2'	32:1a:1361:G:O4'	2.11	0.50
32:1a:1360:A:OP2	45:1n:35:ARG:NH2	2.45	0.50
35:1d:172:PRO:HB2	35:1d:187:ARG:NH2	2.27	0.50
38:1g:41:ARG:O	38:1g:45:ASP:HB2	2.12	0.50
1:2A:882:G:H1	1:2A:894:C:H42	1.59	0.50
1:2A:1069:A:H2'	1:2A:1073:A:N7	2.27	0.50
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.45	0.50
1:2A:2746:U:OP1	7:2H:85:LYS:NZ	2.43	0.50
32:2a:190:U:H2'	32:2a:191:G:H8	1.77	0.50
32:2a:1207:2MG:H2'	32:2a:1208:C:C6	2.46	0.50
32:2a:1400:5MC:C2	53:2y:63:ALA:HA	2.47	0.50
33:2b:50:GLU:O	33:2b:54:THR:N	2.34	0.50
33:2b:180:LEU:HB2	33:2b:182:ILE:HG13	1.94	0.50
34:2c:53:ALA:HB2	34:2c:115:LEU:HD11	1.94	0.50
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.12	0.49
1:1A:2140:C:N3	1:1A:2151:G:O6	2.45	0.49
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.12	0.49
32:1a:1279:A:H5''	41:1j:7:LYS:HZ1	1.77	0.49
33:1b:67:THR:HA	33:1b:90:MET:HE2	1.93	0.49
39:1h:6:ILE:HB	39:1h:85:ARG:NH1	2.26	0.49
39:1h:97:VAL:HG21	39:1h:128:GLY:HA2	1.93	0.49
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.46	0.49
18:2W:71:VAL:HA	18:2W:107:LEU:HD23	1.94	0.49
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.45	0.49
30:28:32:LEU:O	30:28:36:LYS:HE3	2.11	0.49
32:2a:976:G:P	45:2n:32:SER:H	2.35	0.49
41:2j:11:PHE:CE1	41:2j:67:THR:HG22	2.47	0.49
44:2m:33:ALA:HB2	44:2m:64:TRP:HZ3	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:185:U:H4'	1:1A:218:A:H4'	1.95	0.49
1:1A:194:G:N3	61:1A:4284:HOH:O	2.35	0.49
32:1a:17:U:H2'	32:1a:18:C:C6	2.47	0.49
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.94	0.49
1:2A:300:A:P	20:2Y:86:ARG:HH21	2.35	0.49
1:2A:2138:C:H2'	1:2A:2139:C:C6	2.47	0.49
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.13	0.49
8:2I:97:ILE:O	8:2I:101:LEU:HD12	2.12	0.49
11:2P:95:VAL:HG23	11:2P:125:VAL:HA	1.94	0.49
50:2s:50:ALA:HA	50:2s:58:VAL:O	2.13	0.49
1:1A:196:A:N3	61:1A:4282:HOH:O	2.35	0.49
29:17:35:ARG:NH1	61:17:203:HOH:O	2.44	0.49
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.94	0.49
32:2a:316:G:OP2	32:2a:351:G:O2'	2.30	0.49
32:2a:1002:G:N3	32:2a:1003:G:N7	2.59	0.49
47:2p:58:TYR:O	47:2p:61:SER:OG	2.28	0.49
1:1A:604:G:OP2	11:1P:90:ARG:NH1	2.45	0.49
1:1A:1314:C:OP1	61:1A:4110:HOH:O	2.20	0.49
17:1V:80:GLN:OE1	61:1V:301:HOH:O	2.18	0.49
27:15:17:ASP:OD2	61:15:201:HOH:O	2.20	0.49
31:19:15:LYS:HE2	31:19:17:ILE:HD11	1.92	0.49
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.12	0.49
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.93	0.49
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.48	0.49
32:2a:176:C:H2'	32:2a:177:C:C6	2.48	0.49
32:2a:404:U:OP2	35:2d:118:ARG:NH2	2.45	0.49
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.48	0.49
1:1A:2058:MA6:H2	56:1A:4033:ZIT:H181	1.94	0.49
1:1A:2506:U:O2	55:1A:4032:HGR:H23	2.13	0.49
5:1F:116:ASP:OD2	11:1P:1:MET:HB3	2.11	0.49
14:1S:39:ILE:HD11	14:1S:73:LEU:HD21	1.95	0.49
19:1X:35:THR:HG23	19:1X:37:THR:H	1.77	0.49
1:2A:1503:U:H2'	1:2A:1504:C:H6	1.77	0.49
1:2A:1783:A:H5'	1:2A:2608:G:H4'	1.94	0.49
1:2A:2051:A:H8	1:2A:2051:A:OP2	1.96	0.49
3:2D:26:LYS:NZ	3:2D:30:GLU:OE1	2.46	0.49
6:2G:35:GLU:HB3	6:2G:160:VAL:HG12	1.94	0.49
14:2S:101:LEU:HB3	61:2S:201:HOH:O	2.12	0.49
32:2a:1103:C:OP1	33:2b:96:ARG:NH2	2.44	0.49
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.47	0.49
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:110:GLU:OE2	40:2i:113:LYS:NZ	2.41	0.49
1:1A:616:G:H5'	5:1F:205:ARG:HD3	1.94	0.49
42:1k:15:ALA:HA	42:1k:77:MET:HA	1.93	0.49
53:1y:23:ARG:HH11	53:1y:26:LYS:HD2	1.77	0.49
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.47	0.49
1:2A:376:C:OP1	61:2A:3852:HOH:O	2.20	0.49
1:2A:1110:G:H8	1:2A:1110:G:OP2	1.95	0.49
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.59	0.49
30:28:28:GLY:O	30:28:36:LYS:NZ	2.45	0.49
32:2a:779:C:H2'	32:2a:780:A:O4'	2.12	0.49
32:2a:932:C:H2'	32:2a:933:G:C8	2.47	0.49
32:2a:974:A:OP2	45:2n:29:ARG:NH1	2.46	0.49
33:2b:59:GLU:HG3	33:2b:221:LEU:HD11	1.94	0.49
42:2k:13:GLN:HA	42:2k:75:TYR:O	2.13	0.49
1:1A:218:A:OP2	61:1A:4152:HOH:O	2.19	0.49
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.28	0.49
1:1A:1179:C:H2'	1:1A:1180:C:H6	1.76	0.49
1:1A:2167:U:H2'	1:1A:2168:G:C8	2.48	0.49
32:1a:1260:C:H4'	32:1a:1284:C:H5'	1.95	0.49
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.48	0.49
13:2R:9:LYS:O	13:2R:17:ARG:HD3	2.13	0.49
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.31	0.49
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.95	0.49
44:2m:5:ALA:HB2	44:2m:61:GLU:HG2	1.94	0.49
1:1A:244:A:C2	1:1A:255:A:C4	3.01	0.49
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.28	0.49
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.48	0.49
32:1a:998:G:H2'	32:1a:999:C:C6	2.48	0.49
32:1a:1182:G:C4'	32:1a:1183:A:H5'	2.42	0.49
1:2A:1843:C:H5'	3:2D:253:GLN:NE2	2.27	0.49
1:2A:2237:G:OP1	61:2A:3855:HOH:O	2.20	0.49
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.47	0.49
1:2A:2313:C:H2'	1:2A:2314:C:C6	2.48	0.49
1:2A:2887:U:H2'	1:2A:2888:C:H6	1.78	0.49
13:2R:36:THR:HG22	13:2R:37:THR:H	1.78	0.49
14:2S:35:ILE:HG13	14:2S:97:ARG:HH21	1.77	0.49
32:2a:392:G:H2'	32:2a:393:A:C8	2.46	0.49
38:2g:26:PHE:HE1	38:2g:105:VAL:HG22	1.77	0.49
39:2h:9:MET:HG3	39:2h:26:VAL:HG11	1.94	0.49
41:2j:19:SER:O	41:2j:23:ILE:HG12	2.13	0.49
44:2m:89:GLY:HA2	44:2m:92:HIS:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:747:U:O2	1:1A:2014:A:H1'	2.13	0.49
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.13	0.49
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.27	0.49
32:1a:324:G:N7	61:1a:1945:HOH:O	2.35	0.49
32:1a:435:C:H2'	32:1a:436:C:H6	1.77	0.49
32:1a:1320:C:H2'	32:1a:1321:C:O4'	2.13	0.49
33:1b:91:PRO:HG3	33:1b:154:LEU:HD12	1.95	0.49
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.48	0.49
1:2A:1063:G:H1	1:2A:1075:C:H42	1.58	0.49
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.48	0.49
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.48	0.49
34:2c:36:ASP:HA	34:2c:39:ILE:HD12	1.94	0.49
40:2i:4:TYR:HA	40:2i:87:GLN:HE22	1.78	0.49
53:2y:33:HIS:ND1	53:2y:35:ILE:HG12	2.28	0.49
1:1A:2789:C:O3'	1:1A:2790:A:H4'	2.13	0.49
2:1B:50:G:H5''	14:1S:61:ASN:HD21	1.78	0.49
2:1B:66:A:N6	2:1B:108:U:H2'	2.25	0.49
3:1D:137:PRO:HG2	37:1f:81:ILE:HD11	1.95	0.49
18:1W:68:ARG:HH11	18:1W:111:HIS:HA	1.78	0.49
32:1a:377:G:OP1	47:1p:3:LYS:HD3	2.13	0.49
32:1a:1149:C:P	40:1i:9:ARG:HH21	2.36	0.49
32:1a:1304:G:OP2	61:1a:1915:HOH:O	2.20	0.49
33:1b:119:GLU:OE2	33:1b:153:ARG:NH2	2.32	0.49
43:1l:7:ILE:O	43:1l:11:VAL:HG12	2.13	0.49
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.48	0.49
32:2a:611:A:H61	32:2a:629:G:H1	1.59	0.49
48:2q:82:MET:HA	48:2q:85:VAL:HG13	1.95	0.49
1:1A:530:G:N1	1:1A:2023:G:OP1	2.35	0.48
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.95	0.48
15:1T:33:LYS:HG2	15:1T:82:LEU:HD23	1.94	0.48
20:1Y:20:TYR:HB3	20:1Y:23:ARG:HD2	1.95	0.48
32:1a:626:U:H2'	32:1a:627:G:C8	2.49	0.48
32:1a:738:C:H2'	32:1a:739:C:H6	1.78	0.48
32:1a:890:G:O2'	32:1a:906:G:O6	2.19	0.48
33:1b:128:GLU:O	33:1b:130:ARG:N	2.46	0.48
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.27	0.48
1:2A:2136:C:C2	1:2A:2155:G:N2	2.80	0.48
1:2A:2152:G:H2'	1:2A:2153:G:C8	2.48	0.48
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.48	0.48
9:2N:73:THR:HA	9:2N:83:LYS:O	2.13	0.48
31:29:32:HIS:O	31:29:34:GLN:HG3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:9:G:H2'	32:2a:10:A:H8	1.78	0.48
32:2a:100:C:H2'	32:2a:101:A:C8	2.48	0.48
32:2a:584:G:H5'	48:2q:91:ARG:HH22	1.77	0.48
32:2a:952:U:H4'	32:2a:964:A:N1	2.28	0.48
32:2a:1092:A:N3	32:2a:1183:A:N6	2.61	0.48
32:2a:1411:C:H2'	32:2a:1412:C:H6	1.77	0.48
36:2e:78:HIS:CE1	36:2e:142:LEU:HD23	2.47	0.48
44:2m:51:ALA:O	44:2m:55:ARG:HB2	2.12	0.48
1:1A:300:A:OP1	20:1Y:86:ARG:NH2	2.46	0.48
1:1A:2142:C:N3	1:1A:2149:G:C6	2.80	0.48
10:1O:107:ARG:HG3	10:1O:112:MET:HE1	1.95	0.48
32:1a:501:C:H1'	32:1a:549:C:H1'	1.94	0.48
32:1a:1264:C:H2'	32:1a:1265:G:C8	2.48	0.48
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.47	0.48
34:1c:44:GLU:HA	34:1c:52:LEU:HD23	1.93	0.48
37:1f:69:GLU:OE1	37:1f:69:GLU:N	2.46	0.48
48:1q:10:VAL:HG13	48:1q:19:VAL:HB	1.95	0.48
1:2A:855:G:H2'	1:2A:856:C:C6	2.48	0.48
8:2I:104:GLN:HG2	8:2I:105:HIS:CD2	2.48	0.48
32:2a:9:G:H2'	32:2a:10:A:C8	2.48	0.48
33:2b:93:VAL:HG21	33:2b:97:TRP:CD1	2.47	0.48
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.48	0.48
52:2u:17:THR:O	52:2u:22:ARG:NH1	2.39	0.48
53:2y:87:LYS:O	53:2y:91:LYS:HB2	2.14	0.48
1:1A:1805:U:O2	3:1D:50:THR:HB	2.12	0.48
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.13	0.48
4:1E:170:LEU:HD23	4:1E:184:VAL:CG1	2.43	0.48
6:1G:43:LEU:C	6:1G:45:GLU:H	2.22	0.48
17:1V:58:VAL:HG12	17:1V:97:LYS:HB2	1.95	0.48
28:16:6:ARG:HD3	28:16:24:GLU:OE2	2.13	0.48
32:1a:79:G:N1	32:1a:90:U:N3	2.46	0.48
1:2A:1091:G:H2'	1:2A:1091:G:N3	2.27	0.48
1:2A:2295:C:OP1	14:2S:10:ARG:NH1	2.46	0.48
61:2B:313:HOH:O	21:2Z:31:ARG:N	2.44	0.48
6:2G:40:ASN:HB3	6:2G:156:ASP:HB2	1.95	0.48
6:2G:54:GLU:O	6:2G:58:GLN:N	2.45	0.48
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.12	0.48
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.95	0.48
32:2a:551:U:H2'	32:2a:552:U:C6	2.47	0.48
32:2a:728:A:H2'	32:2a:729:A:C8	2.49	0.48
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:446:G:OP1	16:1U:3:ARG:NH1	2.45	0.48
1:1A:1364:G:OP2	23:11:3:LYS:HD3	2.13	0.48
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.13	0.48
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.13	0.48
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.78	0.48
32:1a:1226:C:H4'	32:1a:1227:A:OP1	2.13	0.48
36:1e:50:GLU:HB2	36:1e:53:LEU:HD13	1.95	0.48
1:2A:800:A:H8	1:2A:800:A:OP1	1.97	0.48
1:2A:1818:U:O2'	3:2D:154:LYS:O	2.29	0.48
1:2A:2336:A:H61	22:20:43:THR:CG2	2.26	0.48
24:22:13:ALA:HA	24:22:16:LEU:HD12	1.95	0.48
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.42	0.48
44:2m:95:GLY:O	44:2m:110:ARG:HG3	2.12	0.48
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.95	0.48
1:1A:2336:A:H61	22:10:43:THR:HG22	1.77	0.48
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.10	0.48
26:14:46:GLN:O	26:14:48:ARG:N	2.46	0.48
32:1a:457:C:H2'	32:1a:458:C:C6	2.47	0.48
32:1a:626:U:H2'	32:1a:627:G:H8	1.78	0.48
32:1a:1005:A:H8	32:1a:1005:A:O5'	1.95	0.48
32:1a:1466:C:H2'	32:1a:1467:G:O4'	2.13	0.48
36:1e:12:LEU:HD21	36:1e:14:ARG:HD3	1.94	0.48
43:1l:79:GLU:HG2	43:1l:80:HIS:CD2	2.48	0.48
1:2A:13:A:N1	1:2A:525:U:H2'	2.28	0.48
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.96	0.48
14:2S:15:ARG:HB3	14:2S:19:LYS:HE3	1.94	0.48
32:2a:620:C:C2	35:2d:135:LEU:HG	2.48	0.48
32:2a:921:U:O2	36:2e:19:MET:HB2	2.13	0.48
32:2a:1187:G:OP1	40:2i:113:LYS:HE2	2.13	0.48
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.49	0.48
34:2c:131:ARG:HD2	34:2c:166:GLU:OE1	2.12	0.48
35:2d:25:ARG:NH1	35:2d:30:LYS:O	2.46	0.48
42:2k:21:ILE:HB	42:2k:84:VAL:HG23	1.95	0.48
50:2s:52:TYR:HB2	50:2s:57:HIS:CE1	2.48	0.48
53:2y:7:SER:HB3	53:2y:10:MET:O	2.14	0.48
6:1G:66:GLN:NE2	6:1G:93:THR:O	2.38	0.48
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.76	0.48
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.56	0.48
32:1a:404:U:H2'	32:1a:405:U:H6	1.79	0.48
32:1a:632:A:OP1	39:1h:98:LYS:NZ	2.47	0.48
32:1a:1008:C:H2'	32:1a:1009:G:O4'	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1158:C:H5	32:1a:1181:G:N1	2.11	0.48
32:1a:1251:A:H2'	32:1a:1252:A:C8	2.48	0.48
32:1a:1297:C:O2'	38:1g:114:ARG:NH1	2.39	0.48
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.49	0.48
1:2A:2400:G:H4'	28:26:18:ARG:HG2	1.96	0.48
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.96	0.48
6:2G:126:ASP:CG	6:2G:130:ASN:HB2	2.38	0.48
32:2a:425:G:O3'	35:2d:45:GLN:NE2	2.42	0.48
32:2a:953:G:C2	32:2a:954:G:H1'	2.49	0.48
38:2g:70:LYS:HB3	38:2g:96:GLN:HB3	1.95	0.48
42:2k:59:TYR:CE2	42:2k:63:LEU:HD11	2.49	0.48
1:1A:1131:G:H21	9:1N:73:THR:CG2	2.27	0.48
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.28	0.48
1:1A:2059:A:OP2	61:1A:4145:HOH:O	2.19	0.48
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.49	0.48
44:1m:13:LYS:C	44:1m:44:ARG:HD3	2.39	0.48
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.94	0.48
1:2A:218:A:C2	1:2A:235:U:H4'	2.49	0.48
1:2A:1050:A:H2'	1:2A:1051:G:H8	1.79	0.48
1:2A:1055:G:H2'	1:2A:1056:G:O4'	2.14	0.48
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.49	0.48
1:2A:2805:G:C6	1:2A:2807:G:C6	3.01	0.48
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.45	0.48
3:2D:71:ASP:CG	3:2D:103:ARG:HH22	2.21	0.48
32:2a:1055:A:H2'	34:2c:156:ARG:HD2	1.95	0.48
32:2a:1224:G:O3'	44:2m:102:ARG:NE	2.47	0.48
32:2a:1227:A:H5'	44:2m:111:LYS:HD3	1.94	0.48
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.14	0.48
37:2f:100:ASN:ND2	49:2r:23:LYS:HE2	2.29	0.48
38:2g:72:ARG:NH2	38:2g:142:GLU:OE1	2.46	0.48
1:1A:652(U):G:H3'	1:1A:652(V):C:C6	2.49	0.48
1:1A:848:G:H2'	1:1A:849:A:C8	2.48	0.48
1:1A:1722:A:N3	1:1A:1739:U:O2'	2.45	0.48
1:1A:2887:U:H2'	1:1A:2888:C:H6	1.79	0.48
4:1E:119:ARG:HG2	4:1E:160:TYR:CG	2.49	0.48
29:17:1:MET:HE2	29:17:1:MET:HB3	1.65	0.48
32:1a:109:A:H2'	32:1a:326:G:N2	2.28	0.48
32:1a:629:G:H2'	32:1a:630:G:O4'	2.14	0.48
40:1i:26:VAL:HA	40:1i:61:ALA:HB3	1.96	0.48
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.49	0.48
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:103:LEU:HD23	7:2H:104:GLU:N	2.29	0.48
9:2N:33:LEU:HD12	9:2N:38:HIS:CD2	2.49	0.48
25:23:19:GLN:O	25:23:23:LEU:HD22	2.14	0.48
32:2a:1504:G:OP1	32:2a:1507:A:H4'	2.14	0.48
42:2k:99:GLN:HE21	42:2k:105:VAL:HG21	1.79	0.48
53:2y:32:THR:HG22	53:2y:57:PRO:HD2	1.95	0.48
53:2y:40:ILE:HB	53:2y:51:ASP:HB2	1.94	0.48
1:1A:330:A:H2	1:1A:1210:A:H2'	1.79	0.48
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.49	0.48
32:1a:745:C:H2'	32:1a:746:A:C8	2.49	0.48
32:1a:986:A:H1'	50:1s:55:LYS:HA	1.96	0.48
32:1a:1318:A:H5''	50:1s:3:ARG:NH1	2.28	0.48
1:2A:118:A:C8	1:2A:119:A:C8	3.02	0.48
1:2A:821:A:N1	61:2A:3958:HOH:O	2.35	0.48
1:2A:1076:C:H1'	1:2A:1077:A:H5'	1.96	0.48
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.13	0.48
1:2A:1270:C:H5''	1:2A:1271:G:O5'	2.14	0.48
4:2E:13:ARG:HG2	15:2T:58:ASN:HD21	1.79	0.48
12:2Q:43:THR:N	12:2Q:46:GLN:OE1	2.46	0.48
21:2Z:121:HIS:HB2	21:2Z:171:ILE:HG22	1.96	0.48
32:2a:644:G:H5'	39:2h:92:ARG:HH12	1.78	0.48
32:2a:1402:4OC:HM43	53:2y:83:ARG:CZ	2.43	0.48
1:1A:1721:G:H5'	1:1A:1722:A:OP2	2.14	0.48
1:1A:2038:G:H2'	1:1A:2039:C:O4'	2.14	0.48
5:1F:39:TRP:CH2	5:1F:106:ARG:HD3	2.48	0.48
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.96	0.48
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.95	0.48
32:1a:142:G:H2'	32:1a:143:A:H8	1.78	0.48
1:2A:184:C:H2'	1:2A:185:U:C6	2.48	0.48
1:2A:630:G:N2	1:2A:633:A:OP2	2.42	0.48
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.49	0.48
1:2A:821:A:H2'	1:2A:946:G:H5''	1.95	0.48
4:2E:55:ASN:HB3	4:2E:58:ARG:HG3	1.95	0.48
8:2I:100:ALA:O	8:2I:104:GLN:N	2.47	0.48
20:2Y:21:LYS:HE3	20:2Y:21:LYS:HB2	1.73	0.48
32:2a:1005:A:C5	32:2a:1006:C:H1'	2.49	0.48
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.49	0.48
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.49	0.48
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.29	0.48
33:2b:102:LEU:HB3	33:2b:180:LEU:HD11	1.96	0.48
35:2d:112:VAL:H	35:2d:116:GLN:NE2	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:15:ARG:NH1	61:1P:302:HOH:O	2.46	0.47
12:1Q:109:VAL:HG22	12:1Q:113:GLN:CD	2.39	0.47
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.57	0.47
32:1a:102:G:O2'	32:1a:151:A:N3	2.45	0.47
32:1a:474:G:H2'	32:1a:475:G:C8	2.49	0.47
32:1a:757:U:H2'	32:1a:758:G:O4'	2.14	0.47
32:1a:1054:C:N4	53:1y:46:GLN:OE1	2.46	0.47
32:1a:1329:A:P	44:1m:28:ALA:HB3	2.54	0.47
37:1f:100:ASN:HD21	49:1r:23:LYS:HE2	1.78	0.47
38:1g:126:ASP:HB3	38:1g:131:LYS:HB2	1.94	0.47
48:1q:74:LEU:HD23	48:1q:75:ARG:HG2	1.96	0.47
1:2A:140:G:N3	1:2A:142:A:N6	2.52	0.47
1:2A:635:C:O2'	1:2A:639:U:OP1	2.28	0.47
1:2A:686:G:H21	1:2A:788:A:H61	1.62	0.47
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.14	0.47
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.29	0.47
1:2A:2506:U:O2	55:2A:3712:HGR:H23	2.14	0.47
5:2F:23:ASP:O	5:2F:24:LEU:HD23	2.14	0.47
32:2a:279:A:OP2	48:2q:95:TYR:OH	2.28	0.47
32:2a:540:G:H2'	32:2a:541:G:O4'	2.14	0.47
32:2a:1014:A:H2	32:2a:1219:U:H1'	1.78	0.47
32:2a:1069:C:O2'	32:2a:1192:C:O2	2.32	0.47
33:2b:198:ASP:OD1	39:2h:68:ARG:NH1	2.47	0.47
34:2c:19:GLU:O	34:2c:40:ARG:NH2	2.47	0.47
1:1A:910:A:N1	1:1A:2277:G:H1'	2.29	0.47
1:1A:2038:G:O6	61:1A:4151:HOH:O	2.19	0.47
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.79	0.47
32:1a:104:G:C2	32:1a:105:G:C8	3.03	0.47
32:1a:508:C:OP1	35:1d:209:ARG:NH2	2.46	0.47
32:1a:1158:C:C5	32:1a:1181:G:N1	2.82	0.47
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.49	0.47
34:1c:8:ILE:HG12	34:1c:184:TYR:HB3	1.95	0.47
53:1y:24:LEU:HD11	53:1y:39:ILE:HD11	1.94	0.47
1:2A:874:G:O2'	21:2Z:120:ILE:HD11	2.14	0.47
1:2A:2115:G:N2	1:2A:2119:A:H5'	2.28	0.47
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.50	0.47
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.47	0.47
2:2B:22:U:H2'	2:2B:23:G:C8	2.49	0.47
7:2H:17:VAL:HG22	7:2H:26:VAL:HG22	1.96	0.47
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.95	0.47
32:2a:1291:G:H4'	40:2i:39:GLY:HA3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:30:SER:OG	41:2j:81:THR:HG22	2.15	0.47
42:2k:107:SER:OG	42:2k:108:ILE:N	2.47	0.47
1:1A:652(U):G:H3'	1:1A:652(V):C:H6	1.78	0.47
1:1A:2119:A:N6	1:1A:2171:A:N7	2.62	0.47
1:1A:2135:A:H62	1:1A:2156:G:H21	1.62	0.47
2:1B:66:A:H61	2:1B:109:C:H5'	1.79	0.47
32:1a:1175:G:H2'	32:1a:1176:A:C8	2.49	0.47
33:1b:80:ILE:H	33:1b:80:ILE:HD12	1.78	0.47
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.30	0.47
1:2A:2319:G:N1	14:2S:3:ARG:HA	2.29	0.47
32:2a:981:U:O4	61:2a:3208:HOH:O	2.20	0.47
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.49	0.47
33:2b:83:MET:HE2	33:2b:83:MET:HB3	1.72	0.47
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.96	0.47
1:1A:1069:A:H5'	1:1A:1070:A:C2	2.49	0.47
1:1A:1289:C:H2'	1:1A:1290:C:C6	2.50	0.47
61:1A:4105:HOH:O	4:1E:110:GLY:O	2.20	0.47
15:1T:111:ARG:NH2	32:1a:1464:G:OP2	2.47	0.47
32:1a:45:U:H2'	32:1a:46:G:C8	2.49	0.47
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.96	0.47
43:1l:60:LEU:HD11	43:1l:66:VAL:HG22	1.96	0.47
1:2A:1079:C:N4	1:2A:1080:C:C2	2.82	0.47
1:2A:1639:U:C2'	1:2A:1640:C:H5''	2.44	0.47
33:2b:178:ARG:HB3	39:2h:72:PRO:HA	1.96	0.47
38:2g:133:GLY:HA2	38:2g:136:LYS:HB2	1.96	0.47
44:2m:6:GLY:HA3	44:2m:67:GLU:HB2	1.96	0.47
53:2y:53:THR:HG22	53:2y:62:VAL:HG12	1.97	0.47
1:1A:330:A:H2	1:1A:1210:A:C2'	2.27	0.47
1:1A:1486:A:H2'	1:1A:1487:G:H8	1.80	0.47
6:1G:135:LEU:O	6:1G:154:GLY:HA3	2.15	0.47
8:1I:27:ARG:HD2	23:11:71:TYR:CE2	2.49	0.47
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	1.97	0.47
15:1T:128:GLU:HG2	15:1T:128:GLU:O	2.14	0.47
32:1a:755:G:OP2	46:1o:65:ARG:HD2	2.14	0.47
40:1i:16:ARG:HH11	40:1i:64:THR:HG21	1.79	0.47
1:2A:118:A:N3	1:2A:178:G:H1'	2.29	0.47
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.48	0.47
1:2A:361:G:O2'	1:2A:362:U:H5'	2.14	0.47
1:2A:745:G:O6	61:2A:3853:HOH:O	2.20	0.47
1:2A:1031:G:H21	31:29:36:GLN:HE22	1.62	0.47
1:2A:2119:A:H61	1:2A:2168:G:N2	2.11	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.50	0.47
5:2F:95:ARG:HD3	5:2F:97:TYR:CZ	2.50	0.47
6:2G:3:LEU:HD23	6:2G:3:LEU:H	1.80	0.47
32:2a:755:G:OP2	46:2o:65:ARG:HD2	2.14	0.47
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.45	0.47
35:2d:153:ARG:O	35:2d:155:LEU:N	2.43	0.47
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.14	0.47
44:2m:47:ASP:OD1	44:2m:47:ASP:N	2.45	0.47
1:1A:2139:C:H2'	1:1A:2140:C:C6	2.50	0.47
3:1D:3:VAL:HG13	3:1D:17:THR:HB	1.96	0.47
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.97	0.47
17:1V:21:ARG:HD3	17:1V:91:TYR:CD1	2.49	0.47
32:1a:171:A:H2'	32:1a:172:A:C8	2.50	0.47
32:1a:620:C:C2	35:1d:135:LEU:HG	2.50	0.47
32:1a:1366:C:H2'	32:1a:1367:C:H6	1.80	0.47
1:2A:1087:G:H22	1:2A:1102:C:N4	2.13	0.47
1:2A:1449:A:N3	1:2A:1529:G:H1'	2.30	0.47
1:2A:1533:G:N2	1:2A:1536:C:N3	2.63	0.47
1:2A:2857:G:N2	1:2A:2859:G:H3'	2.30	0.47
32:2a:1255:G:N1	32:2a:1279:A:N7	2.62	0.47
35:2d:118:ARG:HG2	35:2d:136:PRO:HB3	1.97	0.47
41:2j:46:ARG:HA	41:2j:64:GLU:HA	1.96	0.47
1:1A:613:G:N2	1:1A:614(C):A:O2'	2.48	0.47
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.15	0.47
1:1A:1060:U:N3	1:1A:1088:A:N7	2.63	0.47
1:1A:2055:C:O2	61:1A:4154:HOH:O	2.20	0.47
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.50	0.47
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.14	0.47
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.15	0.47
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.60	0.47
5:1F:93:LYS:HD3	5:1F:93:LYS:HA	1.71	0.47
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.64	0.47
10:1O:2:ILE:HB	10:1O:33:ALA:HB3	1.97	0.47
17:1V:22:VAL:HG23	17:1V:23:GLU:O	2.14	0.47
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.96	0.47
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.96	0.47
32:1a:153:C:H2'	32:1a:154:C:C6	2.49	0.47
32:1a:814:A:H2'	32:1a:816:A:H5''	1.96	0.47
32:1a:815:A:N7	32:1a:1509:C:O2'	2.42	0.47
32:1a:1032:G:N2	32:1a:1033:G:N3	2.63	0.47
32:1a:1258:G:H2'	32:1a:1259:C:H6	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:114:ARG:O	33:1b:118:LEU:HG	2.14	0.47
35:1d:190:ASP:OD2	35:1d:191:ARG:N	2.47	0.47
36:1e:140:ARG:O	36:1e:143:ARG:NH2	2.48	0.47
38:1g:32:ARG:NH2	38:1g:109:ASN:OD1	2.47	0.47
44:1m:33:ALA:HA	44:1m:59:TYR:HE2	1.80	0.47
51:1t:14:LYS:O	51:1t:18:GLN:HG3	2.15	0.47
1:2A:539:G:H2'	1:2A:540:C:C6	2.49	0.47
1:2A:927:G:H2'	1:2A:928:G:O4'	2.15	0.47
1:2A:1069:A:C6	1:2A:1095:A:H4'	2.50	0.47
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.50	0.47
1:2A:2165:G:H2'	1:2A:2166:G:O4'	2.15	0.47
1:2A:2224:G:H4'	1:2A:2226:C:C2	2.49	0.47
1:2A:2584:U:H2'	1:2A:2585:U:H2'	1.96	0.47
4:2E:120:TRP:CD2	4:2E:155:LYS:HG2	2.49	0.47
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.13	0.47
15:2T:64:ARG:HH11	15:2T:73:GLU:HG3	1.80	0.47
17:2V:52:VAL:HG23	17:2V:55:ALA:HB3	1.97	0.47
26:24:53:GLU:CD	26:24:54:GLY:H	2.23	0.47
32:2a:409:G:H2'	32:2a:410:G:O4'	2.15	0.47
32:2a:674:G:H2'	32:2a:675:A:C8	2.48	0.47
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.14	0.47
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.47	0.47
32:2a:828:A:H2'	32:2a:829:G:O4'	2.15	0.47
32:2a:932:C:H2'	32:2a:933:G:H8	1.80	0.47
35:2d:108:LEU:HD13	35:2d:174:LEU:HD13	1.96	0.47
38:2g:67:GLU:HA	38:2g:70:LYS:HD3	1.97	0.47
1:1A:93:G:H2'	1:1A:94:C:C6	2.49	0.47
32:1a:115:G:H4'	32:1a:116:A:O5'	2.14	0.47
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.80	0.47
35:1d:60:GLU:OE2	35:1d:63:LYS:NZ	2.38	0.47
1:2A:2459:A:OP2	61:2A:3856:HOH:O	2.20	0.47
61:2A:4907:HOH:O	29:27:43:THR:HB	2.15	0.47
4:2E:1:MET:HB3	4:2E:83:ASP:O	2.14	0.47
32:2a:36:C:OP1	43:2l:123:LYS:NZ	2.48	0.47
32:2a:254:G:H21	48:2q:16:GLN:NE2	2.13	0.47
32:2a:547:A:H5'	61:2a:3207:HOH:O	2.14	0.47
40:2i:23:ASN:HB2	40:2i:25:LYS:HE3	1.96	0.47
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.15	0.47
46:2o:37:ASN:O	46:2o:41:GLU:HG2	2.15	0.47
1:1A:686:G:N2	1:1A:788:A:H61	2.13	0.47
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.14	0.47
1:1A:2804:C:H2'	1:1A:2805:G:C8	2.50	0.47
7:1H:124:GLU:HB2	7:1H:132:ARG:HB3	1.96	0.47
32:1a:736:C:O2'	37:1f:90:VAL:O	2.33	0.47
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.50	0.47
38:1g:66:VAL:O	38:1g:70:LYS:HG3	2.14	0.47
39:1h:12:ARG:NH1	39:1h:25:ASP:O	2.48	0.47
49:1r:45:SER:OG	49:1r:47:THR:HG22	2.15	0.47
1:2A:171:G:H2'	1:2A:172:C:H6	1.80	0.47
1:2A:1063:G:H1	1:2A:1075:C:N4	2.13	0.47
1:2A:1111:A:C2	1:2A:1112:G:H1'	2.50	0.47
1:2A:2262:U:OP1	1:2A:2387:U:O2'	2.28	0.47
1:2A:2706:G:N7	61:2A:3960:HOH:O	2.35	0.47
3:2D:71:ASP:CB	3:2D:103:ARG:HH22	2.28	0.47
12:2Q:25:ASP:CG	21:2Z:78:LYS:HG2	2.40	0.47
32:2a:1252:A:H61	32:2a:1285:A:H61	1.63	0.47
1:1A:404:C:OP1	61:1A:4156:HOH:O	2.21	0.47
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.80	0.47
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.80	0.47
1:1A:2705:A:H2'	1:1A:2706:G:O4'	2.15	0.47
19:1X:60:ARG:HH11	29:17:47:ARG:HH22	1.63	0.47
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.97	0.47
27:15:40:LYS:HE2	61:15:215:HOH:O	2.15	0.47
32:1a:438:G:O2'	32:1a:494:U:O4	2.31	0.47
32:1a:540:G:H2'	32:1a:541:G:O4'	2.15	0.47
32:1a:575:G:O2'	32:1a:821:G:H5'	2.14	0.47
32:1a:674:G:H2'	32:1a:675:A:C8	2.49	0.47
32:1a:1244:C:H2'	32:1a:1245:A:C8	2.50	0.47
49:1r:42:ARG:HA	49:1r:42:ARG:HE	1.81	0.47
1:2A:150:C:H2'	1:2A:151:C:H6	1.80	0.47
1:2A:265:A:N1	1:2A:427:U:O2'	2.43	0.47
1:2A:991:C:OP2	61:2A:3857:HOH:O	2.20	0.47
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.15	0.47
56:2A:3713:ZIT:H191	56:2A:3713:ZIT:H8	1.65	0.47
2:2B:75:G:O3'	21:2Z:10:ARG:NH2	2.48	0.47
6:2G:10:LYS:HG3	6:2G:14:GLU:OE1	2.15	0.47
6:2G:15:VAL:HA	6:2G:175:LEU:HD23	1.97	0.47
7:2H:117:PRO:HG3	7:2H:123:PHE:CE2	2.49	0.47
16:2U:90:VAL:HG12	16:2U:95:LEU:HG	1.97	0.47
32:2a:273:A:H1'	48:2q:16:GLN:HE21	1.80	0.47
32:2a:325:A:H2'	32:2a:326:G:O4'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:415:A:H2'	32:2a:416:G:O4'	2.15	0.47
32:2a:973:G:H3'	32:2a:974:A:H5''	1.97	0.47
1:1A:1057:A:N1	1:1A:1081:U:O4	2.48	0.46
1:1A:2108:C:H42	1:1A:2181:G:H1	1.64	0.46
1:1A:2143:C:N3	1:1A:2148:G:C6	2.83	0.46
4:1E:1:MET:HB3	4:1E:83:ASP:O	2.15	0.46
15:1T:125:ARG:NH1	32:1a:1443:G:H5'	2.30	0.46
21:1Z:75:ASN:O	21:1Z:84:GLU:HG2	2.15	0.46
24:12:65:ASN:O	24:12:69:ARG:HG3	2.15	0.46
33:1b:63:MET:HG3	33:1b:225:ALA:HB1	1.97	0.46
35:1d:168:ARG:HD3	35:1d:168:ARG:HA	1.51	0.46
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.97	0.46
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.96	0.46
6:2G:15:VAL:HG13	6:2G:175:LEU:HB3	1.97	0.46
36:2e:77:PRO:HD2	36:2e:142:LEU:HD22	1.97	0.46
36:2e:146:ALA:HB1	36:2e:150:ARG:HH22	1.79	0.46
1:1A:142:A:N1	1:1A:1595:G:O2'	2.45	0.46
1:1A:1070:A:N7	1:1A:1097:U:H4'	2.30	0.46
1:1A:1171:G:H3'	1:1A:1173:G:H5'	1.97	0.46
1:1A:2181:G:H2'	1:1A:2182:G:C8	2.49	0.46
5:1F:24:LEU:HB3	5:1F:115:ALA:HB2	1.97	0.46
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.38	0.46
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.48	0.46
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	1.96	0.46
16:1U:85:LYS:HE3	16:1U:116:ALA:O	2.16	0.46
32:1a:376:G:H4'	47:1p:5:ARG:HH11	1.80	0.46
32:1a:1003:G:N2	32:1a:1004:A:N3	2.63	0.46
32:1a:1169:A:H2'	32:1a:1170:A:C8	2.50	0.46
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.50	0.46
32:1a:1486:G:H2'	32:1a:1487:G:O4'	2.14	0.46
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.15	0.46
11:2P:2:LYS:HE3	11:2P:4:SER:OG	2.15	0.46
21:2Z:54:HIS:NE2	21:2Z:123:ASP:HB3	2.30	0.46
32:2a:664:G:N2	32:2a:741:G:H1	2.11	0.46
32:2a:818:G:O2'	32:2a:819:A:H5'	2.14	0.46
35:2d:50:ARG:NH1	36:2e:10:MET:HE2	2.29	0.46
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.13	0.46
1:1A:307:G:H21	1:1A:330:A:H62	1.62	0.46
1:1A:2101:G:H2'	1:1A:2102:U:C6	2.51	0.46
1:1A:2612:C:OP2	27:15:2:ALA:N	2.48	0.46
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:136:C:O2'	47:1p:65:GLN:NE2	2.28	0.46
32:1a:523:A:N1	43:1l:92:OTD:H6	2.30	0.46
32:1a:1106:G:H5''	34:1c:172:ARG:HG2	1.97	0.46
48:1q:62:SER:OG	48:1q:72:ARG:HG3	2.15	0.46
50:1s:40:ILE:HA	50:1s:44:MET:SD	2.55	0.46
1:2A:657:U:H2'	1:2A:658:C:C6	2.50	0.46
1:2A:1155:A:OP1	16:2U:55:ARG:HD3	2.16	0.46
1:2A:1762:A:N6	61:2A:4123:HOH:O	2.48	0.46
1:2A:1820:U:H4'	1:2A:1821:A:OP2	2.15	0.46
2:2B:14:U:OP2	2:2B:70:C:O2'	2.28	0.46
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	1.97	0.46
6:2G:66:GLN:OE1	6:2G:98:ARG:NE	2.49	0.46
14:2S:43:GLU:OE2	22:20:49:LYS:NZ	2.46	0.46
33:2b:71:VAL:HG23	33:2b:164:VAL:HA	1.98	0.46
35:2d:173:TRP:CD1	35:2d:189:PRO:HG3	2.50	0.46
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.50	0.46
44:2m:61:GLU:HA	44:2m:66:LEU:HD11	1.97	0.46
1:1A:93:G:H2'	1:1A:94:C:H6	1.80	0.46
1:1A:878:A:H2'	1:1A:879:G:H5'	1.97	0.46
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.81	0.46
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.51	0.46
3:1D:183:ARG:HG3	3:1D:270:ILE:HG12	1.97	0.46
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.51	0.46
32:1a:1277:C:H1'	32:1a:1282:C:O2	2.15	0.46
38:1g:121:ALA:O	38:1g:125:MET:HG3	2.16	0.46
1:2A:1050:A:H2'	1:2A:1051:G:C8	2.50	0.46
1:2A:1055:G:H21	1:2A:1086:A:H8	1.63	0.46
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.14	0.46
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.14	0.46
4:2E:59:VAL:HG21	4:2E:74:PRO:HB2	1.97	0.46
12:2Q:111:GLU:OE1	12:2Q:133:ARG:NH2	2.49	0.46
13:2R:12:ARG:O	13:2R:17:ARG:NH1	2.49	0.46
32:2a:737:A:H2'	32:2a:738:C:H6	1.80	0.46
32:2a:1146:A:H5'	32:2a:1147:C:OP2	2.15	0.46
32:2a:1465:C:H2'	32:2a:1466:C:O4'	2.15	0.46
44:2m:20:THR:C	44:2m:22:ILE:H	2.23	0.46
49:2r:58:LEU:HD22	49:2r:62:GLU:HB3	1.98	0.46
1:1A:886:C:H3'	1:1A:887:A:H5''	1.98	0.46
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.51	0.46
1:1A:2250:G:O2'	1:1A:2496:C:OP1	2.24	0.46
1:2A:9:U:O4	1:2A:2629:A:H2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:644:A:H4'	1:2A:645:C:H5	1.81	0.46
1:2A:1161:C:H4'	17:2V:8:GLY:HA2	1.97	0.46
1:2A:1450:G:H2'	1:2A:1450(A):C:H6	1.80	0.46
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.50	0.46
32:2a:1271:G:H5'	32:2a:1314:C:H5''	1.97	0.46
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.15	0.46
41:2j:32:ALA:HB1	41:2j:33:GLN:CD	2.39	0.46
50:2s:33:THR:HG22	50:2s:35:SER:H	1.80	0.46
1:1A:784:A:C5	3:1D:229:VAL:HG21	2.51	0.46
1:1A:2070:G:OP2	61:1A:4158:HOH:O	2.21	0.46
33:1b:91:PRO:HG2	33:1b:155:LEU:HD13	1.97	0.46
38:1g:111:ARG:HB3	38:1g:113:GLU:HG2	1.98	0.46
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.55	0.46
1:2A:412:A:OP2	1:2A:412:A:H8	1.99	0.46
1:2A:887:A:O2'	1:2A:888:C:H3'	2.15	0.46
1:2A:1064:C:H5	1:2A:1065:U:C6	2.33	0.46
1:2A:1800:C:OP1	3:2D:264:LYS:NZ	2.46	0.46
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.46	0.46
12:2Q:44:ALA:HB2	12:2Q:70:PRO:HG3	1.98	0.46
14:2S:65:VAL:O	14:2S:69:VAL:HG23	2.16	0.46
32:2a:792:A:O2'	32:2a:794:A:N7	2.42	0.46
1:1A:569:U:C4	1:1A:570:G:C6	3.03	0.46
1:1A:1011:G:OP1	16:1U:77:SER:OG	2.29	0.46
1:1A:1252:G:N3	16:1U:33:ARG:HG2	2.31	0.46
1:1A:2028:U:H2'	1:1A:2029:G:O4'	2.16	0.46
1:1A:2615:U:H2'	1:1A:2616:C:C6	2.51	0.46
4:1E:28:ALA:HB3	4:1E:93:VAL:CG1	2.43	0.46
21:1Z:3:TYR:CD2	21:1Z:51:ALA:HB2	2.51	0.46
32:1a:976:G:OP1	45:1n:32:SER:N	2.45	0.46
53:1y:3:MET:HB2	53:1y:37:PRO:HG2	1.96	0.46
1:2A:299:A:N1	1:2A:322:A:O2'	2.42	0.46
1:2A:1359:A:N3	1:2A:1359:A:H5'	2.31	0.46
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.16	0.46
1:2A:2126:A:C5	1:2A:2163:C:H1'	2.51	0.46
34:2c:6:HIS:HB3	45:2n:49:HIS:ND1	2.31	0.46
34:2c:114:PRO:HA	34:2c:185:GLY:HA3	1.98	0.46
39:2h:34:GLU:O	39:2h:37:ARG:HG2	2.15	0.46
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.50	0.46
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.50	0.46
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.49	0.46
12:1Q:63:LYS:HG3	61:1Z:405:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:259:G:OP2	51:1t:83:ARG:NH1	2.47	0.46
32:1a:736:C:H2'	32:1a:737:A:C8	2.51	0.46
32:1a:958:A:C5	50:1s:55:LYS:HD2	2.50	0.46
32:1a:1086:U:H2'	32:1a:1087:G:H8	1.80	0.46
32:1a:1492:A:H4'	32:1a:1493:A:C2	2.50	0.46
33:1b:97:TRP:HH2	33:1b:176:GLU:CD	2.24	0.46
33:1b:218:ALA:O	33:1b:222:ILE:HG13	2.15	0.46
34:1c:55:VAL:HG12	34:1c:68:VAL:HG22	1.97	0.46
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.98	0.46
1:2A:234:C:H2'	1:2A:235:U:C6	2.51	0.46
1:2A:792:G:OP2	61:2A:3858:HOH:O	2.21	0.46
1:2A:2100:G:O6	1:2A:2189:U:O4	2.34	0.46
1:2A:2136:C:OP2	1:2A:2136:C:C6	2.69	0.46
61:2A:4573:HOH:O	5:2F:74:ARG:HG3	2.16	0.46
8:2I:140:LEU:HD22	8:2I:141:LYS:H	1.81	0.46
9:2N:131:GLN:C	9:2N:133:GLN:H	2.23	0.46
31:29:27:CYS:SG	31:29:28:GLU:N	2.89	0.46
32:2a:458:C:H2'	32:2a:460:G:O4'	2.15	0.46
32:2a:543:C:OP2	35:2d:10:ARG:NH2	2.48	0.46
32:2a:560:U:H6	32:2a:560:U:H2'	1.47	0.46
38:2g:16:LEU:HD13	40:2i:45:ALA:HB2	1.98	0.46
46:2o:35:ARG:O	46:2o:39:LEU:HB2	2.16	0.46
53:2y:23:ARG:HG3	53:2y:78:ILE:HD12	1.96	0.46
1:1A:251:A:C5	1:1A:252:G:H1'	2.50	0.46
1:1A:1816:G:H8	3:1D:62:TYR:CZ	2.34	0.46
1:1A:2712:U:H2'	1:1A:2714:G:H5''	1.98	0.46
32:1a:227:G:H2'	32:1a:228:A:O4'	2.16	0.46
32:1a:868:C:H2'	32:1a:869:G:O4'	2.16	0.46
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.83	0.46
33:1b:215:LEU:O	33:1b:219:VAL:HG23	2.16	0.46
44:1m:52:GLU:HG2	44:1m:55:ARG:NH2	2.31	0.46
1:2A:1074:G:C2	1:2A:1075:C:H1'	2.51	0.46
1:2A:2390:U:P	30:28:35:GLN:HE22	2.39	0.46
7:2H:127:GLU:C	7:2H:129:THR:H	2.24	0.46
13:2R:83:ILE:O	13:2R:86:ARG:HG2	2.16	0.46
26:24:62:ARG:HD3	26:24:62:ARG:HA	1.65	0.46
32:2a:766:A:OP2	61:2a:3217:HOH:O	2.20	0.46
32:2a:1527:C:OP1	61:2a:3216:HOH:O	2.20	0.46
33:2b:20:GLU:HB2	33:2b:190:THR:OG1	2.16	0.46
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.47	0.46
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:47:VAL:O	4:1E:80:GLU:HA	2.16	0.46
26:14:50:VAL:HG21	44:1m:64:TRP:C	2.41	0.46
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.51	0.46
32:1a:452:A:H4'	47:1p:72:ARG:CZ	2.45	0.46
32:1a:616:G:OP2	35:1d:141:ARG:NH2	2.49	0.46
33:1b:27:LYS:HB2	33:1b:194:PRO:HD2	1.97	0.46
35:1d:61:LYS:HD3	35:1d:206:PHE:CE2	2.51	0.46
36:1e:84:PHE:CE2	36:1e:133:TYR:HD2	2.34	0.46
53:1y:3:MET:HB3	53:1y:3:MET:HE2	1.67	0.46
1:2A:30:G:H2'	1:2A:31:C:C6	2.50	0.46
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.64	0.46
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.24	0.46
1:2A:2113:U:H2'	1:2A:2114:A:O4'	2.16	0.46
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.31	0.46
13:2R:87:TYR:OH	13:2R:117:VAL:O	2.18	0.46
14:2S:14:VAL:HG11	14:2S:89:ARG:HG2	1.97	0.46
26:24:48:ARG:HD2	26:24:52:THR:HA	1.96	0.46
32:2a:583:A:H2'	32:2a:584:G:O4'	2.16	0.46
32:2a:984:C:H2'	32:2a:985:C:H6	1.81	0.46
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.81	0.46
32:2a:1051:C:H42	32:2a:1207:2MG:HN1	1.63	0.46
34:2c:99:VAL:O	34:2c:101:LEU:N	2.49	0.46
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.80	0.46
1:1A:887:A:H1'	1:1A:888:C:H3'	1.97	0.45
1:1A:969:U:H2'	1:1A:970:C:C6	2.51	0.45
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.50	0.45
1:1A:2019:A:O4'	16:1U:34:LYS:HE2	2.16	0.45
1:1A:2059:A:N1	56:1A:4033:ZIT:H2A1	2.32	0.45
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.16	0.45
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.66	0.45
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.68	0.45
1:2A:606:U:H4'	1:2A:658:C:H4'	1.98	0.45
1:2A:888:C:OP1	44:2m:93:ARG:HD2	2.17	0.45
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.49	0.45
1:2A:2775:A:OP2	61:2A:3854:HOH:O	2.20	0.45
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.52	0.45
32:2a:1172:C:H2'	32:2a:1173:G:C8	2.49	0.45
40:2i:53:VAL:HG21	40:2i:92:TYR:CE1	2.50	0.45
1:1A:1250:G:H5''	61:1U:325:HOH:O	2.16	0.45
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.98	0.45
6:1G:66:GLN:HG3	26:14:1:MET:HE1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:104:ARG:HD2	13:1R:107:ASP:OD1	2.15	0.45
32:1a:404:U:H2'	32:1a:405:U:C6	2.51	0.45
41:1j:31:GLY:HA2	41:1j:32:ALA:HA	1.55	0.45
41:1j:78:ASN:O	41:1j:80:LYS:N	2.49	0.45
47:1p:43:LYS:HA	47:1p:48:TRP:CD1	2.51	0.45
1:2A:69:C:O2	1:2A:73:A:O2'	2.33	0.45
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.14	0.45
1:2A:760:G:H2'	1:2A:761:A:O4'	2.16	0.45
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.51	0.45
7:2H:20:ALA:HB3	7:2H:23:ARG:HB2	1.98	0.45
8:2I:62:LYS:HG2	8:2I:133:HIS:NE2	2.31	0.45
13:2R:72:ASP:HB3	13:2R:75:LEU:HB3	1.96	0.45
21:2Z:5:LEU:HD21	21:2Z:39:VAL:HB	1.98	0.45
21:2Z:73:GLN:H	21:2Z:87:ASP:HB2	1.80	0.45
32:2a:382:A:H2'	32:2a:383:A:C8	2.51	0.45
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.31	0.45
44:2m:74:VAL:O	44:2m:78:ILE:HG12	2.17	0.45
1:1A:219:G:OP2	61:1A:4153:HOH:O	2.20	0.45
1:1A:531:C:H4'	1:1A:532:A:H5''	1.98	0.45
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.51	0.45
1:1A:2119:A:H2	1:1A:2171:A:H5'	1.81	0.45
7:1H:98:LEU:HD22	7:1H:125:VAL:HG23	1.97	0.45
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.97	0.45
28:16:19:ARG:NH1	28:16:52:VAL:HG11	2.32	0.45
32:1a:458:C:H2'	32:1a:460:G:O4'	2.17	0.45
32:1a:1264:C:H2'	32:1a:1265:G:H8	1.80	0.45
34:1c:7:PRO:O	34:1c:11:ARG:NH1	2.48	0.45
42:1k:70:LYS:HE2	42:1k:70:LYS:HB2	1.71	0.45
50:1s:27:GLU:CB	50:1s:28:LYS:HG3	2.46	0.45
1:2A:154(A):C:N4	1:2A:171:G:H1	2.10	0.45
1:2A:614(C):A:C4	5:2F:180:GLY:HA2	2.51	0.45
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.52	0.45
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.99	0.45
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	1.98	0.45
1:2A:2103:C:O2	1:2A:2187:G:N1	2.49	0.45
1:2A:2405:G:H5'	11:2P:75:ILE:HD13	1.98	0.45
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.16	0.45
7:2H:25:LYS:HE3	7:2H:27:LYS:NZ	2.31	0.45
32:2a:539:A:H2'	32:2a:540:G:C8	2.51	0.45
32:2a:684:A:H2'	32:2a:685:G:C8	2.52	0.45
32:2a:1318:A:H1'	50:2s:37:ARG:HH11	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:79:PHE:CE1	35:2d:204:ILE:HD13	2.48	0.45
38:2g:92:SER:O	38:2g:96:GLN:HG3	2.15	0.45
51:2t:50:GLU:HB2	51:2t:99:LEU:HD23	1.98	0.45
1:1A:118:A:C8	1:1A:119:A:C8	3.04	0.45
1:1A:330:A:HO2'	1:1A:331:A:H8	1.62	0.45
1:1A:602:G:N1	1:1A:655:A:OP2	2.42	0.45
1:1A:813:U:H2'	1:1A:814:C:C6	2.52	0.45
1:1A:1210:A:H5''	1:1A:1212:G:O4'	2.17	0.45
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.51	0.45
1:1A:1759:A:H1'	1:1A:2711:A:C2	2.52	0.45
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.51	0.45
1:1A:2190:G:H2'	1:1A:2191:G:O4'	2.17	0.45
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.52	0.45
1:1A:2590:A:H2'	1:1A:2591:C:C6	2.52	0.45
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.49	0.45
4:1E:111:ARG:HA	13:1R:1:MET:SD	2.56	0.45
6:1G:112:PRO:HG3	26:14:43:TYR:CE2	2.51	0.45
26:14:34:GLU:H	26:14:34:GLU:CD	2.25	0.45
32:1a:376:G:H5''	47:1p:5:ARG:HD2	1.98	0.45
32:1a:1366:C:H2'	32:1a:1367:C:C6	2.52	0.45
39:1h:85:ARG:HD2	39:1h:85:ARG:HA	1.70	0.45
1:2A:634:C:H2'	1:2A:635:C:C6	2.51	0.45
1:2A:889:C:O2'	1:2A:890:A:O5'	2.32	0.45
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.40	0.45
1:2A:1525:G:H2'	1:2A:1526:G:C8	2.52	0.45
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.16	0.45
1:2A:2319:G:H22	14:2S:3:ARG:CD	2.29	0.45
1:2A:2462:U:H2'	1:2A:2463:C:C6	2.51	0.45
3:2D:274:ARG:HB3	61:2D:414:HOH:O	2.16	0.45
4:2E:89:ASP:OD2	4:2E:89:ASP:N	2.49	0.45
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	1.98	0.45
6:2G:16:ARG:HB2	6:2G:17:PRO:HD3	1.98	0.45
6:2G:83:ARG:H	6:2G:86:MET:HE3	1.82	0.45
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.46	0.45
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.50	0.45
33:2b:114:ARG:O	33:2b:118:LEU:HB2	2.17	0.45
41:2j:51:ARG:HG3	41:2j:61:GLU:HB2	1.97	0.45
1:1A:644:A:H4'	1:1A:645:C:C5	2.50	0.45
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.31	0.45
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.17	0.45
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:13:A:N1	2:1B:69:G:O2'	2.49	0.45
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.99	0.45
34:1c:130:VAL:HG21	34:1c:157:ILE:HG23	1.99	0.45
35:1d:108:LEU:HD12	35:1d:174:LEU:HD13	1.98	0.45
1:2A:709:U:H2'	1:2A:710:G:C8	2.51	0.45
1:2A:876:C:H2'	1:2A:877:U:O4'	2.16	0.45
1:2A:1354:A:H5''	3:2D:38:LYS:HD3	1.99	0.45
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.52	0.45
1:2A:2115:G:H21	1:2A:2171:A:H61	1.64	0.45
3:2D:275:LYS:HD2	3:2D:275:LYS:HA	1.61	0.45
4:2E:56:PRO:C	4:2E:58:ARG:H	2.24	0.45
26:24:58:ARG:O	26:24:61:ARG:HB2	2.17	0.45
32:2a:731:G:H5'	32:2a:766:A:H4'	1.97	0.45
32:2a:1004:A:OP1	32:2a:1024:G:N2	2.49	0.45
33:2b:83:MET:HE1	33:2b:234:PRO:O	2.16	0.45
36:2e:10:MET:SD	36:2e:13:ILE:HD11	2.57	0.45
1:1A:1270:C:H5''	1:1A:1271:G:O5'	2.16	0.45
1:1A:1289:C:H2'	1:1A:1290:C:H6	1.81	0.45
1:1A:1509:C:H3'	1:1A:1509:C:OP1	2.16	0.45
14:1S:59:LYS:H	14:1S:59:LYS:HG3	1.56	0.45
32:1a:56:U:H2'	32:1a:57:G:C8	2.51	0.45
32:1a:1030(B):C:O2	32:1a:1030(B):C:H2'	2.16	0.45
32:1a:1140:C:H2'	32:1a:1141:C:H6	1.80	0.45
32:1a:1376:U:P	38:1g:94:ARG:HH12	2.40	0.45
32:1a:1498:UR3:H4'	32:1a:1519:MA6:H2	1.99	0.45
47:1p:3:LYS:HG3	47:1p:24:ALA:HB2	1.98	0.45
1:2A:586:A:N1	1:2A:809:G:O2'	2.45	0.45
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.50	0.45
1:2A:900:A:H2'	1:2A:901:A:O4'	2.16	0.45
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.52	0.45
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.50	0.45
1:2A:1384:A:N3	1:2A:1405:U:H1'	2.31	0.45
1:2A:1614:A:P	1:2A:1614:A:H8	2.39	0.45
1:2A:2391:G:O6	1:2A:2425:A:H8	1.99	0.45
2:2B:48:A:H2'	2:2B:49:C:C6	2.51	0.45
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.16	0.45
32:2a:1350:A:H2'	32:2a:1351:U:O4'	2.16	0.45
33:2b:74:LYS:O	33:2b:78:GLN:N	2.50	0.45
40:2i:89:ASN:O	40:2i:92:TYR:HD2	1.99	0.45
44:2m:17:VAL:O	44:2m:20:THR:HG22	2.16	0.45
1:1A:679:C:OP1	61:1A:4114:HOH:O	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:886:C:C3'	1:1A:887:A:H5''	2.47	0.45
1:1A:1166:C:H2'	1:1A:1167:U:H6	1.81	0.45
1:1A:1416:G:O2'	1:1A:1417:C:OP2	2.29	0.45
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.51	0.45
1:1A:2101:G:H2'	1:1A:2102:U:H6	1.81	0.45
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.16	0.45
1:1A:2439:A:H5'	1:1A:2439:A:C8	2.52	0.45
3:1D:112:GLN:O	3:1D:115:GLN:HG2	2.17	0.45
9:1N:48:MET:O	9:1N:48:MET:HE3	2.17	0.45
11:1P:8:PRO:HB2	11:1P:12:ALA:HB3	1.99	0.45
11:1P:71:VAL:HG22	11:1P:72:PRO:HA	1.98	0.45
32:1a:503:C:H2'	32:1a:504:C:H6	1.81	0.45
1:2A:27:G:O2'	1:2A:28:A:OP2	2.31	0.45
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.16	0.45
1:2A:2092:U:H4'	1:2A:2093:G:O5'	2.17	0.45
1:2A:2122:U:O2	1:2A:2176:A:N1	2.50	0.45
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.51	0.45
1:2A:2745:C:C4	1:2A:2746:U:C4	3.05	0.45
2:2B:40:U:H2'	26:24:2:LYS:HE3	1.99	0.45
2:2B:83:G:H1	2:2B:94:C:H42	1.63	0.45
5:2F:24:LEU:HD13	5:2F:115:ALA:HA	1.99	0.45
6:2G:126:ASP:HB3	6:2G:128:ARG:H	1.81	0.45
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.50	0.45
8:2I:81:VAL:HG21	8:2I:88:ILE:HG12	1.99	0.45
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.99	0.45
18:2W:59:VAL:HG23	18:2W:60:ASN:OD1	2.16	0.45
32:2a:653:A:OP1	39:2h:56:LYS:NZ	2.49	0.45
32:2a:1292:U:C2	32:2a:1293:G:C8	3.05	0.45
32:2a:1316:G:N1	32:2a:1319:A:OP2	2.43	0.45
33:2b:216:SER:O	33:2b:220:ASP:N	2.47	0.45
40:2i:78:LYS:HA	40:2i:81:ILE:HG22	1.98	0.45
1:1A:672:C:OP2	11:1P:42:SER:OG	2.34	0.45
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.17	0.45
1:1A:1784:A:H4'	1:1A:1785:A:O5'	2.17	0.45
1:1A:1878:G:H2'	1:1A:1879:C:C6	2.52	0.45
2:1B:39:A:O2'	2:1B:46:A:N1	2.48	0.45
32:1a:142:G:O2'	32:1a:196:A:N1	2.48	0.45
32:1a:174:C:H2'	32:1a:175:C:C6	2.52	0.45
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.99	0.45
42:1k:85:ARG:HD3	42:1k:113:PRO:HD3	1.98	0.45
48:1q:62:SER:HB3	48:1q:72:ARG:HH11	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:747:U:O2	1:2A:2014:A:H1'	2.16	0.45
1:2A:824:A:H2'	1:2A:825:C:O4'	2.17	0.45
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.99	0.45
1:2A:2144:U:H5''	1:2A:2145:C:C5	2.52	0.45
8:2I:72:LEU:HD21	8:2I:107:VAL:HG21	1.98	0.45
23:21:4:VAL:HG12	23:21:11:ARG:HB3	1.98	0.45
32:2a:256:U:H2'	32:2a:257:G:C8	2.51	0.45
32:2a:523:A:H61	43:2I:92:OTD:CG	2.30	0.45
32:2a:839:U:H5''	32:2a:840:C:H5	1.82	0.45
32:2a:1360:A:H2'	32:2a:1361:G:O4'	2.17	0.45
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.52	0.45
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.31	0.45
1:1A:265:A:N1	1:1A:427:U:O2'	2.48	0.45
1:1A:839:U:H2'	1:1A:840:C:C6	2.52	0.45
1:1A:1418:G:O5'	1:1A:1418:G:H8	1.99	0.45
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.17	0.45
56:1A:4033:ZIT:H191	56:1A:4033:ZIT:H8	1.62	0.45
27:15:48:GLU:C	27:15:60:VAL:HG21	2.42	0.45
32:1a:44:G:C2	32:1a:45:U:H1'	2.52	0.45
32:1a:67:C:H2'	32:1a:68:G:C8	2.51	0.45
32:1a:512:U:H2'	32:1a:513:C:C6	2.52	0.45
32:1a:1040:U:H2'	32:1a:1041:A:H8	1.82	0.45
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.51	0.45
39:1h:104:ARG:HD3	39:1h:104:ARG:HA	1.76	0.45
43:1I:88:GLY:O	43:1I:99:HIS:HD2	2.00	0.45
45:1n:3:ARG:O	45:1n:7:ILE:HG13	2.16	0.45
1:2A:1076:C:H4'	1:2A:1077:A:OP1	2.15	0.45
1:2A:2286:A:P	28:26:29:ASN:HD22	2.40	0.45
6:2G:33:ARG:O	6:2G:161:THR:HG23	2.17	0.45
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.51	0.45
31:29:22:ARG:HB3	31:29:24:TYR:HE2	1.82	0.45
32:2a:164:U:H2'	32:2a:165:C:H6	1.82	0.45
32:2a:189(L):G:H2'	32:2a:190:U:C6	2.52	0.45
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.82	0.45
32:2a:1135:U:H4'	32:2a:1136:U:C5	2.51	0.45
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.41	0.45
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.98	0.45
1:1A:2115:G:H2'	1:1A:2117:A:H62	1.81	0.45
19:1X:12:VAL:HG21	19:1X:27:THR:HG22	1.98	0.45
26:14:59:PHE:CZ	50:1s:64:GLU:HG3	2.52	0.45
32:1a:1400:5MC:N3	53:1y:63:ALA:HA	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.49	0.45
1:2A:249:C:O2	30:28:12:LYS:NZ	2.43	0.45
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.17	0.45
1:2A:2261:C:C6	22:20:16:SER:HB3	2.51	0.45
6:2G:77:ILE:HG21	6:2G:80:PHE:CD2	2.52	0.45
32:2a:537:G:H5''	43:2l:113:ARG:NH1	2.32	0.45
32:2a:685:G:O2'	32:2a:686:U:H5'	2.16	0.45
32:2a:976:G:OP1	45:2n:32:SER:N	2.43	0.45
32:2a:1116:C:O2'	40:2i:108:VAL:HG21	2.17	0.45
33:2b:73:THR:HG22	33:2b:95:GLN:O	2.17	0.45
38:2g:101:LEU:O	38:2g:105:VAL:HG23	2.17	0.45
46:2o:8:LYS:O	46:2o:12:ILE:HG13	2.16	0.45
1:1A:724:U:H2'	1:1A:725:G:O4'	2.17	0.44
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.17	0.44
10:1O:18:LYS:HB2	10:1O:45:GLU:HB3	1.99	0.44
10:1O:64:ARG:HD2	10:1O:81:ASP:OD1	2.17	0.44
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	2.00	0.44
32:1a:57:G:H2'	32:1a:58:C:C6	2.52	0.44
32:1a:601:C:H2'	32:1a:602:A:H8	1.81	0.44
32:1a:974:A:OP1	45:1n:29:ARG:NH2	2.50	0.44
32:1a:1112:C:C2	34:1c:178:LEU:HB2	2.52	0.44
32:1a:1347:G:O2'	32:1a:1373:G:O6	2.30	0.44
34:1c:108:ASN:HD21	34:1c:144:SER:HG	1.61	0.44
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.98	0.44
47:1p:71:ARG:HG3	47:1p:80:PHE:CE2	2.52	0.44
1:2A:2887:U:H2'	1:2A:2888:C:C6	2.52	0.44
4:2E:27:LEU:HD22	15:2T:1:MET:SD	2.56	0.44
5:2F:120:GLU:HB2	5:2F:122:LYS:HG2	1.99	0.44
6:2G:42:GLY:HA2	6:2G:89:GLY:HA3	1.98	0.44
18:2W:24:ILE:HA	18:2W:27:LYS:HG3	1.99	0.44
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.82	0.44
32:2a:1190:G:H5'	34:2c:176:HIS:HE1	1.80	0.44
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.32	0.44
46:2o:26:GLU:HG3	46:2o:81:LEU:HD13	1.98	0.44
50:2s:36:ARG:HH12	50:2s:75:ALA:HB3	1.83	0.44
1:1A:271(H):G:O2'	1:1A:271(I):G:OP2	2.29	0.44
1:1A:271(I):G:H2'	1:1A:271(J):C:C6	2.52	0.44
1:1A:478:A:C6	1:1A:480:A:C6	3.05	0.44
1:1A:645:C:O2	1:1A:645:C:H2'	2.17	0.44
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.17	0.44
55:1A:4032:HGR:C16	55:1A:4032:HGR:H3	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:94:GLU:HG3	11:1P:124:LYS:HD3	1.98	0.44
32:1a:77:G:C2'	32:1a:78:G:H5'	2.46	0.44
32:1a:601:C:H2'	32:1a:602:A:C8	2.53	0.44
36:1e:71:LEU:HD11	36:1e:113:ALA:O	2.17	0.44
39:1h:39:LEU:HD12	39:1h:39:LEU:HA	1.76	0.44
44:1m:40:ASN:ND2	44:1m:42:ALA:HB3	2.32	0.44
53:1y:24:LEU:HD23	53:1y:24:LEU:HA	1.88	0.44
1:2A:1047:G:H2'	1:2A:1110:G:H22	1.82	0.44
1:2A:1084:A:N6	1:2A:1086:A:N7	2.64	0.44
1:2A:1138:G:N3	9:2N:106:MET:HE2	2.32	0.44
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.32	0.44
1:2A:2409:G:H2'	1:2A:2410:G:O4'	2.17	0.44
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.17	0.44
2:2B:15:A:H3'	2:2B:16:G:H8	1.82	0.44
7:2H:126:PRO:HG2	7:2H:130:ARG:HE	1.82	0.44
14:2S:26:LEU:HD22	14:2S:87:PHE:CD1	2.52	0.44
21:2Z:144:LEU:HD11	21:2Z:150:LEU:HG	1.98	0.44
32:2a:130:A:O2'	32:2a:131:C:O5'	2.28	0.44
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.50	0.44
32:2a:1070:U:H2'	32:2a:1071:C:C6	2.51	0.44
32:2a:1077:G:N1	32:2a:1081:G:C6	2.85	0.44
32:2a:1212:U:H4'	32:2a:1213:A:C8	2.52	0.44
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.52	0.44
35:2d:30:LYS:HG2	35:2d:35:ARG:HH21	1.80	0.44
35:2d:111:ALA:HB1	35:2d:116:GLN:HG2	2.00	0.44
13:1R:1:MET:HE3	13:1R:1:MET:HB2	1.89	0.44
32:1a:8:A:N6	35:1d:205:GLU:O	2.48	0.44
32:1a:273:A:H1'	48:1q:16:GLN:NE2	2.32	0.44
32:1a:437:U:O2'	35:1d:123:HIS:HD2	2.01	0.44
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.45	0.44
50:1s:15:LEU:O	50:1s:19:VAL:HG23	2.18	0.44
1:2A:150:C:H2'	1:2A:151:C:C6	2.52	0.44
1:2A:620:G:N3	1:2A:620:G:H5'	2.32	0.44
1:2A:890:A:H2'	1:2A:892:G:O4'	2.18	0.44
1:2A:1065:U:H3	1:2A:1073:A:N6	2.09	0.44
1:2A:1112:G:H2'	1:2A:1113:U:O4'	2.18	0.44
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.17	0.44
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.17	0.44
1:2A:2319:G:H4'	1:2A:2320:A:OP1	2.17	0.44
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	2.00	0.44
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:61:LEU:HD12	3:2D:61:LEU:HA	1.83	0.44
3:2D:124:PRO:HB2	3:2D:126:GLN:HG2	1.99	0.44
3:2D:276:LYS:HB2	3:2D:276:LYS:HE3	1.72	0.44
6:2G:60:LEU:HA	6:2G:63:ILE:HB	2.00	0.44
7:2H:11:VAL:CG1	7:2H:15:VAL:HG23	2.46	0.44
10:2O:113:LYS:HB2	10:2O:113:LYS:HE3	1.72	0.44
32:2a:405:U:O4	35:2d:2:GLY:N	2.50	0.44
32:2a:1126:U:O4'	32:2a:1281:U:H1'	2.17	0.44
33:2b:164:VAL:HB	33:2b:186:ALA:HB2	2.00	0.44
33:2b:165:VAL:HG23	33:2b:166:ASP:H	1.82	0.44
34:2c:3:ASN:OD1	34:2c:4:LYS:NZ	2.48	0.44
36:2e:116:THR:HG23	36:2e:117:ASP:CG	2.43	0.44
44:2m:89:GLY:O	44:2m:93:ARG:N	2.40	0.44
1:1A:458:G:O2'	29:17:39:ARG:HD3	2.16	0.44
1:1A:2469:A:H5'	1:1A:2470:G:OP2	2.17	0.44
1:1A:2774:C:H2'	1:1A:2775:A:O4'	2.17	0.44
15:1T:53:ARG:HB3	15:1T:53:ARG:NH1	2.33	0.44
32:1a:316:G:OP2	32:1a:351:G:O2'	2.27	0.44
33:1b:12:GLU:OE2	33:1b:48:MET:HE2	2.17	0.44
34:1c:102:ASN:HD22	34:1c:102:ASN:N	2.15	0.44
53:1y:37:PRO:HA	53:1y:54:ILE:HG12	2.00	0.44
1:2A:1096:A:C4	1:2A:1097:U:H5	2.35	0.44
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.50	0.44
32:2a:1036:G:H3'	32:2a:1037:C:H6	1.82	0.44
32:2a:1438:G:H2'	32:2a:1439:C:C6	2.53	0.44
41:2j:35:SER:HB2	41:2j:73:ASP:HB2	1.99	0.44
1:1A:1041:C:H5'	1:1A:1042:G:OP2	2.17	0.44
1:1A:1301:A:C8	1:1A:1303:G:C8	3.05	0.44
1:1A:2882:A:OP1	13:1R:96:ARG:HD3	2.17	0.44
4:1E:9:VAL:HG22	4:1E:25:VAL:HB	1.98	0.44
12:1Q:17:LEU:HD23	12:1Q:17:LEU:HA	1.84	0.44
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.17	0.44
20:1Y:19:LYS:HB3	20:1Y:19:LYS:HE2	1.85	0.44
21:1Z:198:LYS:HB3	21:1Z:202:GLU:HB3	1.99	0.44
32:1a:1028:C:H2'	32:1a:1029:C:H4'	1.99	0.44
34:1c:95:THR:O	34:1c:97:LYS:HG2	2.18	0.44
35:1d:79:PHE:HE1	35:1d:204:ILE:HD13	1.81	0.44
37:1f:50:TYR:OH	49:1r:74:ARG:O	2.29	0.44
39:1h:6:ILE:O	39:1h:10:LEU:HG	2.18	0.44
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.43	0.44
1:2A:422:A:H2'	1:2A:423:A:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1056:G:H21	1:2A:1103:A:H62	1.66	0.44
1:2A:1890:A:OP2	61:2A:3862:HOH:O	2.21	0.44
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.52	0.44
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.50	0.44
1:2A:2111:C:N4	1:2A:2147:G:H22	2.15	0.44
1:2A:2335:A:C8	1:2A:2337:G:C5	3.06	0.44
4:2E:7:VAL:HG13	4:2E:27:LEU:HB3	1.99	0.44
6:2G:15:VAL:HG11	6:2G:176:LEU:HG	2.00	0.44
7:2H:27:LYS:HG3	7:2H:32:GLU:HB3	2.00	0.44
20:2Y:56:PRO:C	20:2Y:58:GLY:H	2.24	0.44
32:2a:542:G:H5'	35:2d:41:GLY:HA3	1.99	0.44
32:2a:1026:G:N3	32:2a:1026:G:H2'	2.33	0.44
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.52	0.44
32:2a:1370:G:C8	40:2i:109:VAL:HG11	2.53	0.44
32:2a:1379:G:OP1	38:2g:6:ARG:NH1	2.50	0.44
35:2d:108:LEU:HA	35:2d:108:LEU:HD12	1.72	0.44
45:2n:4:LYS:HA	45:2n:7:ILE:HD12	1.99	0.44
1:1A:249:C:HO2'	11:1P:64:LYS:HZ2	1.56	0.44
1:1A:305:U:H2'	1:1A:306:U:C6	2.53	0.44
1:1A:1073:A:N3	1:1A:1073:A:H2'	2.33	0.44
1:1A:1325:G:OP1	1:1A:1647:G:O2'	2.26	0.44
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.53	0.44
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.17	0.44
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.50	0.44
8:1I:77:LEU:HD22	8:1I:101:LEU:HG	2.00	0.44
10:1O:115:VAL:O	57:1a:1882:MPD:H13	2.17	0.44
19:1X:25:LYS:NZ	61:1X:203:HOH:O	2.38	0.44
32:1a:384:G:H2'	32:1a:385:C:H6	1.83	0.44
32:1a:441:A:H3'	32:1a:442:C:H6	1.83	0.44
32:1a:673:G:O3'	37:1f:87:ARG:NH2	2.50	0.44
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.17	0.44
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.52	0.44
42:1k:115:PRO:HB2	42:1k:118:GLY:H	1.82	0.44
1:2A:236:C:H2'	1:2A:237:C:C6	2.53	0.44
1:2A:1057:A:N3	1:2A:1057:A:H2'	2.32	0.44
1:2A:1087:G:H1	1:2A:1102:C:H42	1.65	0.44
7:2H:140:LYS:O	7:2H:144:VAL:HG23	2.18	0.44
19:2X:26:TYR:HB3	19:2X:92:LEU:HD22	2.00	0.44
21:2Z:158:PRO:O	21:2Z:161:VAL:HG22	2.18	0.44
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.18	0.44
34:2c:32:LEU:HB3	34:2c:59:ARG:NH1	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:15:VAL:HG11	44:2m:48:LEU:HD21	1.99	0.44
1:1A:1174:A:N7	61:1A:4232:HOH:O	2.36	0.44
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.18	0.44
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.53	0.44
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.17	0.44
23:11:3:LYS:O	23:11:12:PRO:HD3	2.17	0.44
28:16:33:LYS:HA	28:16:33:LYS:HD3	1.84	0.44
32:1a:1216:G:H5''	45:1n:5:ALA:HB2	1.99	0.44
35:1d:43:HIS:HB3	35:1d:46:LYS:HD2	2.00	0.44
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.50	0.44
1:2A:523:C:H4'	1:2A:540:C:O2	2.17	0.44
1:2A:2119:A:H2	1:2A:2171:A:H5'	1.82	0.44
1:2A:2377:A:N3	61:2A:3970:HOH:O	2.36	0.44
1:2A:2839:G:C5'	13:2R:46:GLY:HA2	2.47	0.44
32:2a:1225:A:P	44:2m:102:ARG:HE	2.41	0.44
36:2e:40:ARG:HA	36:2e:67:VAL:O	2.17	0.44
46:2o:82:ILE:O	46:2o:86:GLY:N	2.47	0.44
1:1A:383:U:H2'	1:1A:385:C:H5	1.82	0.44
1:1A:645:C:H5'	1:1A:646:A:OP2	2.17	0.44
1:1A:800:A:H8	1:1A:800:A:OP1	2.01	0.44
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.52	0.44
1:1A:1802:A:N1	1:1A:1822:G:H1'	2.33	0.44
1:1A:1938:A:N6	61:1A:4211:HOH:O	2.29	0.44
1:1A:2119:A:C2	1:1A:2171:A:H5'	2.53	0.44
1:1A:2171:A:N3	1:1A:2172:U:N3	2.65	0.44
3:1D:142:VAL:HG12	3:1D:193:VAL:HA	1.99	0.44
19:1X:94:GLY:HA3	19:1X:95:LEU:C	2.43	0.44
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.53	0.44
32:1a:441:A:H8	32:1a:441:A:OP2	2.01	0.44
51:1t:101:GLY:HA3	51:1t:102:GLY:HA2	1.64	0.44
1:2A:1011:G:H5''	16:2U:77:SER:OG	2.18	0.44
1:2A:1075:C:H2'	1:2A:1076:C:H5'	2.00	0.44
1:2A:2123:G:N1	1:2A:2175:C:O2	2.35	0.44
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	2.00	0.44
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.99	0.44
6:2G:167:GLU:OE1	6:2G:167:GLU:N	2.49	0.44
32:2a:118:U:H3'	32:2a:288:A:H61	1.83	0.44
32:2a:189(F):U:C4	48:2q:72:ARG:NH1	2.86	0.44
32:2a:848:C:H2'	32:2a:849:C:H6	1.83	0.44
32:2a:961:U:OP2	32:2a:1223:C:O2'	2.24	0.44
32:2a:1028:C:C2	32:2a:1033:G:N2	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.18	0.44
32:2a:1317:C:OP1	45:2n:17:LYS:HG2	2.18	0.44
35:2d:173:TRP:CD1	35:2d:174:LEU:HG	2.52	0.44
39:2h:104:ARG:HA	39:2h:104:ARG:HD3	1.79	0.44
42:2k:103:LEU:HD12	42:2k:103:LEU:HA	1.87	0.44
1:1A:903:C:H2'	1:1A:904:C:C6	2.53	0.44
1:1A:2059:A:O2'	5:1F:69:HIS:HD2	1.99	0.44
1:1A:2064:C:H2'	1:1A:2065:C:C6	2.53	0.44
1:1A:2119:A:H61	1:1A:2168:G:H21	1.65	0.44
1:1A:2133:G:C2	1:1A:2157:G:H2'	2.53	0.44
1:1A:2181:G:H2'	1:1A:2182:G:H8	1.83	0.44
3:1D:242:ARG:HG3	3:1D:242:ARG:NH1	2.26	0.44
7:1H:23:ARG:HD2	7:1H:34:GLU:OE1	2.18	0.44
32:1a:201:C:N4	32:1a:216:G:H1	2.02	0.44
32:1a:328:C:H4'	32:1a:329:A:H5''	2.00	0.44
32:1a:405:U:O4	35:1d:2:GLY:N	2.50	0.44
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.32	0.44
32:1a:1202:G:N2	45:1n:46:GLU:OE2	2.49	0.44
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	2.00	0.44
41:1j:5:ARG:NE	41:1j:73:ASP:OD1	2.42	0.44
48:1q:81:ARG:NH1	48:1q:83:ASP:OD2	2.51	0.44
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.17	0.44
1:2A:2115:G:N2	1:2A:2171:A:H61	2.15	0.44
1:2A:2350:C:H5''	30:28:42:ARG:HD3	2.00	0.44
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	1.98	0.44
14:2S:99:LYS:HE2	14:2S:103:GLU:OE2	2.18	0.44
21:2Z:9:TYR:HE2	21:2Z:61:LEU:HD13	1.83	0.44
32:2a:190:U:C2	32:2a:191:G:C8	3.06	0.44
32:2a:622:A:C8	32:2a:623:C:C6	3.06	0.44
32:2a:1060:C:O2'	41:2j:56:HIS:ND1	2.46	0.44
32:2a:1277:C:O2'	32:2a:1279:A:C8	2.71	0.44
33:2b:14:GLY:O	33:2b:15:VAL:HG13	2.18	0.44
33:2b:16:HIS:O	33:2b:18:GLY:N	2.51	0.44
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.50	0.44
35:2d:109:GLY:HA3	35:2d:165:MET:HG3	1.99	0.44
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.33	0.44
53:2y:23:ARG:HG3	53:2y:78:ILE:CD1	2.48	0.44
53:2y:42:SER:O	53:2y:49:VAL:N	2.48	0.44
1:1A:606:U:H4'	1:1A:658:C:H4'	1.99	0.43
1:1A:1058:G:O6	1:1A:1080:C:N3	2.51	0.43
1:1A:1098:A:H2'	1:1A:1099:G:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2107:C:O2	1:1A:2182:G:N1	2.36	0.43
1:1A:2590:A:H2'	1:1A:2591:C:H6	1.83	0.43
4:1E:181:LEU:HD23	4:1E:181:LEU:HA	1.81	0.43
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	2.01	0.43
10:1O:116:SER:O	57:1a:1882:MPD:H11	2.18	0.43
14:1S:59:LYS:NZ	14:1S:68:GLN:HE22	2.16	0.43
22:10:10:THR:HA	61:10:209:HOH:O	2.18	0.43
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.40	0.43
35:1d:153:ARG:O	35:1d:181:MET:HE1	2.17	0.43
40:1i:127:LYS:HE2	40:1i:127:LYS:HB3	1.91	0.43
42:1k:124:LYS:HE3	42:1k:125:PHE:CE2	2.53	0.43
1:2A:359:A:H2'	1:2A:360:G:O4'	2.17	0.43
1:2A:480:A:OP2	20:2Y:47:LYS:HD3	2.18	0.43
1:2A:1262:A:O2'	61:2A:3861:HOH:O	2.21	0.43
4:2E:170:LEU:HB3	4:2E:184:VAL:HG13	1.99	0.43
10:2O:9:GLU:O	10:2O:83:ALA:HA	2.18	0.43
12:2Q:7:MET:HE3	12:2Q:7:MET:HB2	1.72	0.43
15:2T:5:ALA:HA	15:2T:8:LYS:HE3	2.00	0.43
32:2a:56:U:H2'	32:2a:57:G:C8	2.53	0.43
32:2a:109:A:H2'	32:2a:326:G:N2	2.32	0.43
32:2a:411:A:O2'	32:2a:413:G:H5'	2.18	0.43
32:2a:453:A:C5	32:2a:454:C:C4	3.06	0.43
32:2a:1035:A:O2'	32:2a:1036:G:H8	2.01	0.43
34:2c:180:ALA:HB1	34:2c:203:PHE:HE1	1.84	0.43
44:2m:60:VAL:HG23	44:2m:64:TRP:HE3	1.83	0.43
44:2m:92:HIS:CE1	44:2m:98:VAL:HG21	2.53	0.43
46:2o:10:LYS:HB2	46:2o:10:LYS:HE3	1.70	0.43
50:2s:3:ARG:NH2	50:2s:10:PHE:HB2	2.33	0.43
51:2t:43:LEU:HB3	51:2t:52:ALA:HB2	2.00	0.43
53:2y:85:LEU:O	53:2y:89:GLN:HG2	2.18	0.43
1:1A:644:A:H4'	1:1A:645:C:H5	1.83	0.43
1:1A:1066:U:O4	1:1A:1069:A:H2'	2.18	0.43
13:1R:83:ILE:O	13:1R:86:ARG:HG2	2.18	0.43
32:1a:79:G:O6	32:1a:90:U:O4	2.36	0.43
32:1a:174:C:H2'	32:1a:175:C:H6	1.83	0.43
32:1a:506:G:OP1	61:1a:1918:HOH:O	2.21	0.43
33:1b:55:PHE:CD1	33:1b:58:ILE:HD12	2.52	0.43
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.29	0.43
35:1d:53:ASP:HB3	35:1d:57:ARG:NH1	2.33	0.43
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.18	0.43
6:2G:14:GLU:C	6:2G:17:PRO:HD2	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:4:U:C4	39:2h:105:ARG:HD3	2.53	0.43
32:2a:555:C:H2'	32:2a:556:C:C6	2.53	0.43
32:2a:1129:C:H1'	32:2a:1130:A:N7	2.33	0.43
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.18	0.43
34:2c:131:ARG:NH1	36:2e:50:GLU:HG3	2.33	0.43
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	2.00	0.43
39:2h:121:ASP:HB2	39:2h:125:ARG:NH2	2.33	0.43
1:1A:278:A:H2'	1:1A:279:C:C6	2.53	0.43
3:1D:221:VAL:HG22	3:1D:226:MET:HE3	2.00	0.43
5:1F:179:GLU:CD	5:1F:179:GLU:H	2.26	0.43
9:1N:30:ILE:HG22	9:1N:34:LEU:HD22	1.99	0.43
9:1N:94:HIS:HB3	9:1N:97:ARG:HG3	1.99	0.43
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.53	0.43
32:1a:130:A:C8	48:1q:63:ARG:HD3	2.53	0.43
32:1a:131:C:H2'	32:1a:132:C:C6	2.54	0.43
32:1a:178:C:H2'	32:1a:179:A:H8	1.84	0.43
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.53	0.43
38:1g:116:ALA:O	38:1g:120:ILE:HG12	2.19	0.43
44:1m:4:ILE:HD11	44:1m:19:LEU:HD21	2.00	0.43
50:1s:12:ASP:O	50:1s:14:HIS:N	2.44	0.43
51:1t:91:LEU:HD23	51:1t:91:LEU:HA	1.91	0.43
1:2A:2484:G:C2	1:2A:2485:G:C8	3.06	0.43
55:2A:3712:HGR:C16	55:2A:3712:HGR:H3	2.48	0.43
14:2S:28:VAL:HG21	14:2S:98:VAL:HG13	2.01	0.43
15:2T:1:MET:HE2	15:2T:3:ARG:HG3	2.00	0.43
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.99	0.43
21:2Z:106:GLY:O	21:2Z:141:VAL:HG23	2.17	0.43
32:2a:901:A:O2'	32:2a:1513:A:OP1	2.29	0.43
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.33	0.43
32:2a:1151:A:O4'	41:2j:39:PRO:HB2	2.18	0.43
32:2a:1286:A:H2'	32:2a:1287:A:H4'	2.01	0.43
33:2b:165:VAL:HG23	33:2b:166:ASP:N	2.33	0.43
34:2c:117:ALA:HB2	34:2c:200:ALA:HB2	2.00	0.43
38:2g:111:ARG:HB2	38:2g:119:ARG:HD2	1.99	0.43
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.54	0.43
1:1A:1359:A:N1	1:1A:1372:U:O4	2.52	0.43
1:1A:2165:G:H2'	1:1A:2166:G:C8	2.53	0.43
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.53	0.43
4:1E:9:VAL:HB	15:1T:3:ARG:HG2	2.00	0.43
29:17:30:VAL:O	29:17:34:ARG:HG3	2.18	0.43
32:1a:399:G:H2'	32:1a:400:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:689:C:H2'	32:1a:690:G:O4'	2.18	0.43
32:1a:1014:A:C2	32:1a:1219:U:H1'	2.53	0.43
32:1a:1104:G:O5'	33:1b:111:ARG:HD3	2.18	0.43
32:1a:1258:G:H2'	32:1a:1259:C:C6	2.52	0.43
35:1d:122:ARG:HA	35:1d:122:ARG:HD2	1.63	0.43
35:1d:178:VAL:C	35:1d:180:GLY:H	2.26	0.43
50:1s:52:TYR:HA	50:1s:56:GLN:O	2.19	0.43
1:2A:271(F):C:H2'	1:2A:271(G):C:C6	2.54	0.43
1:2A:631:A:N3	1:2A:2415:G:O2'	2.47	0.43
1:2A:2134:A:N7	1:2A:2157:G:H5'	2.34	0.43
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.17	0.43
6:2G:19:LEU:HD11	6:2G:172:LEU:HB2	1.99	0.43
10:2O:64:ARG:HB2	10:2O:79:PHE:CG	2.54	0.43
19:2X:50:LYS:N	19:2X:87:GLN:OE1	2.48	0.43
32:2a:19:C:H5''	36:2e:86:ALA:HB3	2.00	0.43
32:2a:424:G:H2'	32:2a:425:G:H8	1.83	0.43
32:2a:551:U:H2'	32:2a:552:U:H6	1.82	0.43
32:2a:943:U:H1'	40:2i:124:GLN:HE22	1.83	0.43
32:2a:999:C:H2'	32:2a:1000:U:C6	2.53	0.43
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.51	0.43
32:2a:1349:A:C4	32:2a:1350:A:C8	3.06	0.43
32:2a:1492:A:H2'	32:2a:1493:A:O4'	2.18	0.43
34:2c:28:GLN:HE21	34:2c:32:LEU:HD21	1.84	0.43
35:2d:152:SER:O	35:2d:155:LEU:HB3	2.18	0.43
53:2y:78:ILE:HG22	53:2y:82:GLU:HG3	2.00	0.43
1:1A:184:C:H2'	1:1A:185:U:H6	1.82	0.43
1:1A:548:A:O2'	1:1A:549:G:OP1	2.35	0.43
1:1A:579:G:H2'	1:1A:580:C:C6	2.53	0.43
1:1A:922:U:H2'	1:1A:923:C:C6	2.53	0.43
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.54	0.43
1:1A:1639:U:O2'	1:1A:1640:C:H5'	2.18	0.43
1:1A:2892:A:N6	1:1A:2893:G:N1	2.67	0.43
9:1N:1:MET:HE3	9:1N:1:MET:HB2	1.88	0.43
30:18:8:LYS:NZ	61:18:208:HOH:O	2.49	0.43
32:1a:953:G:N7	44:1m:104:ARG:NH2	2.56	0.43
34:1c:189:ALA:HB3	34:1c:196:LEU:HB2	1.99	0.43
44:1m:59:TYR:CE1	44:1m:63:THR:HG21	2.54	0.43
47:1p:29:ASP:OD1	47:1p:29:ASP:N	2.51	0.43
1:2A:1031:G:N2	31:29:36:GLN:HE22	2.16	0.43
1:2A:2593:U:OP1	61:2A:3864:HOH:O	2.21	0.43
2:2B:8:U:H5'	14:2S:15:ARG:NH1	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:3:VAL:HG13	3:2D:17:THR:HB	2.00	0.43
18:2W:68:ARG:NH1	18:2W:111:HIS:HA	2.34	0.43
20:2Y:56:PRO:O	20:2Y:57:GLN:HB2	2.18	0.43
27:25:16:ARG:HD2	27:25:20:ARG:NH1	2.33	0.43
32:2a:303:A:H2'	32:2a:304:U:O4'	2.19	0.43
32:2a:420:U:H2'	32:2a:422:C:C5	2.54	0.43
32:2a:624:C:H2'	32:2a:625:G:H8	1.84	0.43
32:2a:662:G:O2'	32:2a:836:G:OP1	2.36	0.43
32:2a:1150:U:C2'	32:2a:1151:A:H5'	2.49	0.43
32:2a:1220:G:O2'	50:2s:52:TYR:O	2.36	0.43
32:2a:1248:A:N3	40:2i:70:LYS:NZ	2.65	0.43
34:2c:5:ILE:HD12	34:2c:5:ILE:HA	1.86	0.43
39:2h:92:ARG:HD3	39:2h:92:ARG:HA	1.69	0.43
48:2q:94:ASN:O	48:2q:98:LEU:HD13	2.18	0.43
1:1A:2461:C:H2'	1:1A:2462:U:C6	2.54	0.43
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	2.01	0.43
6:1G:7:LEU:HD23	6:1G:7:LEU:HA	1.87	0.43
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	2.00	0.43
15:1T:64:ARG:HB2	15:1T:73:GLU:HG2	2.00	0.43
32:1a:313:A:H2'	32:1a:314:C:C6	2.53	0.43
32:1a:390:C:H2'	32:1a:391:G:C8	2.53	0.43
32:1a:1003:G:H8	32:1a:1003:G:O5'	2.02	0.43
33:1b:15:VAL:HG22	33:1b:209:ARG:HB3	2.01	0.43
35:1d:121:VAL:O	35:1d:134:ASP:HA	2.19	0.43
38:1g:54:THR:O	38:1g:56:GLN:N	2.50	0.43
1:2A:655:A:H8	1:2A:656:G:O4'	2.01	0.43
1:2A:1059:G:OP2	1:2A:1060:U:H2'	2.18	0.43
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.19	0.43
1:2A:2601:C:H2'	1:2A:2602:A:H8	1.84	0.43
27:25:33:CYS:HB2	27:25:40:LYS:HD3	2.00	0.43
32:2a:748:C:H4'	32:2a:749:C:O5'	2.19	0.43
32:2a:950:U:H2'	32:2a:951:G:C8	2.53	0.43
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.54	0.43
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.33	0.43
33:2b:195:ASP:O	39:2h:68:ARG:NH2	2.46	0.43
40:2i:89:ASN:HB3	40:2i:92:TYR:HE2	1.84	0.43
1:1A:491:G:H5''	61:1A:4364:HOH:O	2.18	0.43
1:1A:746:A:H2'	1:1A:2612:C:H5''	2.01	0.43
1:1A:1086:A:H3'	1:1A:1086:A:N3	2.34	0.43
6:1G:16:ARG:HB2	6:1G:17:PRO:HD3	1.99	0.43
17:1V:71:LEU:HA	17:1V:71:LEU:HD23	1.75	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.32	0.43
32:1a:533:A:O2'	32:1a:535:A:OP2	2.27	0.43
32:1a:587:G:N7	61:1a:1950:HOH:O	2.36	0.43
36:1e:91:LEU:HB3	36:1e:118:ILE:HD11	2.01	0.43
40:1i:5:TYR:OH	40:1i:7:THR:HG22	2.18	0.43
49:1r:47:THR:HG23	49:1r:49:LYS:HG3	2.00	0.43
50:1s:6:LYS:HB3	50:1s:6:LYS:HE2	1.87	0.43
1:2A:578:A:H3'	61:2A:3866:HOH:O	2.18	0.43
1:2A:1111:A:N3	1:2A:1112:G:H1'	2.34	0.43
1:2A:1359:A:H61	1:2A:1372:U:H3	1.67	0.43
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.54	0.43
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.34	0.43
1:2A:2316:C:O2'	6:2G:128:ARG:NH1	2.51	0.43
2:2B:2:C:H2'	2:2B:3:C:C6	2.53	0.43
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.83	0.43
5:2F:188:ARG:HA	11:2P:3:LEU:HD13	2.01	0.43
6:2G:116:ASP:O	6:2G:118:ARG:N	2.51	0.43
10:2O:64:ARG:HG2	10:2O:83:ALA:HB3	1.99	0.43
32:2a:102:G:O2'	32:2a:151:A:N3	2.51	0.43
32:2a:353:A:H5'	32:2a:353:A:H8	1.82	0.43
32:2a:685:G:C2	32:2a:686:U:C4	3.07	0.43
32:2a:1306:A:H2'	32:2a:1307:U:C6	2.54	0.43
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.18	0.43
1:1A:271(H):G:O2'	1:1A:271(I):G:C8	2.72	0.43
1:1A:655:A:H5''	1:1A:656:G:OP2	2.19	0.43
1:1A:876:C:H2'	1:1A:877:U:O4'	2.19	0.43
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.84	0.43
1:1A:1448:G:O2'	1:1A:1528(A):A:N1	2.49	0.43
1:1A:2186:G:H5'	1:1A:2187:G:OP2	2.19	0.43
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	2.00	0.43
4:1E:182:LEU:HD12	4:1E:182:LEU:HA	1.90	0.43
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.18	0.43
32:1a:165:C:H2'	32:1a:166:G:C8	2.53	0.43
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.33	0.43
32:1a:826:C:O2	39:1h:15:ASN:ND2	2.52	0.43
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.33	0.43
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	2.01	0.43
40:1i:22:GLY:HA3	40:1i:60:ASP:OD2	2.19	0.43
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.82	0.43
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.18	0.43
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:95:C:H2'	2:2B:96:U:C6	2.54	0.43
6:2G:33:ARG:CZ	6:2G:162:THR:HG21	2.49	0.43
12:2Q:132:VAL:HG11	21:2Z:81:ARG:HE	1.84	0.43
32:2a:540:G:C6	32:2a:541:G:C5	3.07	0.43
32:2a:684:A:C2	32:2a:685:G:C4	3.06	0.43
32:2a:972:C:O2'	41:2j:55:LYS:O	2.37	0.43
32:2a:1154:G:H2'	32:2a:1155:G:C8	2.53	0.43
35:2d:155:LEU:HD12	35:2d:156:GLU:H	1.83	0.43
38:2g:23:VAL:HG13	38:2g:43:PHE:CE2	2.54	0.43
53:2y:16:ILE:O	53:2y:20:VAL:HG23	2.19	0.43
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.54	0.43
2:1B:81:G:O6	58:1B:230:ARG:NH1	2.47	0.43
14:1S:10:ARG:HG2	14:1S:91:PRO:HA	2.01	0.43
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.18	0.43
24:12:29:LYS:HG2	24:12:57:ILE:HD13	2.00	0.43
32:1a:130:A:N7	48:1q:63:ARG:HB2	2.34	0.43
32:1a:381:C:H2'	32:1a:382:A:O4'	2.18	0.43
32:1a:572:A:OP1	61:1a:1919:HOH:O	2.21	0.43
33:1b:230:VAL:HG22	33:1b:231:GLU:H	1.83	0.43
44:1m:33:ALA:HA	44:1m:59:TYR:CE2	2.54	0.43
50:1s:52:TYR:HB2	50:1s:57:HIS:CE1	2.54	0.43
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.54	0.43
1:2A:873:G:H1	1:2A:904:C:H42	1.65	0.43
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.34	0.43
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.34	0.43
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.54	0.43
1:2A:2331:G:O2'	22:20:43:THR:HG22	2.19	0.43
5:2F:108:LYS:HE2	5:2F:108:LYS:HB3	1.86	0.43
7:2H:117:PRO:HA	7:2H:118:PRO:HD3	1.91	0.43
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.18	0.43
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.37	0.43
33:2b:74:LYS:C	33:2b:76:GLN:H	2.26	0.43
36:2e:51:VAL:O	36:2e:55:VAL:HG23	2.19	0.43
40:2i:50:LEU:HB3	40:2i:56:LEU:HA	2.00	0.43
50:2s:41:VAL:HG13	50:2s:43:GLU:N	2.33	0.43
50:2s:58:VAL:O	50:2s:60:VAL:HG23	2.19	0.43
1:1A:1131:G:H21	9:1N:73:THR:HG21	1.84	0.43
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.80	0.43
1:1A:1865:G:OP1	61:1A:4162:HOH:O	2.22	0.43
5:1F:158:THR:O	5:1F:164:ARG:NH1	2.51	0.43
31:19:7:VAL:HG12	31:19:34:GLN:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:472:A:O3'	47:1p:81:ARG:HA	2.19	0.43
32:1a:615:C:C2	32:1a:616:G:C8	3.07	0.43
32:1a:664:G:N2	32:1a:741:G:H1	2.07	0.43
32:1a:977:A:O2'	32:1a:979:C:OP2	2.34	0.43
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.54	0.43
33:1b:55:PHE:HD1	33:1b:58:ILE:HD12	1.84	0.43
33:1b:217:ARG:HD3	33:1b:217:ARG:HA	1.71	0.43
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	2.00	0.43
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.19	0.43
1:2A:1359:A:N1	1:2A:1372:U:O4	2.51	0.43
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.53	0.43
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.54	0.43
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.19	0.43
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.19	0.43
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.52	0.43
1:2A:2836:U:C4	1:2A:2883:A:N6	2.87	0.43
3:2D:71:ASP:HB3	3:2D:103:ARG:NH2	2.33	0.43
6:2G:38:VAL:HG22	6:2G:93:THR:HG22	2.01	0.43
18:2W:68:ARG:HH12	18:2W:112:GLY:H	1.66	0.43
32:2a:316:G:H4'	61:2a:3382:HOH:O	2.18	0.43
32:2a:512:U:H2'	32:2a:513:C:C6	2.54	0.43
32:2a:857:C:H2'	32:2a:858:G:O4'	2.19	0.43
40:2i:42:ARG:HE	40:2i:42:ARG:HB3	1.53	0.43
41:2j:46:ARG:NH2	41:2j:64:GLU:OE1	2.51	0.43
46:2o:6:GLU:OE1	46:2o:6:GLU:N	2.50	0.43
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.18	0.42
1:1A:194:G:H3'	61:1A:4510:HOH:O	2.19	0.42
1:1A:271(L):U:OP1	8:1I:50:ARG:NH2	2.50	0.42
1:1A:1056:G:H5''	1:1A:1057:A:O4'	2.18	0.42
1:1A:2308:G:O2'	1:1A:2310:A:N7	2.43	0.42
4:1E:170:LEU:HD23	4:1E:184:VAL:HG11	2.01	0.42
5:1F:102:PRO:O	5:1F:106:ARG:HG3	2.18	0.42
7:1H:3:ARG:NH1	7:1H:4:ILE:H	2.15	0.42
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.35	0.42
25:13:23:LEU:HD13	25:13:50:VAL:HG11	2.00	0.42
32:1a:141:A:H1'	32:1a:182:U:O2	2.19	0.42
32:1a:620:C:H2'	32:1a:621:A:O4'	2.19	0.42
32:1a:1166:G:H5'	32:1a:1168:A:OP2	2.19	0.42
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	2.00	0.42
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.84	0.42
40:1i:108:VAL:HG12	40:1i:109:VAL:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:84:ILE:HB	50:1s:66:MET:HE2	2.01	0.42
1:2A:656:G:H2'	1:2A:657:U:O4'	2.18	0.42
1:2A:740:U:H2'	1:2A:741:G:C8	2.54	0.42
1:2A:1087:G:H22	1:2A:1102:C:H42	1.66	0.42
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.84	0.42
1:2A:2104:G:H2'	1:2A:2104:G:N3	2.34	0.42
1:2A:2118:U:C3'	1:2A:2119:A:H5''	2.49	0.42
1:2A:2341:G:H2'	1:2A:2342:C:C6	2.54	0.42
1:2A:2872:G:C2	1:2A:2873:A:N6	2.87	0.42
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	2.01	0.42
6:2G:166:ASP:HA	6:2G:169:ALA:HB3	2.01	0.42
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.50	0.42
16:2U:110:VAL:O	16:2U:114:LYS:HG3	2.18	0.42
22:20:53:MET:HA	22:20:58:THR:O	2.19	0.42
32:2a:21:G:H2'	32:2a:22:G:C8	2.54	0.42
32:2a:109:A:C6	32:2a:326:G:C6	3.08	0.42
36:2e:80:ILE:HG22	36:2e:91:LEU:HB2	2.01	0.42
1:1A:628:G:H5''	30:18:18:ALA:HB2	2.00	0.42
1:1A:657:U:H2'	1:1A:658:C:C6	2.54	0.42
1:1A:1371:G:N7	61:1A:4298:HOH:O	2.37	0.42
1:1A:1816:G:H3'	3:1D:62:TYR:CE1	2.53	0.42
2:1B:30:C:H2'	2:1B:31:C:H5'	2.01	0.42
2:1B:42:C:O2'	6:1G:66:GLN:HG2	2.20	0.42
3:1D:245:PRO:HA	3:1D:246:PRO:HD3	1.92	0.42
6:1G:109:VAL:HG11	6:1G:142:PRO:HB3	2.01	0.42
9:1N:36:GLY:HA2	9:1N:38:HIS:CE1	2.53	0.42
20:1Y:56:PRO:C	20:1Y:58:GLY:H	2.27	0.42
32:1a:472:A:H2'	32:1a:473:G:O4'	2.18	0.42
32:1a:719:C:O2'	49:1r:49:LYS:HB3	2.19	0.42
32:1a:1015:A:C6	32:1a:1016:A:C6	3.07	0.42
32:1a:1220:G:N2	50:1s:54:GLY:O	2.48	0.42
49:1r:42:ARG:HA	49:1r:42:ARG:NE	2.34	0.42
1:2A:1319:G:C6	1:2A:1320:C:N4	2.87	0.42
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.54	0.42
2:2B:42:C:N3	6:2G:91:ARG:NH1	2.48	0.42
6:2G:67:LYS:HE3	26:24:5:ILE:HD12	2.01	0.42
6:2G:96:ARG:N	6:2G:99:MET:HE2	2.32	0.42
7:2H:3:ARG:HH11	7:2H:4:ILE:H	1.66	0.42
21:2Z:43:GLU:O	21:2Z:47:VAL:HG12	2.19	0.42
21:2Z:157:LEU:HD11	21:2Z:163:LEU:HD13	2.01	0.42
32:2a:67:C:H2'	32:2a:68:G:H8	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:177:C:H2'	32:2a:178:C:H6	1.84	0.42
32:2a:443:C:H2'	32:2a:444:C:H6	1.83	0.42
32:2a:1108:G:H5'	34:2c:176:HIS:CD2	2.53	0.42
35:2d:61:LYS:HD2	35:2d:207:TYR:OH	2.19	0.42
47:2p:25:ARG:H	47:2p:25:ARG:HG3	1.62	0.42
1:1A:1287:A:H8	13:1R:104:ARG:HD3	1.84	0.42
1:1A:2119:A:O2'	1:1A:2120:G:H5'	2.19	0.42
1:1A:2242:G:N3	61:1A:4297:HOH:O	2.36	0.42
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.54	0.42
1:1A:2662:A:H8	1:1A:2662:A:O5'	2.02	0.42
6:1G:28:VAL:O	6:1G:31:VAL:HG13	2.18	0.42
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.54	0.42
13:1R:95:THR:HG22	13:1R:116:LEU:HD23	2.00	0.42
26:14:9:LEU:HD23	26:14:27:THR:HG23	2.01	0.42
27:15:45:VAL:HG11	27:15:58:LEU:CD1	2.49	0.42
32:1a:1054:C:H4'	32:1a:1055:A:O5'	2.20	0.42
32:1a:1371:G:O3'	40:1i:69:GLY:HA3	2.20	0.42
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	2.01	0.42
37:1f:42:GLU:OE2	37:1f:59:TYR:OH	2.32	0.42
41:1j:84:GLN:NE2	41:1j:85:LEU:HG	2.34	0.42
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.31	0.42
1:2A:566:U:H2'	1:2A:567:A:O4'	2.19	0.42
1:2A:690:G:H2'	1:2A:691:C:C6	2.54	0.42
1:2A:1204:A:H61	1:2A:1240:U:H2'	1.84	0.42
1:2A:1530:C:H42	1:2A:1539:G:H1	1.66	0.42
1:2A:2180:U:H2'	1:2A:2181:G:C8	2.55	0.42
1:2A:2467:C:H4'	12:2Q:123:HIS:CG	2.54	0.42
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.54	0.42
1:2A:2808:U:H5''	1:2A:2891:G:O6	2.19	0.42
4:2E:28:ALA:HB3	4:2E:93:VAL:CG1	2.48	0.42
6:2G:41:GLN:O	6:2G:43:LEU:N	2.52	0.42
21:2Z:10:ARG:NH1	21:2Z:26:GLY:H	2.17	0.42
21:2Z:27:VAL:HG12	21:2Z:85:HIS:CE1	2.55	0.42
21:2Z:152:ALA:O	21:2Z:155:LEU:HB2	2.19	0.42
26:24:44:THR:C	26:24:46:GLN:H	2.25	0.42
26:24:48:ARG:HB3	26:24:52:THR:HA	2.02	0.42
32:2a:321:A:C2	32:2a:333:G:C2	3.08	0.42
32:2a:1117:G:H4'	40:2i:104:ARG:NH1	2.35	0.42
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.34	0.42
37:2f:69:GLU:O	37:2f:72:VAL:HG13	2.19	0.42
1:1A:214:G:O2'	1:1A:216:A:O2'	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:222:A:H3'	1:1A:421:U:H5'	2.01	0.42
1:1A:829:A:N7	1:1A:2248:C:H5'	2.35	0.42
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.33	0.42
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	2.00	0.42
20:1Y:81:LYS:HE2	20:1Y:81:LYS:HB3	1.78	0.42
32:1a:408:A:H2'	32:1a:409:G:O4'	2.19	0.42
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.55	0.42
33:1b:139:LYS:HE3	33:1b:139:LYS:HB2	1.88	0.42
35:1d:162:LEU:HD13	35:1d:181:MET:HG2	2.01	0.42
35:1d:176:LEU:HG	35:1d:178:VAL:HG22	2.01	0.42
40:1i:99:LEU:HD12	40:1i:99:LEU:H	1.83	0.42
1:2A:42:G:H2'	1:2A:43:A:O4'	2.19	0.42
1:2A:297:C:H2'	1:2A:298:G:O4'	2.19	0.42
1:2A:1494:A:H2'	1:2A:1495:A:C8	2.54	0.42
1:2A:1510:G:H2'	1:2A:1511:C:C6	2.53	0.42
3:2D:16:MET:HG3	3:2D:206:LEU:O	2.19	0.42
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.50	0.42
5:2F:133:ASN:N	5:2F:138:GLU:OE1	2.52	0.42
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	2.02	0.42
17:2V:82:ARG:HH11	17:2V:82:ARG:HG3	1.84	0.42
22:20:43:THR:OG1	22:20:46:LYS:HG2	2.19	0.42
32:2a:388:G:H5''	61:2a:3285:HOH:O	2.19	0.42
32:2a:684:A:C6	32:2a:685:G:C6	3.08	0.42
33:2b:28:PHE:HE1	33:2b:192:SER:HB2	1.84	0.42
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.84	0.42
1:1A:27:G:C2	1:1A:512:G:N3	2.87	0.42
1:1A:378:C:O2'	61:1A:4134:HOH:O	2.17	0.42
1:1A:2830:G:H4'	61:1A:4990:HOH:O	2.19	0.42
6:1G:82:LEU:HD23	6:1G:82:LEU:HA	1.92	0.42
18:1W:18:ARG:HG3	18:1W:76:VAL:HB	2.00	0.42
26:14:56:VAL:HB	26:14:60:GLN:HE21	1.84	0.42
32:1a:309:G:H1'	32:1a:608:A:C2	2.55	0.42
32:1a:743:U:H2'	32:1a:744:C:C6	2.54	0.42
32:1a:1267:C:O2	52:1u:20:LYS:HD2	2.20	0.42
34:1c:35:GLU:CD	34:1c:59:ARG:HH22	2.27	0.42
35:1d:14:ARG:HG3	35:1d:59:ARG:NH1	2.34	0.42
50:1s:11:VAL:O	50:1s:13:ASP:N	2.53	0.42
1:2A:315:G:H2'	1:2A:316:C:C6	2.54	0.42
1:2A:509:C:OP1	61:2A:3863:HOH:O	2.21	0.42
1:2A:888:C:H2'	1:2A:889:C:N3	2.34	0.42
1:2A:1180:C:H2'	1:2A:1181:C:C6	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.31	0.42
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.19	0.42
1:2A:2893:G:H5''	1:2A:2894:G:O4'	2.20	0.42
4:2E:9:VAL:HB	15:2T:3:ARG:HG2	2.00	0.42
32:2a:189(D):C:H2'	32:2a:189(E):U:O4'	2.19	0.42
32:2a:294:U:OP1	32:2a:610:G:O2'	2.32	0.42
32:2a:501:C:OP1	43:2l:117:ARG:NH2	2.33	0.42
32:2a:1075:C:H5''	33:2b:179:LYS:HE2	2.00	0.42
32:2a:1090:U:H2'	32:2a:1091:U:H6	1.83	0.42
32:2a:1188:A:H2'	32:2a:1189:C:O4'	2.20	0.42
33:2b:134:GLU:O	33:2b:138:LEU:HD22	2.20	0.42
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.39	0.42
36:2e:144:THR:H	36:2e:147:ASP:HB2	1.84	0.42
43:2l:82:VAL:O	43:2l:106:ASP:HB2	2.19	0.42
48:2q:62:SER:HB3	48:2q:72:ARG:HH11	1.85	0.42
1:1A:253:C:OP1	61:1A:4159:HOH:O	2.21	0.42
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.55	0.42
1:1A:1359:A:N1	1:1A:1372:U:C4	2.88	0.42
1:1A:2134:A:N6	1:1A:2157:G:H4'	2.35	0.42
3:1D:88:ARG:HB2	61:1D:450:HOH:O	2.19	0.42
14:1S:25:ARG:HD3	14:1S:42:ASP:OD1	2.20	0.42
23:11:60:PHE:HE1	23:11:95:LEU:HD21	1.84	0.42
26:14:16:CYS:HA	26:14:33:VAL:HG23	2.00	0.42
32:1a:376:G:OP1	47:1p:5:ARG:HB2	2.19	0.42
32:1a:418:C:H1'	32:1a:540:G:O2'	2.20	0.42
32:1a:865:A:H2'	32:1a:866:C:C6	2.54	0.42
32:1a:1014:A:H4'	50:1s:14:HIS:CE1	2.55	0.42
39:1h:104:ARG:O	39:1h:106:GLY:N	2.52	0.42
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.19	0.42
45:1n:58:LYS:HE2	45:1n:58:LYS:HB3	1.76	0.42
1:2A:854:G:H2'	1:2A:855:G:H8	1.85	0.42
1:2A:1540:U:H2'	1:2A:1541:G:O4'	2.19	0.42
1:2A:1714:G:H2'	1:2A:1717:G:C8	2.48	0.42
1:2A:2109:U:H2'	1:2A:2110:G:C8	2.54	0.42
1:2A:2131:G:H5'	1:2A:2133:G:O4'	2.19	0.42
1:2A:2370:G:C6	1:2A:2371:G:C6	3.08	0.42
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.20	0.42
3:2D:239:ARG:NH1	61:2D:413:HOH:O	2.52	0.42
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.52	0.42
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	2.01	0.42
24:22:16:LEU:HB3	24:22:20:GLU:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:116:A:H61	32:2a:313:A:H1'	1.83	0.42
32:2a:309:G:H1'	32:2a:608:A:C2	2.54	0.42
32:2a:328:C:H4'	32:2a:329:A:H5'	2.00	0.42
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.46	0.42
34:2c:123:GLN:O	34:2c:128:PHE:HB2	2.20	0.42
38:2g:20:ASP:HB3	38:2g:23:VAL:HB	2.02	0.42
38:2g:105:VAL:HG12	38:2g:109:ASN:ND2	2.35	0.42
45:2n:24:CYS:O	45:2n:28:GLY:N	2.41	0.42
1:1A:1069:A:H5'	1:1A:1070:A:H2	1.85	0.42
6:1G:74:LYS:O	6:1G:84:LYS:HG3	2.20	0.42
8:1I:72:LEU:O	8:1I:73:GLU:HB2	2.18	0.42
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.54	0.42
32:1a:233:C:H2'	32:1a:234:C:H6	1.85	0.42
32:1a:309:G:O2'	32:1a:607:A:N1	2.52	0.42
32:1a:600:C:H4'	39:1h:128:GLY:O	2.19	0.42
32:1a:841:U:C6	32:1a:848:C:H1'	2.55	0.42
32:1a:933:G:OP2	38:1g:3:ARG:HB2	2.20	0.42
32:1a:1119:C:H2'	32:1a:1120:G:C8	2.54	0.42
32:1a:1216:G:OP1	45:1n:2:ALA:HA	2.20	0.42
34:1c:148:GLY:HA3	34:1c:172:ARG:O	2.19	0.42
44:1m:108:ARG:HA	44:1m:108:ARG:HD3	1.91	0.42
1:2A:244:A:C2	1:2A:255:A:C4	3.08	0.42
1:2A:415:A:H2'	1:2A:416:C:O4'	2.20	0.42
1:2A:784:A:C8	1:2A:792:G:C5	3.08	0.42
1:2A:1452:A:OP2	61:2A:3859:HOH:O	2.21	0.42
1:2A:1501:C:O4'	3:2D:100:GLY:HA2	2.20	0.42
1:2A:2756:U:H1'	1:2A:2757:A:H5''	2.01	0.42
2:2B:66:A:H61	2:2B:109:C:H5'	1.85	0.42
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.20	0.42
32:2a:141:A:H1'	32:2a:182:U:O2	2.20	0.42
32:2a:1003:G:C6	32:2a:1004:A:H1'	2.54	0.42
32:2a:1044:A:C5	32:2a:1045:C:H1'	2.55	0.42
34:2c:91:LEU:C	34:2c:93:LYS:H	2.28	0.42
35:2d:105:VAL:HG13	35:2d:110:PHE:HB2	2.02	0.42
42:2k:85:ARG:HG2	42:2k:112:THR:HA	2.01	0.42
52:2u:2:GLY:C	52:2u:4:GLY:H	2.27	0.42
53:2y:37:PRO:HB3	53:2y:54:ILE:HG12	2.00	0.42
1:1A:621:A:H5'	11:1P:108:LYS:NZ	2.34	0.42
1:1A:711:G:O6	61:1A:4161:HOH:O	2.21	0.42
1:1A:957:A:N1	1:1A:2458:G:H4'	2.35	0.42
1:1A:2145:C:H2'	1:1A:2147:G:N2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2183:C:O2'	1:1A:2184:G:H5'	2.20	0.42
32:1a:580:U:H2'	32:1a:581:G:O4'	2.19	0.42
32:1a:600:C:H2'	32:1a:601:C:C6	2.53	0.42
33:1b:69:LEU:HD12	33:1b:91:PRO:HB2	2.02	0.42
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.20	0.42
1:2A:729:G:C5	3:2D:208:LYS:HB2	2.55	0.42
1:2A:1071:G:H1'	1:2A:1089:G:C8	2.54	0.42
1:2A:1106:G:H2'	1:2A:1107:G:C8	2.52	0.42
1:2A:2641:G:P	9:2N:74:ARG:HH21	2.42	0.42
2:2B:73:A:C4	2:2B:105:A:C2	3.07	0.42
4:2E:119:ARG:CG	4:2E:160:TYR:HB2	2.49	0.42
9:2N:34:LEU:O	9:2N:49:GLY:HA3	2.20	0.42
13:2R:29:LEU:HD12	13:2R:29:LEU:HA	1.81	0.42
23:21:52:ARG:NH1	23:21:55:GLY:O	2.52	0.42
32:2a:1005:A:H1'	32:2a:1025:U:O2	2.20	0.42
39:2h:122:ARG:HG3	39:2h:123:GLU:N	2.34	0.42
43:2l:110:VAL:HG23	43:2l:120:TYR:HB3	2.02	0.42
50:2s:61:TYR:CE2	50:2s:63:THR:HG23	2.53	0.42
1:1A:459:U:H4'	29:17:40:TRP:CZ3	2.55	0.42
1:1A:493:G:H2'	1:1A:494:G:O4'	2.20	0.42
1:1A:919:G:N2	1:1A:2269:A:OP2	2.53	0.42
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.20	0.42
1:1A:2245:U:O2'	1:1A:2436:G:OP2	2.31	0.42
61:1A:5808:HOH:O	11:1P:70:GLN:HG2	2.20	0.42
3:1D:133:LEU:HB3	3:1D:173:VAL:HG11	2.02	0.42
26:14:35:VAL:HG22	26:14:36:CYS:H	1.85	0.42
31:19:25:VAL:O	31:19:33:LYS:HA	2.20	0.42
32:1a:262:A:C6	32:1a:263:A:C6	3.07	0.42
32:1a:708:C:H2'	32:1a:709:G:H8	1.84	0.42
47:1p:15:PRO:HD2	47:1p:42:ARG:HD3	2.01	0.42
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	2.00	0.42
1:2A:828:U:H4'	1:2A:831:G:N1	2.34	0.42
1:2A:1073:A:C8	1:2A:1073:A:H3'	2.54	0.42
1:2A:1263:U:C4	1:2A:1264:G:C6	3.07	0.42
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.53	0.42
7:2H:55:PRO:HG2	7:2H:61:HIS:CE1	2.55	0.42
7:2H:103:LEU:HD22	7:2H:105:LEU:HD22	2.02	0.42
19:2X:18:TYR:C	19:2X:20:GLY:H	2.28	0.42
21:2Z:6:LYS:HA	21:2Z:60:GLU:HB2	2.02	0.42
21:2Z:69:THR:HG21	21:2Z:88:PHE:HB3	2.01	0.42
32:2a:396:G:O2'	32:2a:398:C:OP1	2.26	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:544:G:OP1	35:2d:59:ARG:NH2	2.53	0.42
32:2a:926:G:N3	53:2y:91:LYS:HG3	2.35	0.42
32:2a:938:A:C6	32:2a:939:G:C5	3.07	0.42
32:2a:1002:G:H2'	32:2a:1003:G:C8	2.55	0.42
32:2a:1371:G:C6	32:2a:1372:U:C4	3.07	0.42
33:2b:229:VAL:HG12	33:2b:230:VAL:H	1.84	0.42
34:2c:59:ARG:H	41:2j:92:THR:CG2	2.32	0.42
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	2.02	0.42
47:2p:43:LYS:HG2	47:2p:48:TRP:CE2	2.55	0.42
48:2q:22:LEU:HD11	48:2q:39:SER:HB2	2.01	0.42
48:2q:40:LYS:HD3	48:2q:42:TYR:CZ	2.55	0.42
1:1A:228:A:H8	1:1A:229:A:H5'	1.84	0.42
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.20	0.42
32:1a:250:A:H4'	32:1a:251:G:O5'	2.20	0.42
32:1a:266:G:N3	32:1a:266:G:H2'	2.35	0.42
32:1a:765:G:C6	32:1a:812:C:C2	3.08	0.42
32:1a:1236:A:H4'	32:1a:1304:G:H4'	2.00	0.42
37:1f:69:GLU:O	37:1f:72:VAL:HG12	2.20	0.42
37:1f:97:PHE:HD2	49:1r:31:LEU:HD12	1.85	0.42
38:1g:36:LYS:HA	38:1g:39:ALA:HB3	2.02	0.42
1:2A:35:G:H2'	1:2A:36:G:O4'	2.19	0.42
1:2A:455:C:N3	1:2A:472:A:H2'	2.35	0.42
1:2A:1131:G:C2	1:2A:1132:A:C4	3.08	0.42
1:2A:1638:C:H2'	1:2A:1639:U:O4'	2.19	0.42
1:2A:2262:U:H4'	1:2A:2328:A:H2	1.85	0.42
1:2A:2336:A:H61	22:20:43:THR:HG21	1.85	0.42
3:2D:106:ILE:HD11	3:2D:143:HIS:HD2	1.84	0.42
8:2I:57:ARG:O	8:2I:61:ARG:HG2	2.20	0.42
32:2a:57:G:H2'	32:2a:58:C:C6	2.55	0.42
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.55	0.42
32:2a:1240:U:C2	38:2g:32:ARG:HG3	2.55	0.42
32:2a:1288:A:H5''	52:2u:9:ARG:HH21	1.84	0.42
37:2f:3:ARG:HD3	37:2f:64:GLN:NE2	2.34	0.42
41:2j:21:GLN:O	41:2j:25:GLU:HG2	2.20	0.42
45:2n:3:ARG:O	45:2n:7:ILE:HG13	2.19	0.42
1:1A:784:A:H5'	1:1A:785:G:OP1	2.20	0.41
1:1A:996:A:H4'	16:1U:91:ASP:OD2	2.20	0.41
1:1A:1469:A:H2'	1:1A:1470:G:O4'	2.20	0.41
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.20	0.41
1:1A:2667:C:H2'	1:1A:2668:G:O4'	2.20	0.41
4:1E:34:VAL:HB	4:1E:48:GLN:HE21	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:51:ARG:HG3	15:1T:98:LYS:HE3	2.02	0.41
19:1X:35:THR:H	19:1X:38:GLU:HG2	1.85	0.41
26:14:62:ARG:HA	26:14:62:ARG:HD3	1.80	0.41
32:1a:108:G:C6	51:1t:15:ARG:HG2	2.55	0.41
32:1a:674:G:H2'	32:1a:675:A:H8	1.85	0.41
39:1h:95:VAL:HB	39:1h:99:GLU:HG3	2.01	0.41
41:1j:30:SER:CB	41:1j:81:THR:HG22	2.50	0.41
46:1o:69:TYR:HA	46:1o:72:ARG:NH2	2.35	0.41
47:1p:70:ALA:O	47:1p:74:LEU:HD12	2.20	0.41
1:2A:1055:G:N2	1:2A:1086:A:H8	2.18	0.41
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.19	0.41
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.55	0.41
4:2E:72:VAL:HG12	4:2E:73:GLU:O	2.19	0.41
4:2E:101:ARG:NH2	4:2E:171:GLU:HB2	2.35	0.41
13:2R:26:LYS:HE2	13:2R:70:LEU:O	2.20	0.41
29:27:47:ARG:HE	29:27:47:ARG:HB3	1.74	0.41
32:2a:41:G:H2'	32:2a:42:G:H8	1.83	0.41
32:2a:660:G:H2'	32:2a:661:G:O4'	2.20	0.41
32:2a:859:A:H2'	32:2a:860:A:O4'	2.19	0.41
32:2a:976:G:N2	32:2a:1363:C:OP2	2.53	0.41
32:2a:1002:G:N2	32:2a:1039:C:C2	2.87	0.41
32:2a:1170:A:C5	32:2a:1171:G:H1'	2.54	0.41
34:2c:111:LEU:HD22	34:2c:146:ALA:HB2	2.02	0.41
35:2d:78:LEU:HD23	35:2d:78:LEU:HA	1.91	0.41
40:2i:92:TYR:HB3	40:2i:96:LEU:HD12	2.01	0.41
42:2k:48:ILE:HD12	42:2k:63:LEU:HB2	2.01	0.41
44:2m:13:LYS:O	44:2m:45:VAL:HG23	2.20	0.41
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	2.01	0.41
1:1A:271(K):U:O2	8:1I:50:ARG:HG3	2.20	0.41
1:1A:1494:A:H2'	1:1A:1495:A:C8	2.56	0.41
1:1A:2149:G:H2'	1:1A:2150:U:O4'	2.20	0.41
12:1Q:7:MET:HB2	12:1Q:7:MET:HE3	1.51	0.41
17:1V:49:THR:HG22	17:1V:49:THR:O	2.19	0.41
32:1a:370:C:H2'	32:1a:371:G:C8	2.55	0.41
32:1a:489:C:OP1	35:1d:132:ARG:NH2	2.53	0.41
39:1h:20:TYR:HA	39:1h:65:TYR:CZ	2.54	0.41
40:1i:16:ARG:HB2	40:1i:64:THR:HG22	2.02	0.41
1:2A:444:C:H4'	5:2F:49:ALA:HB2	2.03	0.41
1:2A:1111:A:O2'	1:2A:1112:G:H4'	2.19	0.41
1:2A:2111:C:N3	1:2A:2145:C:O2'	2.52	0.41
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:50:GLY:HA2	4:2E:77:ILE:O	2.20	0.41
20:2Y:26:LYS:HB3	20:2Y:26:LYS:HE3	1.92	0.41
21:2Z:183:LEU:HD23	21:2Z:186:GLU:OE1	2.20	0.41
28:26:39:TYR:HB2	28:26:46:HIS:CE1	2.55	0.41
30:28:52:LYS:HE2	30:28:52:LYS:HB3	1.84	0.41
32:2a:229:U:O2'	47:2p:23:ASP:OD2	2.34	0.41
32:2a:614:A:H2'	32:2a:615:C:C6	2.55	0.41
32:2a:986:A:N3	50:2s:52:TYR:OH	2.34	0.41
32:2a:1275:A:H2'	32:2a:1276:G:O4'	2.20	0.41
32:2a:1340:A:OP1	53:2y:57:PRO:HB3	2.19	0.41
33:2b:48:MET:HE3	33:2b:48:MET:HB2	1.90	0.41
34:2c:143:GLU:C	34:2c:145:GLY:H	2.27	0.41
35:2d:61:LYS:HA	35:2d:203:VAL:HG22	2.02	0.41
40:2i:42:ARG:NH2	40:2i:71:SER:HB2	2.35	0.41
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.27	0.41
1:1A:2354:G:H21	22:10:36:ILE:HD11	1.85	0.41
1:1A:2400:G:O6	61:1A:4157:HOH:O	2.21	0.41
1:1A:2441:C:OP2	1:1A:2586:C:O2'	2.34	0.41
2:1B:74:U:H2'	2:1B:75:G:O4'	2.20	0.41
8:1I:57:ARG:O	8:1I:61:ARG:HG2	2.19	0.41
8:1I:140:LEU:HD12	8:1I:140:LEU:HA	1.78	0.41
11:1P:101:VAL:HG12	11:1P:106:LEU:HB3	2.02	0.41
15:1T:53:ARG:HB3	15:1T:53:ARG:HH11	1.85	0.41
20:1Y:86:ARG:NH1	20:1Y:100:ALA:O	2.53	0.41
32:1a:189(K):U:H2'	32:1a:189(L):G:H8	1.83	0.41
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.39	0.41
32:1a:1118:C:H1'	32:1a:1179:A:C5	2.55	0.41
49:1r:73:ALA:HB3	49:1r:79:LEU:HD12	2.03	0.41
1:2A:1506:C:H2'	1:2A:1507:A:H5'	2.01	0.41
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	2.02	0.41
4:2E:4:ILE:HG21	4:2E:28:ALA:HB1	2.02	0.41
5:2F:140:LEU:HD13	5:2F:140:LEU:HA	1.88	0.41
5:2F:207:GLY:O	61:2F:401:HOH:O	2.22	0.41
11:2P:114:ILE:HG13	11:2P:125:VAL:HG21	2.02	0.41
11:2P:124:LYS:HA	11:2P:144:GLU:O	2.20	0.41
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	2.03	0.41
29:27:5:TRP:CD1	29:27:7:PRO:HD3	2.54	0.41
32:2a:187:C:O2'	51:2t:89:ARG:HD3	2.20	0.41
32:2a:377:G:OP1	47:2p:3:LYS:HD3	2.19	0.41
33:2b:77:ALA:O	33:2b:81:VAL:HG22	2.21	0.41
34:2c:5:ILE:HD11	45:2n:49:HIS:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:28:GLN:HG2	34:2c:32:LEU:HD21	2.01	0.41
34:2c:45:LYS:HD3	34:2c:45:LYS:HA	1.77	0.41
45:2n:32:SER:OG	45:2n:41:ARG:HG2	2.20	0.41
49:2r:45:SER:OG	49:2r:47:THR:HG22	2.21	0.41
1:1A:324:A:H2'	1:1A:325:G:O4'	2.20	0.41
1:1A:476:G:H4'	1:1A:502:A:N1	2.36	0.41
1:1A:1083:U:H1'	1:1A:1086:A:N6	2.34	0.41
1:1A:1439:A:OP1	61:1A:4133:HOH:O	2.22	0.41
1:1A:2142:C:H2'	1:1A:2143:C:C6	2.56	0.41
1:1A:2180:U:H2'	1:1A:2181:G:O4'	2.21	0.41
9:1N:15:LEU:HB2	9:1N:135:PRO:HB2	2.01	0.41
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.54	0.41
18:1W:20:VAL:O	18:1W:23:LEU:HB2	2.20	0.41
26:14:41:PRO:HB3	26:14:47:GLN:O	2.21	0.41
27:15:37:LYS:HA	27:15:37:LYS:HD3	1.80	0.41
32:1a:1029:C:N3	32:1a:1032:G:O6	2.53	0.41
41:1j:47:PHE:HB2	41:1j:63:PHE:HB2	2.02	0.41
1:2A:539:G:H2'	1:2A:540:C:H6	1.85	0.41
1:2A:582:G:H2'	1:2A:583:G:C8	2.55	0.41
1:2A:900:A:O2'	1:2A:901:A:OP1	2.38	0.41
1:2A:1062:G:N7	1:2A:1070:A:H1'	2.35	0.41
1:2A:2103:C:N4	1:2A:2104:G:O6	2.53	0.41
1:2A:2104:G:N2	1:2A:2105:C:C2	2.89	0.41
1:2A:2117:A:H4'	1:2A:2148:G:OP1	2.19	0.41
1:2A:2572:A:N7	4:2E:145:LYS:HB2	2.35	0.41
3:2D:102:LYS:C	3:2D:103:ARG:HG2	2.45	0.41
4:2E:151:TYR:HB3	9:2N:79:PRO:HG3	2.02	0.41
9:2N:37:LYS:HG3	9:2N:42:TRP:CE2	2.55	0.41
11:2P:138:LEU:HD23	11:2P:145:PRO:HB3	2.03	0.41
15:2T:6:LEU:HD12	15:2T:6:LEU:HA	1.80	0.41
21:2Z:130:PRO:C	21:2Z:132:ASN:H	2.29	0.41
32:2a:61:G:N7	51:2t:11:SER:OG	2.46	0.41
32:2a:673:G:O3'	37:2f:87:ARG:NH2	2.53	0.41
32:2a:1244:C:H2'	32:2a:1245:A:C8	2.55	0.41
32:2a:1372:U:OP1	40:2i:71:SER:OG	2.28	0.41
33:2b:83:MET:SD	33:2b:234:PRO:HB2	2.60	0.41
34:2c:6:HIS:HE1	34:2c:184:TYR:HD2	1.68	0.41
35:2d:57:ARG:HG3	35:2d:202:LEU:HD13	2.02	0.41
39:2h:103:VAL:HG21	39:2h:110:ALA:HB2	2.02	0.41
44:2m:5:ALA:HB1	44:2m:66:LEU:HD13	2.02	0.41
1:1A:888:C:H6	1:1A:888:C:H2'	1.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1170:G:N2	1:1A:1180:C:C2	2.88	0.41
1:1A:1509(B):A:H2'	1:1A:1510:G:O4'	2.20	0.41
1:1A:2196:C:O2'	1:1A:2197:U:H5'	2.19	0.41
1:1A:2418:A:H2'	1:1A:2419:U:C6	2.55	0.41
1:1A:2499:C:N3	61:1A:4300:HOH:O	2.37	0.41
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.56	0.41
6:1G:181:ARG:HG3	6:1G:182:LYS:N	2.30	0.41
7:1H:55:PRO:HG2	7:1H:61:HIS:CE1	2.56	0.41
8:1I:109:ILE:HD12	8:1I:109:ILE:HA	1.64	0.41
11:1P:96:THR:HG22	11:1P:126:VAL:HB	2.01	0.41
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.21	0.41
32:1a:138:G:H1	32:1a:225:C:H42	1.67	0.41
32:1a:674:G:N2	32:1a:717:C:O2	2.54	0.41
32:1a:938:A:C6	32:1a:939:G:C5	3.08	0.41
32:1a:1186:G:H21	45:1n:61:TRP:C	2.27	0.41
32:1a:1479:C:H2'	32:1a:1480:G:H8	1.86	0.41
33:1b:100:GLY:N	33:1b:176:GLU:OE2	2.28	0.41
35:1d:85:LYS:HG3	35:1d:86:LYS:H	1.85	0.41
1:2A:207:A:H2'	1:2A:208:C:O4'	2.20	0.41
1:2A:453:C:O2	1:2A:457:A:O2'	2.38	0.41
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.56	0.41
1:2A:1653:G:C4	13:2R:9:LYS:HD2	2.56	0.41
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.21	0.41
4:2E:37:ARG:HA	4:2E:42:ASP:OD2	2.20	0.41
6:2G:97:ASP:O	6:2G:101:ILE:HG13	2.21	0.41
6:2G:144:ILE:HA	6:2G:148:MET:SD	2.60	0.41
15:2T:25:GLY:O	15:2T:92:GLY:HA3	2.20	0.41
20:2Y:19:LYS:HZ3	20:2Y:20:TYR:HE2	1.68	0.41
21:2Z:7:ALA:O	21:2Z:62:PRO:HD3	2.20	0.41
23:21:81:LYS:HB3	23:21:81:LYS:HE2	1.74	0.41
32:2a:266:G:H3'	48:2q:67:LYS:HB2	2.02	0.41
32:2a:707:C:H2'	32:2a:708:C:C6	2.55	0.41
32:2a:945:G:H2'	32:2a:945:G:N3	2.35	0.41
32:2a:1323:G:H4'	32:2a:1363:C:C2	2.55	0.41
33:2b:38:GLY:C	33:2b:39:ILE:HG13	2.45	0.41
33:2b:155:LEU:HD21	33:2b:159:PRO:HG3	2.03	0.41
35:2d:171:GLY:HA2	35:2d:172:PRO:HD3	1.92	0.41
36:2e:69:VAL:HA	36:2e:70:PRO:HD3	1.85	0.41
40:2i:89:ASN:HA	40:2i:90:PRO:HD3	1.97	0.41
52:2u:11:GLY:O	52:2u:15:ARG:HG3	2.20	0.41
1:1A:757:U:H2'	1:1A:758:C:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1185:C:H5''	1:1A:1186:G:OP1	2.21	0.41
1:1A:1766:U:H2'	1:1A:1767:C:H6	1.86	0.41
1:1A:1766:U:H2'	1:1A:1767:C:C6	2.56	0.41
1:1A:2801(A):A:N3	1:1A:2895:U:H1'	2.35	0.41
22:10:32:ARG:H	22:10:35:ASN:ND2	2.19	0.41
22:10:43:THR:O	22:10:43:THR:HG23	2.21	0.41
26:14:13:ARG:HA	26:14:22:ILE:O	2.21	0.41
32:1a:833:U:H2'	32:1a:834:C:C6	2.56	0.41
32:1a:1010:G:H22	32:1a:1020:U:H1'	1.85	0.41
42:1k:18:ARG:HB2	42:1k:33:THR:OG1	2.21	0.41
44:1m:49:THR:HB	44:1m:52:GLU:HG3	2.03	0.41
47:1p:75:ARG:HG3	47:1p:80:PHE:HD2	1.85	0.41
1:2A:26:G:C6	1:2A:27:G:N1	2.89	0.41
1:2A:330:A:HO2'	1:2A:331:A:H8	1.61	0.41
1:2A:954:G:H5''	12:2Q:13:GLN:HB3	2.02	0.41
1:2A:1056:G:N2	1:2A:1103:A:H62	2.19	0.41
1:2A:1063:G:H2'	1:2A:1063:G:OP2	2.21	0.41
1:2A:1459:G:O2'	1:2A:1461:G:H5'	2.21	0.41
1:2A:2184:G:H2'	1:2A:2185:C:C6	2.55	0.41
1:2A:2494:G:O2'	12:2Q:80:GLU:HA	2.20	0.41
8:2I:38:LEU:HD23	8:2I:38:LEU:HA	1.84	0.41
8:2I:140:LEU:HD22	8:2I:141:LYS:N	2.36	0.41
12:2Q:118:LEU:HB2	12:2Q:131:ILE:HD13	2.00	0.41
20:2Y:15:VAL:HG21	20:2Y:42:VAL:HG11	2.02	0.41
21:2Z:3:TYR:O	21:2Z:57:ILE:HA	2.20	0.41
32:2a:790:A:H4'	53:2y:31:GLN:OE1	2.20	0.41
32:2a:972:C:O3'	41:2j:57:LYS:HD2	2.19	0.41
32:2a:1002:G:C2	32:2a:1003:G:N7	2.89	0.41
32:2a:1423:G:H2'	32:2a:1424:C:C6	2.56	0.41
33:2b:30:ARG:NH2	33:2b:194:PRO:HB2	2.35	0.41
34:2c:37:GLN:NE2	45:2n:52:GLN:HB3	2.35	0.41
35:2d:153:ARG:H	35:2d:153:ARG:HG3	1.61	0.41
44:2m:106:ASN:O	44:2m:106:ASN:ND2	2.53	0.41
45:2n:14:PRO:HG2	45:2n:16:PHE:O	2.21	0.41
49:2r:52:PRO:O	49:2r:56:THR:HG23	2.21	0.41
1:1A:272:G:O2'	1:1A:421:U:OP2	2.22	0.41
1:1A:1067:A:H2'	1:1A:1067:A:N3	2.36	0.41
1:1A:1495:A:C6	1:1A:1496:A:C6	3.08	0.41
1:1A:1583:A:H5'	1:1A:1584:C:OP1	2.20	0.41
1:1A:1756:G:H4'	1:1A:1758:G:O4'	2.21	0.41
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2140:C:O2	1:1A:2151:G:N1	2.51	0.41
1:1A:2674:G:H2'	1:1A:2675:A:C8	2.56	0.41
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.55	0.41
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	2.03	0.41
57:1A:4034:MPD:H4	57:1A:4034:MPD:HM2	1.81	0.41
2:1B:24:G:N7	2:1B:56:G:H2'	2.36	0.41
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.69	0.41
4:1E:7:VAL:HG13	4:1E:27:LEU:HB3	2.03	0.41
9:1N:67:LEU:HD12	9:1N:67:LEU:HA	1.93	0.41
32:1a:186:C:H2'	32:1a:187:C:H6	1.83	0.41
33:1b:42:ILE:HG21	33:1b:202:PRO:O	2.21	0.41
38:1g:89:MET:HE1	38:1g:156:TRP:CZ2	2.55	0.41
1:2A:1590:U:H2'	1:2A:1591:G:C8	2.56	0.41
1:2A:2108:C:H5'	1:2A:2109:U:OP2	2.21	0.41
1:2A:2109:U:O2	1:2A:2181:G:N2	2.54	0.41
1:2A:2689:U:OP2	1:2A:2719:G:N2	2.49	0.41
1:2A:2840:C:O3'	13:2R:53:HIS:NE2	2.53	0.41
5:2F:117:ARG:NH2	5:2F:189:THR:O	2.51	0.41
11:2P:39:LYS:HD2	11:2P:45:LEU:HD11	2.03	0.41
13:2R:70:LEU:HD23	13:2R:70:LEU:HA	1.92	0.41
23:21:30:VAL:HG13	61:21:207:HOH:O	2.20	0.41
32:2a:103:C:O2'	32:2a:172:A:N1	2.51	0.41
32:2a:126:G:OP1	32:2a:605:U:O2'	2.35	0.41
32:2a:156:G:C2	32:2a:157:G:C8	3.09	0.41
32:2a:925:G:H1'	32:2a:1502:A:C4	2.56	0.41
32:2a:1122:U:H2'	32:2a:1123:A:O4'	2.21	0.41
32:2a:1400:5MC:N3	53:2y:63:ALA:HA	2.36	0.41
33:2b:98:LEU:HD23	33:2b:98:LEU:HA	1.67	0.41
34:2c:39:ILE:HG23	34:2c:91:LEU:HD11	2.03	0.41
36:2e:69:VAL:HG11	36:2e:113:ALA:HB1	2.02	0.41
36:2e:143:ARG:HH11	39:2h:77:GLU:CD	2.28	0.41
38:2g:113:GLU:H	38:2g:113:GLU:HG2	1.33	0.41
40:2i:125:TYR:HE1	40:2i:127:LYS:HB3	1.86	0.41
41:2j:40:LEU:HB2	41:2j:69:ASN:HB3	2.01	0.41
1:1A:121:G:H4'	1:1A:149:A:H5'	2.03	0.41
1:1A:817:C:H4'	1:1A:932:G:C5	2.56	0.41
1:1A:1045:A:O2'	1:1A:1047:G:C4	2.70	0.41
1:1A:1071:G:H1'	1:1A:1089:G:C8	2.56	0.41
1:1A:1383:C:H5	61:1A:7095:HOH:O	2.04	0.41
1:1A:1514:U:H2'	1:1A:1515:G:H8	1.86	0.41
1:1A:1698:A:C8	1:1A:1700:A:O4'	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2518:A:N3	1:1A:2518:A:H2'	2.35	0.41
3:1D:43:ARG:HA	3:1D:48:ARG:O	2.21	0.41
10:1O:1:MET:HE3	10:1O:32:TYR:CE2	2.56	0.41
12:1Q:32:TYR:O	12:1Q:105:GLU:HA	2.21	0.41
13:1R:65:LEU:HD12	13:1R:65:LEU:HA	1.88	0.41
25:13:55:ARG:NH1	61:13:204:HOH:O	2.53	0.41
32:1a:129(A):G:C6	32:1a:189(E):U:H4'	2.56	0.41
32:1a:1228:C:P	44:1m:108:ARG:HH22	2.43	0.41
33:1b:21:ARG:HG3	33:1b:22:LYS:H	1.86	0.41
37:1f:99:ALA:HB1	49:1r:23:LYS:HE3	2.02	0.41
43:1l:47:LYS:HA	43:1l:48:PRO:HA	1.83	0.41
53:1y:87:LYS:O	53:1y:91:LYS:HB2	2.20	0.41
1:2A:735:A:N7	1:2A:761:A:H2	2.19	0.41
1:2A:945:A:C4	1:2A:2448:A:C2	3.08	0.41
1:2A:1006:C:C2	1:2A:1138:G:N2	2.89	0.41
10:2O:64:ARG:HD3	10:2O:79:PHE:CD1	2.55	0.41
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	2.02	0.41
19:2X:31:HIS:HD2	19:2X:33:LYS:H	1.67	0.41
19:2X:44:GLU:O	19:2X:48:LYS:N	2.52	0.41
23:21:62:VAL:HG22	23:21:63:ALA:O	2.21	0.41
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.55	0.41
32:2a:1263:C:H2'	32:2a:1264:C:C6	2.56	0.41
33:2b:18:GLY:HA2	33:2b:42:ILE:HD12	2.01	0.41
33:2b:80:ILE:HD11	33:2b:212:GLN:HA	2.02	0.41
33:2b:122:PHE:HA	33:2b:127:ILE:HG12	2.02	0.41
34:2c:29:TYR:OH	45:2n:54:PRO:HD2	2.21	0.41
35:2d:122:ARG:HH11	35:2d:122:ARG:HA	1.86	0.41
42:2k:38:ASN:HA	42:2k:39:PRO:HD3	1.96	0.41
43:2l:5:PRO:HD2	43:2l:15:ARG:NH2	2.36	0.41
1:1A:438:G:H2'	1:1A:440:G:C8	2.56	0.41
1:1A:1171:G:C3'	1:1A:1173:G:H5'	2.51	0.41
1:1A:1315:C:O2'	1:1A:1392:A:N3	2.52	0.41
1:1A:1913:A:C2	32:1a:1493:A:H8	2.39	0.41
1:1A:2287:A:C8	1:1A:2289:G:C8	3.08	0.41
1:1A:2319:G:N2	14:1S:3:ARG:HA	2.36	0.41
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.56	0.41
61:1A:6091:HOH:O	4:1E:145:LYS:HD2	2.21	0.41
2:1B:2:C:H2'	2:1B:3:C:C6	2.55	0.41
3:1D:79:VAL:HG11	3:1D:111:LEU:HD13	2.02	0.41
5:1F:102:PRO:HB2	5:1F:105:VAL:HG23	2.03	0.41
8:1I:77:LEU:HA	8:1I:77:LEU:HD12	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:15:29:THR:O	27:15:30:LEU:HD23	2.21	0.41
32:1a:437:U:O2	35:1d:119:GLN:NE2	2.54	0.41
32:1a:616:G:O2'	32:1a:617:G:H5'	2.21	0.41
32:1a:651:C:H2'	32:1a:652:U:C6	2.55	0.41
32:1a:963:G:H5'	61:1a:2144:HOH:O	2.20	0.41
32:1a:1096:C:H2'	32:1a:1097:C:H6	1.85	0.41
32:1a:1304:G:C6	32:1a:1305:G:N1	2.89	0.41
32:1a:1312:G:N7	50:1s:2:PRO:HD2	2.35	0.41
33:1b:21:ARG:HA	33:1b:39:ILE:HG12	2.03	0.41
33:1b:208:ILE:HA	33:1b:211:ILE:HD12	2.03	0.41
38:1g:106:GLN:O	38:1g:110:GLN:HG2	2.20	0.41
41:1j:30:SER:HB2	41:1j:81:THR:HG22	2.03	0.41
42:1k:20:TYR:O	42:1k:30:VAL:HA	2.21	0.41
44:1m:20:THR:C	44:1m:22:ILE:H	2.29	0.41
51:1t:47:GLY:CA	51:1t:48:LYS:HB2	2.51	0.41
1:2A:218:A:OP2	61:2A:3865:HOH:O	2.22	0.41
1:2A:262:A:H2'	1:2A:263:C:O4'	2.21	0.41
1:2A:854:G:H2'	1:2A:855:G:C8	2.55	0.41
1:2A:904:C:H2'	1:2A:905:U:C6	2.56	0.41
1:2A:1203:G:C6	1:2A:1204:A:N6	2.89	0.41
1:2A:1756:G:H4'	1:2A:1758:G:O4'	2.21	0.41
1:2A:2321:G:N3	1:2A:2321:G:H2'	2.34	0.41
1:2A:2330:G:H2'	1:2A:2331:G:O4'	2.21	0.41
1:2A:2732:G:H3'	1:2A:2733:A:O4'	2.21	0.41
3:2D:235:GLY:O	61:2D:401:HOH:O	2.21	0.41
4:2E:13:ARG:O	15:2T:57:PHE:HE2	2.03	0.41
6:2G:44:GLY:N	6:2G:88:ILE:O	2.52	0.41
9:2N:21:LYS:NZ	9:2N:140:VAL:OXT	2.50	0.41
16:2U:11:ARG:O	16:2U:15:LYS:HG3	2.21	0.41
25:23:11:SER:HA	25:23:31:LEU:HD11	2.02	0.41
32:2a:413:G:N7	35:2d:35:ARG:NH1	2.68	0.41
32:2a:439:A:C5	32:2a:441:A:H1'	2.56	0.41
32:2a:546:G:OP1	35:2d:73:ARG:HG2	2.21	0.41
32:2a:570:G:H1'	32:2a:820:U:C4	2.55	0.41
32:2a:786:G:C2	32:2a:797:C:C2	3.09	0.41
32:2a:983:A:H2	32:2a:984:C:C6	2.39	0.41
32:2a:1024:G:H2'	32:2a:1025:U:H5''	2.01	0.41
32:2a:1256:A:N6	32:2a:1278:U:H1'	2.36	0.41
33:2b:167:PRO:HG3	33:2b:188:ALA:HB2	2.02	0.41
33:2b:178:ARG:HA	33:2b:178:ARG:HD2	1.91	0.41
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:71:ALA:HA	34:2c:106:VAL:HB	2.01	0.41
39:2h:25:ASP:HB3	39:2h:58:TYR:HB3	2.03	0.41
45:2n:6:LEU:HA	45:2n:9:LYS:HB3	2.02	0.41
1:1A:185:U:H2'	1:1A:186:G:C8	2.56	0.41
1:1A:362:U:H6	1:1A:362:U:H2'	1.70	0.41
1:1A:651:G:OP1	30:18:19:SER:OG	2.30	0.41
1:1A:1814:G:C4'	3:1D:51:VAL:HG21	2.51	0.41
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.21	0.41
1:1A:2076:U:OP2	1:1A:2238:G:N2	2.47	0.41
2:1B:66:A:N6	2:1B:109:C:H5'	2.36	0.41
6:1G:53:LEU:HD12	6:1G:54:GLU:N	2.35	0.41
9:1N:73:THR:HG23	9:1N:82:LEU:HD11	2.03	0.41
14:1S:110:LEU:HD12	14:1S:110:LEU:HA	1.92	0.41
32:1a:266:G:C5'	32:1a:268:C:H41	2.34	0.41
32:1a:481:G:O2'	32:1a:483:C:N4	2.52	0.41
32:1a:645:C:H2'	32:1a:646:U:C6	2.56	0.41
32:1a:1004:A:O2'	32:1a:1038:C:O2	2.16	0.41
32:1a:1095:U:H2'	32:1a:1096:C:C6	2.56	0.41
38:1g:104:LEU:HD13	38:1g:104:LEU:HA	1.87	0.41
40:1i:16:ARG:HH11	40:1i:64:THR:CG2	2.33	0.41
41:1j:33:GLN:O	41:1j:75:ILE:N	2.54	0.41
44:1m:49:THR:HB	44:1m:52:GLU:CG	2.51	0.41
1:2A:878:A:H2'	1:2A:879:G:O4'	2.20	0.41
1:2A:1021:A:O2'	1:2A:1123:C:OP1	2.37	0.41
1:2A:1495:A:H2'	1:2A:1496:A:H8	1.86	0.41
1:2A:2023:G:H4'	1:2A:2617:C:O3'	2.20	0.41
1:2A:2188:C:H2'	1:2A:2189:U:O4'	2.20	0.41
1:2A:2298:A:C4	1:2A:2321:G:N2	2.89	0.41
1:2A:2636:U:H1'	1:2A:2783:G:N2	2.36	0.41
1:2A:2740:A:C6	1:2A:2764:A:C8	3.09	0.41
6:2G:80:PHE:O	6:2G:82:LEU:N	2.54	0.41
6:2G:179:PRO:HG3	26:24:43:TYR:CZ	2.56	0.41
15:2T:15:VAL:HG13	15:2T:79:HIS:CE1	2.56	0.41
21:2Z:157:LEU:HB3	21:2Z:161:VAL:HG23	2.02	0.41
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.59	0.41
32:2a:102:G:H2'	32:2a:103:C:H6	1.85	0.41
32:2a:179:A:H2'	32:2a:180:U:C6	2.56	0.41
32:2a:443:C:H2'	32:2a:444:C:C6	2.56	0.41
32:2a:587:G:OP1	39:2h:89:PRO:HB3	2.21	0.41
32:2a:1122:U:C4	32:2a:1123:A:N7	2.89	0.41
32:2a:1135:U:H2'	32:2a:1137:C:N3	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:17:THR:HG22	39:2h:63:LEU:HG	2.03	0.41
52:2u:6:ARG:C	52:2u:8:THR:H	2.29	0.41
1:1A:12:U:O2	1:1A:12:U:H2'	2.21	0.40
1:1A:666:G:N2	30:18:2:PRO:O	2.54	0.40
1:1A:685:A:H1'	1:1A:688:U:O4	2.20	0.40
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.21	0.40
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.21	0.40
1:1A:2650:U:H2'	1:1A:2651:C:C6	2.56	0.40
3:1D:233:HIS:HA	61:1D:457:HOH:O	2.20	0.40
10:1O:70:LYS:HB3	10:1O:70:LYS:HE2	1.91	0.40
26:14:61:ARG:HH21	50:1s:42:PRO:CD	2.31	0.40
32:1a:7:G:H21	36:1e:121:LYS:HG2	1.87	0.40
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.55	0.40
38:1g:146:GLU:OE2	38:1g:149:ARG:NE	2.54	0.40
39:1h:48:TYR:HA	39:1h:60:ARG:O	2.21	0.40
40:1i:111:ARG:HG2	40:1i:112:LYS:N	2.35	0.40
44:1m:107:ALA:O	44:1m:111:LYS:HB2	2.20	0.40
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	2.03	0.40
1:2A:570:G:H2'	1:2A:2030:A:C5	2.56	0.40
1:2A:1848:A:C6	32:2a:702:A:C6	3.09	0.40
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.36	0.40
1:2A:2028:U:H2'	1:2A:2029:G:O4'	2.22	0.40
3:2D:132:PRO:HG3	3:2D:190:TYR:CE2	2.55	0.40
5:2F:161:GLU:O	5:2F:165:ARG:HG3	2.19	0.40
5:2F:176:LEU:HA	5:2F:176:LEU:HD23	1.85	0.40
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.54	0.40
13:2R:30:THR:HG22	13:2R:31:HIS:CD2	2.56	0.40
17:2V:5:VAL:HG11	17:2V:57:VAL:HG21	2.03	0.40
32:2a:161:A:H2'	32:2a:162:A:C8	2.56	0.40
32:2a:519:C:H2'	32:2a:520:A:O4'	2.20	0.40
32:2a:620:C:H2'	32:2a:621:A:O4'	2.21	0.40
32:2a:645:C:H2'	32:2a:646:U:C6	2.56	0.40
33:2b:133:LYS:HD3	33:2b:133:LYS:HA	1.89	0.40
34:2c:5:ILE:HD11	45:2n:49:HIS:HE1	1.86	0.40
38:2g:26:PHE:O	38:2g:30:ILE:HG13	2.22	0.40
39:2h:4:ASP:OD2	39:2h:85:ARG:NH1	2.53	0.40
52:2u:6:ARG:H	52:2u:6:ARG:HG3	1.62	0.40
17:1V:1:MET:HE2	17:1V:43:GLU:OE1	2.21	0.40
21:1Z:54:HIS:ND1	21:1Z:101:PRO:HG3	2.36	0.40
32:1a:738:C:H2'	32:1a:739:C:C6	2.55	0.40
32:1a:1347:G:H22	32:1a:1373:G:H2'	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:65:ARG:HD2	35:1d:72:GLU:HA	2.03	0.40
41:1j:67:THR:O	41:1j:67:THR:OG1	2.33	0.40
50:1s:12:ASP:C	50:1s:14:HIS:H	2.29	0.40
1:2A:1092:C:O2	1:2A:1092:C:H2'	2.22	0.40
1:2A:1431:U:H2'	1:2A:1432:C:C6	2.55	0.40
1:2A:1450:G:H2'	1:2A:1450(A):C:C6	2.56	0.40
1:2A:2133:G:N2	1:2A:2157:G:H2'	2.35	0.40
1:2A:2377:A:N6	61:2A:3816:HOH:O	2.10	0.40
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.56	0.40
1:2A:2580:U:C5	1:2A:2581:G:C6	3.09	0.40
2:2B:80:U:H2'	2:2B:81:G:C8	2.57	0.40
5:2F:178:PRO:HG2	5:2F:179:GLU:OE2	2.22	0.40
7:2H:30:LYS:NZ	7:2H:81:GLU:O	2.53	0.40
11:2P:135:LEU:HD23	11:2P:135:LEU:HA	1.82	0.40
32:2a:841:U:H3'	32:2a:848:C:O4'	2.21	0.40
32:2a:983:A:N3	32:2a:983:A:H3'	2.36	0.40
32:2a:1121:U:H2'	32:2a:1122:U:C6	2.56	0.40
33:2b:178:ARG:HH22	39:2h:74:PRO:HB3	1.87	0.40
36:2e:77:PRO:HG2	36:2e:78:HIS:CD2	2.56	0.40
38:2g:102:ARG:HG2	38:2g:106:GLN:NE2	2.36	0.40
44:2m:54:VAL:HA	44:2m:57:ARG:HB3	2.03	0.40
51:2t:42:GLN:O	51:2t:45:GLN:HB3	2.21	0.40
1:1A:411:G:C5	11:1P:72:PRO:HB3	2.56	0.40
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.22	0.40
1:1A:2322:A:H2'	1:1A:2323:G:O4'	2.22	0.40
4:1E:134:ILE:C	4:1E:134:ILE:HD12	2.47	0.40
9:1N:62:VAL:CG1	9:1N:66:LYS:HB2	2.52	0.40
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.54	0.40
18:1W:23:LEU:HD12	18:1W:23:LEU:HA	1.88	0.40
23:11:34:THR:HG21	23:11:37:ILE:HD11	2.04	0.40
32:1a:509:A:H5''	35:1d:55:ALA:HB2	2.04	0.40
32:1a:690:G:C6	32:1a:691:G:C6	3.10	0.40
36:1e:69:VAL:HA	36:1e:70:PRO:HD3	1.82	0.40
51:1t:96:GLY:HA2	51:1t:97:ALA:HA	1.78	0.40
1:2A:127:A:H5''	1:2A:128:C:C6	2.56	0.40
1:2A:336:C:H5''	20:2Y:6:HIS:ND1	2.36	0.40
1:2A:2261:C:C2	1:2A:2280:G:C2	3.09	0.40
1:2A:2503:2MA:H4'	1:2A:2504:U:OP1	2.21	0.40
1:2A:2563:U:O2	1:2A:2565:A:H8	2.05	0.40
6:2G:19:LEU:HD23	6:2G:19:LEU:HA	1.87	0.40
9:2N:120:LEU:HA	9:2N:120:LEU:HD12	1.81	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:338:A:H2	32:2a:351:G:H22	1.69	0.40
32:2a:373:A:O2'	32:2a:451:A:N7	2.54	0.40
32:2a:382:A:H2'	32:2a:383:A:H8	1.86	0.40
32:2a:691:G:H2'	32:2a:692:U:C6	2.57	0.40
32:2a:978:A:O2'	32:2a:1322:C:N3	2.50	0.40
32:2a:1151:A:N3	41:2j:39:PRO:HG3	2.36	0.40
32:2a:1170:A:N6	32:2a:1171:G:N3	2.69	0.40
32:2a:1481:U:H2'	32:2a:1482:G:C8	2.57	0.40
50:2s:18:LYS:HA	50:2s:21:GLU:HB3	2.03	0.40
1:1A:453:C:O2	1:1A:457:A:O2'	2.36	0.40
1:1A:570:G:H2'	1:1A:2030:A:N7	2.35	0.40
1:1A:1001:A:H2'	1:1A:1002:G:O4'	2.22	0.40
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.21	0.40
1:1A:1668:A:H4'	1:1A:1669:A:O5'	2.20	0.40
1:1A:1693:U:H1'	3:1D:14:ARG:NH1	2.37	0.40
1:1A:2251:OMG:HM23	1:1A:2251:OMG:H1'	1.89	0.40
14:1S:25:ARG:HD3	14:1S:25:ARG:HH11	1.76	0.40
16:1U:79:PHE:CZ	16:1U:83:LEU:HD11	2.57	0.40
17:1V:62:LEU:HD11	17:1V:95:LEU:HB2	2.03	0.40
23:11:56:GLN:HE21	23:11:87:PRO:HG3	1.85	0.40
26:14:53:GLU:HG3	26:14:54:GLY:N	2.37	0.40
26:14:68:ARG:HD3	26:14:69:LYS:N	2.37	0.40
32:1a:1003:G:H2'	32:1a:1004:A:C4'	2.37	0.40
32:1a:1479:C:H2'	32:1a:1480:G:C8	2.57	0.40
33:1b:10:LEU:HA	33:1b:48:MET:HE1	2.04	0.40
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.21	0.40
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.85	0.40
40:1i:50:LEU:O	40:1i:54:ASP:N	2.54	0.40
47:1p:14:ASN:OD1	47:1p:16:HIS:HE1	2.05	0.40
53:1y:23:ARG:NH1	53:1y:26:LYS:HD2	2.36	0.40
1:2A:1048:A:N1	1:2A:1112:G:O2'	2.43	0.40
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.29	0.40
1:2A:2136:C:O2	1:2A:2156:G:O2'	2.27	0.40
1:2A:2352:A:N6	1:2A:2365:G:O2'	2.54	0.40
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.21	0.40
8:2I:78:THR:H	8:2I:104:GLN:HE22	1.69	0.40
8:2I:129:THR:HA	8:2I:138:ILE:O	2.21	0.40
15:2T:92:GLY:O	15:2T:120:ARG:NH2	2.54	0.40
32:2a:227:G:H2'	32:2a:228:A:C8	2.57	0.40
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.53	0.40
32:2a:741:G:H2'	32:2a:742:G:O4'	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:936:C:H2'	32:2a:937:A:O4'	2.22	0.40
32:2a:952:U:O4	44:2m:104:ARG:HD3	2.21	0.40
35:2d:67:ILE:HD13	35:2d:196:LEU:HD23	2.03	0.40
49:2r:41:LYS:HE2	49:2r:41:LYS:HB3	1.73	0.40
1:1A:1096:A:H3'	1:1A:1097:U:H5''	2.02	0.40
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.22	0.40
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.86	0.40
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.33	0.40
1:1A:2740:A:C6	1:1A:2764:A:C8	3.10	0.40
3:1D:175:LEU:HD12	3:1D:185:VAL:HG21	2.04	0.40
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.22	0.40
11:1P:94:GLU:HA	11:1P:124:LYS:O	2.21	0.40
18:1W:1:MET:HE2	18:1W:62:HIS:HB3	2.03	0.40
32:1a:191:G:N3	51:1t:103:GLY:HA3	2.36	0.40
32:1a:355:C:H2'	32:1a:356:A:O4'	2.22	0.40
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.54	0.40
37:1f:38:GLU:HB2	37:1f:64:GLN:HG2	2.04	0.40
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.57	0.40
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.51	0.40
1:2A:994:C:O2'	1:2A:996:A:OP1	2.28	0.40
1:2A:1104:C:H2'	1:2A:1105:U:H6	1.82	0.40
2:2B:90:A:N7	2:2B:91:C:H1'	2.37	0.40
5:2F:158:THR:O	5:2F:164:ARG:NH1	2.49	0.40
5:2F:192:LEU:HD13	5:2F:194:MET:HE2	2.03	0.40
6:2G:48:GLU:HA	6:2G:51:ARG:CZ	2.51	0.40
9:2N:19:GLU:HG3	9:2N:59:LYS:HB3	2.03	0.40
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	2.03	0.40
15:2T:119:LYS:O	15:2T:123:GLN:HG3	2.22	0.40
20:2Y:7:VAL:CG1	20:2Y:27:VAL:HG21	2.51	0.40
20:2Y:73:ARG:HH11	20:2Y:73:ARG:HG2	1.86	0.40
32:2a:600:C:H2'	32:2a:601:C:C6	2.56	0.40
32:2a:657:G:C2	32:2a:750:G:C5	3.10	0.40
32:2a:1077:G:O6	36:2e:47:LYS:NZ	2.54	0.40
33:2b:144:ARG:NH1	33:2b:148:TYR:OH	2.54	0.40
35:2d:191:ARG:HA	35:2d:191:ARG:HD2	1.90	0.40
37:2f:50:TYR:OH	49:2r:74:ARG:O	2.39	0.40
38:2g:49:ILE:H	38:2g:49:ILE:HG13	1.62	0.40
39:2h:36:LEU:HD23	39:2h:36:LEU:HA	1.94	0.40
47:2p:18:ARG:NH1	47:2p:32:TYR:OH	2.55	0.40
48:2q:28:PRO:HA	48:2q:35:VAL:HA	2.03	0.40
51:2t:54:LYS:HA	51:2t:57:ARG:CZ	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	39
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	39
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	39
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	39
6	1G	179/182 (98%)	161 (90%)	12 (7%)	6 (3%)	3	4
6	2G	179/182 (98%)	159 (89%)	15 (8%)	5 (3%)	4	6
7	1H	172/180 (96%)	161 (94%)	11 (6%)	0	100	100
7	2H	171/180 (95%)	152 (89%)	16 (9%)	3 (2%)	6	11
8	1I	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
8	2I	144/148 (97%)	132 (92%)	10 (7%)	2 (1%)	9	14
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	134 (97%)	2 (1%)	2 (1%)	9	14
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	27
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	30
11	2P	147/150 (98%)	138 (94%)	6 (4%)	3 (2%)	6	10
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	104 (96%)	2 (2%)	2 (2%)	6	10
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12	20
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	20
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%)	90 (97%)	2 (2%)	1 (1%)	11	19
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	19
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
21	1Z	201/206 (98%)	185 (92%)	14 (7%)	2 (1%)	12	20
21	2Z	199/206 (97%)	179 (90%)	20 (10%)	0	100	100
22	10	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
22	20	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	19
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	19
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	0
26	24	67/71 (94%)	41 (61%)	21 (31%)	5 (8%)	1	0
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	197 (86%)	25 (11%)	7 (3%)	3	5
33	2b	229/256 (90%)	197 (86%)	26 (11%)	6 (3%)	4	6
34	1c	204/239 (85%)	184 (90%)	19 (9%)	1 (0%)	24	39
34	2c	204/239 (85%)	169 (83%)	33 (16%)	2 (1%)	12	20
35	1d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	24	39
35	2d	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	12	20
36	1e	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
36	2e	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	18	30
38	2g	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	6	10
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	18	30
40	1i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
40	2i	124/128 (97%)	106 (86%)	14 (11%)	4 (3%)	3	4
41	1j	95/105 (90%)	83 (87%)	7 (7%)	5 (5%)	1	2
41	2j	94/105 (90%)	77 (82%)	12 (13%)	5 (5%)	1	2
42	1k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	24
42	2k	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16	27
44	1m	114/126 (90%)	106 (93%)	5 (4%)	3 (3%)	4	6
44	2m	112/126 (89%)	96 (86%)	14 (12%)	2 (2%)	6	11
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	1o	86/89 (97%)	79 (92%)	4 (5%)	3 (4%)	3	4
46	2o	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	5	8
47	1p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	70 (86%)	9 (11%)	2 (2%)	4	7
50	2s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	10	17
51	1t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	5	9
51	2t	96/106 (91%)	88 (92%)	6 (6%)	2 (2%)	5	9
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2	2
53	1y	95/113 (84%)	93 (98%)	2 (2%)	0	100	100
53	2y	94/113 (83%)	93 (99%)	1 (1%)	0	100	100
All	All	11629/12354 (94%)	10830 (93%)	694 (6%)	105 (1%)	14	24

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
21	1Z	53	ILE
26	14	55	ARG
33	1b	17	PHE
33	1b	21	ARG
33	1b	129	GLU
44	1m	67	GLU
8	2I	10	GLU
11	2P	36	LYS
26	24	60	GLN
33	2b	17	PHE
40	2i	43	ALA
40	2i	55	ALA
41	2j	56	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	79	ARG
6	1G	126	ASP
19	1X	94	GLY
26	14	47	GLN
26	14	49	PHE
26	14	57	GLU
33	1b	8	LYS
41	1j	55	LYS
44	1m	106	ASN
51	1t	47	GLY
5	2F	130	ALA
6	2G	78	SER
6	2G	81	LYS
6	2G	117	PHE
7	2H	126	PRO
14	2S	81	GLY
17	2V	79	VAL
19	2X	94	GLY
23	21	3	LYS
26	24	62	ARG
33	2b	125	PRO
34	2c	100	ALA
40	2i	54	ASP
44	2m	106	ASN
46	2o	88	ARG
6	1G	54	GLU
21	1Z	52	SER
34	1c	107	GLN
35	1d	85	LYS
41	1j	77	PRO
41	1j	79	ARG
46	1o	88	ARG
50	1s	12	ASP
50	1s	27	GLU
6	2G	42	GLY
6	2G	47	LYS
7	2H	65	HIS
8	2I	117	GLU
10	2O	5	GLN
11	2P	29	LYS
14	2S	96	GLY
26	24	47	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	10	LEU
33	2b	22	LYS
34	2c	156	ARG
35	2d	156	GLU
38	2g	7	ALA
41	2j	78	ASN
51	2t	100	ILE
4	1E	52	LEU
6	1G	50	ALA
17	1V	79	VAL
23	11	3	LYS
33	1b	20	GLU
44	1m	12	ASN
46	1o	87	ILE
4	2E	52	LEU
7	2H	47	GLU
9	2N	132	ALA
26	24	55	ARG
38	2g	33	ASP
43	2l	105	TYR
6	1G	49	ASP
26	24	53	GLU
33	2b	9	GLU
33	2b	20	GLU
38	2g	131	LYS
39	2h	133	LEU
40	2i	96	LEU
41	2j	29	ARG
44	2m	67	GLU
52	2u	3	LYS
6	1G	74	LYS
11	1P	29	LYS
33	1b	127	ILE
41	1j	78	ASN
35	2d	154	ASN
38	1g	55	GLY
41	1j	82	ILE
51	1t	100	ILE
46	2o	87	ILE
50	2s	9	VAL
26	14	19	GLY
42	1k	105	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	1o	19	PRO
9	2N	129	PRO
41	2j	75	ILE
11	2P	122	PRO
51	2t	102	GLY
33	1b	125	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	197 (92%)	17 (8%)	11	19
3	2D	215/218 (99%)	198 (92%)	17 (8%)	11	19
4	1E	164/166 (99%)	156 (95%)	8 (5%)	22	38
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19	33
5	1F	160/166 (96%)	146 (91%)	14 (9%)	9	15
5	2F	159/166 (96%)	146 (92%)	13 (8%)	10	18
6	1G	144/156 (92%)	127 (88%)	17 (12%)	5	7
6	2G	142/156 (91%)	124 (87%)	18 (13%)	4	6
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	14
7	2H	143/148 (97%)	125 (87%)	18 (13%)	4	6
8	1I	111/124 (90%)	101 (91%)	10 (9%)	9	14
8	2I	108/124 (87%)	95 (88%)	13 (12%)	5	7
9	1N	119/119 (100%)	105 (88%)	14 (12%)	5	7
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8	13
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	47
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	57
11	1P	115/116 (99%)	102 (89%)	13 (11%)	5	8
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26	44
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	16	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	2Q	111/111 (100%)	101 (91%)	10 (9%)	9	14
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11	19
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	15
14	1S	87/88 (99%)	75 (86%)	12 (14%)	3	5
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6	10
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	24
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16	29
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	27
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10	16
17	1V	81/82 (99%)	77 (95%)	4 (5%)	22	38
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9	15
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	20
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11	20
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	48
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	63
20	1Y	86/91 (94%)	81 (94%)	5 (6%)	18	31
20	2Y	86/91 (94%)	82 (95%)	4 (5%)	23	40
21	1Z	169/179 (94%)	155 (92%)	14 (8%)	10	18
21	2Z	165/179 (92%)	152 (92%)	13 (8%)	11	19
22	10	61/67 (91%)	58 (95%)	3 (5%)	22	38
22	20	61/67 (91%)	59 (97%)	2 (3%)	33	55
23	11	79/83 (95%)	75 (95%)	4 (5%)	21	36
23	21	81/83 (98%)	73 (90%)	8 (10%)	7	11
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	56
24	22	66/67 (98%)	61 (92%)	5 (8%)	12	21
25	13	51/52 (98%)	48 (94%)	3 (6%)	18	30
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	30
26	14	58/63 (92%)	55 (95%)	3 (5%)	21	36
26	24	54/63 (86%)	47 (87%)	7 (13%)	4	6
27	15	51/52 (98%)	46 (90%)	5 (10%)	7	11
27	25	50/52 (96%)	49 (98%)	1 (2%)	48	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	20
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	11
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	11
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	22
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	32
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	32
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	58
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	30
33	1b	191/220 (87%)	173 (91%)	18 (9%)	8	13
33	2b	187/220 (85%)	159 (85%)	28 (15%)	3	4
34	1c	144/188 (77%)	131 (91%)	13 (9%)	9	14
34	2c	140/188 (74%)	124 (89%)	16 (11%)	5	8
35	1d	171/181 (94%)	159 (93%)	12 (7%)	14	24
35	2d	172/181 (95%)	158 (92%)	14 (8%)	11	18
36	1e	114/123 (93%)	104 (91%)	10 (9%)	9	15
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	12
37	1f	85/90 (94%)	77 (91%)	8 (9%)	8	13
37	2f	85/90 (94%)	75 (88%)	10 (12%)	5	7
38	1g	120/127 (94%)	111 (92%)	9 (8%)	12	21
38	2g	119/127 (94%)	103 (87%)	16 (13%)	4	5
39	1h	116/119 (98%)	108 (93%)	8 (7%)	14	24
39	2h	114/119 (96%)	101 (89%)	13 (11%)	5	8
40	1i	91/99 (92%)	83 (91%)	8 (9%)	9	15
40	2i	88/99 (89%)	74 (84%)	14 (16%)	2	3
41	1j	68/92 (74%)	65 (96%)	3 (4%)	25	43
41	2j	68/92 (74%)	56 (82%)	12 (18%)	2	2
42	1k	83/99 (84%)	81 (98%)	2 (2%)	43	65
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10	17
43	1l	96/108 (89%)	94 (98%)	2 (2%)	47	69
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8	13
44	1m	90/101 (89%)	85 (94%)	5 (6%)	19	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	2m	87/101 (86%)	82 (94%)	5 (6%)	18	32
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	7
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	10
46	1o	78/80 (98%)	72 (92%)	6 (8%)	12	20
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16	28
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	4
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2	3
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20	35
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	28
49	1r	59/77 (77%)	52 (88%)	7 (12%)	5	7
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	53
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7	10
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	5
51	1t	71/82 (87%)	68 (96%)	3 (4%)	26	45
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10	16
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	32
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	32
53	1y	82/98 (84%)	81 (99%)	1 (1%)	63	79
53	2y	79/98 (81%)	67 (85%)	12 (15%)	3	4
All	All	9524/10260 (93%)	8730 (92%)	794 (8%)	10	18

All (794) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	35	LYS
3	1D	37	LEU
3	1D	39	LYS
3	1D	99	ASP
3	1D	111	LEU
3	1D	113	VAL
3	1D	141	VAL
3	1D	155	LEU
3	1D	173	VAL
3	1D	193	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	275	LYS
4	1E	9	VAL
4	1E	47	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	116	VAL
4	1E	119	ARG
4	1E	184	VAL
4	1E	195	LEU
5	1F	12	LEU
5	1F	24	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	103	LYS
5	1F	110	LEU
5	1F	126	VAL
5	1F	132	VAL
5	1F	140	LEU
5	1F	145	GLU
5	1F	158	THR
5	1F	183	VAL
5	1F	192	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	47	LYS
6	1G	52	ILE
6	1G	58	GLN
6	1G	78	SER
6	1G	79	ASN
6	1G	86	MET
6	1G	130	ASN
6	1G	137	GLU
6	1G	140	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	1G	152	LEU
6	1G	153	ARG
6	1G	159	VAL
7	1H	24	VAL
7	1H	49	VAL
7	1H	58	GLU
7	1H	62	LYS
7	1H	71	LEU
7	1H	98	LEU
7	1H	107	VAL
7	1H	119	GLU
7	1H	122	THR
7	1H	127	GLU
7	1H	132	ARG
7	1H	149	ARG
7	1H	172	LYS
8	1I	15	VAL
8	1I	20	ASP
8	1I	41	GLU
8	1I	44	LEU
8	1I	75	LEU
8	1I	78	THR
8	1I	87	LYS
8	1I	92	VAL
8	1I	109	ILE
8	1I	117	GLU
9	1N	5	VAL
9	1N	8	GLN
9	1N	9	VAL
9	1N	14	VAL
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	67	LEU
9	1N	73	THR
9	1N	99	LEU
9	1N	121	LYS
10	1O	10	VAL
10	1O	23	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	1O	94	ARG
10	1O	113	LYS
11	1P	3	LEU
11	1P	15	ARG
11	1P	56	SER
11	1P	59	LEU
11	1P	71	VAL
11	1P	75	ILE
11	1P	95	VAL
11	1P	99	LEU
11	1P	101	VAL
11	1P	125	VAL
11	1P	133	SER
11	1P	147	LEU
11	1P	149	GLU
12	1Q	5	ARG
12	1Q	7	MET
12	1Q	21	THR
12	1Q	75	THR
12	1Q	80	GLU
12	1Q	109	VAL
12	1Q	129	THR
13	1R	6	SER
13	1R	8	ARG
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	65	LEU
13	1R	96	ARG
13	1R	114	VAL
14	1S	14	VAL
14	1S	43	GLU
14	1S	46	VAL
14	1S	49	VAL
14	1S	50	SER
14	1S	52	SER
14	1S	59	LYS
14	1S	69	VAL
14	1S	73	LEU
14	1S	75	GLU
14	1S	85	VAL
14	1S	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	1T	16	ARG
15	1T	28	VAL
15	1T	33	LYS
15	1T	34	VAL
15	1T	53	ARG
15	1T	75	ILE
15	1T	96	ARG
15	1T	107	ASP
16	1U	52	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	104	GLN
16	1U	114	LYS
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	59	VAL
18	1W	82	LEU
18	1W	100	THR
19	1X	35	THR
19	1X	66	LEU
19	1X	88	LYS
20	1Y	23	ARG
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	61	LEU
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	93	ASP
21	1Z	94	GLU
21	1Z	119	GLU
21	1Z	120	ILE
21	1Z	126	VAL
21	1Z	138	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	161	VAL
21	1Z	162	GLU
21	1Z	170	THR
21	1Z	191	VAL
21	1Z	203	GLU
22	10	11	ARG
22	10	53	MET
22	10	74	ARG
23	11	21	ARG
23	11	30	VAL
23	11	46	LEU
23	11	85	LEU
24	12	53	LEU
24	12	70	GLN
25	13	6	VAL
25	13	23	LEU
25	13	54	VAL
26	14	1	MET
26	14	13	ARG
26	14	49	PHE
27	15	6	VAL
27	15	16	ARG
27	15	26	THR
27	15	40	LYS
27	15	58	LEU
28	16	19	ARG
28	16	44	ARG
28	16	47	THR
28	16	52	VAL
29	17	1	MET
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	29	LYS
30	18	58	ILE
31	19	17	ILE
33	1b	9	GLU
33	1b	10	LEU
33	1b	15	VAL
33	1b	39	ILE
33	1b	59	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	67	THR
33	1b	111	ARG
33	1b	126	GLU
33	1b	146	GLN
33	1b	158	LEU
33	1b	160	ASP
33	1b	185	ILE
33	1b	187	LEU
33	1b	189	ASP
33	1b	200	ILE
33	1b	206	ASP
33	1b	221	LEU
33	1b	229	VAL
34	1c	3	ASN
34	1c	4	LYS
34	1c	55	VAL
34	1c	64	VAL
34	1c	70	VAL
34	1c	82	GLU
34	1c	98	ASN
34	1c	102	ASN
34	1c	132	ARG
34	1c	144	SER
34	1c	154	SER
34	1c	188	LEU
34	1c	204	LEU
35	1d	8	VAL
35	1d	17	VAL
35	1d	26	CYS
35	1d	94	LEU
35	1d	135	LEU
35	1d	157	LEU
35	1d	168	ARG
35	1d	175	SER
35	1d	178	VAL
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
36	1e	10	MET
36	1e	34	VAL
36	1e	41	VAL
36	1e	47	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1e	68	GLU
36	1e	69	VAL
36	1e	101	ILE
36	1e	126	ARG
36	1e	144	THR
36	1e	147	ASP
37	1f	17	SER
37	1f	45	LEU
37	1f	61	LEU
37	1f	64	GLN
37	1f	69	GLU
37	1f	72	VAL
37	1f	78	GLU
37	1f	86	ARG
38	1g	6	ARG
38	1g	13	GLN
38	1g	45	ASP
38	1g	51	GLN
38	1g	56	GLN
38	1g	59	LEU
38	1g	89	MET
38	1g	104	LEU
38	1g	113	GLU
39	1h	25	ASP
39	1h	26	VAL
39	1h	54	ASP
39	1h	61	VAL
39	1h	95	VAL
39	1h	99	GLU
39	1h	107	LEU
39	1h	120	THR
40	1i	14	VAL
40	1i	47	LEU
40	1i	56	LEU
40	1i	64	THR
40	1i	65	VAL
40	1i	81	ILE
40	1i	108	VAL
40	1i	109	VAL
41	1j	49	VAL
41	1j	67	THR
41	1j	84	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	1k	16	SER
42	1k	114	VAL
43	1l	11	VAL
43	1l	83	VAL
44	1m	4	ILE
44	1m	11	ARG
44	1m	14	ARG
44	1m	70	LEU
44	1m	106	ASN
45	1n	3	ARG
45	1n	4	LYS
45	1n	9	LYS
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
46	1o	6	GLU
46	1o	39	LEU
46	1o	40	SER
46	1o	83	GLU
46	1o	87	ILE
46	1o	88	ARG
47	1p	6	LEU
47	1p	20	VAL
47	1p	21	VAL
47	1p	29	ASP
47	1p	42	ARG
47	1p	50	LYS
47	1p	53	VAL
47	1p	61	SER
47	1p	72	ARG
47	1p	74	LEU
48	1q	26	GLN
48	1q	61	GLU
48	1q	74	LEU
48	1q	77	VAL
48	1q	97	SER
49	1r	25	THR
49	1r	26	LEU
49	1r	28	GLU
49	1r	37	VAL
49	1r	69	THR
49	1r	82	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	1r	86	VAL
50	1s	5	LEU
50	1s	30	LEU
50	1s	35	SER
50	1s	37	ARG
50	1s	41	VAL
50	1s	55	LYS
50	1s	79	THR
51	1t	24	LEU
51	1t	30	LYS
51	1t	100	ILE
52	1u	24	ARG
53	1y	42	SER
3	2D	3	VAL
3	2D	61	LEU
3	2D	71	ASP
3	2D	89	SER
3	2D	103	ARG
3	2D	106	ILE
3	2D	113	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	169	GLU
3	2D	183	ARG
3	2D	211	ARG
3	2D	217	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	274	ARG
4	2E	7	VAL
4	2E	9	VAL
4	2E	47	VAL
4	2E	52	LEU
4	2E	73	GLU
4	2E	75	VAL
4	2E	116	VAL
4	2E	119	ARG
4	2E	170	LEU
5	2F	20	LEU
5	2F	33	LEU
5	2F	57	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	2F	60	SER
5	2F	74	ARG
5	2F	126	VAL
5	2F	140	LEU
5	2F	157	VAL
5	2F	165	ARG
5	2F	175	THR
5	2F	183	VAL
5	2F	192	LEU
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	13	GLU
6	2G	28	VAL
6	2G	31	VAL
6	2G	39	ILE
6	2G	43	LEU
6	2G	60	LEU
6	2G	70	VAL
6	2G	77	ILE
6	2G	88	ILE
6	2G	106	LEU
6	2G	113	ARG
6	2G	115	ARG
6	2G	123	ASN
6	2G	133	LEU
6	2G	139	LEU
6	2G	145	THR
7	2H	18	GLU
7	2H	24	VAL
7	2H	33	LEU
7	2H	43	VAL
7	2H	47	GLU
7	2H	49	VAL
7	2H	50	VAL
7	2H	56	SER
7	2H	68	THR
7	2H	71	LEU
7	2H	95	ARG
7	2H	105	LEU
7	2H	122	THR
7	2H	124	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	2H	127	GLU
7	2H	133	VAL
7	2H	136	ILE
7	2H	139	GLN
8	2I	12	LEU
8	2I	38	LEU
8	2I	47	LEU
8	2I	48	GLU
8	2I	50	ARG
8	2I	73	GLU
8	2I	76	THR
8	2I	92	VAL
8	2I	108	THR
8	2I	114	LEU
8	2I	117	GLU
8	2I	127	VAL
8	2I	142	VAL
9	2N	16	ILE
9	2N	28	THR
9	2N	33	LEU
9	2N	38	HIS
9	2N	62	VAL
9	2N	67	LEU
9	2N	68	GLU
9	2N	71	ILE
9	2N	87	LEU
9	2N	100	GLU
9	2N	140	VAL
10	2O	10	VAL
10	2O	23	ARG
10	2O	116	SER
11	2P	15	ARG
11	2P	35	HIS
11	2P	99	LEU
11	2P	125	VAL
11	2P	149	GLU
12	2Q	2	LEU
12	2Q	7	MET
12	2Q	21	THR
12	2Q	22	LYS
12	2Q	35	VAL
12	2Q	85	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	112	GLU
12	2Q	135	ASP
13	2R	29	LEU
13	2R	33	ARG
13	2R	36	THR
13	2R	65	LEU
13	2R	73	VAL
13	2R	86	ARG
13	2R	96	ARG
13	2R	114	VAL
13	2R	117	VAL
14	2S	12	PHE
14	2S	13	ARG
14	2S	21	THR
14	2S	35	ILE
14	2S	40	ILE
14	2S	44	LYS
14	2S	64	GLU
14	2S	84	GLN
14	2S	85	VAL
15	2T	6	LEU
15	2T	28	VAL
15	2T	34	VAL
15	2T	53	ARG
15	2T	85	LYS
15	2T	96	ARG
15	2T	119	LYS
16	2U	5	LYS
16	2U	31	SER
16	2U	55	ARG
16	2U	63	VAL
16	2U	74	LEU
16	2U	77	SER
16	2U	104	GLN
16	2U	117	GLN
17	2V	5	VAL
17	2V	32	THR
17	2V	35	LEU
17	2V	46	VAL
17	2V	66	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	2V	72	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	63	ASP
18	2W	85	VAL
18	2W	100	THR
19	2X	35	THR
19	2X	57	LEU
20	2Y	2	ARG
20	2Y	19	LYS
20	2Y	28	LYS
20	2Y	72	VAL
21	2Z	33	LEU
21	2Z	46	LYS
21	2Z	47	VAL
21	2Z	66	SER
21	2Z	74	VAL
21	2Z	107	THR
21	2Z	117	LEU
21	2Z	126	VAL
21	2Z	141	VAL
21	2Z	142	SER
21	2Z	163	LEU
21	2Z	165	VAL
21	2Z	175	VAL
22	20	10	THR
22	20	36	ILE
23	21	11	ARG
23	21	21	ARG
23	21	30	VAL
23	21	35	THR
23	21	40	ARG
23	21	46	LEU
23	21	51	VAL
23	21	59	THR
24	22	16	LEU
24	22	32	LEU
24	22	44	LEU
24	22	52	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	22	53	LEU
25	23	23	LEU
25	23	31	LEU
25	23	38	GLU
26	24	10	VAL
26	24	15	ILE
26	24	27	THR
26	24	40	HIS
26	24	50	VAL
26	24	53	GLU
26	24	63	TYR
27	25	6	VAL
28	26	5	VAL
28	26	14	THR
28	26	40	CYS
28	26	48	VAL
28	26	50	ARG
29	27	1	MET
29	27	24	THR
29	27	46	VAL
30	28	14	VAL
30	28	23	VAL
30	28	46	ARG
31	29	4	ARG
31	29	7	VAL
33	2b	7	VAL
33	2b	8	LYS
33	2b	11	LEU
33	2b	15	VAL
33	2b	16	HIS
33	2b	28	PHE
33	2b	44	LEU
33	2b	47	THR
33	2b	49	GLU
33	2b	52	GLU
33	2b	67	THR
33	2b	80	ILE
33	2b	81	VAL
33	2b	83	MET
33	2b	93	VAL
33	2b	96	ARG
33	2b	98	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	111	ARG
33	2b	118	LEU
33	2b	124	SER
33	2b	126	GLU
33	2b	138	LEU
33	2b	157	ARG
33	2b	160	ASP
33	2b	187	LEU
33	2b	208	ILE
33	2b	210	SER
33	2b	229	VAL
34	2c	3	ASN
34	2c	8	ILE
34	2c	14	ILE
34	2c	47	LEU
34	2c	52	LEU
34	2c	82	GLU
34	2c	105	GLU
34	2c	126	ARG
34	2c	131	ARG
34	2c	136	GLN
34	2c	152	ILE
34	2c	161	GLU
34	2c	166	GLU
34	2c	195	VAL
34	2c	204	LEU
34	2c	207	VAL
35	2d	5	ILE
35	2d	8	VAL
35	2d	17	VAL
35	2d	28	SER
35	2d	59	ARG
35	2d	108	LEU
35	2d	115	ARG
35	2d	135	LEU
35	2d	153	ARG
35	2d	158	ILE
35	2d	170	VAL
35	2d	175	SER
35	2d	202	LEU
35	2d	209	ARG
36	2e	16	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2e	34	VAL
36	2e	41	VAL
36	2e	68	GLU
36	2e	69	VAL
36	2e	75	THR
36	2e	79	GLU
36	2e	120	THR
36	2e	135	THR
36	2e	140	ARG
36	2e	143	ARG
37	2f	10	LEU
37	2f	22	GLU
37	2f	61	LEU
37	2f	69	GLU
37	2f	70	ASP
37	2f	72	VAL
37	2f	75	LEU
37	2f	78	GLU
37	2f	91	VAL
37	2f	92	LYS
38	2g	8	GLU
38	2g	9	VAL
38	2g	13	GLN
38	2g	16	LEU
38	2g	27	ILE
38	2g	49	ILE
38	2g	51	GLN
38	2g	59	LEU
38	2g	89	MET
38	2g	95	ARG
38	2g	104	LEU
38	2g	113	GLU
38	2g	115	ARG
38	2g	131	LYS
38	2g	138	LYS
38	2g	155	ARG
39	2h	2	LEU
39	2h	3	THR
39	2h	33	GLU
39	2h	63	LEU
39	2h	64	LYS
39	2h	84	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	2h	85	ARG
39	2h	109	ILE
39	2h	112	LEU
39	2h	114	THR
39	2h	121	ASP
39	2h	133	LEU
39	2h	137	VAL
40	2i	17	VAL
40	2i	23	ASN
40	2i	27	THR
40	2i	28	VAL
40	2i	47	LEU
40	2i	50	LEU
40	2i	53	VAL
40	2i	56	LEU
40	2i	64	THR
40	2i	75	ASP
40	2i	99	LEU
40	2i	108	VAL
40	2i	109	VAL
40	2i	125	TYR
41	2j	9	ARG
41	2j	30	SER
41	2j	34	VAL
41	2j	38	ILE
41	2j	47	PHE
41	2j	69	ASN
41	2j	72	VAL
41	2j	74	ILE
41	2j	84	GLN
41	2j	94	VAL
41	2j	98	ILE
41	2j	100	THR
42	2k	26	ASN
42	2k	79	SER
42	2k	103	LEU
42	2k	104	GLN
42	2k	105	VAL
42	2k	109	VAL
42	2k	117	ASN
43	2l	28	LYS
43	2l	47	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	2l	55	VAL
43	2l	57	LYS
43	2l	67	THR
43	2l	81	SER
43	2l	82	VAL
43	2l	83	VAL
43	2l	104	VAL
44	2m	17	VAL
44	2m	47	ASP
44	2m	62	ASN
44	2m	69	GLU
44	2m	102	ARG
45	2n	4	LYS
45	2n	18	VAL
45	2n	29	ARG
45	2n	33	VAL
45	2n	42	ILE
46	2o	3	ILE
46	2o	5	LYS
46	2o	39	LEU
46	2o	76	GLU
46	2o	88	ARG
47	2p	1	MET
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	25	ARG
47	2p	28	ARG
47	2p	38	TYR
47	2p	45	THR
47	2p	47	ASP
47	2p	67	THR
47	2p	69	THR
48	2q	16	GLN
48	2q	24	GLU
48	2q	53	LEU
48	2q	56	VAL
48	2q	85	VAL
48	2q	99	SER
49	2r	25	THR
49	2r	37	VAL
50	2s	5	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	2s	22	LEU
50	2s	33	THR
50	2s	41	VAL
50	2s	48	THR
50	2s	49	ILE
50	2s	63	THR
50	2s	71	LEU
50	2s	79	THR
51	2t	10	LEU
51	2t	24	LEU
51	2t	42	GLN
51	2t	71	THR
51	2t	84	LEU
51	2t	99	LEU
52	2u	6	ARG
53	2y	5	ILE
53	2y	6	THR
53	2y	13	THR
53	2y	16	ILE
53	2y	29	LYS
53	2y	32	THR
53	2y	42	SER
53	2y	46	GLN
53	2y	61	LEU
53	2y	75	ASN
53	2y	78	ILE
53	2y	95	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	253	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	40	ASN
8	1I	104	GLN
8	1I	105	HIS
9	1N	8	GLN
10	1O	3	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1R	13	HIS
13	1R	31	HIS
13	1R	50	HIS
13	1R	71	GLN
14	1S	68	GLN
14	1S	95	HIS
15	1T	58	ASN
15	1T	123	GLN
16	1U	72	HIS
16	1U	81	HIS
16	1U	94	ASN
17	1V	80	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	32	HIS
21	1Z	73	GLN
21	1Z	121	HIS
21	1Z	151	HIS
23	11	19	GLN
23	11	56	GLN
25	13	32	GLN
26	14	60	GLN
28	16	20	ASN
33	1b	76	GLN
33	1b	135	GLN
34	1c	6	HIS
34	1c	31	HIS
34	1c	69	HIS
34	1c	102	ASN
34	1c	104	GLN
34	1c	108	ASN
35	1d	45	GLN
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	129	ASN
35	1d	201	GLN
36	1e	38	GLN
36	1e	56	GLN
37	1f	7	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	1f	100	ASN
38	1g	28	ASN
38	1g	64	GLN
38	1g	86	GLN
38	1g	148	ASN
40	1i	3	GLN
40	1i	73	GLN
40	1i	87	GLN
40	1i	117	HIS
41	1j	13	HIS
41	1j	56	HIS
41	1j	84	GLN
42	1k	62	GLN
42	1k	93	GLN
43	1l	80	HIS
43	1l	99	HIS
44	1m	40	ASN
45	1n	52	GLN
46	1o	13	GLN
46	1o	28	GLN
47	1p	16	HIS
48	1q	16	GLN
48	1q	26	GLN
48	1q	45	HIS
50	1s	57	HIS
50	1s	83	HIS
51	1t	16	HIS
51	1t	18	GLN
53	1y	89	GLN
3	2D	126	GLN
3	2D	253	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	75	HIS
5	2F	203	GLN
8	2I	43	ASN
8	2I	104	GLN
8	2I	105	HIS
9	2N	94	HIS
9	2N	133	GLN
13	2R	50	HIS
13	2R	71	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	2S	68	GLN
15	2T	58	ASN
15	2T	84	GLN
15	2T	123	GLN
16	2U	72	HIS
16	2U	94	ASN
16	2U	117	GLN
17	2V	64	HIS
19	2X	31	HIS
19	2X	82	GLN
21	2Z	32	HIS
21	2Z	50	GLN
21	2Z	73	GLN
21	2Z	75	ASN
21	2Z	132	ASN
25	23	32	GLN
29	27	36	GLN
30	28	35	GLN
33	2b	40	HIS
33	2b	76	GLN
33	2b	146	GLN
33	2b	212	GLN
34	2c	6	HIS
34	2c	28	GLN
34	2c	139	GLN
34	2c	176	HIS
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	161	ASN
35	2d	201	GLN
36	2e	38	GLN
36	2e	56	GLN
37	2f	13	ASN
37	2f	100	ASN
38	2g	11	GLN
38	2g	13	GLN
38	2g	97	GLN
38	2g	106	GLN
39	2h	82	HIS
40	2i	58	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	2i	117	HIS
41	2j	68	HIS
41	2j	84	GLN
42	2k	93	GLN
42	2k	99	GLN
43	2l	99	HIS
44	2m	12	ASN
44	2m	40	ASN
44	2m	92	HIS
46	2o	13	GLN
46	2o	28	GLN
46	2o	50	HIS
47	2p	13	HIS
48	2q	16	GLN
48	2q	26	GLN
51	2t	18	GLN
53	2y	36	ASN
53	2y	38	HIS
53	2y	79	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	399 (13%)	33 (1%)
1	2A	2858/2915 (98%)	464 (16%)	35 (1%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	119/121 (98%)	15 (12%)	0
32	1a	1497/1521 (98%)	242 (16%)	0
32	2a	1501/1521 (98%)	240 (15%)	0
All	All	8959/9114 (98%)	1373 (15%)	68 (0%)

All (1373) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	153	C
1	1A	181	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	229	A
1	1A	248	G
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	280	C
1	1A	311	A
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	428	A
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	456	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	457	A
1	1A	481	G
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	654	A
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	740	U
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	792	G
1	1A	805	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	882	G
1	1A	886	C
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1039	G
1	1A	1041	C
1	1A	1042	G
1	1A	1043	C
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1053	C
1	1A	1054	A
1	1A	1060	U
1	1A	1061	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1062	G
1	1A	1065	U
1	1A	1066	U
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1076	C
1	1A	1077	A
1	1A	1079	C
1	1A	1083	U
1	1A	1084	A
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1096	A
1	1A	1097	U
1	1A	1109	C
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1139	G
1	1A	1155	A
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1210	A
1	1A	1211	U
1	1A	1220	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1320	C
1	1A	1352	U
1	1A	1359	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C
1	1A	1508	A
1	1A	1509(A)	A
1	1A	1542	A
1	1A	1543	C
1	1A	1545	A
1	1A	1554	A
1	1A	1558	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1610	A
1	1A	1648	C
1	1A	1653	G
1	1A	1654	A
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1740	G
1	1A	1746	G
1	1A	1756	G
1	1A	1757	U
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1858	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1971	A
1	1A	1972	A
1	1A	1981	A
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2099	U
1	1A	2103	C
1	1A	2106	G
1	1A	2107	C
1	1A	2108	C
1	1A	2112	G
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2119	A
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2139	C
1	1A	2142	C
1	1A	2145	C
1	1A	2146	C
1	1A	2152	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2171	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2173	A
1	1A	2180	U
1	1A	2181	G
1	1A	2184	G
1	1A	2186	G
1	1A	2187	G
1	1A	2189	U
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2279	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2321	G
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2469	A
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2498	C
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2758	A
1	1A	2761	G
1	1A	2764	A
1	1A	2765	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2803	C
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	15	A
2	1B	42	C
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G
32	1a	6	G
32	1a	7	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	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	97	G
32	1a	101	A
32	1a	115	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	116	A
32	1a	117	G
32	1a	121	C
32	1a	131	C
32	1a	143	A
32	1a	144	G
32	1a	159	G
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	195	A
32	1a	197	A
32	1a	200	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	262	A
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	388	G
32	1a	397	A
32	1a	406	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	412	A
32	1a	413	G
32	1a	414	A
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	470	C
32	1a	475	G
32	1a	484	G
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	521	G
32	1a	532	A
32	1a	536	C
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	564	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	633	G
32	1a	642	A
32	1a	653	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	661	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	702	A
32	1a	723	U
32	1a	731	G
32	1a	755	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	836	G
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	966	M2G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	999	C
32	1a	1001(A)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1006	C
32	1a	1009	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	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(B)	C
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1039	C
32	1a	1040	U
32	1a	1044	A
32	1a	1053	G
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	1121	U
32	1a	1124	G
32	1a	1125	U
32	1a	1126	U
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1152	A
32	1a	1159	U
32	1a	1168	A
32	1a	1183	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1224	G
32	1a	1225	A
32	1a	1227	A
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	9	U
1	2A	10	G
1	2A	11	G
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	265	A
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	308	G
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	370	G
1	2A	372	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	470	A
1	2A	481	G
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	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	669	G
1	2A	686	G
1	2A	730	C
1	2A	751	A
1	2A	752	A
1	2A	753	C
1	2A	765	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	802	A
1	2A	805	G
1	2A	811	U
1	2A	812	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	880	G
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	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1042	G
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1047	G
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1070	A
1	2A	1071	G
1	2A	1072	C
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1095	A
1	2A	1097	U
1	2A	1098	A
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1319	G
1	2A	1321	A
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	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1509(A)	A
1	2A	1510	G
1	2A	1525	G
1	2A	1537	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1629	U
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1664	A
1	2A	1670	C
1	2A	1674	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1750	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1975	G
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	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	2096	U
1	2A	2099	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2100	G
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2111	C
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2144	U
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2150	U
1	2A	2151	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2175	C
1	2A	2180	U
1	2A	2181	G
1	2A	2183	C
1	2A	2186	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2187	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
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	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2407	G
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2473	U
1	2A	2474	C
1	2A	2476	A
1	2A	2487	G
1	2A	2491	U
1	2A	2492	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2744	G
1	2A	2757	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2789	C
1	2A	2802	G
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	2880	C
1	2A	2891	G
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2896	C
2	2B	2	C
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	30	C
2	2B	32	C
2	2B	35	U
2	2B	45	A
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	106	G
2	2B	109	C
2	2B	110	G
32	2a	5	U
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	60	A
32	2a	61	G
32	2a	66	G
32	2a	78	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	156	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	227	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	306	G
32	2a	318	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
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	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
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	631	G
32	2a	632	A
32	2a	653	A
32	2a	661	G
32	2a	665	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	703	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	859	A
32	2a	902	G
32	2a	914	A
32	2a	919	A
32	2a	920	U
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	980	C
32	2a	984	C
32	2a	989	C
32	2a	990	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1017	G
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1041	A
32	2a	1043	C
32	2a	1046	A
32	2a	1047	G
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1139	G
32	2a	1140	C
32	2a	1147	C
32	2a	1151	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1183	A
32	2a	1184	G
32	2a	1194	U
32	2a	1196	U
32	2a	1197	G
32	2a	1211	U
32	2a	1212	U
32	2a	1214	C
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1248	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1278	U
32	2a	1279	A
32	2a	1281	U
32	2a	1282	C
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1312	G
32	2a	1317	C
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1354	C
32	2a	1363	C
32	2a	1364	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1370	G
32	2a	1375	A
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1460	A
32	2a	1492	A
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	1528	U
32	2a	1529	G
32	2a	1530	G

All (68) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	839	U
1	1A	840	C
1	1A	888	C
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1142(A)	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1300	U
1	1A	1301	A
1	1A	1379	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	2116	G
1	1A	2126	A
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2602	A
1	1A	2689	U
1	2A	9	U
1	2A	195	A
1	2A	196	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	752	A
1	2A	764	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1608	A
1	2A	1992	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2406	U
1	2A	2439	A
1	2A	2601	C
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	5MC	2A	1942	1	19,22,23	1.62	3 (15%)	26,32,35	1.28	3 (11%)
1	5MC	1A	1942	1,54	19,22,23	1.54	3 (15%)	26,32,35	1.12	3 (11%)
32	5MC	1a	967	32	19,22,23	1.66	3 (15%)	26,32,35	1.07	2 (7%)
43	0TD	1l	92	43	8,9,10	4.50	1 (12%)	6,11,13	5.92	3 (50%)
32	4OC	2a	1402	32	20,23,24	0.76	1 (5%)	25,32,35	0.95	1 (4%)
1	PSU	1A	2605	1	18,21,22	1.35	3 (16%)	21,30,33	2.08	4 (19%)
32	2MG	1a	1207	32	23,26,27	1.26	2 (8%)	33,38,41	2.44	9 (27%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.02	3 (14%)
32	UR3	2a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.76	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
1	5MC	1A	1962	1,54	19,22,23	1.51	3 (15%)	26,32,35	1.06	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.36	3 (16%)	21,30,33	2.17	4 (19%)
43	0TD	2l	92	43	8,9,10	4.42	1 (12%)	6,11,13	2.32	3 (50%)
1	5MU	1A	1915	1,54	19,22,23	1.46	5 (26%)	27,32,35	2.29	8 (29%)
32	5MC	1a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.16	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1915	1	19,22,23	1.49	4 (21%)	27,32,35	2.27	9 (33%)
32	5MC	2a	967	32	19,22,23	2.01	3 (15%)	26,32,35	1.15	3 (11%)
1	5MU	2A	1939	1,54	19,22,23	1.47	6 (31%)	27,32,35	2.28	6 (22%)
32	G7M	2a	527	32	23,26,27	2.39	5 (21%)	34,39,42	3.05	10 (29%)
32	M2G	2a	966	32,54	24,27,28	1.27	3 (12%)	33,40,43	1.82	5 (15%)
32	4OC	1a	1402	32	20,23,24	0.75	1 (5%)	25,32,35	1.03	1 (4%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.11	9 (27%)
32	G7M	1a	527	32,54	23,26,27	2.33	5 (21%)	34,39,42	3.02	10 (29%)
32	2MG	2a	1207	32	23,26,27	1.25	4 (17%)	33,38,41	2.15	9 (27%)
1	5MC	2A	1962	1,54	19,22,23	1.57	3 (15%)	26,32,35	1.09	2 (7%)
32	5MC	2a	1400	32	19,22,23	1.60	3 (15%)	26,32,35	1.21	3 (11%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.85	6 (18%)
1	OMG	2A	2251	1,54	23,26,27	1.22	3 (13%)	32,38,41	1.95	5 (15%)
1	OMC	1A	1920	1,54	19,22,23	0.79	0	25,31,34	0.94	1 (4%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	1.93	8 (24%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.98	1 (4%)
32	UR3	1a	1498	32	19,22,23	0.94	1 (5%)	26,32,35	1.83	3 (11%)
1	2MA	2A	2503	1,54	22,25,26	1.44	4 (18%)	32,37,40	2.41	9 (28%)
1	OMU	2A	2552	1,54	19,22,23	1.30	2 (10%)	25,31,34	1.89	6 (24%)
1	MA6	1A	2058	1,54	23,26,27	0.40	0	33,38,41	2.04	9 (27%)
1	5MU	1A	1939	1	19,22,23	1.41	5 (26%)	27,32,35	2.19	6 (22%)
32	PSU	1a	516	32,54	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
32	PSU	2a	516	32,54	18,21,22	1.34	2 (11%)	21,30,33	2.08	5 (23%)
32	5MC	2a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.24	4 (15%)
1	PSU	2A	1911	1	18,21,22	1.41	3 (16%)	21,30,33	2.06	5 (23%)
32	MA6	2a	1518	32	23,26,27	0.41	0	33,38,41	2.02	9 (27%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	1.86	4 (19%)
1	OMG	1A	2251	1,54	23,26,27	1.26	3 (13%)	32,38,41	1.99	6 (18%)
1	2MA	1A	2503	1,54	22,25,26	1.50	5 (22%)	32,37,40	2.38	10 (31%)
32	5MC	1a	1407	32	19,22,23	1.71	3 (15%)	26,32,35	1.19	4 (15%)
1	OMU	1A	2552	1,54	19,22,23	1.33	4 (21%)	25,31,34	1.81	6 (24%)
1	MA6	2A	2058	1	23,26,27	0.38	0	33,38,41	1.95	9 (27%)
32	5MC	2a	1407	32	19,22,23	1.53	2 (10%)	26,32,35	1.09	3 (11%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.13	5 (23%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.17	9 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,54	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
1	5MU	1A	1915	1,54	-	2/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,54	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	0/7/25/26	0/3/3/3
32	M2G	2a	966	32,54	-	0/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
32	MA6	1a	1519	32	-	1/11/29/30	0/3/3/3
32	G7M	1a	527	32,54	-	1/7/25/26	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	OMG	2A	2251	1,54	-	0/9/27/28	0/3/3/3
1	OMC	1A	1920	1,54	-	1/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	OMC	2A	1920	1	-	2/9/27/28	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	1/7/25/26	0/3/3/3
1	OMU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
1	MA6	1A	2058	1,54	-	0/11/29/30	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,54	-	0/9/27/28	0/3/3/3
1	2MA	1A	2503	1,54	-	1/7/25/26	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
1	MA6	2A	2058	1	-	0/11/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	1/11/29/30	0/3/3/3

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.18	1.70	1.82
43	2l	92	0TD	CB-SB	-12.14	1.70	1.82
32	2a	527	G7M	C8-N7	7.77	1.46	1.33
32	2a	967	5MC	C5-C4	7.62	1.49	1.44
32	1a	527	G7M	C8-N7	7.31	1.45	1.33
32	2a	1404	5MC	C5-C4	6.40	1.49	1.44
32	1a	1407	5MC	C5-C4	6.32	1.48	1.44
32	1a	1400	5MC	C5-C4	6.21	1.48	1.44
32	1a	967	5MC	C5-C4	6.15	1.48	1.44
1	2A	1942	5MC	C5-C4	5.81	1.48	1.44
32	1a	1404	5MC	C5-C4	5.77	1.48	1.44
32	2a	1400	5MC	C5-C4	5.75	1.48	1.44
1	2A	1962	5MC	C5-C4	5.67	1.48	1.44
32	2a	1407	5MC	C5-C4	5.36	1.48	1.44
1	1A	1942	5MC	C5-C4	5.32	1.48	1.44
1	1A	1962	5MC	C5-C4	4.99	1.47	1.44
32	1a	527	G7M	C5-N7	-4.86	1.33	1.39
32	2a	527	G7M	C5-N7	-4.60	1.33	1.39
1	1A	2503	2MA	C5-C4	4.42	1.47	1.39
32	2a	527	G7M	C8-N9	4.36	1.47	1.35
1	2A	2503	2MA	C5-C4	4.25	1.46	1.39
32	1a	527	G7M	C8-N9	4.09	1.46	1.35
32	1a	527	G7M	C5-C4	3.76	1.47	1.38
32	2a	527	G7M	C5-C4	3.75	1.47	1.38
1	1A	1917	PSU	C6-C5	3.49	1.39	1.35
32	2a	516	PSU	C6-C5	3.48	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1911	PSU	C6-C5	3.46	1.39	1.35
1	2A	1911	PSU	C6-C5	3.42	1.39	1.35
32	1a	516	PSU	C6-C5	3.31	1.39	1.35
32	2a	1207	2MG	C5-C4	3.30	1.47	1.38
1	2A	1915	5MU	C2-N1	3.30	1.43	1.38
1	2A	1917	PSU	C6-C5	3.28	1.38	1.35
32	2a	966	M2G	C5-C4	3.27	1.47	1.38
32	1a	966	M2G	C5-C4	3.19	1.47	1.38
32	2a	967	5MC	C6-C5	3.14	1.39	1.34
1	1A	1915	5MU	C2-N1	3.13	1.43	1.38
1	1A	2251	OMG	C5-C4	3.11	1.47	1.38
1	2A	2251	OMG	C5-C4	3.07	1.47	1.38
1	2A	2605	PSU	C6-C5	3.01	1.38	1.35
32	1a	1207	2MG	C5-C4	3.01	1.47	1.38
1	2A	2552	OMU	C4-N3	-2.97	1.33	1.38
1	1A	1939	5MU	C6-C5	2.94	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.94	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.90	1.33	1.38
32	1a	1400	5MC	C6-C5	2.88	1.39	1.34
1	2A	1915	5MU	C6-C5	2.87	1.39	1.34
1	1A	2552	OMU	C4-N3	-2.85	1.33	1.38
32	1a	966	M2G	C6-N1	-2.84	1.33	1.38
32	1a	1404	5MC	C6-C5	2.82	1.39	1.34
32	2a	1400	5MC	C6-C5	2.81	1.39	1.34
32	2a	1407	5MC	C6-C5	2.80	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.79	1.33	1.38
1	2A	1939	5MU	C6-C5	2.77	1.39	1.34
1	2A	2503	2MA	C5-C6	2.76	1.48	1.41
1	1A	1962	5MC	C6-N1	-2.73	1.33	1.38
1	1A	1915	5MU	C4-N3	-2.73	1.33	1.38
1	2A	1942	5MC	C6-C5	2.72	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.71	1.33	1.38
1	1A	1962	5MC	C6-C5	2.69	1.39	1.34
1	1A	2251	OMG	C6-N1	-2.69	1.33	1.38
32	2a	1404	5MC	C6-C5	2.67	1.39	1.34
1	2A	1911	PSU	C4-N3	-2.67	1.33	1.38
32	1a	966	M2G	C2-N2	2.66	1.40	1.35
1	1A	2503	2MA	C5-C6	2.65	1.48	1.41
32	2a	966	M2G	C2-N2	2.65	1.40	1.35
1	2A	1962	5MC	C6-C5	2.64	1.38	1.34
1	1A	1942	5MC	C6-N1	-2.64	1.33	1.38
1	1A	1917	PSU	C4-N3	-2.63	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2605	PSU	C4-N3	-2.58	1.34	1.38
1	1A	1915	5MU	C6-C5	2.58	1.38	1.34
1	2A	1917	PSU	C4-N3	-2.57	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.57	1.34	1.38
32	1a	1407	5MC	C6-C5	2.57	1.38	1.34
1	1A	2251	OMG	C5-N7	-2.55	1.34	1.39
32	1a	967	5MC	C6-C5	2.54	1.38	1.34
1	1A	2503	2MA	C8-N7	2.53	1.36	1.31
1	2A	1939	5MU	C2-N3	-2.53	1.33	1.38
1	2A	1939	5MU	C4-C5	2.52	1.48	1.44
1	1A	2503	2MA	C5-N7	-2.52	1.34	1.39
32	1a	1207	2MG	C6-N1	-2.51	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.51	1.34	1.38
32	2a	516	PSU	C4-N3	-2.48	1.34	1.38
32	1a	516	PSU	C4-N3	-2.47	1.34	1.38
1	1A	1942	5MC	C6-C5	2.46	1.38	1.34
1	1A	2552	OMU	C2-N3	-2.44	1.33	1.38
1	2A	2552	OMU	C2-N3	-2.43	1.33	1.38
1	1A	1939	5MU	C6-N1	-2.42	1.33	1.38
1	2A	1915	5MU	C4-C5	2.41	1.48	1.44
1	1A	2605	PSU	C6-C5	2.39	1.37	1.35
32	2a	527	G7M	C6-N1	-2.36	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.33	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.30	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.29	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.29	1.34	1.38
1	1A	2552	OMU	C5-C4	2.28	1.48	1.43
1	1A	1915	5MU	C4-C5	2.28	1.48	1.44
32	2a	966	M2G	C6-N1	-2.27	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.26	1.34	1.39
1	2A	2503	2MA	C8-N7	2.26	1.36	1.31
32	2a	1404	5MC	C6-N1	-2.22	1.34	1.38
32	1a	527	G7M	C6-N1	-2.20	1.34	1.38
32	1a	966	M2G	C5-N7	-2.18	1.34	1.39
32	2a	1207	2MG	C2-N3	2.16	1.36	1.32
1	2A	2605	PSU	C2-N3	-2.16	1.33	1.37
32	1a	1407	5MC	C6-N1	-2.16	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.15	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.15	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.14	1.34	1.38
1	1A	1939	5MU	C4-C5	2.14	1.48	1.44
1	2A	1962	5MC	C6-N1	-2.13	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1498	UR3	C6-C5	2.09	1.39	1.35
32	1a	967	5MC	C6-N1	-2.09	1.34	1.38
1	2A	1939	5MU	C2-N1	2.09	1.41	1.38
1	2A	2503	2MA	C5-N7	-2.09	1.35	1.39
32	2a	1498	UR3	C6-C5	2.08	1.39	1.35
32	1a	1402	4OC	C6-C5	2.08	1.39	1.35
32	2a	1207	2MG	C5-N7	-2.07	1.34	1.39
1	1A	2605	PSU	C2-N1	-2.05	1.34	1.36
1	2A	1911	PSU	C2-N3	-2.05	1.34	1.37
32	2a	967	5MC	C6-N1	-2.05	1.34	1.38
1	1A	1915	5MU	C2-N3	-2.05	1.34	1.38
1	1A	2503	2MA	C4-N9	-2.04	1.33	1.37
1	1A	2552	OMU	C2-N1	2.01	1.41	1.38
32	2a	1402	4OC	C6-C5	2.00	1.39	1.35

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	13.66	126.92	102.36
1	2A	2503	2MA	C5-C4-N3	-8.38	118.35	127.18
32	2a	527	G7M	CN7-N7-C8	-8.36	112.13	124.79
32	1a	527	G7M	CN7-N7-C8	-8.34	112.16	124.79
1	1A	2503	2MA	C5-C4-N3	-8.31	118.42	127.18
32	1a	1498	UR3	C4-N3-C2	-7.47	118.57	124.58
32	1a	1207	2MG	C2-N3-C4	7.28	121.10	112.00
32	2a	1498	UR3	C4-N3-C2	-7.15	118.83	124.58
32	2a	527	G7M	N9-C8-N7	-6.91	95.70	112.48
32	2a	527	G7M	C8-N7-C5	6.88	116.39	107.78
32	2a	1207	2MG	C2-N3-C4	6.85	120.57	112.00
1	1A	1911	PSU	N1-C2-N3	6.73	122.27	115.17
32	1a	527	G7M	N9-C8-N7	-6.73	96.15	112.48
1	2A	2605	PSU	N1-C2-N3	6.62	122.16	115.17
1	2A	1911	PSU	N1-C2-N3	6.59	122.12	115.17
32	1a	527	G7M	C8-N7-C5	6.42	115.81	107.78
1	2A	2503	2MA	N3-C4-N9	6.39	135.10	126.99
1	2A	1917	PSU	N1-C2-N3	6.28	121.79	115.17
32	2a	516	PSU	N1-C2-N3	6.25	121.76	115.17
1	1A	2605	PSU	N1-C2-N3	6.24	121.75	115.17
1	2A	2251	OMG	C5-C4-N3	-6.24	118.46	128.39
32	1a	966	M2G	C5-C4-N3	-6.23	118.48	128.39
1	1A	2251	OMG	C5-C4-N3	-6.20	118.53	128.39
32	1a	527	G7M	N9-C4-N3	6.15	138.25	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	G7M	N9-C4-N3	6.06	138.07	125.95
32	1a	516	PSU	N1-C2-N3	6.06	121.56	115.17
32	2a	1207	2MG	C5-C4-N3	-6.04	118.78	128.39
32	1a	1207	2MG	C5-C4-N3	-5.92	118.98	128.39
32	2a	966	M2G	C5-C4-N3	-5.86	119.07	128.39
1	2A	1939	5MU	C4-N3-C2	-5.75	119.80	127.34
1	1A	2503	2MA	N3-C4-N9	5.72	134.25	126.99
1	1A	1917	PSU	N1-C2-N3	5.58	121.05	115.17
1	2A	1939	5MU	N3-C2-N1	5.53	122.09	114.89
32	2a	527	G7M	C5-C4-N3	-5.35	118.03	128.15
1	1A	1939	5MU	C4-N3-C2	-5.30	120.40	127.34
1	1A	2058	MA6	N1-C2-N3	-5.27	120.60	128.58
1	1A	1939	5MU	N3-C2-N1	5.25	121.72	114.89
32	1a	527	G7M	C5-C4-N3	-5.22	118.30	128.15
1	1A	2251	OMG	C2-N3-C4	5.00	120.91	112.30
1	2A	1915	5MU	N3-C2-N1	4.99	121.39	114.89
1	1A	2552	OMU	N3-C2-N1	4.99	121.39	114.89
1	2A	2552	OMU	N3-C2-N1	4.93	121.31	114.89
1	1A	1915	5MU	N3-C2-N1	4.91	121.29	114.89
32	1a	1519	MA6	C5-C4-N3	-4.89	119.99	126.72
1	2A	2251	OMG	C2-N3-C4	4.84	120.64	112.30
32	2a	1519	MA6	C5-C4-N3	-4.83	120.06	126.72
1	2A	1939	5MU	C5-C4-N3	4.82	119.52	115.32
32	1a	1518	MA6	N1-C2-N3	-4.78	121.34	128.58
1	1A	1915	5MU	C4-N3-C2	-4.76	121.10	127.34
1	2A	2552	OMU	C4-N3-C2	-4.75	120.71	126.61
32	2a	1518	MA6	N1-C2-N3	-4.75	121.39	128.58
32	1a	966	M2G	N9-C4-N3	4.72	135.38	125.95
1	1A	1939	5MU	C5-C4-N3	4.70	119.41	115.32
32	1a	1519	MA6	N1-C2-N3	-4.69	121.49	128.58
32	2a	1519	MA6	N1-C2-N3	-4.67	121.52	128.58
1	2A	1939	5MU	C5-C6-N1	-4.64	118.28	123.31
1	2A	2058	MA6	N1-C2-N3	-4.58	121.65	128.58
1	2A	1915	5MU	C4-N3-C2	-4.56	121.37	127.34
1	2A	2605	PSU	C4-N3-C2	-4.51	120.15	126.37
1	2A	2251	OMG	N9-C4-N3	4.51	134.97	125.95
1	1A	1915	5MU	C5-C4-N3	4.50	119.23	115.32
1	2A	1915	5MU	C1'-N1-C2	4.43	125.55	117.59
1	1A	2605	PSU	C4-N3-C2	-4.43	120.27	126.37
32	2a	527	G7M	C2-N3-C4	4.43	119.93	112.30
32	2a	966	M2G	C2-N3-C4	4.39	120.63	112.51
1	1A	2251	OMG	N9-C4-N3	4.39	134.74	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2058	MA6	C5-C4-N3	-4.37	120.70	126.72
32	2a	1207	2MG	N9-C4-N3	4.37	134.69	125.95
32	1a	966	M2G	C2-N3-C4	4.33	120.52	112.51
1	1A	1911	PSU	C4-N3-C2	-4.31	120.44	126.37
1	1A	1915	5MU	C1'-N1-C2	4.31	125.33	117.59
32	1a	527	G7M	C8-N9-C4	4.29	117.72	107.09
32	2a	516	PSU	C4-N3-C2	-4.28	120.48	126.37
32	2a	1519	MA6	C4-C5-N7	-4.25	105.72	110.58
1	1A	1939	5MU	O4-C4-C5	-4.23	120.08	124.92
32	2a	1519	MA6	C5-N7-C8	4.22	110.09	103.45
32	2a	527	G7M	C8-N9-C4	4.22	117.54	107.09
32	1a	527	G7M	C2-N3-C4	4.22	119.56	112.30
43	2l	92	0TD	CSB-SB-CB	4.22	109.94	102.36
1	1A	2058	MA6	C5-C4-N3	-4.20	120.94	126.72
32	1a	527	G7M	CN7-N7-C5	4.19	132.02	126.80
32	2a	966	M2G	N9-C4-N3	4.16	134.27	125.95
1	1A	2503	2MA	C4-C5-N7	-4.14	105.85	110.58
32	2a	1518	MA6	C2-N1-C6	4.13	121.92	111.83
32	1a	516	PSU	C4-N3-C2	-4.09	120.73	126.37
32	2a	1518	MA6	C5-N7-C8	4.02	109.77	103.45
32	1a	1207	2MG	C6-C5-N7	4.02	137.60	130.29
32	1a	1518	MA6	C2-N1-C6	4.01	121.62	111.83
1	2A	2503	2MA	C4-C5-N7	-4.00	106.01	110.58
1	2A	1917	PSU	C4-N3-C2	-4.00	120.87	126.37
1	2A	1911	PSU	C4-N3-C2	-3.99	120.88	126.37
1	2A	1942	5MC	C5-C6-N1	-3.99	118.98	123.31
32	2a	1518	MA6	C5-C4-N3	-3.96	121.27	126.72
32	2a	1518	MA6	C4-C5-N7	-3.93	106.09	110.58
1	1A	2605	PSU	O2-C2-N1	-3.93	118.74	122.79
1	1A	2552	OMU	C4-N3-C2	-3.90	121.77	126.61
32	2a	1519	MA6	C2-N1-C6	3.89	121.32	111.83
32	1a	1519	MA6	C5-N7-C8	3.87	109.54	103.45
32	1a	1519	MA6	C2-N1-C6	3.86	121.25	111.83
1	2A	1915	5MU	C5-C4-N3	3.84	118.66	115.32
1	2A	2058	MA6	C2-N1-C6	3.83	121.20	111.83
32	1a	1519	MA6	C4-C5-N7	-3.83	106.20	110.58
1	1A	2058	MA6	C2-N1-C6	3.82	121.16	111.83
1	2A	1917	PSU	O2-C2-N1	-3.79	118.88	122.79
1	2A	1915	5MU	O4-C4-C5	-3.78	120.59	124.92
32	2a	527	G7M	CN7-N7-C5	3.76	131.48	126.80
1	1A	1939	5MU	C5-C6-N1	-3.75	119.24	123.31
32	1a	1518	MA6	C5-N7-C8	3.75	109.35	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1915	5MU	O4-C4-C5	-3.75	120.62	124.92
1	1A	1911	PSU	O2-C2-N1	-3.75	118.92	122.79
32	1a	1400	5MC	C5-C6-N1	-3.73	119.27	123.31
43	1l	92	0TD	OD2-CG-CB	3.72	121.18	113.15
32	1a	1404	5MC	C5-C6-N1	-3.71	119.28	123.31
32	2a	967	5MC	C5-C6-N1	-3.71	119.28	123.31
1	1A	1917	PSU	C4-N3-C2	-3.70	121.27	126.37
32	2a	1400	5MC	C5-C6-N1	-3.70	119.30	123.31
1	1A	1915	5MU	C1'-N1-C6	-3.68	115.09	121.15
1	1A	2058	MA6	C2-N3-C4	3.66	120.78	111.83
1	1A	2058	MA6	C5-N7-C8	3.66	109.20	103.45
32	2a	1519	MA6	N9-C8-N7	-3.66	108.75	113.94
32	1a	1207	2MG	N9-C4-N3	3.64	133.24	125.95
32	1a	527	G7M	C1'-N9-C8	-3.63	114.48	126.74
1	2A	1915	5MU	C1'-N1-C6	-3.62	115.20	121.15
1	2A	1911	PSU	O2-C2-N1	-3.60	119.07	122.79
32	1a	1518	MA6	C4-C5-N7	-3.60	106.47	110.58
1	2A	2058	MA6	C5-N7-C8	3.58	109.08	103.45
1	2A	2058	MA6	C4-C5-N7	-3.53	106.55	110.58
1	1A	2058	MA6	N9-C8-N7	-3.52	108.94	113.94
32	1a	1518	MA6	C5-C4-N3	-3.52	121.88	126.72
32	2a	1518	MA6	N9-C8-N7	-3.50	108.97	113.94
32	2a	516	PSU	O2-C2-N1	-3.50	119.18	122.79
1	2A	1962	5MC	C5-C6-N1	-3.49	119.53	123.31
32	1a	1519	MA6	C2-N3-C4	3.48	120.33	111.83
1	2A	1939	5MU	O4-C4-C5	-3.48	120.94	124.92
32	2a	1519	MA6	C2-N3-C4	3.46	120.28	111.83
32	1a	1519	MA6	N9-C8-N7	-3.40	109.11	113.94
1	1A	1962	5MC	C5-C6-N1	-3.40	119.62	123.31
32	1a	1518	MA6	N9-C8-N7	-3.40	109.12	113.94
32	2a	1498	UR3	C5-C4-N3	3.40	119.51	115.04
32	2a	966	M2G	C6-C5-N7	3.36	136.41	130.29
32	1a	1498	UR3	C5-C4-N3	3.36	119.47	115.04
1	1A	1942	5MC	C5-C6-N1	-3.36	119.67	123.31
1	2A	2605	PSU	O2-C2-N1	-3.33	119.36	122.79
32	1a	1207	2MG	N1-C2-N2	3.32	119.95	116.56
1	1A	2503	2MA	N6-C6-N1	3.30	121.47	117.03
1	2A	2058	MA6	C2-N3-C4	3.28	119.84	111.83
1	1A	2552	OMU	C2'-C1'-N1	-3.27	108.04	114.24
32	1a	967	5MC	C5-C6-N1	-3.25	119.78	123.31
1	2A	2552	OMU	C5-C4-N3	3.24	119.34	114.80
1	1A	2058	MA6	C4-C5-N7	-3.24	106.88	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	516	PSU	O2-C2-N1	-3.22	119.47	122.79
32	2a	527	G7M	C1'-N9-C8	-3.21	115.91	126.74
1	1A	2251	OMG	C6-C5-N7	3.19	136.10	130.29
32	2a	1207	2MG	C6-C5-N7	3.18	136.07	130.29
32	2a	1518	MA6	C2-N3-C4	3.18	119.59	111.83
1	1A	1939	5MU	O2-C2-N1	-3.17	118.67	122.80
1	1A	1917	PSU	O2-C2-N1	-3.16	119.53	122.79
1	2A	2503	2MA	C4-N9-C8	3.12	109.01	105.74
32	1a	1207	2MG	C4-C5-N7	-3.11	105.74	110.67
1	2A	2058	MA6	N9-C8-N7	-3.09	109.55	113.94
32	1a	1518	MA6	C2-N3-C4	3.08	119.36	111.83
1	2A	2251	OMG	C6-C5-N7	3.06	135.85	130.29
32	1a	1519	MA6	N3-C4-N9	3.05	132.36	127.17
32	2a	1404	5MC	C5-C6-N1	-3.03	120.02	123.31
32	2a	1407	5MC	C5-C6-N1	-3.03	120.03	123.31
1	2A	2503	2MA	C5-N7-C8	3.00	108.17	103.45
32	1a	1519	MA6	C4-C5-C6	2.97	118.98	115.91
32	2a	1404	5MC	C5-C4-N3	-2.93	118.76	121.75
1	2A	2552	OMU	C2'-C1'-N1	-2.92	108.70	114.24
32	1a	1407	5MC	C5-C6-N1	-2.92	120.15	123.31
1	1A	2503	2MA	C5-N7-C8	2.90	108.01	103.45
1	1A	2058	MA6	N3-C4-N9	2.89	132.08	127.17
32	2a	1519	MA6	N3-C4-N9	2.87	132.05	127.17
32	1a	966	M2G	C6-C5-N7	2.87	135.52	130.29
1	2A	2503	2MA	N6-C6-N1	2.87	120.89	117.03
43	2l	92	0TD	OD2-CG-CB	2.87	119.34	113.15
32	2a	1519	MA6	C4-C5-C6	2.86	118.87	115.91
32	1a	1402	4OC	C6-C5-C4	2.86	120.44	117.00
1	1A	1915	5MU	O2-C2-N3	-2.80	116.33	121.49
32	1a	1407	5MC	C5-C4-N3	-2.78	118.90	121.75
1	1A	2503	2MA	CM2-C2-N1	2.78	121.29	117.13
32	1a	527	G7M	O6-C6-C5	-2.73	121.92	128.01
1	1A	2251	OMG	C4-C5-N7	-2.71	106.38	110.67
32	1a	1207	2MG	N2-C2-N3	-2.71	117.06	120.51
32	2a	1400	5MC	C5-C4-N3	-2.69	119.00	121.75
1	2A	2605	PSU	C5-C6-N1	-2.69	118.41	122.14
32	1a	1400	5MC	C5-C4-N3	-2.68	119.00	121.75
1	2A	1939	5MU	O2-C2-N1	-2.66	119.33	122.80
1	2A	1942	5MC	O2-C2-N3	-2.66	118.14	122.33
32	2a	1407	5MC	C5-C4-N3	-2.65	119.03	121.75
1	2A	2058	MA6	N3-C4-N9	2.65	131.67	127.17
32	2a	966	M2G	C4-C5-N7	-2.64	106.49	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	967	5MC	C5-C4-N3	-2.63	119.05	121.75
1	1A	1942	5MC	C5-C4-N3	-2.61	119.08	121.75
32	2a	1207	2MG	C4-C5-N7	-2.61	106.53	110.67
1	2A	2503	2MA	N9-C8-N7	-2.59	110.26	113.94
1	2A	2552	OMU	O2-C2-N1	-2.59	119.43	122.80
1	1A	1920	OMC	O2-C2-N3	-2.57	118.27	122.33
1	1A	1915	5MU	C5-C6-N1	-2.57	120.52	123.31
1	2A	2251	OMG	C4-C5-N7	-2.54	106.65	110.67
1	2A	1942	5MC	C5-C4-N3	-2.54	119.16	121.75
1	1A	2503	2MA	C6-C5-N7	2.53	136.96	132.09
32	2a	1404	5MC	O2-C2-N3	-2.51	118.37	122.33
1	2A	1915	5MU	O2-C2-N3	-2.51	116.86	121.49
32	1a	1498	UR3	C3U-N3-C2	2.51	121.70	117.33
32	1a	1207	2MG	CM2-N2-C2	-2.50	118.27	123.65
32	2a	516	PSU	O4'-C1'-C2'	2.48	108.58	105.15
32	1a	967	5MC	C5-C4-N3	-2.48	119.21	121.75
1	1A	2552	OMU	C5-C4-N3	2.48	118.27	114.80
43	1l	92	0TD	OD1-CG-CB	-2.47	117.27	122.44
32	2a	1402	4OC	C6-C5-C4	2.45	119.96	117.00
1	2A	2552	OMU	O4-C4-C5	-2.45	120.93	125.16
1	2A	2503	2MA	C6-C5-N7	2.45	136.82	132.09
32	1a	1207	2MG	O3'-C3'-C2'	2.45	119.66	111.82
32	1a	1407	5MC	CM5-C5-C6	-2.44	119.55	122.85
1	2A	2503	2MA	C2-N1-C6	2.42	121.82	118.10
32	2a	527	G7M	O6-C6-C5	-2.40	122.64	128.01
1	2A	1915	5MU	C5-C6-N1	-2.40	120.70	123.31
1	1A	2605	PSU	C5-C6-N1	-2.39	118.82	122.14
32	1a	1404	5MC	C5-C4-N3	-2.39	119.31	121.75
1	1A	2251	OMG	O6-C6-C5	-2.34	120.35	126.53
32	1a	1407	5MC	O2-C2-N3	-2.34	118.65	122.33
32	2a	1518	MA6	N3-C4-N9	2.32	131.11	127.17
1	2A	1920	OMC	O2-C2-N3	-2.30	118.71	122.33
32	2a	1404	5MC	CM5-C5-C6	-2.30	119.74	122.85
1	2A	2058	MA6	C4-C5-C6	2.29	118.28	115.91
32	1a	966	M2G	C4-C5-N7	-2.28	107.05	110.67
1	1A	2503	2MA	C2-N1-C6	2.28	121.61	118.10
32	2a	1400	5MC	O2-C2-N3	-2.27	118.75	122.33
32	2a	516	PSU	C5-C6-N1	-2.23	119.05	122.14
1	2A	1962	5MC	C5-C4-N3	-2.23	119.47	121.75
1	1A	1962	5MC	C5-C4-N3	-2.23	119.47	121.75
32	2a	1407	5MC	O2-C2-N3	-2.22	118.82	122.33
32	2a	1518	MA6	C4-C5-C6	2.22	118.20	115.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	N9-C8-N7	-2.22	110.79	113.94
1	1A	2503	2MA	C4-N9-C8	2.18	108.02	105.74
1	1A	1911	PSU	C5-C6-N1	-2.17	119.13	122.14
1	1A	2058	MA6	C4-N9-C8	2.14	107.99	105.74
1	1A	2552	OMU	O4-C4-C5	-2.13	121.48	125.16
1	1A	1942	5MC	CM5-C5-C6	-2.12	119.98	122.85
32	1a	966	M2G	O6-C6-C5	-2.10	121.00	126.53
32	2a	1207	2MG	N1-C2-N2	2.09	118.70	116.56
1	2A	1915	5MU	C6-N1-C2	-2.09	119.22	121.30
32	1a	1518	MA6	N3-C4-N9	2.06	130.68	127.17
1	2A	1911	PSU	O4'-C1'-C2'	2.06	108.01	105.15
32	1a	516	PSU	C5-C6-N1	-2.06	119.28	122.14
43	2l	92	0TD	OD1-CG-CB	-2.05	118.14	122.44
1	1A	2552	OMU	O2-C2-N1	-2.04	120.14	122.80
32	2a	1207	2MG	O6-C6-C5	-2.04	121.15	126.53
1	2A	1911	PSU	C5-C6-N1	-2.03	119.32	122.14
32	2a	1498	UR3	C3U-N3-C2	2.03	120.86	117.33
32	2a	1207	2MG	N2-C2-N3	-2.02	117.94	120.51
1	1A	1911	PSU	O4'-C1'-C2'	2.01	107.94	105.15
32	2a	1207	2MG	CM2-N2-C2	-2.00	119.34	123.65
32	2a	967	5MC	CM5-C5-C6	-2.00	120.14	122.85
1	1A	1917	PSU	C6-C5-C4	-2.00	116.82	118.17

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1519	MA6	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C2'-O2'-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CA-CB-SB-CSB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	2a	1402	4OC	C1'-C2'-O2'-CM2
1	1A	1920	OMC	C3'-C2'-O2'-CM2
1	2A	1920	OMC	C3'-C2'-O2'-CM2
1	2A	1920	OMC	C2'-C1'-N1-C2

There are no ring outliers.

21 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	1l	92	0TD	1	0
32	2a	1402	4OC	3	0
43	2l	92	0TD	1	0
32	1a	1400	5MC	2	0
32	2a	967	5MC	1	0
1	2A	1939	5MU	1	0
32	1a	1402	4OC	1	0
32	1a	1519	MA6	3	0
32	2a	1207	2MG	3	0
32	2a	1400	5MC	2	0
1	1A	1920	OMC	1	0
32	1a	1518	MA6	2	0
1	2A	1920	OMC	1	0
32	1a	1498	UR3	1	0
1	2A	2503	2MA	1	0
1	1A	2058	MA6	3	0
32	2a	1518	MA6	1	0
1	1A	1917	PSU	1	0
1	1A	2251	OMG	1	0
1	2A	2058	MA6	1	0
32	2a	1519	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2493 ligands modelled in this entry, 2478 are monoatomic - leaving 15 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
56	ZIT	2A	3713	-	54,54,54	0.91	1 (1%)	82,83,83	1.66	16 (19%)
55	HGR	2A	3712	-	39,39,39	2.39	8 (20%)	48,58,58	1.66	13 (27%)
57	MPD	2A	3714	-	7,7,7	0.36	0	9,10,10	0.35	0
57	MPD	2B	219	-	7,7,7	0.33	0	9,10,10	0.24	0
57	MPD	1A	4034	-	7,7,7	0.36	0	9,10,10	0.38	0
58	ARG	1F	319	54	10,11,11	0.71	1 (10%)	9,13,13	0.99	1 (11%)
55	HGR	1A	4032	-	39,39,39	2.42	9 (23%)	48,58,58	1.70	13 (27%)
56	ZIT	1A	4033	-	54,54,54	0.90	1 (1%)	82,83,83	1.45	11 (13%)
58	ARG	1B	230	-	10,11,11	0.76	1 (10%)	9,13,13	1.10	1 (11%)
57	MPD	18	103	-	7,7,7	0.32	0	9,10,10	0.37	0
57	MPD	2A	3715	-	7,7,7	0.32	0	9,10,10	0.25	0
57	MPD	1T	207	-	7,7,7	0.35	0	9,10,10	0.30	0
57	MPD	1a	1882	32	7,7,7	0.41	0	9,10,10	0.61	0
60	SF4	2d	501	35	0,12,12	-	-	-	-	-
60	SF4	1d	303	35	0,12,12	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	ZIT	2A	3713	-	-	15/72/107/107	0/3/3/3
55	HGR	2A	3712	-	-	5/20/79/79	0/4/4/4
57	MPD	2A	3714	-	-	0/5/5/5	-
57	MPD	2B	219	-	-	5/5/5/5	-
57	MPD	1A	4034	-	-	2/5/5/5	-
58	ARG	1F	319	54	-	5/11/11/11	-
55	HGR	1A	4032	-	-	5/20/79/79	0/4/4/4
56	ZIT	1A	4033	-	-	9/72/107/107	0/3/3/3
58	ARG	1B	230	-	-	5/11/11/11	-
57	MPD	18	103	-	-	3/5/5/5	-
57	MPD	2A	3715	-	-	5/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	1T	207	-	-	1/5/5/5	-
57	MPD	1a	1882	32	-	3/5/5/5	-
60	SF4	2d	501	35	-	-	0/6/5/5
60	SF4	1d	303	35	-	-	0/6/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4032	HGR	C12-C14	9.06	1.55	1.33
55	2A	3712	HGR	C12-C14	8.98	1.54	1.33
55	1A	4032	HGR	C5-C4	-5.56	1.39	1.49
55	2A	3712	HGR	C5-C4	-5.54	1.39	1.49
56	2A	3713	ZIT	O14-C1	5.35	1.46	1.34
55	1A	4032	HGR	C5-C6	-5.30	1.39	1.50
55	2A	3712	HGR	C5-C6	-5.28	1.39	1.50
56	1A	4033	ZIT	O14-C1	5.27	1.46	1.34
55	2A	3712	HGR	C3-C2	-4.90	1.39	1.48
55	1A	4032	HGR	C3-C2	-4.67	1.39	1.48
55	1A	4032	HGR	O4-C2	4.44	1.36	1.24
55	2A	3712	HGR	O4-C2	4.28	1.35	1.24
55	1A	4032	HGR	O8-C23	2.79	1.46	1.41
55	1A	4032	HGR	C8-C7	-2.52	1.50	1.53
55	2A	3712	HGR	O8-C23	2.33	1.45	1.41
55	2A	3712	HGR	O1-C10	2.17	1.45	1.41
55	1A	4032	HGR	O1-C10	2.17	1.45	1.41
58	1B	230	ARG	OXT-C	-2.17	1.23	1.30
55	2A	3712	HGR	C1-C2	-2.07	1.39	1.44
55	1A	4032	HGR	C1-C2	-2.07	1.39	1.44
58	1F	319	ARG	OXT-C	-2.04	1.24	1.30

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	4033	ZIT	O1A-C5-C6	4.82	112.14	106.40
56	2A	3713	ZIT	O3B-C3B-C2B	-4.47	106.07	112.95
55	2A	3712	HGR	C4-C5-C6	4.31	121.56	112.35
55	1A	4032	HGR	C4-C5-C6	4.30	121.53	112.35
56	1A	4033	ZIT	O3B-C3B-C4B	4.27	110.05	103.86
55	1A	4032	HGR	C23-O9-C22	-4.00	100.21	106.31
56	2A	3713	ZIT	O3B-C3B-C4B	3.89	109.50	103.86
56	2A	3713	ZIT	C2B-C3B-C4B	3.85	114.23	107.64
56	2A	3713	ZIT	C4A-C3A-N3A	-3.79	104.95	115.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2A	3713	ZIT	O1A-C5-C6	3.52	110.60	106.40
56	1A	4033	ZIT	O14-C1-C2	3.48	118.96	111.53
56	1A	4033	ZIT	C14-O14-C1	-3.29	112.46	118.20
56	1A	4033	ZIT	C8B-O3B-C3B	3.28	124.19	117.51
55	1A	4032	HGR	C4-C3-C2	-3.27	118.99	121.81
56	2A	3713	ZIT	C15-C14-C13	-3.20	109.34	115.20
56	2A	3713	ZIT	O14-C1-C2	3.18	118.33	111.53
58	1B	230	ARG	OXT-C-O	-3.16	116.90	124.08
55	2A	3712	HGR	O9-C22-C18	-3.08	99.51	106.03
55	2A	3712	HGR	O1-C10-C9	-2.99	101.17	104.98
55	2A	3712	HGR	O8-C18-C22	-2.99	99.71	106.03
55	2A	3712	HGR	C4-C3-C2	-2.97	119.25	121.81
55	2A	3712	HGR	O4-C2-C3	-2.95	116.85	121.28
56	1A	4033	ZIT	O3B-C3B-C2B	-2.95	108.41	112.95
56	2A	3713	ZIT	C3B-C4B-C5B	2.92	115.36	111.12
55	1A	4032	HGR	O3-C3-C2	2.88	117.74	112.51
56	2A	3713	ZIT	O1B-C3-C4	2.88	111.63	108.23
55	1A	4032	HGR	O3-C10-C9	2.88	111.36	106.69
58	1F	319	ARG	OXT-C-O	-2.85	117.62	124.08
56	2A	3713	ZIT	C6-C5-C4	-2.82	109.80	113.89
55	1A	4032	HGR	O1-C10-C9	-2.81	101.41	104.98
55	2A	3712	HGR	O3-C10-C9	2.72	111.11	106.69
55	1A	4032	HGR	C10-C9-C8	-2.71	98.91	102.29
56	2A	3713	ZIT	C6A-C5A-C4A	-2.71	109.18	113.27
55	2A	3712	HGR	C10-C9-C8	-2.66	98.97	102.29
55	1A	4032	HGR	O9-C22-C18	-2.64	100.45	106.03
55	2A	3712	HGR	C12-C6-C1	-2.60	116.45	119.35
55	1A	4032	HGR	C1-C2-C3	2.59	120.93	116.06
55	2A	3712	HGR	C1-C2-C3	2.57	120.88	116.06
55	1A	4032	HGR	C12-C6-C1	-2.56	116.50	119.35
55	2A	3712	HGR	O3-C3-C2	2.55	117.14	112.51
56	2A	3713	ZIT	O5B-C5B-C6B	2.53	112.36	106.74
56	1A	4033	ZIT	O5B-C5B-C4B	2.52	114.38	110.04
56	1A	4033	ZIT	O1B-C3-C4	2.52	111.21	108.23
56	1A	4033	ZIT	C9-N10-C11	-2.45	107.99	112.06
56	2A	3713	ZIT	C1B-O5B-C5B	2.41	120.43	113.82
55	1A	4032	HGR	O4-C2-C3	-2.39	117.69	121.28
55	2A	3712	HGR	C23-O9-C22	-2.37	102.70	106.31
55	1A	4032	HGR	O8-C18-C22	-2.27	101.23	106.03
55	1A	4032	HGR	C19-C17-N1	2.26	114.78	110.62
55	2A	3712	HGR	C10-O3-C3	-2.14	110.78	115.41
56	2A	3713	ZIT	O14-C1-O1	-2.09	120.18	123.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2A	3713	ZIT	O5A-C5A-C6A	2.04	110.70	106.88
56	1A	4033	ZIT	C6-C5-C4	-2.03	110.94	113.89
56	2A	3713	ZIT	C8B-O3B-C3B	2.00	121.59	117.51
56	1A	4033	ZIT	C4A-C3A-N3A	-2.00	109.97	115.59

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	1A	4033	ZIT	C19-C6-C7-C8
56	1A	4033	ZIT	O6-C6-C7-C8
56	1A	4033	ZIT	C12-C11-N10-C21
56	1A	4033	ZIT	C22-C11-N10-C21
56	1A	4033	ZIT	C4B-C3B-O3B-C8B
56	2A	3713	ZIT	C7-C8-C9-N10
56	2A	3713	ZIT	C20-C8-C9-N10
56	2A	3713	ZIT	C2B-C3B-O3B-C8B
56	2A	3713	ZIT	C4B-C3B-O3B-C8B
56	2A	3713	ZIT	C7B-C3B-O3B-C8B
57	1a	1882	MPD	C2-C3-C4-O4
57	1a	1882	MPD	C2-C3-C4-C5
57	2A	3715	MPD	C2-C3-C4-O4
57	2A	3715	MPD	C2-C3-C4-C5
58	1B	230	ARG	NE-CD-CG-CB
58	1F	319	ARG	NE-CD-CG-CB
58	1F	319	ARG	OXT-C-CA-CB
56	1A	4033	ZIT	C2B-C3B-O3B-C8B
58	1F	319	ARG	O-C-CA-CB
58	1F	319	ARG	OXT-C-CA-N
56	1A	4033	ZIT	O1A-C5-C6-C7
56	1A	4033	ZIT	C4-C5-C6-O6
58	1B	230	ARG	CA-CB-CG-CD
58	1B	230	ARG	O-C-CA-N
58	1F	319	ARG	O-C-CA-N
56	2A	3713	ZIT	C22-C11-C12-C13
55	1A	4032	HGR	C12-C14-C15-O7
55	2A	3712	HGR	C12-C14-C15-O7
55	2A	3712	HGR	C12-C14-C15-N1
58	1B	230	ARG	C-CA-CB-CG
57	1A	4034	MPD	O2-C2-C3-C4
57	2A	3715	MPD	O2-C2-C3-C4
55	1A	4032	HGR	C2-C3-O3-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	2A	3712	HGR	C2-C3-O3-C10
57	2B	219	MPD	C2-C3-C4-O4
57	2A	3715	MPD	C1-C2-C3-C4
57	2A	3715	MPD	CM-C2-C3-C4
57	2B	219	MPD	CM-C2-C3-C4
56	2A	3713	ZIT	O12-C12-C13-O13
56	2A	3713	ZIT	N10-C11-C12-O12
56	2A	3713	ZIT	C22-C11-C12-O12
57	2B	219	MPD	C2-C3-C4-C5
55	1A	4032	HGR	C12-C14-C15-N1
56	1A	4033	ZIT	C2A-C3A-N3A-C8A
55	1A	4032	HGR	C16-C14-C15-O7
55	2A	3712	HGR	C16-C14-C15-O7
56	2A	3713	ZIT	C19-C6-C7-C8
56	2A	3713	ZIT	O14-C14-C15-C16
56	2A	3713	ZIT	O12-C12-C13-C14
55	2A	3712	HGR	C16-C14-C15-N1
58	1B	230	ARG	OXT-C-CA-N
57	18	103	MPD	O2-C2-C3-C4
57	2B	219	MPD	O2-C2-C3-C4
57	1A	4034	MPD	C2-C3-C4-O4
57	1T	207	MPD	C2-C3-C4-O4
57	18	103	MPD	C1-C2-C3-C4
57	18	103	MPD	CM-C2-C3-C4
57	1a	1882	MPD	CM-C2-C3-C4
57	2B	219	MPD	C1-C2-C3-C4
56	2A	3713	ZIT	C12-C11-N10-C9
56	2A	3713	ZIT	C11-C12-C13-C23
56	2A	3713	ZIT	C11-C12-C13-O13
55	1A	4032	HGR	C16-C14-C15-N1

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	2A	3713	ZIT	2	0
55	2A	3712	HGR	2	0
57	1A	4034	MPD	1	0
58	1F	319	ARG	1	0
55	1A	4032	HGR	2	0
56	1A	4033	ZIT	6	0
58	1B	230	ARG	3	0

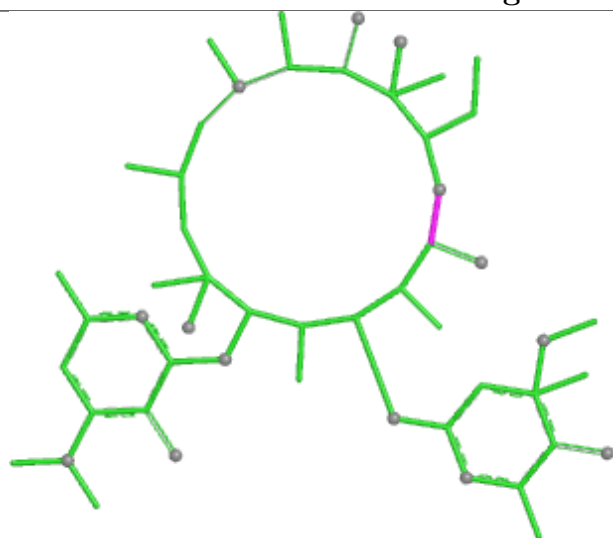
Continued on next page...

Continued from previous page...

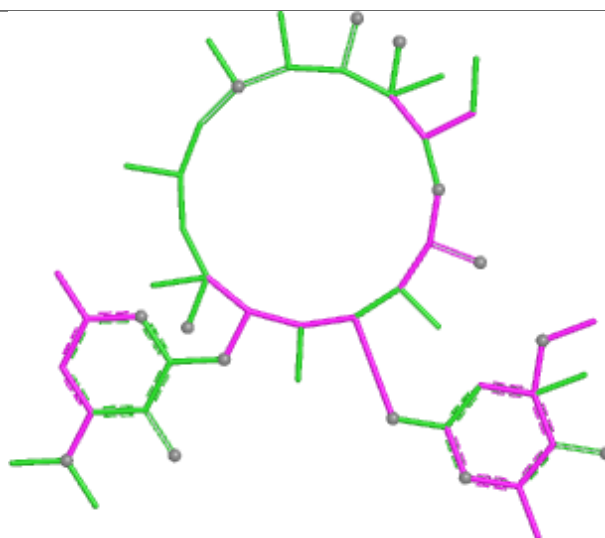
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1a	1882	MPD	5	0
60	1d	303	SF4	1	0

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

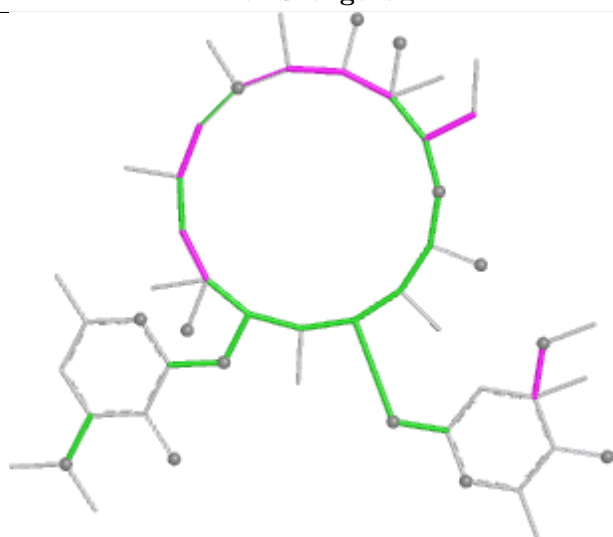
Ligand ZIT 2A 3713



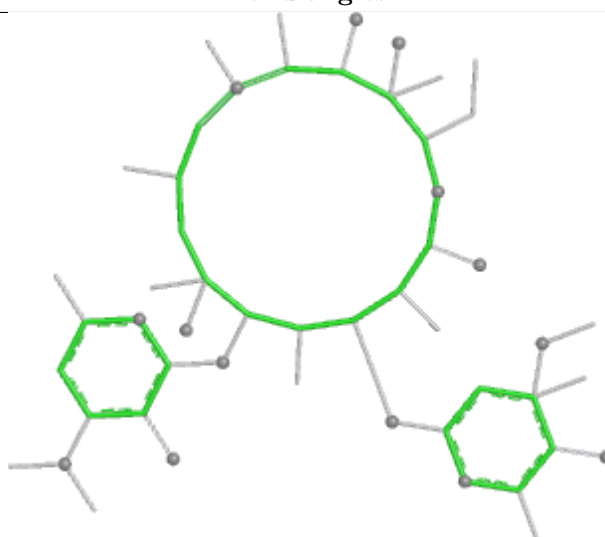
Bond lengths



Bond angles

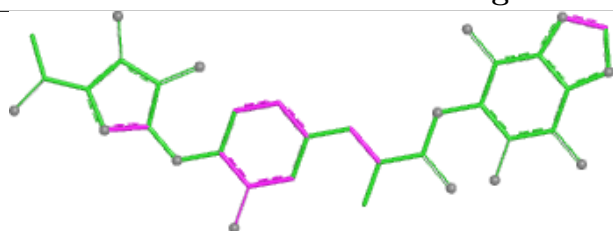


Torsions

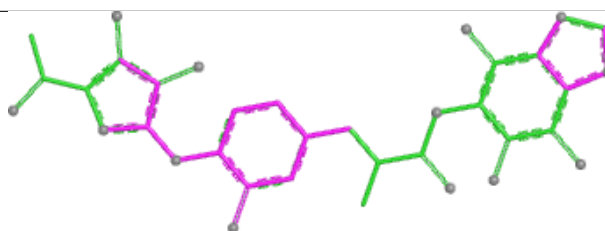


Rings

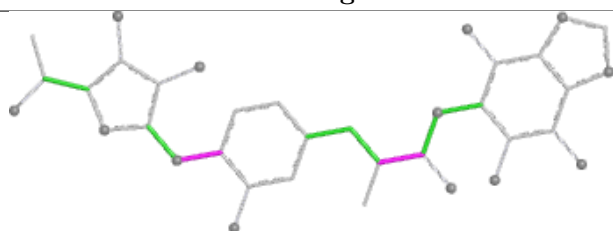
Ligand HGR 2A 3712



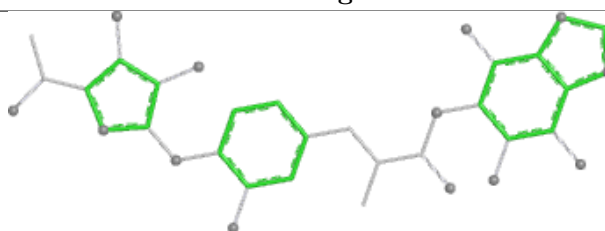
Bond lengths



Bond angles

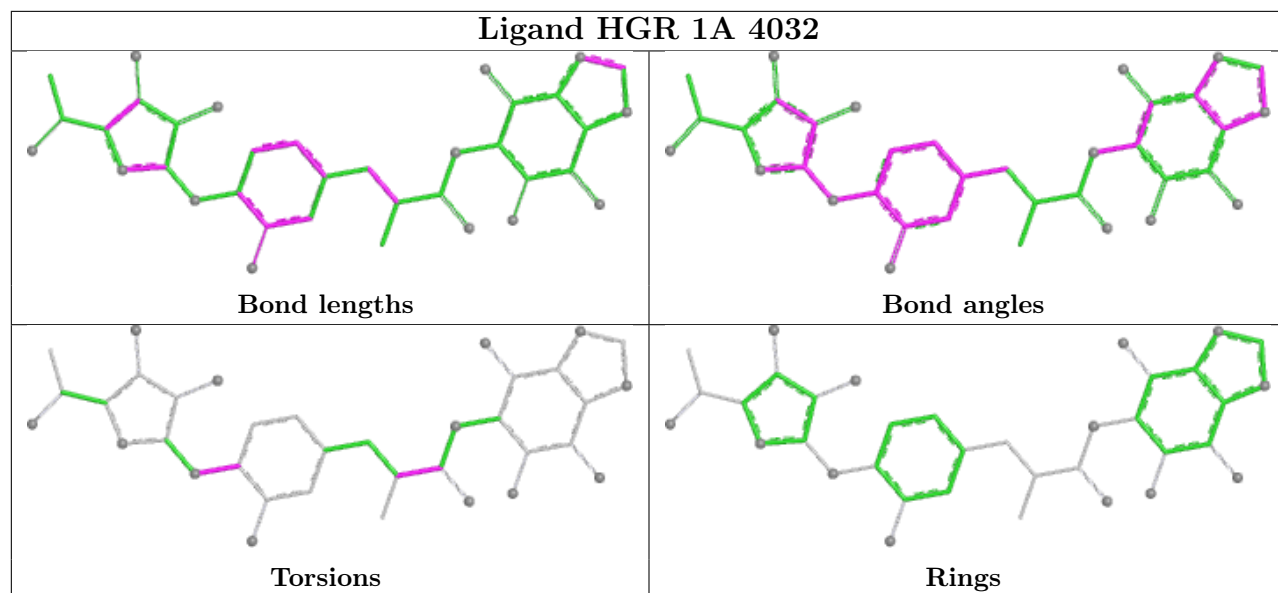


Torsions

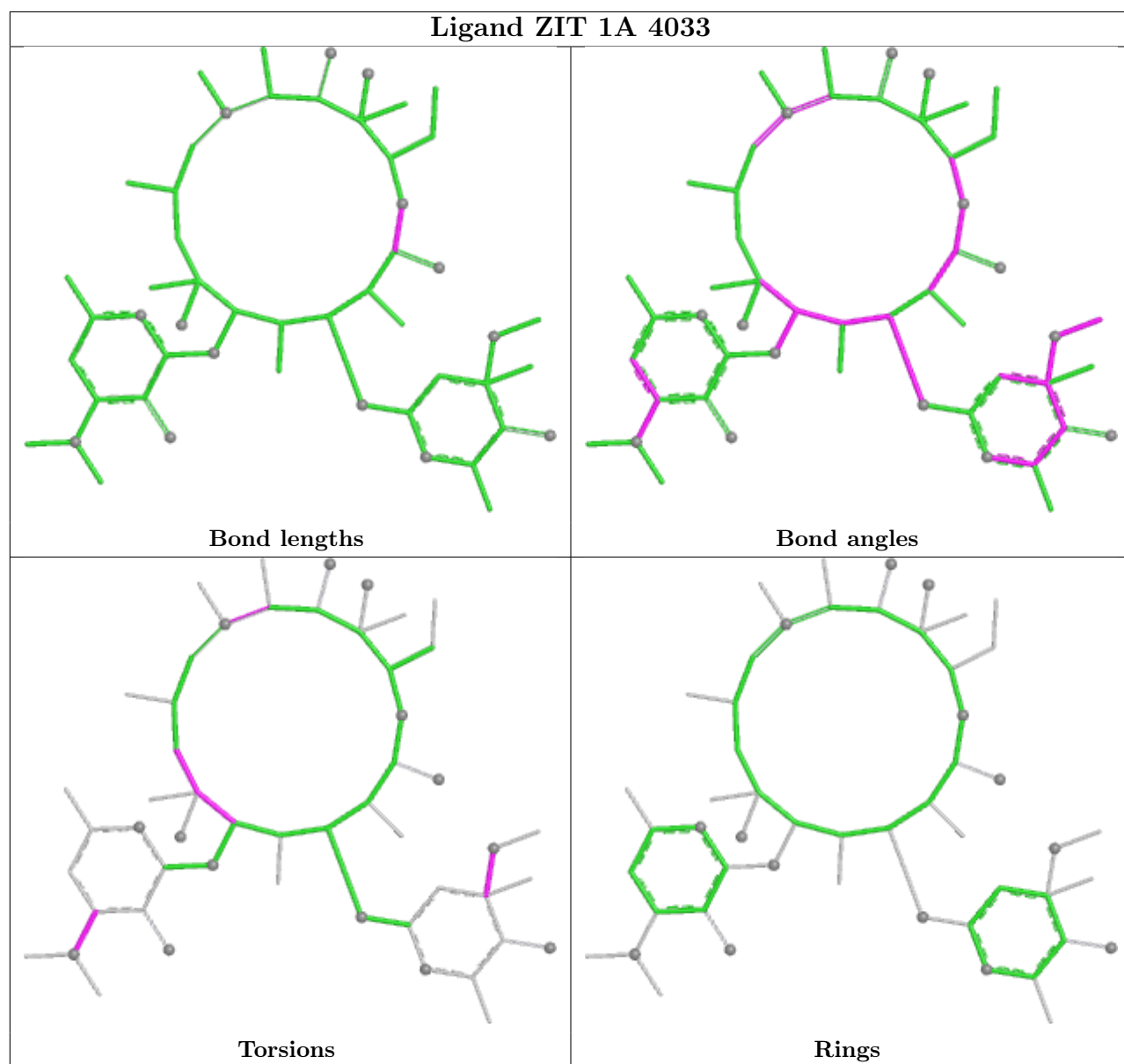


Rings

Ligand HGR 1A 4032



Ligand ZIT 1A 4033



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%)	-0.58	133 (4%)	36	28	24, 40, 101, 113	0
1	2A	2855/2915 (97%)	-0.17	150 (5%)	32	25	34, 57, 103, 114	0
2	1B	120/121 (99%)	-0.41	1 (0%)	82	79	36, 56, 70, 89	0
2	2B	120/121 (99%)	0.35	1 (0%)	82	79	63, 82, 90, 100	0
3	1D	275/276 (99%)	-0.17	3 (1%)	78	75	24, 40, 55, 81	0
3	2D	275/276 (99%)	0.09	5 (1%)	67	63	32, 51, 64, 87	0
4	1E	204/206 (99%)	-0.19	1 (0%)	87	85	23, 43, 66, 79	0
4	2E	204/206 (99%)	0.16	3 (1%)	72	67	34, 57, 74, 86	0
5	1F	203/210 (96%)	-0.05	3 (1%)	72	67	24, 46, 72, 89	0
5	2F	203/210 (96%)	0.38	3 (1%)	72	67	35, 68, 82, 91	0
6	1G	181/182 (99%)	0.48	8 (4%)	39	31	54, 73, 85, 93	0
6	2G	181/182 (99%)	1.64	58 (32%)	1	0	77, 89, 96, 99	0
7	1H	174/180 (96%)	0.17	2 (1%)	78	75	39, 56, 70, 75	0
7	2H	173/180 (96%)	0.92	13 (7%)	20	15	71, 84, 91, 95	0
8	1I	147/148 (99%)	0.63	6 (4%)	41	33	46, 74, 84, 90	0
8	2I	146/148 (98%)	0.74	6 (4%)	41	33	58, 77, 88, 92	0
9	1N	140/140 (100%)	-0.16	1 (0%)	84	82	30, 43, 65, 81	0
9	2N	140/140 (100%)	0.51	2 (1%)	73	69	47, 65, 78, 87	0
10	1O	122/122 (100%)	-0.28	0	100	100	33, 43, 63, 69	0
10	2O	122/122 (100%)	0.23	0	100	100	45, 57, 70, 77	0
11	1P	149/150 (99%)	0.05	0	100	100	25, 50, 70, 88	0
11	2P	149/150 (99%)	0.34	3 (2%)	65	59	40, 68, 84, 91	0
12	1Q	141/141 (100%)	-0.20	1 (0%)	84	82	30, 44, 56, 71	0
12	2Q	141/141 (100%)	0.60	4 (2%)	55	48	48, 67, 79, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.24	0 100 100	30, 40, 57, 65	0
13	2R	118/118 (100%)	0.10	1 (0%) 82 79	39, 53, 66, 71	0
14	1S	110/112 (98%)	0.07	1 (0%) 81 78	45, 57, 71, 75	0
14	2S	110/112 (98%)	1.15	18 (16%) 4 3	66, 77, 84, 87	0
15	1T	131/146 (89%)	0.06	4 (3%) 51 43	36, 48, 71, 86	0
15	2T	131/146 (89%)	0.31	4 (3%) 51 43	50, 60, 78, 86	0
16	1U	116/118 (98%)	-0.38	0 100 100	28, 35, 52, 67	0
16	2U	116/118 (98%)	0.32	1 (0%) 81 78	42, 61, 76, 85	0
17	1V	101/101 (100%)	-0.29	0 100 100	25, 46, 62, 76	0
17	2V	101/101 (100%)	0.44	0 100 100	43, 73, 81, 87	0
18	1W	112/113 (99%)	-0.21	2 (1%) 67 63	28, 36, 56, 86	0
18	2W	112/113 (99%)	-0.01	1 (0%) 81 78	39, 51, 71, 93	0
19	1X	95/96 (98%)	0.01	3 (3%) 50 42	33, 45, 70, 78	0
19	2X	95/96 (98%)	0.41	3 (3%) 50 42	46, 62, 77, 85	0
20	1Y	107/110 (97%)	0.10	2 (1%) 66 61	40, 53, 69, 78	0
20	2Y	107/110 (97%)	0.61	4 (3%) 45 37	59, 71, 82, 87	0
21	1Z	203/206 (98%)	0.37	3 (1%) 72 67	47, 63, 77, 87	0
21	2Z	201/206 (97%)	0.75	3 (1%) 72 67	66, 79, 88, 94	0
22	10	77/85 (90%)	-0.09	1 (1%) 75 71	34, 42, 62, 69	0
22	20	77/85 (90%)	0.64	6 (7%) 19 14	53, 66, 77, 81	0
23	11	97/98 (98%)	0.09	1 (1%) 79 76	31, 50, 74, 84	0
23	21	97/98 (98%)	0.29	2 (2%) 63 57	43, 56, 75, 84	0
24	12	70/72 (97%)	0.11	2 (2%) 53 46	41, 53, 65, 89	0
24	22	70/72 (97%)	0.48	1 (1%) 73 69	61, 72, 79, 80	0
25	13	59/60 (98%)	-0.09	1 (1%) 69 64	32, 41, 68, 76	0
25	23	59/60 (98%)	0.75	4 (6%) 23 17	53, 64, 78, 85	0
26	14	69/71 (97%)	0.77	8 (11%) 9 8	66, 85, 95, 98	0
26	24	69/71 (97%)	1.89	23 (33%) 1 0	86, 95, 100, 103	0
27	15	59/60 (98%)	-0.30	0 100 100	27, 39, 61, 71	0
27	25	59/60 (98%)	-0.15	0 100 100	36, 53, 70, 77	0
28	16	53/54 (98%)	-0.23	0 100 100	37, 47, 61, 65	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%)	0.26	1 (1%) 66 61	53, 62, 73, 77	0
29	17	48/49 (97%)	-0.10	4 (8%) 17 12	26, 33, 57, 66	0
29	27	48/49 (97%)	-0.05	4 (8%) 17 12	36, 41, 64, 75	0
30	18	64/65 (98%)	-0.23	0 100 100	33, 40, 46, 60	0
30	28	64/65 (98%)	0.41	0 100 100	48, 57, 64, 71	0
31	19	37/37 (100%)	-0.03	0 100 100	36, 45, 63, 64	0
31	29	37/37 (100%)	1.13	4 (10%) 11 9	59, 70, 78, 80	0
32	1a	1488/1521 (97%)	0.21	49 (3%) 49 40	39, 73, 98, 112	0
32	2a	1492/1521 (98%)	0.41	56 (3%) 44 36	47, 78, 101, 113	0
33	1b	231/256 (90%)	0.94	35 (15%) 5 4	69, 83, 92, 96	0
33	2b	231/256 (90%)	1.22	28 (12%) 8 7	77, 87, 94, 98	0
34	1c	206/239 (86%)	0.81	12 (5%) 29 22	65, 78, 89, 94	0
34	2c	206/239 (86%)	1.28	32 (15%) 5 4	77, 88, 93, 97	0
35	1d	208/209 (99%)	0.75	11 (5%) 32 25	57, 73, 82, 92	0
35	2d	208/209 (99%)	0.77	8 (3%) 44 36	61, 74, 82, 87	0
36	1e	148/162 (91%)	0.37	1 (0%) 84 82	49, 67, 77, 91	0
36	2e	148/162 (91%)	0.77	6 (4%) 41 33	60, 75, 85, 92	0
37	1f	100/101 (99%)	0.43	1 (1%) 79 76	53, 70, 79, 85	0
37	2f	100/101 (99%)	0.44	1 (1%) 79 76	58, 71, 81, 85	0
38	1g	155/156 (99%)	0.66	7 (4%) 38 31	70, 78, 85, 90	0
38	2g	155/156 (99%)	0.92	15 (9%) 13 10	78, 85, 90, 94	0
39	1h	137/138 (99%)	0.59	2 (1%) 72 67	57, 70, 78, 83	0
39	2h	137/138 (99%)	0.65	2 (1%) 72 67	65, 76, 82, 87	0
40	1i	127/128 (99%)	1.38	22 (17%) 4 3	70, 85, 91, 93	0
40	2i	126/128 (98%)	1.91	53 (42%) 0 0	80, 90, 95, 97	0
41	1j	97/105 (92%)	1.11	7 (7%) 21 16	68, 85, 91, 95	0
41	2j	96/105 (91%)	1.81	34 (35%) 1 0	81, 90, 95, 97	0
42	1k	114/129 (88%)	0.40	4 (3%) 47 38	46, 67, 78, 85	0
42	2k	114/129 (88%)	0.97	14 (12%) 8 7	59, 75, 84, 88	0
43	1l	121/132 (91%)	0.44	5 (4%) 41 33	49, 62, 74, 80	0
43	2l	121/132 (91%)	0.58	7 (5%) 29 22	57, 68, 76, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.74	7 (6%) 27 21	66, 80, 86, 90	0
44	2m	114/126 (90%)	1.62	35 (30%) 1 0	82, 90, 95, 98	0
45	1n	60/61 (98%)	1.06	9 (15%) 5 4	71, 76, 85, 89	0
45	2n	60/61 (98%)	1.99	25 (41%) 0 0	82, 89, 94, 99	0
46	1o	88/89 (98%)	0.74	4 (4%) 38 31	49, 70, 81, 86	0
46	2o	88/89 (98%)	0.92	7 (7%) 18 14	60, 74, 82, 89	0
47	1p	82/88 (93%)	1.13	6 (7%) 21 15	63, 74, 83, 88	0
47	2p	82/88 (93%)	1.06	7 (8%) 16 12	63, 72, 82, 88	0
48	1q	99/105 (94%)	0.95	4 (4%) 42 34	55, 71, 81, 84	0
48	2q	99/105 (94%)	0.75	3 (3%) 52 45	59, 73, 81, 87	0
49	1r	68/88 (77%)	0.40	1 (1%) 72 67	61, 68, 83, 87	0
49	2r	68/88 (77%)	0.70	3 (4%) 39 31	65, 73, 83, 86	0
50	1s	83/93 (89%)	1.08	10 (12%) 9 7	74, 82, 89, 92	0
50	2s	83/93 (89%)	1.99	45 (54%) 0 0	84, 92, 96, 100	0
51	1t	96/106 (90%)	0.96	11 (11%) 9 8	65, 75, 87, 92	0
51	2t	98/106 (92%)	0.63	4 (4%) 41 33	59, 73, 84, 86	0
52	1u	23/27 (85%)	1.11	4 (17%) 4 3	77, 79, 83, 84	0
52	2u	23/27 (85%)	2.54	16 (69%) 0 0	84, 88, 91, 93	0
53	1y	97/113 (85%)	0.59	6 (6%) 26 20	59, 69, 79, 82	0
53	2y	96/113 (84%)	1.59	27 (28%) 1 1	70, 83, 90, 92	0
All	All	20764/21468 (96%)	0.25	1165 (5%) 30 24	23, 66, 93, 114	0

All (1165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	653	A	9.5
1	2A	653	A	9.1
1	2A	652(U)	G	9.1
45	2n	2	ALA	8.1
1	2A	652(T)	C	8.0
53	1y	98	ALA	8.0
1	1A	654	A	8.0
1	2A	654	A	7.8
1	2A	652(C)	G	7.7
1	2A	652(V)	C	7.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	652(V)	C	7.4
1	1A	652(C)	G	7.2
1	1A	1087	G	6.8
53	2y	98	ALA	6.7
1	1A	1076	C	6.7
40	1i	106	ALA	6.3
51	1t	103	GLY	6.3
1	1A	652(D)	C	6.2
26	24	56	VAL	6.2
1	1A	1509	C	6.1
1	1A	652(E)	G	5.8
1	2A	2602	A	5.7
1	1A	1091	G	5.5
1	2A	1509	C	5.5
1	2A	652(E)	G	5.4
1	2A	652(D)	C	5.4
3	1D	276	LYS	5.3
40	2i	127	LYS	5.2
1	1A	652(U)	G	5.1
51	2t	6	PRO	5.1
25	23	2	PRO	5.1
40	1i	126	SER	5.0
1	1A	1090	U	5.0
32	2a	1030(A)	G	4.9
15	1T	131	ALA	4.9
1	1A	2805	G	4.9
32	2a	1202	G	4.9
23	11	2	SER	4.9
40	2i	2	GLU	4.9
1	2A	1536	C	4.9
6	2G	87	PRO	4.9
1	1A	1092	C	4.8
40	2i	125	TYR	4.8
38	1g	84	ASN	4.8
46	2o	86	GLY	4.7
1	1A	2602	A	4.7
1	1A	2804	C	4.7
40	1i	56	LEU	4.7
50	2s	2	PRO	4.7
45	2n	33	VAL	4.7
29	27	48	LYS	4.7
7	1H	2	SER	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
53	2y	97	ALA	4.7
40	2i	126	SER	4.7
26	24	49	PHE	4.6
44	2m	98	VAL	4.6
23	2l	2	SER	4.6
1	1A	652(T)	C	4.6
41	2j	75	ILE	4.6
33	2b	237	ALA	4.6
1	1A	1089	G	4.6
1	1A	1077	A	4.5
1	2A	1091	G	4.4
1	1A	1072	C	4.4
1	1A	1088	A	4.4
45	2n	18	VAL	4.4
1	1A	1078	U	4.3
1	1A	1102	C	4.3
40	2i	7	THR	4.3
1	1A	1064	C	4.3
1	1A	1104	C	4.3
1	2A	652(B)	A	4.3
53	1y	97	ALA	4.2
39	2h	2	LEU	4.2
15	1T	104	ASN	4.2
1	1A	2107	C	4.2
6	2G	20	ILE	4.2
1	1A	1176	G	4.2
45	2n	34	TYR	4.1
15	1T	130	ALA	4.1
1	1A	1103	A	4.1
52	2u	24	ARG	4.1
45	2n	13	THR	4.1
32	2a	1030(B)	C	4.1
5	1F	207	GLY	4.1
14	2S	35	ILE	4.1
44	1m	102	ARG	4.1
24	12	70	GLN	4.1
41	2j	34	VAL	4.1
1	1A	652(F)	G	4.0
20	2Y	1	MET	4.0
1	2A	2147	G	4.0
1	2A	2117	A	4.0
45	1n	2	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	102	LEU	4.0
1	1A	1075	C	4.0
15	1T	37	GLY	4.0
8	1I	147	GLN	3.9
1	2A	2139	C	3.9
1	1A	1066	U	3.9
35	1d	167	GLY	3.9
43	1l	126	LYS	3.9
12	2Q	104	PHE	3.9
52	2u	14	TRP	3.9
52	2u	16	GLY	3.9
33	1b	7	VAL	3.9
1	2A	34	C	3.9
40	2i	109	VAL	3.9
41	2j	37	PRO	3.8
47	1p	19	ILE	3.8
1	1A	652(S)	C	3.8
33	1b	10	LEU	3.8
8	2I	146	ALA	3.8
1	2A	2133	G	3.8
44	2m	100	GLY	3.8
1	1A	1086	A	3.8
15	2T	130	ALA	3.8
50	2s	76	PRO	3.8
33	1b	236	TYR	3.8
1	2A	1064	C	3.8
1	2A	1076	C	3.8
33	2b	136	VAL	3.8
1	2A	2168	G	3.7
1	1A	2803	C	3.7
51	2t	103	GLY	3.7
1	2A	1046	A	3.7
32	1a	1286	A	3.7
1	1A	1065	U	3.7
11	2P	15	ARG	3.7
1	2A	2116	G	3.7
14	2S	32	LEU	3.7
1	2A	2146	C	3.7
26	14	56	VAL	3.7
34	1c	90	GLU	3.7
40	2i	105	ASP	3.6
43	2l	17	LYS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2145	C	3.6
40	2i	101	PHE	3.6
33	2b	7	VAL	3.6
6	2G	53	LEU	3.6
1	2A	1067	A	3.6
1	2A	2135	A	3.6
3	2D	276	LYS	3.6
26	24	63	TYR	3.6
40	1i	125	TYR	3.6
42	1k	25	TYR	3.6
1	1A	1080	C	3.6
1	2A	2153	G	3.6
1	2A	2155	G	3.6
1	2A	2174	C	3.6
50	2s	67	VAL	3.6
3	1D	275	LYS	3.6
52	2u	6	ARG	3.6
2	2B	1	U	3.6
1	2A	2145	C	3.6
1	1A	1071	G	3.6
51	1t	9	ASN	3.6
18	2W	112	GLY	3.6
32	1a	1257	U	3.6
47	2p	82	GLN	3.6
50	2s	9	VAL	3.6
38	2g	16	LEU	3.6
45	1n	7	ILE	3.5
1	2A	2124	G	3.5
1	2A	2152	G	3.5
21	1Z	192	ALA	3.5
44	2m	76	ALA	3.5
50	2s	82	GLY	3.5
1	1A	888	C	3.5
6	2G	2	PRO	3.5
33	2b	236	TYR	3.5
1	2A	614(A)	U	3.5
40	2i	75	ASP	3.5
45	2n	59	ALA	3.5
1	2A	2803	C	3.5
6	2G	52	ILE	3.5
14	2S	59	LYS	3.5
1	2A	1084	A	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	160	ALA	3.5
50	2s	59	PRO	3.5
22	20	84	LEU	3.5
43	1l	64	TYR	3.4
2	1B	1	U	3.4
41	2j	76	ASN	3.4
40	1i	19	LEU	3.4
40	2i	117	HIS	3.4
26	14	63	TYR	3.4
6	1G	76	SER	3.4
1	1A	2143	C	3.4
1	1A	2794	C	3.4
25	13	2	PRO	3.4
42	2k	13	GLN	3.4
47	1p	82	GLN	3.4
33	2b	165	VAL	3.4
1	1A	2793	G	3.4
1	2A	2805	G	3.4
32	1a	1036	G	3.4
46	1o	3	ILE	3.4
1	1A	2139	C	3.4
1	2A	2140	C	3.4
5	1F	6	VAL	3.4
26	14	52	THR	3.4
40	2i	10	ARG	3.4
41	1j	4	ILE	3.3
22	20	8	GLY	3.3
1	1A	2117	A	3.3
1	2A	2893	G	3.3
32	2a	1031	G	3.3
26	24	35	VAL	3.3
6	2G	90	LEU	3.3
52	2u	2	GLY	3.3
33	1b	17	PHE	3.3
1	2A	1070	A	3.3
32	2a	1357	A	3.3
34	2c	77	ILE	3.3
34	1c	10	PHE	3.3
38	2g	80	VAL	3.3
40	2i	18	PHE	3.3
32	1a	1001	A	3.3
52	2u	15	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2112	G	3.3
32	1a	1032	G	3.3
6	2G	155	MET	3.3
47	2p	38	TYR	3.3
26	24	54	GLY	3.3
34	2c	159	GLY	3.3
40	2i	46	ALA	3.3
6	2G	147	ASP	3.3
1	1A	2174	C	3.2
1	2A	2136	C	3.2
14	2S	3	ARG	3.2
6	2G	3	LEU	3.2
41	2j	62	HIS	3.2
48	1q	100	LYS	3.2
26	24	67	TYR	3.2
1	2A	1171	G	3.2
32	1a	1030(B)	C	3.2
40	1i	46	ALA	3.2
26	24	65	ASP	3.2
38	2g	5	ARG	3.2
1	2A	2172	U	3.2
32	2a	1257	U	3.2
52	2u	20	LYS	3.2
53	2y	38	HIS	3.2
50	2s	63	THR	3.2
6	1G	44	GLY	3.2
1	2A	2107	C	3.2
15	2T	131	ALA	3.2
6	2G	109	VAL	3.2
41	2j	47	PHE	3.2
40	1i	127	LYS	3.2
4	1E	163	GLU	3.2
6	2G	62	LEU	3.2
1	1A	1093	G	3.2
32	2a	1003	G	3.2
29	17	45	ALA	3.2
40	2i	43	ALA	3.2
40	2i	76	ALA	3.2
1	2A	1075	C	3.1
32	1a	63	C	3.1
45	2n	3	ARG	3.1
26	14	69	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
18	1W	112	GLY	3.1
31	29	21	GLY	3.1
1	2A	1026	U	3.1
6	2G	76	SER	3.1
32	1a	1030(A)	G	3.1
32	1a	1031	G	3.1
42	2k	75	TYR	3.1
52	2u	18	TYR	3.1
1	2A	2142	C	3.1
35	1d	179	GLU	3.1
26	14	54	GLY	3.1
33	2b	230	VAL	3.1
1	2A	2130	U	3.1
41	2j	46	ARG	3.1
41	2j	78	ASN	3.1
6	2G	152	LEU	3.1
52	2u	5	ASP	3.1
1	1A	2147	G	3.1
33	1b	131	PRO	3.1
1	1A	2146	C	3.1
32	2a	1027	C	3.1
3	2D	262	ARG	3.1
51	1t	70	SER	3.1
39	1h	2	LEU	3.1
32	1a	1001(A)	G	3.1
32	2a	1001(A)	G	3.1
46	1o	89	GLY	3.1
14	2S	33	LYS	3.1
26	24	28	LYS	3.1
26	24	58	ARG	3.1
1	1A	34	C	3.1
32	1a	1030	C	3.1
32	2a	1030	C	3.1
33	1b	165	VAL	3.1
1	2A	6	A	3.0
35	1d	155	LEU	3.0
35	1d	166	LYS	3.0
41	2j	48	THR	3.0
26	14	49	PHE	3.0
19	1X	95	LEU	3.0
42	2k	117	ASN	3.0
1	2A	2801(A)	A	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
53	2y	9	GLN	3.0
6	1G	52	ILE	3.0
53	2y	7	SER	3.0
6	1G	48	GLU	3.0
1	2A	2112	G	3.0
1	2A	2125	G	3.0
1	2A	2165	G	3.0
1	2A	2119	A	3.0
32	2a	1447	A	3.0
44	2m	6	GLY	3.0
5	2F	21	ALA	3.0
1	2A	2118	U	3.0
32	1a	1000	U	3.0
21	2Z	191	VAL	3.0
34	2c	207	VAL	3.0
50	2s	16	LEU	3.0
26	24	57	GLU	3.0
26	24	66	SER	3.0
12	2Q	59	ARG	3.0
40	1i	7	THR	3.0
1	2A	2793	G	3.0
1	1A	1079	C	3.0
1	2A	2804	C	3.0
45	2n	20	ALA	3.0
1	2A	1085	A	3.0
26	14	59	PHE	3.0
40	2i	56	LEU	2.9
44	2m	66	LEU	2.9
20	1Y	1	MET	2.9
34	2c	79	ARG	2.9
36	2e	13	ILE	2.9
41	2j	36	GLY	2.9
44	2m	24	GLY	2.9
26	24	59	PHE	2.9
50	2s	30	LEU	2.9
1	2A	2802	G	2.9
32	1a	630	G	2.9
32	1a	1033	G	2.9
32	2a	1286	A	2.9
36	2e	10	MET	2.9
6	2G	146	TYR	2.9
46	2o	89	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	71	LEU	2.9
1	1A	2108	C	2.9
1	2A	229	A	2.9
1	2A	2111	C	2.9
1	2A	2896	C	2.9
1	2A	2150	U	2.9
1	2A	2897	U	2.9
34	2c	124	ILE	2.9
43	2l	126	LYS	2.9
1	1A	1081	U	2.9
1	1A	1101	U	2.9
1	1A	2142	C	2.9
1	2A	645	C	2.9
1	2A	1073	A	2.9
1	2A	1090	U	2.9
1	2A	2144	U	2.9
32	1a	1030(D)	A	2.9
1	2A	614(B)	G	2.9
1	2A	2151	G	2.9
8	1I	3	VAL	2.9
7	2H	136	ILE	2.8
34	2c	5	ILE	2.8
38	2g	154	TYR	2.8
40	2i	11	LYS	2.8
28	26	11	LEU	2.8
53	2y	73	ALA	2.8
1	1A	2119	A	2.8
1	1A	2167	U	2.8
1	2A	2169	A	2.8
1	2A	2129	C	2.8
1	2A	2138	C	2.8
8	1I	117	GLU	2.8
41	2j	64	GLU	2.8
44	2m	113	PRO	2.8
1	1A	2116	G	2.8
1	2A	2154	G	2.8
1	2A	2162	G	2.8
6	2G	118	ARG	2.8
40	1i	128	ARG	2.8
44	2m	91	ARG	2.8
50	2s	29	ARG	2.8
36	2e	20	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	139	LEU	2.8
41	2j	67	THR	2.8
44	2m	72	ALA	2.8
3	2D	113	VAL	2.8
34	1c	207	VAL	2.8
1	1A	1084	A	2.8
32	1a	1041	A	2.8
31	29	17	ILE	2.8
33	1b	22	LYS	2.8
53	2y	54	ILE	2.8
1	1A	1074	G	2.8
1	1A	2115	G	2.8
1	2A	2160	G	2.8
33	1b	11	LEU	2.8
50	2s	15	LEU	2.8
20	2Y	91	GLU	2.8
7	2H	21	PRO	2.8
33	2b	21	ARG	2.8
40	1i	123	PRO	2.8
1	2A	2113	U	2.8
1	1A	887	A	2.8
6	2G	88	ILE	2.8
32	1a	1027	C	2.8
32	1a	1037	C	2.8
32	2a	1116	C	2.8
19	2X	95	LEU	2.8
34	2c	196	LEU	2.8
49	2r	85	LEU	2.8
26	24	51	ASP	2.8
29	17	1	MET	2.8
42	2k	105	VAL	2.8
47	1p	1	MET	2.8
12	2Q	65	PHE	2.8
1	2A	2106	G	2.8
32	1a	79	G	2.8
44	2m	87	TYR	2.8
51	1t	18	GLN	2.7
45	2n	7	ILE	2.7
50	2s	31	ILE	2.7
1	1A	2132	U	2.7
26	24	9	LEU	2.7
41	2j	65	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	2l	95	GLY	2.7
6	1G	50	ALA	2.7
50	2s	19	VAL	2.7
50	2s	33	THR	2.7
53	2y	51	ASP	2.7
6	1G	83	ARG	2.7
33	2b	152	PHE	2.7
38	2g	32	ARG	2.7
6	2G	12	TYR	2.7
40	2i	88	TYR	2.7
53	2y	57	PRO	2.7
1	1A	1062	G	2.7
32	2a	1373	G	2.7
33	2b	11	LEU	2.7
35	1d	157	LEU	2.7
8	1I	20	ASP	2.7
40	2i	104	ARG	2.7
1	1A	2158	A	2.7
1	2A	655	A	2.7
1	2A	2126	A	2.7
40	1i	21	PRO	2.7
41	2j	57	LYS	2.7
1	1A	2166	G	2.7
1	1A	2792	G	2.7
1	2A	2148	G	2.7
34	2c	2	GLY	2.7
52	1u	16	GLY	2.7
7	2H	3	ARG	2.7
14	1S	3	ARG	2.7
53	2y	4	ASN	2.7
14	2S	49	VAL	2.7
21	1Z	51	ALA	2.7
26	24	50	VAL	2.7
33	1b	237	ALA	2.7
33	2b	15	VAL	2.7
37	1f	90	VAL	2.7
41	2j	54	PHE	2.7
1	1A	655	A	2.7
1	2A	1096	A	2.7
32	1a	1492	A	2.7
41	1j	74	ILE	2.7
1	2A	2789	C	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	136	C	2.7
32	1a	1029	C	2.7
5	2F	181	LEU	2.7
6	2G	43	LEU	2.7
36	2e	22	GLY	2.7
52	2u	9	ARG	2.7
50	2s	35	SER	2.7
7	2H	45	VAL	2.7
33	2b	22	LYS	2.7
35	1d	110	PHE	2.7
38	1g	83	ALA	2.7
40	2i	106	ALA	2.7
41	2j	72	VAL	2.7
45	1n	22	THR	2.7
53	1y	2	THR	2.7
32	1a	380	G	2.6
32	2a	1036	G	2.6
1	1A	2144	U	2.6
51	1t	100	ILE	2.6
1	1A	1085	A	2.6
33	1b	187	LEU	2.6
48	2q	98	LEU	2.6
25	23	29	ARG	2.6
43	1l	19	ARG	2.6
1	2A	2179	C	2.6
14	2S	29	PHE	2.6
34	2c	92	ALA	2.6
41	1j	44	VAL	2.6
41	2j	63	PHE	2.6
44	1m	2	ALA	2.6
50	2s	74	PHE	2.6
33	1b	127	ILE	2.6
35	2d	5	ILE	2.6
1	1A	275	G	2.6
1	2A	2159	G	2.6
32	1a	1023	G	2.6
32	2a	1026	G	2.6
32	2a	1030(C)	G	2.6
32	2a	1240	U	2.6
8	1I	38	LEU	2.6
34	1c	87	LEU	2.6
34	2c	94	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	24	55	ARG	2.6
29	17	48	LYS	2.6
1	2A	1509(A)	A	2.6
4	2E	204	ALA	2.6
44	2m	106	ASN	2.6
33	2b	97	TRP	2.6
41	2j	30	SER	2.6
45	1n	33	VAL	2.6
1	2A	888	C	2.6
32	2a	1363	C	2.6
48	1q	63	ARG	2.6
45	2n	17	LYS	2.6
1	2A	171	G	2.6
1	2A	1074	G	2.6
32	1a	1026	G	2.6
32	2a	630	G	2.6
32	2a	1022	G	2.6
32	2a	1024	G	2.6
44	2m	75	ALA	2.6
1	2A	887	A	2.6
32	1a	1447	A	2.6
32	2a	532	A	2.6
32	2a	1030(D)	A	2.6
6	2G	7	LEU	2.6
33	1b	36	ARG	2.6
44	1m	115	LYS	2.6
44	2m	31	LYS	2.6
45	1n	4	LYS	2.6
14	2S	60	GLY	2.6
33	1b	38	GLY	2.6
1	2A	1083	U	2.6
6	2G	50	ALA	2.6
34	2c	149	ALA	2.6
40	2i	17	VAL	2.6
40	2i	53	VAL	2.6
40	2i	108	VAL	2.6
40	2i	119	ALA	2.6
49	2r	20	ALA	2.6
50	2s	58	VAL	2.6
24	22	70	GLN	2.6
1	1A	614(B)	G	2.5
1	1A	2125	G	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	1089	G	2.5
1	2A	2166	G	2.5
32	2a	1033	G	2.5
32	2a	1058	G	2.5
50	2s	66	MET	2.5
40	2i	81	ILE	2.5
44	2m	22	ILE	2.5
53	2y	5	ILE	2.5
1	1A	1057	A	2.5
11	2P	6	LEU	2.5
40	2i	99	LEU	2.5
13	2R	68	ARG	2.5
20	2Y	54	LYS	2.5
33	2b	133	LYS	2.5
40	2i	83	ARG	2.5
33	1b	19	HIS	2.5
40	2i	36	TYR	2.5
6	2G	42	GLY	2.5
33	1b	14	GLY	2.5
6	2G	80	PHE	2.5
6	2G	151	ALA	2.5
33	2b	17	PHE	2.5
44	1m	116	THR	2.5
1	1A	1026	U	2.5
1	2A	2167	U	2.5
53	2y	10	MET	2.5
33	1b	39	ILE	2.5
34	2c	157	ILE	2.5
44	2m	102	ARG	2.5
1	1A	2141	G	2.5
1	1A	2155	G	2.5
32	2a	1002	G	2.5
32	2a	1032	G	2.5
1	2A	1088	A	2.5
33	1b	33	TYR	2.5
42	2k	25	TYR	2.5
52	2u	23	PRO	2.5
49	1r	24	ALA	2.5
1	2A	2143	C	2.5
32	2a	470	C	2.5
51	1t	11	SER	2.5
6	2G	140	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	44	LEU	2.5
35	1d	188	LEU	2.5
44	2m	90	LEU	2.5
40	1i	39	GLY	2.5
40	2i	123	PRO	2.5
1	1A	1067	A	2.5
1	1A	1073	A	2.5
1	1A	2159	G	2.5
1	2A	2127	G	2.5
1	2A	2892	A	2.5
32	1a	1030(C)	G	2.5
32	2a	1013	G	2.5
33	1b	230	VAL	2.5
42	2k	15	ALA	2.5
42	2k	125	PHE	2.5
51	1t	97	ALA	2.5
6	2G	145	THR	2.5
41	2j	40	LEU	2.5
45	2n	6	LEU	2.5
45	2n	39	LEU	2.5
1	1A	2138	C	2.5
1	2A	2103	C	2.5
1	2A	2105	C	2.5
32	2a	1038	C	2.5
40	1i	91	ASP	2.5
40	2i	91	ASP	2.5
1	1A	1175	U	2.5
32	2a	1000	U	2.5
34	2c	90	GLU	2.5
35	2d	23	GLY	2.5
40	2i	114	TYR	2.5
41	2j	53	PRO	2.5
53	2y	14	PRO	2.5
6	2G	28	VAL	2.5
6	2G	70	VAL	2.5
34	1c	76	VAL	2.5
4	2E	114	ALA	2.5
33	2b	57	PHE	2.5
40	2i	45	ALA	2.5
45	2n	15	LYS	2.4
46	2o	48	LYS	2.4
26	24	52	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	529	A	2.4
1	1A	1508	A	2.4
1	1A	1509(A)	A	2.4
1	2A	2170	A	2.4
1	2A	2176	A	2.4
14	2S	61	ASN	2.4
32	2a	994	A	2.4
40	2i	42	ARG	2.4
41	1j	78	ASN	2.4
42	1k	117	ASN	2.4
45	2n	29	ARG	2.4
51	1t	8	ARG	2.4
6	2G	77	ILE	2.4
50	2s	5	LEU	2.4
1	1A	2148	G	2.4
1	2A	2207	G	2.4
32	1a	1003	G	2.4
6	2G	49	ASP	2.4
33	1b	128	GLU	2.4
1	1A	154(A)	C	2.4
1	2A	886	C	2.4
1	1A	1061	U	2.4
1	1A	1963	U	2.4
45	2n	14	PRO	2.4
50	2s	42	PRO	2.4
52	2u	11	GLY	2.4
19	1X	69	TYR	2.4
45	2n	21	TYR	2.4
7	2H	52	VAL	2.4
33	2b	93	VAL	2.4
35	1d	169	LYS	2.4
40	1i	95	LYS	2.4
40	2i	86	VAL	2.4
44	2m	101	GLN	2.4
22	20	69	PHE	2.4
45	1n	5	ALA	2.4
38	2g	79	ARG	2.4
40	1i	107	ARG	2.4
22	10	84	LEU	2.4
50	2s	65	ASN	2.4
1	1A	548	A	2.4
1	2A	1086	A	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2158	A	2.4
33	1b	134	GLU	2.4
1	2A	1047	G	2.4
1	2A	1087	G	2.4
1	2A	2894	G	2.4
32	1a	102	G	2.4
32	2a	973	G	2.4
20	2Y	5	MET	2.4
48	2q	100	LYS	2.4
1	2A	1092	C	2.4
1	2A	2108	C	2.4
1	2A	2132	U	2.4
14	2S	7	TYR	2.4
38	1g	85	TYR	2.4
38	2g	85	TYR	2.4
40	2i	4	TYR	2.4
14	2S	12	PHE	2.4
29	27	47	ARG	2.4
33	1b	62	ALA	2.4
33	1b	130	ARG	2.4
40	2i	94	ALA	2.4
52	2u	10	ARG	2.4
40	2i	19	LEU	2.4
40	2i	96	LEU	2.4
38	2g	84	ASN	2.4
1	2A	2114	A	2.4
44	2m	65	LYS	2.4
6	2G	149	VAL	2.4
6	2G	160	VAL	2.4
8	2I	92	VAL	2.4
9	2N	140	VAL	2.4
34	2c	153	VAL	2.4
44	2m	60	VAL	2.4
50	1s	9	VAL	2.4
50	2s	45	VAL	2.4
1	1A	1063	G	2.4
1	2A	2318	G	2.4
6	2G	72	ARG	2.4
34	2c	163	ALA	2.4
38	2g	2	ALA	2.4
50	2s	75	ALA	2.4
51	1t	76	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2150	U	2.4
1	2A	2109	U	2.4
6	2G	157	ILE	2.4
7	2H	89	ILE	2.4
33	2b	10	LEU	2.4
41	1j	75	ILE	2.4
44	2m	84	ILE	2.4
9	1N	68	GLU	2.4
40	2i	110	GLU	2.4
50	2s	64	GLU	2.4
43	2l	23	LYS	2.4
6	2G	134	GLY	2.4
45	2n	38	GLY	2.4
53	2y	92	GLY	2.4
43	2l	89	ARG	2.4
44	1m	117	VAL	2.4
53	1y	95	ARG	2.4
1	1A	2173	A	2.4
19	2X	66	LEU	2.3
35	1d	138	TYR	2.3
42	2k	103	LEU	2.3
6	2G	39	ILE	2.3
41	2j	38	ILE	2.3
52	2u	13	ILE	2.3
53	2y	12	ILE	2.3
1	1A	2130	U	2.3
1	2A	2122	U	2.3
1	2A	2808	U	2.3
21	1Z	203	GLU	2.3
26	24	30	GLU	2.3
33	1b	126	GLU	2.3
34	1c	62	ASP	2.3
38	2g	33	ASP	2.3
53	2y	8	LYS	2.3
53	2y	64	SER	2.3
34	2c	162	GLN	2.3
40	2i	6	GLY	2.3
6	2G	51	ARG	2.3
22	20	74	ARG	2.3
41	2j	45	ARG	2.3
48	1q	91	ARG	2.3
9	2N	9	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	41	VAL	2.3
6	2G	102	PHE	2.3
33	1b	13	ALA	2.3
45	2n	37	PHE	2.3
44	2m	96	LEU	2.3
1	1A	2126	A	2.3
50	2s	48	THR	2.3
50	2s	69	HIS	2.3
40	2i	118	LYS	2.3
1	1A	271(K)	U	2.3
1	1A	2113	U	2.3
1	1A	2118	U	2.3
26	14	51	ASP	2.3
44	2m	64	TRP	2.3
1	2A	2115	G	2.3
32	1a	1024	G	2.3
32	1a	1034	G	2.3
32	2a	1190	G	2.3
32	2a	1347	G	2.3
1	2A	2161	C	2.3
32	1a	221	C	2.3
35	1d	2	GLY	2.3
53	2y	46	GLN	2.3
53	2y	83	ARG	2.3
8	2I	5	LEU	2.3
33	2b	122	PHE	2.3
41	2j	90	LEU	2.3
48	2q	71	PHE	2.3
33	1b	214	ILE	2.3
33	2b	208	ILE	2.3
7	2H	129	THR	2.3
14	2S	92	TYR	2.3
6	2G	45	GLU	2.3
6	2G	48	GLU	2.3
33	1b	8	LYS	2.3
40	1i	12	GLU	2.3
1	1A	2629	A	2.3
1	2A	652(A)	A	2.3
1	2A	2173	A	2.3
32	1a	1035	A	2.3
32	2a	1035	A	2.3
41	2j	19	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	17	ARG	2.3
47	2p	48	TRP	2.3
4	2E	115	GLY	2.3
5	1F	208	GLY	2.3
1	1A	12	U	2.3
1	1A	1082	U	2.3
45	2n	25	VAL	2.3
3	1D	2	ALA	2.3
6	2G	46	ALA	2.3
41	2j	26	ALA	2.3
1	2A	1072	C	2.3
1	2A	2131	G	2.3
1	2A	2149	G	2.3
32	2a	1034	G	2.3
33	1b	200	ILE	2.3
53	2y	39	ILE	2.3
1	2A	2183	C	2.3
22	20	43	THR	2.3
12	1Q	32	TYR	2.3
35	2d	54	TYR	2.3
44	2m	23	TYR	2.3
50	2s	80	TYR	2.3
36	2e	130	ASN	2.3
50	1s	23	ASN	2.3
19	1X	60	ARG	2.3
22	20	9	SER	2.3
33	2b	131	PRO	2.3
38	1g	77	SER	2.3
45	2n	32	SER	2.3
1	1A	229	A	2.3
1	2A	1095	A	2.3
6	2G	100	TRP	2.3
33	1b	97	TRP	2.3
34	1c	2	GLY	2.3
50	2s	8	GLY	2.3
50	2s	34	TRP	2.3
50	2s	20	LEU	2.3
1	1A	2109	U	2.2
1	1A	2172	U	2.2
6	2G	63	ILE	2.2
33	2b	200	ILE	2.2
38	2g	83	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	55	LYS	2.2
50	2s	25	LYS	2.2
53	2y	3	MET	2.2
42	2k	87	THR	2.2
45	1n	13	THR	2.2
47	2p	69	THR	2.2
6	2G	137	GLU	2.2
1	2A	2163	C	2.2
1	2A	2175	C	2.2
1	2A	2178	C	2.2
1	1A	2106	G	2.2
1	1A	2133	G	2.2
1	1A	2807	G	2.2
1	2A	2121	G	2.2
38	2g	76	ARG	2.2
33	2b	232	PRO	2.2
38	2g	14	PRO	2.2
40	2i	49	PRO	2.2
50	1s	13	ASP	2.2
35	2d	183	GLY	2.2
7	2H	49	VAL	2.2
34	2c	33	LEU	2.2
41	2j	71	LEU	2.2
1	1A	2176	A	2.2
1	2A	2134	A	2.2
25	23	25	ALA	2.2
26	24	22	ILE	2.2
32	2a	1004	A	2.2
40	2i	37	PHE	2.2
41	2j	32	ALA	2.2
53	2y	66	LYS	2.2
33	1b	12	GLU	2.2
40	1i	64	THR	2.2
41	1j	87	THR	2.2
44	2m	58	GLU	2.2
12	2Q	60	ARG	2.2
45	1n	12	ARG	2.2
45	2n	31	ARG	2.2
47	2p	26	ARG	2.2
6	2G	142	PRO	2.2
33	1b	232	PRO	2.2
46	2o	75	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2111	C	2.2
1	1A	2136	C	2.2
1	2A	2128	C	2.2
1	2A	2137	C	2.2
20	1Y	57	GLN	2.2
32	2a	1028	C	2.2
1	1A	2123	G	2.2
1	1A	2153	G	2.2
1	1A	2894	G	2.2
1	2A	2104	G	2.2
1	2A	2141	G	2.2
7	2H	120	GLY	2.2
14	2S	48	LEU	2.2
14	2S	80	LEU	2.2
32	1a	1042	G	2.2
53	1y	92	GLY	2.2
41	1j	88	LEU	2.2
41	2j	8	LEU	2.2
7	1H	175	LYS	2.2
33	1b	133	LYS	2.2
50	2s	11	VAL	2.2
44	2m	78	ILE	2.2
44	2m	82	MET	2.2
8	2I	7	GLU	2.2
1	1A	652(A)	A	2.2
32	2a	968	A	2.2
44	2m	43	THR	2.2
1	1A	272(A)	U	2.2
32	1a	841	U	2.2
32	2a	1025	U	2.2
32	2a	1358	U	2.2
49	2r	87	ARG	2.2
40	1i	5	TYR	2.2
35	2d	74	GLN	2.2
6	2G	74	LYS	2.2
6	2G	107	LEU	2.2
26	24	45	GLY	2.2
26	24	64	GLY	2.2
40	2i	40	LEU	2.2
40	2i	79	LEU	2.2
41	2j	16	LEU	2.2
43	1l	63	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	4	LYS	2.2
52	1u	2	GLY	2.2
52	2u	3	LYS	2.2
6	2G	86	MET	2.2
7	2H	44	VAL	2.2
1	1A	1584	C	2.2
26	24	40	HIS	2.2
32	1a	1007	C	2.2
32	2a	1029	C	2.2
32	2a	1267	C	2.2
33	2b	70	PHE	2.2
35	2d	70	ILE	2.2
21	2Z	192	ALA	2.2
29	27	45	ALA	2.2
45	2n	5	ALA	2.2
34	2c	190	ARG	2.2
50	2s	3	ARG	2.2
50	2s	78	ARG	2.2
1	1A	1046	A	2.2
1	1A	2135	A	2.2
26	24	7	PRO	2.2
32	2a	1001	A	2.2
32	2a	1256	A	2.2
41	2j	91	PRO	2.2
51	2t	98	PRO	2.2
1	1A	1105	U	2.2
1	2A	271(K)	U	2.2
1	2A	1065	U	2.2
1	2A	2180	U	2.2
14	2S	58	LEU	2.2
40	1i	105	ASP	2.2
8	2I	71	ILE	2.2
40	2i	41	VAL	2.2
53	2y	33	HIS	2.2
3	2D	2	ALA	2.1
14	2S	79	ALA	2.1
50	2s	24	ALA	2.1
44	2m	67	GLU	2.1
1	1A	1053	C	2.1
1	1A	2161	C	2.1
1	2A	2185	C	2.1
3	2D	259	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	219	C	2.1
52	2u	17	THR	2.1
53	1y	53	THR	2.1
1	1A	2149	G	2.1
44	1m	113	PRO	2.1
35	2d	166	LYS	2.1
43	2l	20	LYS	2.1
33	2b	121	LEU	2.1
50	1s	5	LEU	2.1
51	1t	10	LEU	2.1
1	1A	2114	A	2.1
8	1I	13	GLY	2.1
15	2T	69	GLY	2.1
32	2a	975	A	2.1
40	2i	115	GLY	2.1
1	2A	1082	U	2.1
6	2G	92	VAL	2.1
32	1a	992	U	2.1
34	1c	84	ILE	2.1
34	2c	152	ILE	2.1
34	2c	173	VAL	2.1
40	1i	14	VAL	2.1
40	2i	14	VAL	2.1
41	2j	58	ASP	2.1
42	1k	36	ASP	2.1
42	2k	36	ASP	2.1
47	1p	51	VAL	2.1
40	1i	122	ALA	2.1
29	17	47	ARG	2.1
33	1b	23	ARG	2.1
44	1m	114	ARG	2.1
34	2c	95	THR	2.1
42	2k	31	THR	2.1
1	2A	885	C	2.1
16	2U	117	GLN	2.1
6	1G	53	LEU	2.1
35	2d	20	TYR	2.1
51	1t	99	LEU	2.1
50	1s	46	GLY	2.1
1	1A	1537	G	2.1
1	1A	2157	G	2.1
6	2G	101	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	2I	20	ASP	2.1
32	1a	376	G	2.1
32	1a	1021	G	2.1
32	2a	971	G	2.1
32	2a	976	G	2.1
38	2g	120	ILE	2.1
42	1k	14	VAL	2.1
45	1n	32	SER	2.1
1	1A	9	U	2.1
1	2A	1098	A	2.1
1	2A	1111	A	2.1
6	2G	69	ALA	2.1
32	1a	1020	U	2.1
33	2b	123	ALA	2.1
6	2G	29	TRP	2.1
24	12	69	ARG	2.1
38	1g	5	ARG	2.1
52	1u	24	ARG	2.1
53	2y	95	ARG	2.1
34	2c	192	THR	2.1
42	2k	28	THR	2.1
45	2n	22	THR	2.1
50	2s	77	THR	2.1
47	1p	15	PRO	2.1
48	1q	82	MET	2.1
7	2H	7	LEU	2.1
34	2c	47	LEU	2.1
39	1h	133	LEU	2.1
50	2s	22	LEU	2.1
33	1b	37	ASN	2.1
6	1G	85	GLY	2.1
14	2S	36	TYR	2.1
40	2i	5	TYR	2.1
42	2k	90	GLY	2.1
50	1s	26	GLY	2.1
50	2s	26	GLY	2.1
1	1A	2140	C	2.1
33	2b	127	ILE	2.1
34	1c	86	VAL	2.1
44	2m	7	VAL	2.1
50	2s	60	VAL	2.1
40	1i	75	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	189	ALA	2.1
41	2j	35	SER	2.1
6	2G	91	ARG	2.1
19	2X	68	ARG	2.1
44	2m	28	ALA	2.1
44	2m	69	GLU	2.1
44	2m	88	ARG	2.1
50	1s	29	ARG	2.1
1	1A	2127	G	2.1
1	2A	1533	G	2.1
1	2A	2123	G	2.1
1	2A	2792	G	2.1
6	2G	81	LYS	2.1
23	2l	48	LYS	2.1
32	1a	220	G	2.1
32	1a	378	G	2.1
32	1a	1117	G	2.1
43	1l	47	LYS	2.1
29	27	1	MET	2.1
11	2P	3	LEU	2.1
34	1c	91	LEU	2.1
38	1g	16	LEU	2.1
31	29	20	HIS	2.1
34	2c	80	GLY	2.1
36	1e	85	GLY	2.1
44	2m	68	GLY	2.1
50	1s	47	HIS	2.1
44	2m	9	ILE	2.1
47	2p	33	ILE	2.1
50	2s	61	TYR	2.1
33	1b	15	VAL	2.1
43	2l	18	VAL	2.1
6	2G	116	ASP	2.0
6	2G	141	PHE	2.1
7	2H	116	GLU	2.0
37	2f	47	ARG	2.0
40	2i	9	ARG	2.0
44	2m	80	ARG	2.0
46	2o	68	ARG	2.0
21	2Z	189	ALA	2.0
33	2b	225	ALA	2.0
1	1A	1116	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	132	C	2.0
33	1b	234	PRO	2.0
40	2i	21	PRO	2.0
40	2i	90	PRO	2.0
1	2A	1097	U	2.0
32	2a	1065	U	2.0
32	2a	1205	U	2.0
34	1c	42	LEU	2.0
38	2g	12	LEU	2.0
42	2k	98	LEU	2.0
53	2y	27	LEU	2.0
1	1A	1056	G	2.0
1	1A	1058	G	2.0
1	2A	2110	G	2.0
1	2A	2120	G	2.0
1	2A	2807	G	2.0
32	2a	1224	G	2.0
34	2c	3	ASN	2.0
50	2s	53	ASN	2.0
34	2c	84	ILE	2.0
34	2c	155	GLY	2.0
51	2t	96	GLY	2.0
53	2y	35	ILE	2.0
7	2H	19	VAL	2.0
25	23	6	VAL	2.0
34	1c	99	VAL	2.0
47	1p	17	TYR	2.0
6	2G	136	ARG	2.0
31	29	22	ARG	2.0
45	2n	12	ARG	2.0
50	2s	10	PHE	2.0
52	1u	6	ARG	2.0
6	2G	35	GLU	2.0
34	2c	129	ALA	2.0
36	2e	94	ALA	2.0
41	2j	27	ALA	2.0
53	2y	63	ALA	2.0
15	2T	1	MET	2.0
38	1g	156	TRP	2.0
32	1a	379	C	2.0
32	1a	1354	C	2.0
32	2a	1195	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	188	LEU	2.0
39	2h	70	GLN	2.0
46	2o	71	GLN	2.0
50	1s	22	LEU	2.0
18	1W	111	HIS	2.0
1	1A	1420	U	2.0
32	1a	1040	U	2.0
35	1d	70	ILE	2.0
46	1o	20	GLY	2.0
46	2o	3	ILE	2.0
47	2p	10	GLY	2.0
1	1A	2170	A	2.0
1	2A	1077	A	2.0
32	1a	1493	A	2.0
32	2a	1191	A	2.0
32	2a	1363(A)	A	2.0
34	2c	103	VAL	2.0
46	1o	88	ARG	2.0
50	1s	19	VAL	2.0
50	2s	51	VAL	2.0
5	2F	7	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5MU	2A	1915	21/22	0.83	0.11	82,90,98,107	0
1	5MU	1A	1915	21/22	0.85	0.12	75,82,90,97	0
32	2MG	2a	1207	24/25	0.86	0.13	88,95,99,101	0
32	M2G	2a	966	25/26	0.89	0.16	72,77,93,104	0
32	5MC	2a	967	21/22	0.89	0.14	75,79,87,92	0
32	2MG	1a	1207	24/25	0.89	0.11	71,78,82,89	0
1	PSU	2A	1917	20/21	0.90	0.08	77,83,93,95	0
43	0TD	2l	92	10/11	0.90	0.12	66,69,72,88	0
1	PSU	1A	1917	20/21	0.91	0.10	68,76,83,84	0
1	PSU	2A	1911	20/21	0.91	0.08	72,77,88,89	0
32	PSU	2a	516	20/21	0.93	0.08	79,82,86,86	0
32	G7M	2a	527	24/25	0.93	0.10	64,74,76,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	1a	967	21/22	0.94	0.11	65,73,82,86	0
1	PSU	1A	1911	20/21	0.94	0.07	65,71,77,77	0
43	0TD	1l	92	10/11	0.94	0.09	53,60,63,71	0
32	5MC	1a	1407	21/22	0.95	0.10	47,54,61,64	0
32	PSU	1a	516	20/21	0.95	0.08	64,68,72,78	0
1	OMC	2A	1920	21/22	0.95	0.08	69,73,78,82	0
1	5MC	2A	1942	21/22	0.95	0.09	51,55,60,64	0
32	4OC	2a	1402	22/23	0.95	0.10	63,70,73,79	0
32	5MC	2a	1404	21/22	0.95	0.09	61,65,69,70	0
32	5MC	2a	1407	21/22	0.95	0.09	61,67,72,78	0
32	UR3	2a	1498	21/22	0.95	0.09	56,62,68,71	0
32	MA6	2a	1518	24/25	0.95	0.11	57,70,75,76	0
32	MA6	2a	1519	24/25	0.95	0.13	58,67,72,75	0
32	M2G	1a	966	25/26	0.95	0.10	61,67,71,75	0
32	G7M	1a	527	24/25	0.96	0.09	48,57,62,71	0
1	OMC	1A	1920	21/22	0.96	0.09	49,61,65,67	0
1	5MU	2A	1939	21/22	0.96	0.09	36,41,45,48	0
32	4OC	1a	1402	22/23	0.96	0.09	52,58,61,71	0
32	5MC	2a	1400	21/22	0.96	0.12	71,78,80,84	0
32	5MC	1a	1404	21/22	0.96	0.08	48,51,55,58	0
1	5MC	2A	1962	21/22	0.97	0.07	44,49,54,68	0
1	MA6	2A	2058	24/25	0.97	0.09	33,40,45,49	0
1	2MA	2A	2503	23/24	0.97	0.08	34,38,40,43	0
32	UR3	1a	1498	21/22	0.97	0.07	47,51,55,64	0
32	MA6	1a	1518	24/25	0.97	0.09	46,49,56,56	0
32	MA6	1a	1519	24/25	0.97	0.08	42,52,56,57	0
32	5MC	1a	1400	21/22	0.97	0.08	47,58,62,67	0
1	5MC	1A	1942	21/22	0.97	0.07	36,42,47,48	0
1	2MA	1A	2503	23/24	0.98	0.06	21,28,31,32	0
1	OMU	1A	2552	21/22	0.98	0.06	30,34,38,43	0
1	PSU	1A	2605	20/21	0.98	0.07	28,32,35,37	0
1	OMG	2A	2251	24/25	0.98	0.09	39,43,46,49	0
1	5MU	1A	1939	21/22	0.98	0.06	28,33,37,38	0
1	OMU	2A	2552	21/22	0.98	0.08	38,43,49,51	0
1	PSU	2A	2605	20/21	0.98	0.07	35,41,46,46	0
1	5MC	1A	1962	21/22	0.98	0.07	28,36,42,49	0
1	MA6	1A	2058	24/25	0.98	0.06	19,27,36,43	0
1	OMG	1A	2251	24/25	0.98	0.06	23,29,31,33	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
54	MG	2a	3085	1/1	0.21	0.66	97,97,97,97	0
54	MG	2a	3045	1/1	0.22	0.21	91,91,91,91	0
54	MG	2A	3414	1/1	0.39	0.20	82,82,82,82	0
54	MG	1A	3656	1/1	0.46	0.29	85,85,85,85	0
54	MG	2G	201	1/1	0.46	0.25	90,90,90,90	0
54	MG	1A	3854	1/1	0.51	0.27	76,76,76,76	0
54	MG	1A	3657	1/1	0.54	0.30	74,74,74,74	0
54	MG	1A	3983	1/1	0.55	0.16	61,61,61,61	0
54	MG	2G	202	1/1	0.55	0.20	88,88,88,88	0
54	MG	2A	3108	1/1	0.57	0.17	78,78,78,78	0
54	MG	1A	3984	1/1	0.57	0.18	41,41,41,41	0
54	MG	1A	3685	1/1	0.58	0.29	74,74,74,74	0
54	MG	2A	3206	1/1	0.62	0.41	81,81,81,81	0
54	MG	1A	3282	1/1	0.63	0.10	91,91,91,91	0
54	MG	1B	227	1/1	0.64	0.11	79,79,79,79	0
54	MG	2B	206	1/1	0.64	0.40	85,85,85,85	0
54	MG	2A	3355	1/1	0.64	0.17	92,92,92,92	0
54	MG	2n	3101	1/1	0.64	0.30	88,88,88,88	0
54	MG	2B	213	1/1	0.65	0.16	77,77,77,77	0
54	MG	1A	3027	1/1	0.65	0.16	75,75,75,75	0
54	MG	1a	1877	1/1	0.66	0.16	90,90,90,90	0
54	MG	2a	3066	1/1	0.66	0.22	81,81,81,81	0
54	MG	1a	1791	1/1	0.66	0.20	80,80,80,80	0
54	MG	1a	1813	1/1	0.66	0.28	80,80,80,80	0
54	MG	1A	4026	1/1	0.67	0.27	84,84,84,84	0
54	MG	1A	3556	1/1	0.67	0.21	43,43,43,43	0
54	MG	2A	3529	1/1	0.67	0.17	77,77,77,77	0
54	MG	2a	3055	1/1	0.67	0.35	89,89,89,89	0
54	MG	2A	3607	1/1	0.67	0.15	80,80,80,80	0
54	MG	1a	1744	1/1	0.67	0.15	97,97,97,97	0
54	MG	1A	3875	1/1	0.67	0.20	76,76,76,76	0
54	MG	1S	201	1/1	0.68	0.20	68,68,68,68	0
54	MG	2A	3347	1/1	0.68	0.21	82,82,82,82	0
54	MG	1a	1685	1/1	0.68	0.22	76,76,76,76	0
54	MG	1a	1874	1/1	0.68	0.16	79,79,79,79	0
54	MG	1a	1714	1/1	0.68	0.22	81,81,81,81	0
54	MG	2A	3085	1/1	0.68	0.36	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2B	204	1/1	0.68	0.21	85,85,85,85	0
54	MG	1A	3895	1/1	0.68	0.19	64,64,64,64	0
54	MG	2a	3008	1/1	0.69	0.29	81,81,81,81	0
54	MG	2A	3471	1/1	0.69	0.17	84,84,84,84	0
54	MG	2A	3359	1/1	0.69	0.27	71,71,71,71	0
54	MG	2A	3556	1/1	0.69	0.23	68,68,68,68	0
54	MG	2A	3601	1/1	0.69	0.21	88,88,88,88	0
54	MG	2A	3449	1/1	0.69	0.20	75,75,75,75	0
54	MG	1A	3863	1/1	0.70	0.20	76,76,76,76	0
54	MG	1A	3963	1/1	0.70	0.25	72,72,72,72	0
54	MG	2A	3439	1/1	0.70	0.26	65,65,65,65	0
54	MG	1A	3988	1/1	0.70	0.22	82,82,82,82	0
57	MPD	2B	219	8/8	0.70	0.30	70,79,82,82	0
54	MG	1n	103	1/1	0.71	0.19	85,85,85,85	0
54	MG	2a	3056	1/1	0.71	0.30	74,74,74,74	0
54	MG	1A	3910	1/1	0.71	0.15	61,61,61,61	0
54	MG	1A	3887	1/1	0.72	0.15	64,64,64,64	0
54	MG	1A	3998	1/1	0.72	0.30	66,66,66,66	0
54	MG	2a	3113	1/1	0.72	0.23	79,79,79,79	0
54	MG	2a	3164	1/1	0.72	0.15	97,97,97,97	0
54	MG	1A	4000	1/1	0.72	0.32	83,83,83,83	0
54	MG	2A	3430	1/1	0.72	0.15	77,77,77,77	0
54	MG	2A	3089	1/1	0.73	0.20	80,80,80,80	0
54	MG	2a	3061	1/1	0.73	0.13	91,91,91,91	0
54	MG	2A	3090	1/1	0.73	0.43	75,75,75,75	0
54	MG	1A	4020	1/1	0.73	0.19	79,79,79,79	0
54	MG	2A	3572	1/1	0.73	0.13	59,59,59,59	0
54	MG	1a	1850	1/1	0.73	0.22	86,86,86,86	0
54	MG	2A	3267	1/1	0.73	0.34	66,66,66,66	0
54	MG	1A	3300	1/1	0.73	0.14	93,93,93,93	0
54	MG	1A	3165	1/1	0.74	0.23	62,62,62,62	0
54	MG	1A	3542	1/1	0.74	0.15	66,66,66,66	0
54	MG	1a	1693	1/1	0.74	0.29	79,79,79,79	0
54	MG	2A	3470	1/1	0.74	0.18	70,70,70,70	0
54	MG	2A	3185	1/1	0.74	0.21	84,84,84,84	0
54	MG	2A	3371	1/1	0.74	0.17	51,51,51,51	0
54	MG	2A	3409	1/1	0.74	0.13	85,85,85,85	0
54	MG	2I	201	1/1	0.74	0.12	80,80,80,80	0
54	MG	2N	201	1/1	0.74	0.11	75,75,75,75	0
54	MG	1A	3727	1/1	0.74	0.26	57,57,57,57	0
54	MG	1a	1708	1/1	0.75	0.13	98,98,98,98	0
54	MG	2A	3209	1/1	0.75	0.32	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3651	1/1	0.75	0.31	36,36,36,36	0
54	MG	2A	3493	1/1	0.75	0.14	74,74,74,74	0
54	MG	2A	3502	1/1	0.75	0.17	51,51,51,51	0
54	MG	1A	3759	1/1	0.75	0.15	70,70,70,70	0
54	MG	2A	3051	1/1	0.75	0.28	68,68,68,68	0
54	MG	1a	1638	1/1	0.75	0.27	72,72,72,72	0
54	MG	1a	1794	1/1	0.75	0.26	79,79,79,79	0
54	MG	1A	3272	1/1	0.75	0.16	57,57,57,57	0
54	MG	1a	1814	1/1	0.75	0.20	81,81,81,81	0
54	MG	2a	3117	1/1	0.75	0.22	74,74,74,74	0
54	MG	2A	3424	1/1	0.75	0.16	56,56,56,56	0
54	MG	2A	3124	1/1	0.75	0.27	76,76,76,76	0
54	MG	1A	3693	1/1	0.75	0.29	79,79,79,79	0
54	MG	2A	3254	1/1	0.76	0.18	59,59,59,59	0
54	MG	1A	3979	1/1	0.76	0.21	74,74,74,74	0
54	MG	1A	3385	1/1	0.76	0.15	70,70,70,70	0
54	MG	2a	3065	1/1	0.76	0.26	78,78,78,78	0
54	MG	1A	3840	1/1	0.76	0.19	61,61,61,61	0
54	MG	2a	3067	1/1	0.76	0.20	80,80,80,80	0
54	MG	1A	3601	1/1	0.76	0.43	50,50,50,50	0
54	MG	2A	3462	1/1	0.76	0.16	56,56,56,56	0
54	MG	1B	224	1/1	0.76	0.14	64,64,64,64	0
54	MG	2a	3016	1/1	0.76	0.14	94,94,94,94	0
54	MG	2A	3219	1/1	0.76	0.18	70,70,70,70	0
57	MPD	1T	207	8/8	0.76	0.23	73,77,81,82	0
54	MG	2a	3047	1/1	0.76	0.34	72,72,72,72	0
58	ARG	1F	319	12/12	0.76	0.22	60,72,89,89	0
54	MG	1H	201	1/1	0.77	0.17	76,76,76,76	0
54	MG	1A	3237	1/1	0.77	0.29	79,79,79,79	0
54	MG	2A	3153	1/1	0.77	0.18	77,77,77,77	0
54	MG	2A	3376	1/1	0.77	0.21	60,60,60,60	0
54	MG	1a	1879	1/1	0.77	0.15	90,90,90,90	0
54	MG	2a	3103	1/1	0.77	0.12	73,73,73,73	0
54	MG	1n	101	1/1	0.77	0.17	72,72,72,72	0
54	MG	1A	3731	1/1	0.77	0.13	48,48,48,48	0
54	MG	1a	1642	1/1	0.77	0.16	76,76,76,76	0
54	MG	1A	3736	1/1	0.77	0.09	74,74,74,74	0
54	MG	1A	3975	1/1	0.77	0.19	63,63,63,63	0
54	MG	1A	3978	1/1	0.77	0.20	67,67,67,67	0
54	MG	2a	3059	1/1	0.77	0.34	85,85,85,85	0
54	MG	2A	3512	1/1	0.78	0.11	79,79,79,79	0
54	MG	1A	3562	1/1	0.78	0.15	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3797	1/1	0.78	0.24	73,73,73,73	0
54	MG	1a	1647	1/1	0.78	0.30	71,71,71,71	0
54	MG	15	106	1/1	0.78	0.19	58,58,58,58	0
54	MG	2a	3180	1/1	0.78	0.16	86,86,86,86	0
54	MG	2A	3398	1/1	0.78	0.16	70,70,70,70	0
54	MG	2A	3675	1/1	0.78	0.20	55,55,55,55	0
54	MG	2A	3448	1/1	0.78	0.22	67,67,67,67	0
54	MG	2a	3033	1/1	0.78	0.18	84,84,84,84	0
54	MG	1A	3476	1/1	0.79	0.13	58,58,58,58	0
54	MG	2A	3597	1/1	0.79	0.20	48,48,48,48	0
54	MG	2A	3415	1/1	0.79	0.23	71,71,71,71	0
54	MG	1a	1747	1/1	0.79	0.17	78,78,78,78	0
54	MG	1A	3341	1/1	0.79	0.14	49,49,49,49	0
54	MG	1D	318	1/1	0.79	0.19	68,68,68,68	0
54	MG	1a	1652	1/1	0.79	0.25	81,81,81,81	0
54	MG	2a	3080	1/1	0.79	0.20	70,70,70,70	0
54	MG	2A	3282	1/1	0.79	0.17	61,61,61,61	0
54	MG	2A	3292	1/1	0.79	0.14	65,65,65,65	0
54	MG	2A	3465	1/1	0.79	0.18	80,80,80,80	0
54	MG	1A	3733	1/1	0.79	0.22	68,68,68,68	0
54	MG	1a	1821	1/1	0.79	0.17	88,88,88,88	0
54	MG	1A	3814	1/1	0.79	0.24	68,68,68,68	0
54	MG	1T	202	1/1	0.79	0.17	59,59,59,59	0
54	MG	1a	1875	1/1	0.79	0.18	82,82,82,82	0
54	MG	1A	3964	1/1	0.79	0.15	70,70,70,70	0
54	MG	2A	3186	1/1	0.79	0.29	59,59,59,59	0
54	MG	1g	202	1/1	0.80	0.14	69,69,69,69	0
54	MG	1A	3696	1/1	0.80	0.15	71,71,71,71	0
54	MG	2a	3032	1/1	0.80	0.24	74,74,74,74	0
54	MG	1A	3396	1/1	0.80	0.26	71,71,71,71	0
54	MG	1A	3614	1/1	0.80	0.18	75,75,75,75	0
54	MG	2A	3334	1/1	0.80	0.15	83,83,83,83	0
54	MG	2A	3345	1/1	0.80	0.22	81,81,81,81	0
54	MG	1a	1793	1/1	0.80	0.13	71,71,71,71	0
54	MG	2A	3517	1/1	0.80	0.12	61,61,61,61	0
54	MG	1A	3675	1/1	0.80	0.14	34,34,34,34	0
54	MG	1a	1671	1/1	0.80	0.21	81,81,81,81	0
54	MG	1a	1679	1/1	0.80	0.28	71,71,71,71	0
54	MG	1A	3626	1/1	0.80	0.15	85,85,85,85	0
54	MG	1A	3749	1/1	0.80	0.15	59,59,59,59	0
54	MG	2A	3162	1/1	0.80	0.21	68,68,68,68	0
54	MG	2A	3671	1/1	0.80	0.14	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
54	MG	2a	3111	1/1	0.80	0.23	75,75,75,75	0
54	MG	2A	3171	1/1	0.80	0.15	80,80,80,80	0
54	MG	1a	1865	1/1	0.80	0.25	85,85,85,85	0
54	MG	1a	1706	1/1	0.80	0.44	81,81,81,81	0
54	MG	2A	3195	1/1	0.80	0.22	67,67,67,67	0
54	MG	1A	3445	1/1	0.80	0.14	78,78,78,78	0
54	MG	1a	1618	1/1	0.80	0.15	66,66,66,66	0
54	MG	1a	1723	1/1	0.80	0.27	79,79,79,79	0
54	MG	2A	3452	1/1	0.80	0.18	70,70,70,70	0
54	MG	2a	3028	1/1	0.81	0.26	87,87,87,87	0
54	MG	2A	3498	1/1	0.81	0.21	46,46,46,46	0
54	MG	1A	3236	1/1	0.81	0.28	74,74,74,74	0
54	MG	2a	3035	1/1	0.81	0.26	74,74,74,74	0
54	MG	1A	3150	1/1	0.81	0.23	76,76,76,76	0
54	MG	1A	3751	1/1	0.81	0.12	55,55,55,55	0
54	MG	2A	3194	1/1	0.81	0.16	64,64,64,64	0
54	MG	1A	3701	1/1	0.81	0.14	74,74,74,74	0
54	MG	2a	3058	1/1	0.81	0.20	92,92,92,92	0
54	MG	1a	1756	1/1	0.81	0.11	84,84,84,84	0
54	MG	2A	3593	1/1	0.81	0.14	50,50,50,50	0
54	MG	2A	3208	1/1	0.81	0.21	65,65,65,65	0
54	MG	1a	1660	1/1	0.81	0.38	79,79,79,79	0
54	MG	1a	1666	1/1	0.81	0.12	77,77,77,77	0
54	MG	2A	3240	1/1	0.81	0.37	72,72,72,72	0
54	MG	2A	3445	1/1	0.81	0.11	84,84,84,84	0
54	MG	1A	3304	1/1	0.81	0.18	51,51,51,51	0
54	MG	1A	3319	1/1	0.81	0.17	74,74,74,74	0
54	MG	1A	3185	1/1	0.81	0.15	71,71,71,71	0
54	MG	1a	1816	1/1	0.81	0.13	76,76,76,76	0
54	MG	1l	102	1/1	0.81	0.31	63,63,63,63	0
54	MG	1A	3845	1/1	0.81	0.11	53,53,53,53	0
54	MG	2e	202	1/1	0.81	0.34	79,79,79,79	0
54	MG	1A	3972	1/1	0.81	0.13	51,51,51,51	0
54	MG	2A	3477	1/1	0.81	0.27	75,75,75,75	0
54	MG	2a	3011	1/1	0.81	0.33	77,77,77,77	0
54	MG	1a	1871	1/1	0.81	0.15	76,76,76,76	0
54	MG	1A	3856	1/1	0.82	0.16	61,61,61,61	0
54	MG	1A	3318	1/1	0.82	0.19	69,69,69,69	0
54	MG	2A	3043	1/1	0.82	0.32	80,80,80,80	0
54	MG	1a	1798	1/1	0.82	0.31	72,72,72,72	0
54	MG	2A	3264	1/1	0.82	0.19	75,75,75,75	0
54	MG	2A	3052	1/1	0.82	0.28	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3084	1/1	0.82	0.18	80,80,80,80	0
54	MG	13	102	1/1	0.82	0.21	67,67,67,67	0
54	MG	2A	3293	1/1	0.82	0.18	56,56,56,56	0
54	MG	1A	3870	1/1	0.82	0.20	45,45,45,45	0
54	MG	2A	3506	1/1	0.82	0.20	92,92,92,92	0
54	MG	2A	3510	1/1	0.82	0.18	79,79,79,79	0
54	MG	1A	3457	1/1	0.82	0.13	53,53,53,53	0
54	MG	2a	3057	1/1	0.82	0.30	86,86,86,86	0
54	MG	1B	203	1/1	0.82	0.25	67,67,67,67	0
54	MG	1a	1827	1/1	0.82	0.19	88,88,88,88	0
54	MG	1a	1836	1/1	0.82	0.29	74,74,74,74	0
54	MG	2A	3161	1/1	0.82	0.20	83,83,83,83	0
54	MG	1A	3377	1/1	0.82	0.15	61,61,61,61	0
54	MG	2A	3392	1/1	0.82	0.21	78,78,78,78	0
54	MG	1A	3591	1/1	0.82	0.14	76,76,76,76	0
54	MG	2A	3179	1/1	0.82	0.23	82,82,82,82	0
54	MG	1A	3509	1/1	0.82	0.12	29,29,29,29	0
54	MG	2a	3104	1/1	0.82	0.10	85,85,85,85	0
54	MG	1A	3713	1/1	0.82	0.33	54,54,54,54	0
54	MG	2A	3680	1/1	0.82	0.18	64,64,64,64	0
54	MG	2A	3689	1/1	0.82	0.25	70,70,70,70	0
54	MG	1a	1662	1/1	0.82	0.14	70,70,70,70	0
54	MG	2a	3167	1/1	0.82	0.24	89,89,89,89	0
54	MG	1a	1773	1/1	0.82	0.22	64,64,64,64	0
54	MG	2B	208	1/1	0.82	0.29	85,85,85,85	0
54	MG	2B	209	1/1	0.82	0.29	80,80,80,80	0
54	MG	2A	3203	1/1	0.82	0.30	72,72,72,72	0
54	MG	1a	1788	1/1	0.82	0.12	86,86,86,86	0
54	MG	1A	3992	1/1	0.82	0.25	55,55,55,55	0
54	MG	2A	3291	1/1	0.83	0.14	59,59,59,59	0
54	MG	2a	3018	1/1	0.83	0.42	74,74,74,74	0
54	MG	1A	3574	1/1	0.83	0.27	46,46,46,46	0
54	MG	1A	3540	1/1	0.83	0.14	66,66,66,66	0
54	MG	1a	1795	1/1	0.83	0.15	66,66,66,66	0
54	MG	2A	3106	1/1	0.83	0.20	62,62,62,62	0
54	MG	1A	3592	1/1	0.83	0.27	52,52,52,52	0
54	MG	1a	1684	1/1	0.83	0.31	76,76,76,76	0
54	MG	1A	3970	1/1	0.83	0.19	51,51,51,51	0
54	MG	1A	4009	1/1	0.83	0.10	84,84,84,84	0
54	MG	1a	1704	1/1	0.83	0.20	74,74,74,74	0
54	MG	1A	3336	1/1	0.83	0.16	63,63,63,63	0
54	MG	1a	1707	1/1	0.83	0.20	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1615	1/1	0.83	0.10	79,79,79,79	0
54	MG	2A	3612	1/1	0.83	0.20	72,72,72,72	0
54	MG	1A	4024	1/1	0.83	0.17	61,61,61,61	0
54	MG	2A	3187	1/1	0.83	0.25	74,74,74,74	0
54	MG	1a	1717	1/1	0.83	0.33	80,80,80,80	0
54	MG	2A	3686	1/1	0.83	0.18	82,82,82,82	0
54	MG	2a	3099	1/1	0.83	0.13	78,78,78,78	0
54	MG	1a	1720	1/1	0.83	0.41	77,77,77,77	0
54	MG	2A	3691	1/1	0.83	0.20	83,83,83,83	0
54	MG	1a	1626	1/1	0.83	0.09	66,66,66,66	0
54	MG	1a	1727	1/1	0.83	0.16	70,70,70,70	0
54	MG	1A	3551	1/1	0.83	0.30	62,62,62,62	0
54	MG	2a	3145	1/1	0.83	0.16	88,88,88,88	0
54	MG	1A	3621	1/1	0.83	0.14	46,46,46,46	0
54	MG	1B	210	1/1	0.83	0.15	65,65,65,65	0
54	MG	2a	3173	1/1	0.83	0.23	72,72,72,72	0
54	MG	1a	1765	1/1	0.83	0.19	67,67,67,67	0
54	MG	1A	3261	1/1	0.83	0.22	81,81,81,81	0
54	MG	1a	1777	1/1	0.83	0.10	69,69,69,69	0
54	MG	1A	3331	1/1	0.83	0.32	81,81,81,81	0
54	MG	2A	3268	1/1	0.83	0.17	78,78,78,78	0
54	MG	1A	3725	1/1	0.83	0.18	26,26,26,26	0
54	MG	1A	3799	1/1	0.84	0.16	34,34,34,34	0
54	MG	1a	1680	1/1	0.84	0.14	86,86,86,86	0
54	MG	1B	226	1/1	0.84	0.10	78,78,78,78	0
54	MG	1A	3405	1/1	0.84	0.14	51,51,51,51	0
54	MG	1A	3834	1/1	0.84	0.21	47,47,47,47	0
54	MG	1a	1698	1/1	0.84	0.24	78,78,78,78	0
54	MG	1A	3443	1/1	0.84	0.29	82,82,82,82	0
54	MG	1N	203	1/1	0.84	0.14	70,70,70,70	0
54	MG	1A	3707	1/1	0.84	0.15	70,70,70,70	0
54	MG	2A	3227	1/1	0.84	0.27	65,65,65,65	0
54	MG	2A	3234	1/1	0.84	0.26	73,73,73,73	0
54	MG	1A	3981	1/1	0.84	0.25	59,59,59,59	0
54	MG	1A	3145	1/1	0.84	0.17	69,69,69,69	0
54	MG	1A	3454	1/1	0.84	0.23	65,65,65,65	0
54	MG	1d	302	1/1	0.84	0.20	74,74,74,74	0
54	MG	1A	3986	1/1	0.84	0.10	75,75,75,75	0
54	MG	19	103	1/1	0.84	0.21	67,67,67,67	0
54	MG	2A	3548	1/1	0.84	0.14	37,37,37,37	0
54	MG	1a	1603	1/1	0.84	0.22	77,77,77,77	0
54	MG	1a	1612	1/1	0.84	0.20	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3325	1/1	0.84	0.18	66,66,66,66	0
54	MG	2a	3072	1/1	0.84	0.36	67,67,67,67	0
54	MG	1A	3061	1/1	0.84	0.23	64,64,64,64	0
54	MG	2A	3053	1/1	0.84	0.28	69,69,69,69	0
54	MG	1A	3667	1/1	0.84	0.17	65,65,65,65	0
54	MG	2a	3101	1/1	0.84	0.14	71,71,71,71	0
54	MG	1a	1769	1/1	0.84	0.18	63,63,63,63	0
54	MG	1A	3491	1/1	0.84	0.12	60,60,60,60	0
54	MG	1A	4008	1/1	0.84	0.14	61,61,61,61	0
54	MG	1a	1782	1/1	0.84	0.12	76,76,76,76	0
54	MG	1A	3676	1/1	0.84	0.12	49,49,49,49	0
54	MG	2a	3119	1/1	0.84	0.13	65,65,65,65	0
54	MG	1A	3898	1/1	0.84	0.27	40,40,40,40	0
54	MG	2A	3406	1/1	0.84	0.20	92,92,92,92	0
54	MG	2B	202	1/1	0.84	0.16	73,73,73,73	0
54	MG	1A	3107	1/1	0.84	0.15	36,36,36,36	0
54	MG	2a	3178	1/1	0.84	0.19	81,81,81,81	0
54	MG	1A	3931	1/1	0.84	0.17	64,64,64,64	0
54	MG	1a	1665	1/1	0.84	0.17	76,76,76,76	0
54	MG	1A	3530	1/1	0.84	0.12	79,79,79,79	0
54	MG	1a	1809	1/1	0.84	0.28	74,74,74,74	0
54	MG	2A	3438	1/1	0.84	0.37	64,64,64,64	0
54	MG	1A	3694	1/1	0.84	0.23	78,78,78,78	0
54	MG	1a	1869	1/1	0.85	0.13	84,84,84,84	0
54	MG	1a	1729	1/1	0.85	0.19	74,74,74,74	0
54	MG	2A	3228	1/1	0.85	0.16	66,66,66,66	0
54	MG	1a	1872	1/1	0.85	0.11	89,89,89,89	0
54	MG	2A	3632	1/1	0.85	0.12	87,87,87,87	0
54	MG	1A	3699	1/1	0.85	0.16	41,41,41,41	0
54	MG	1A	3926	1/1	0.85	0.15	30,30,30,30	0
54	MG	2A	3259	1/1	0.85	0.20	57,57,57,57	0
54	MG	1a	1749	1/1	0.85	0.13	65,65,65,65	0
54	MG	1a	1750	1/1	0.85	0.20	73,73,73,73	0
54	MG	1d	301	1/1	0.85	0.26	74,74,74,74	0
54	MG	2A	3707	1/1	0.85	0.12	73,73,73,73	0
54	MG	2A	3708	1/1	0.85	0.21	64,64,64,64	0
54	MG	2A	3269	1/1	0.85	0.18	39,39,39,39	0
54	MG	2B	203	1/1	0.85	0.27	74,74,74,74	0
54	MG	1a	1752	1/1	0.85	0.33	71,71,71,71	0
54	MG	1e	201	1/1	0.85	0.21	72,72,72,72	0
54	MG	1A	3479	1/1	0.85	0.12	50,50,50,50	0
54	MG	1h	201	1/1	0.85	0.16	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3297	1/1	0.85	0.21	82,82,82,82	0
54	MG	2E	305	1/1	0.85	0.21	62,62,62,62	0
54	MG	2A	3333	1/1	0.85	0.10	36,36,36,36	0
54	MG	1i	3100	1/1	0.85	0.14	80,80,80,80	0
54	MG	1a	1757	1/1	0.85	0.20	50,50,50,50	0
54	MG	1A	3035	1/1	0.85	0.34	68,68,68,68	0
54	MG	2a	3002	1/1	0.85	0.13	66,66,66,66	0
54	MG	1t	201	1/1	0.85	0.14	70,70,70,70	0
54	MG	1y	203	1/1	0.85	0.11	75,75,75,75	0
54	MG	2A	3012	1/1	0.85	0.14	71,71,71,71	0
54	MG	2A	3024	1/1	0.85	0.24	77,77,77,77	0
54	MG	2a	3020	1/1	0.85	0.28	66,66,66,66	0
54	MG	2a	3021	1/1	0.85	0.20	76,76,76,76	0
54	MG	2a	3022	1/1	0.85	0.22	60,60,60,60	0
54	MG	2A	3036	1/1	0.85	0.20	57,57,57,57	0
54	MG	1A	3189	1/1	0.85	0.13	76,76,76,76	0
54	MG	1A	4019	1/1	0.85	0.12	66,66,66,66	0
54	MG	2A	3408	1/1	0.85	0.18	59,59,59,59	0
54	MG	1a	1774	1/1	0.85	0.14	73,73,73,73	0
54	MG	1A	3583	1/1	0.85	0.12	63,63,63,63	0
54	MG	2a	3049	1/1	0.85	0.34	69,69,69,69	0
54	MG	2A	3073	1/1	0.85	0.28	65,65,65,65	0
54	MG	1a	1682	1/1	0.85	0.12	69,69,69,69	0
54	MG	1a	1601	1/1	0.85	0.15	89,89,89,89	0
54	MG	1A	3659	1/1	0.85	0.23	42,42,42,42	0
54	MG	1A	3079	1/1	0.85	0.18	60,60,60,60	0
54	MG	1A	3538	1/1	0.85	0.10	62,62,62,62	0
54	MG	1A	3866	1/1	0.85	0.12	56,56,56,56	0
54	MG	2A	3120	1/1	0.85	0.23	63,63,63,63	0
54	MG	1a	1796	1/1	0.85	0.18	90,90,90,90	0
54	MG	1A	3600	1/1	0.85	0.18	65,65,65,65	0
54	MG	2A	3160	1/1	0.85	0.14	72,72,72,72	0
54	MG	1a	1630	1/1	0.85	0.16	63,63,63,63	0
54	MG	2a	3086	1/1	0.85	0.28	81,81,81,81	0
54	MG	1A	3455	1/1	0.85	0.14	34,34,34,34	0
54	MG	1a	1710	1/1	0.85	0.25	71,71,71,71	0
54	MG	2A	3486	1/1	0.85	0.15	74,74,74,74	0
54	MG	2A	3491	1/1	0.85	0.09	76,76,76,76	0
54	MG	1a	1641	1/1	0.85	0.17	79,79,79,79	0
54	MG	2A	3180	1/1	0.85	0.19	71,71,71,71	0
54	MG	2a	3116	1/1	0.85	0.22	82,82,82,82	0
54	MG	1A	3610	1/1	0.85	0.30	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3402	1/1	0.85	0.17	72,72,72,72	0
54	MG	2a	3143	1/1	0.85	0.17	70,70,70,70	0
54	MG	1a	1829	1/1	0.85	0.24	74,74,74,74	0
54	MG	2a	3158	1/1	0.85	0.15	88,88,88,88	0
54	MG	1a	1831	1/1	0.85	0.13	62,62,62,62	0
54	MG	2A	3515	1/1	0.85	0.21	82,82,82,82	0
54	MG	1A	3363	1/1	0.85	0.12	71,71,71,71	0
54	MG	2A	3202	1/1	0.85	0.24	63,63,63,63	0
54	MG	2A	3531	1/1	0.85	0.12	87,87,87,87	0
54	MG	1a	1841	1/1	0.85	0.22	79,79,79,79	0
54	MG	2j	201	1/1	0.85	0.08	84,84,84,84	0
54	MG	1a	1849	1/1	0.85	0.15	66,66,66,66	0
57	MPD	1A	4034	8/8	0.85	0.26	54,59,62,65	0
54	MG	1a	1724	1/1	0.85	0.18	64,64,64,64	0
54	MG	2A	3591	1/1	0.85	0.13	55,55,55,55	0
54	MG	1a	1657	1/1	0.85	0.21	84,84,84,84	0
54	MG	2D	308	1/1	0.86	0.10	37,37,37,37	0
54	MG	1A	3036	1/1	0.86	0.10	51,51,51,51	0
54	MG	1a	1867	1/1	0.86	0.12	87,87,87,87	0
54	MG	1a	1659	1/1	0.86	0.24	47,47,47,47	0
54	MG	1a	1870	1/1	0.86	0.17	69,69,69,69	0
54	MG	1A	3152	1/1	0.86	0.19	50,50,50,50	0
54	MG	2O	202	1/1	0.86	0.14	76,76,76,76	0
54	MG	2O	101	1/1	0.86	0.16	78,78,78,78	0
54	MG	1A	3524	1/1	0.86	0.16	56,56,56,56	0
54	MG	1A	3646	1/1	0.86	0.13	30,30,30,30	0
54	MG	2A	3451	1/1	0.86	0.15	67,67,67,67	0
54	MG	1A	3787	1/1	0.86	0.09	24,24,24,24	0
54	MG	1a	1668	1/1	0.86	0.25	82,82,82,82	0
54	MG	1A	3648	1/1	0.86	0.20	55,55,55,55	0
54	MG	1a	1673	1/1	0.86	0.17	61,61,61,61	0
54	MG	1a	1770	1/1	0.86	0.12	68,68,68,68	0
54	MG	1A	3398	1/1	0.86	0.13	53,53,53,53	0
54	MG	2a	3030	1/1	0.86	0.34	72,72,72,72	0
54	MG	2A	3482	1/1	0.86	0.17	65,65,65,65	0
54	MG	2A	3204	1/1	0.86	0.15	67,67,67,67	0
54	MG	2a	3034	1/1	0.86	0.23	92,92,92,92	0
54	MG	2A	3205	1/1	0.86	0.16	74,74,74,74	0
54	MG	1A	3809	1/1	0.86	0.24	59,59,59,59	0
54	MG	1A	3587	1/1	0.86	0.14	57,57,57,57	0
54	MG	2A	3499	1/1	0.86	0.12	67,67,67,67	0
54	MG	2a	3052	1/1	0.86	0.20	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
54	MG	1A	3941	1/1	0.86	0.18	53,53,53,53	0
54	MG	1A	3947	1/1	0.86	0.13	48,48,48,48	0
54	MG	1a	1690	1/1	0.86	0.39	69,69,69,69	0
54	MG	1A	3956	1/1	0.86	0.12	55,55,55,55	0
54	MG	1y	202	1/1	0.86	0.15	68,68,68,68	0
54	MG	2a	3060	1/1	0.86	0.32	80,80,80,80	0
54	MG	1A	4023	1/1	0.86	0.15	60,60,60,60	0
54	MG	1A	3817	1/1	0.86	0.18	77,77,77,77	0
54	MG	2A	3016	1/1	0.86	0.32	74,74,74,74	0
54	MG	1A	3131	1/1	0.86	0.18	45,45,45,45	0
54	MG	2A	3551	1/1	0.86	0.13	51,51,51,51	0
54	MG	2a	3074	1/1	0.86	0.25	75,75,75,75	0
54	MG	2a	3078	1/1	0.86	0.39	71,71,71,71	0
54	MG	2A	3552	1/1	0.86	0.14	44,44,44,44	0
54	MG	2A	3025	1/1	0.86	0.13	62,62,62,62	0
54	MG	2A	3034	1/1	0.86	0.23	77,77,77,77	0
54	MG	2a	3092	1/1	0.86	0.12	89,89,89,89	0
54	MG	2a	3096	1/1	0.86	0.10	63,63,63,63	0
54	MG	1A	3719	1/1	0.86	0.14	60,60,60,60	0
54	MG	1a	1801	1/1	0.86	0.32	85,85,85,85	0
54	MG	2a	3102	1/1	0.86	0.10	67,67,67,67	0
54	MG	1a	1803	1/1	0.86	0.16	80,80,80,80	0
54	MG	1a	1631	1/1	0.86	0.20	54,54,54,54	0
54	MG	1a	1635	1/1	0.86	0.20	76,76,76,76	0
54	MG	2A	3059	1/1	0.86	0.28	58,58,58,58	0
54	MG	1A	3461	1/1	0.86	0.23	74,74,74,74	0
54	MG	2A	3076	1/1	0.86	0.14	63,63,63,63	0
54	MG	2a	3118	1/1	0.86	0.20	61,61,61,61	0
54	MG	2A	3340	1/1	0.86	0.17	50,50,50,50	0
54	MG	1a	1716	1/1	0.86	0.26	65,65,65,65	0
54	MG	1A	3087	1/1	0.86	0.17	59,59,59,59	0
54	MG	1B	225	1/1	0.86	0.12	72,72,72,72	0
54	MG	1a	1721	1/1	0.86	0.11	75,75,75,75	0
54	MG	2A	3100	1/1	0.86	0.17	71,71,71,71	0
54	MG	2a	3171	1/1	0.86	0.13	83,83,83,83	0
54	MG	2A	3101	1/1	0.86	0.27	61,61,61,61	0
54	MG	2B	201	1/1	0.86	0.14	82,82,82,82	0
54	MG	1a	1644	1/1	0.86	0.27	68,68,68,68	0
54	MG	1A	3543	1/1	0.86	0.08	26,26,26,26	0
54	MG	2A	3112	1/1	0.86	0.35	73,73,73,73	0
54	MG	2A	3113	1/1	0.86	0.19	67,67,67,67	0
54	MG	1A	3148	1/1	0.86	0.11	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1728	1/1	0.86	0.29	65,65,65,65	0
57	MPD	2A	3714	8/8	0.86	0.28	49,56,62,62	0
54	MG	1a	1653	1/1	0.86	0.28	70,70,70,70	0
54	MG	2B	214	1/1	0.86	0.11	76,76,76,76	0
54	MG	2B	212	1/1	0.87	0.09	97,97,97,97	0
54	MG	2A	3375	1/1	0.87	0.12	60,60,60,60	0
54	MG	2A	3082	1/1	0.87	0.16	50,50,50,50	0
54	MG	1a	1805	1/1	0.87	0.17	79,79,79,79	0
54	MG	1a	1806	1/1	0.87	0.18	70,70,70,70	0
54	MG	2A	3404	1/1	0.87	0.15	60,60,60,60	0
54	MG	2A	3088	1/1	0.87	0.21	77,77,77,77	0
54	MG	1A	3822	1/1	0.87	0.11	45,45,45,45	0
54	MG	1a	1810	1/1	0.87	0.21	71,71,71,71	0
54	MG	1a	1811	1/1	0.87	0.16	63,63,63,63	0
54	MG	1a	1812	1/1	0.87	0.19	77,77,77,77	0
54	MG	2A	3423	1/1	0.87	0.15	69,69,69,69	0
54	MG	15	108	1/1	0.87	0.18	76,76,76,76	0
54	MG	1A	3982	1/1	0.87	0.15	68,68,68,68	0
54	MG	1a	1705	1/1	0.87	0.22	75,75,75,75	0
54	MG	1a	1819	1/1	0.87	0.23	68,68,68,68	0
54	MG	2A	3441	1/1	0.87	0.13	68,68,68,68	0
54	MG	1A	3180	1/1	0.87	0.43	67,67,67,67	0
54	MG	2A	3446	1/1	0.87	0.18	69,69,69,69	0
54	MG	2a	3027	1/1	0.87	0.20	77,77,77,77	0
54	MG	2A	3121	1/1	0.87	0.17	70,70,70,70	0
54	MG	1a	1602	1/1	0.87	0.13	81,81,81,81	0
54	MG	2A	3131	1/1	0.87	0.14	71,71,71,71	0
54	MG	2A	3152	1/1	0.87	0.19	66,66,66,66	0
54	MG	1A	3837	1/1	0.87	0.10	54,54,54,54	0
54	MG	2A	3154	1/1	0.87	0.21	62,62,62,62	0
54	MG	2a	3039	1/1	0.87	0.20	80,80,80,80	0
54	MG	1a	1610	1/1	0.87	0.32	60,60,60,60	0
54	MG	1A	3647	1/1	0.87	0.21	69,69,69,69	0
54	MG	1a	1840	1/1	0.87	0.19	51,51,51,51	0
54	MG	1A	3408	1/1	0.87	0.27	68,68,68,68	0
54	MG	1a	1848	1/1	0.87	0.15	65,65,65,65	0
54	MG	2A	3489	1/1	0.87	0.12	83,83,83,83	0
54	MG	1A	3503	1/1	0.87	0.09	33,33,33,33	0
54	MG	1A	3652	1/1	0.87	0.12	59,59,59,59	0
54	MG	1A	3437	1/1	0.87	0.16	76,76,76,76	0
54	MG	1a	1722	1/1	0.87	0.17	64,64,64,64	0
54	MG	1A	4007	1/1	0.87	0.16	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
54	MG	1A	3098	1/1	0.87	0.09	63,63,63,63	0
54	MG	1A	3525	1/1	0.87	0.15	66,66,66,66	0
54	MG	1A	3737	1/1	0.87	0.17	45,45,45,45	0
54	MG	1A	3528	1/1	0.87	0.10	51,51,51,51	0
54	MG	1A	3596	1/1	0.87	0.10	31,31,31,31	0
54	MG	1A	3155	1/1	0.87	0.14	47,47,47,47	0
54	MG	1A	3763	1/1	0.87	0.17	43,43,43,43	0
54	MG	2a	3084	1/1	0.87	0.22	69,69,69,69	0
54	MG	1A	3764	1/1	0.87	0.23	56,56,56,56	0
54	MG	1a	1656	1/1	0.87	0.33	61,61,61,61	0
54	MG	1A	3783	1/1	0.87	0.10	45,45,45,45	0
54	MG	1B	221	1/1	0.87	0.11	59,59,59,59	0
54	MG	2A	3558	1/1	0.87	0.10	78,78,78,78	0
54	MG	1A	3933	1/1	0.87	0.13	61,61,61,61	0
54	MG	1A	3066	1/1	0.87	0.19	57,57,57,57	0
54	MG	1a	1663	1/1	0.87	0.20	75,75,75,75	0
54	MG	1A	3790	1/1	0.87	0.10	30,30,30,30	0
54	MG	2A	3260	1/1	0.87	0.22	68,68,68,68	0
54	MG	1A	3792	1/1	0.87	0.11	45,45,45,45	0
54	MG	1A	3284	1/1	0.87	0.32	74,74,74,74	0
54	MG	2A	3613	1/1	0.87	0.22	81,81,81,81	0
54	MG	2A	3631	1/1	0.87	0.13	53,53,53,53	0
54	MG	1a	1779	1/1	0.87	0.16	72,72,72,72	0
54	MG	2a	3134	1/1	0.87	0.09	80,80,80,80	0
54	MG	2A	3656	1/1	0.87	0.10	78,78,78,78	0
54	MG	2A	3006	1/1	0.87	0.21	71,71,71,71	0
54	MG	1a	1780	1/1	0.87	0.20	78,78,78,78	0
54	MG	1a	1670	1/1	0.87	0.30	61,61,61,61	0
54	MG	1G	203	1/1	0.87	0.12	63,63,63,63	0
54	MG	1a	1789	1/1	0.87	0.17	83,83,83,83	0
54	MG	1A	3297	1/1	0.87	0.13	53,53,53,53	0
54	MG	2a	3175	1/1	0.87	0.09	79,79,79,79	0
54	MG	2A	3330	1/1	0.87	0.13	39,39,39,39	0
54	MG	1A	3803	1/1	0.87	0.23	69,69,69,69	0
54	MG	2e	201	1/1	0.87	0.20	75,75,75,75	0
54	MG	1A	3400	1/1	0.87	0.18	56,56,56,56	0
54	MG	1A	3810	1/1	0.87	0.16	65,65,65,65	0
54	MG	1T	204	1/1	0.87	0.18	67,67,67,67	0
54	MG	1A	3298	1/1	0.87	0.16	74,74,74,74	0
54	MG	2B	205	1/1	0.87	0.20	64,64,64,64	0
54	MG	1a	1799	1/1	0.87	0.11	73,73,73,73	0
54	MG	1a	1689	1/1	0.87	0.27	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3631	1/1	0.87	0.20	53,53,53,53	0
54	MG	2A	3031	1/1	0.88	0.14	68,68,68,68	0
54	MG	1a	1674	1/1	0.88	0.32	66,66,66,66	0
54	MG	2A	3692	1/1	0.88	0.10	89,89,89,89	0
54	MG	2A	3300	1/1	0.88	0.15	63,63,63,63	0
54	MG	2A	3307	1/1	0.88	0.12	54,54,54,54	0
54	MG	2A	3319	1/1	0.88	0.10	48,48,48,48	0
54	MG	2A	3324	1/1	0.88	0.18	65,65,65,65	0
54	MG	1a	1676	1/1	0.88	0.13	75,75,75,75	0
54	MG	2A	3041	1/1	0.88	0.13	50,50,50,50	0
54	MG	1R	205	1/1	0.88	0.19	49,49,49,49	0
54	MG	2A	3046	1/1	0.88	0.11	65,65,65,65	0
54	MG	1A	3974	1/1	0.88	0.19	59,59,59,59	0
54	MG	1a	1681	1/1	0.88	0.15	62,62,62,62	0
54	MG	1A	3430	1/1	0.88	0.15	54,54,54,54	0
54	MG	2A	3357	1/1	0.88	0.09	35,35,35,35	0
54	MG	1A	3198	1/1	0.88	0.14	61,61,61,61	0
54	MG	2A	3361	1/1	0.88	0.20	69,69,69,69	0
54	MG	2D	309	1/1	0.88	0.21	55,55,55,55	0
54	MG	2A	3367	1/1	0.88	0.14	42,42,42,42	0
54	MG	2A	3070	1/1	0.88	0.20	65,65,65,65	0
54	MG	10	103	1/1	0.88	0.13	60,60,60,60	0
54	MG	1A	3616	1/1	0.88	0.12	45,45,45,45	0
54	MG	2A	3388	1/1	0.88	0.09	71,71,71,71	0
54	MG	1A	3536	1/1	0.88	0.11	28,28,28,28	0
54	MG	2P	201	1/1	0.88	0.25	72,72,72,72	0
54	MG	1a	1808	1/1	0.88	0.28	70,70,70,70	0
54	MG	2I	101	1/1	0.88	0.09	88,88,88,88	0
54	MG	1a	1692	1/1	0.88	0.19	62,62,62,62	0
54	MG	1A	3344	1/1	0.88	0.28	51,51,51,51	0
54	MG	1A	3843	1/1	0.88	0.11	54,54,54,54	0
54	MG	1a	1703	1/1	0.88	0.38	78,78,78,78	0
54	MG	1A	3351	1/1	0.88	0.14	70,70,70,70	0
54	MG	1A	3204	1/1	0.88	0.23	64,64,64,64	0
54	MG	1A	3008	1/1	0.88	0.15	50,50,50,50	0
54	MG	1A	3859	1/1	0.88	0.17	54,54,54,54	0
54	MG	2A	3429	1/1	0.88	0.15	62,62,62,62	0
54	MG	1a	1604	1/1	0.88	0.38	78,78,78,78	0
54	MG	2a	3029	1/1	0.88	0.29	64,64,64,64	0
54	MG	2A	3431	1/1	0.88	0.12	66,66,66,66	0
54	MG	1A	3116	1/1	0.88	0.23	47,47,47,47	0
54	MG	2A	3116	1/1	0.88	0.16	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1712	1/1	0.88	0.33	80,80,80,80	0
54	MG	1a	1611	1/1	0.88	0.28	71,71,71,71	0
54	MG	1a	1834	1/1	0.88	0.10	84,84,84,84	0
54	MG	2a	3041	1/1	0.88	0.22	65,65,65,65	0
54	MG	2a	3043	1/1	0.88	0.32	70,70,70,70	0
54	MG	2A	3127	1/1	0.88	0.21	58,58,58,58	0
54	MG	1A	3392	1/1	0.88	0.10	40,40,40,40	0
54	MG	1A	4001	1/1	0.88	0.30	45,45,45,45	0
54	MG	1a	1719	1/1	0.88	0.47	75,75,75,75	0
54	MG	2a	3054	1/1	0.88	0.21	72,72,72,72	0
54	MG	1a	1843	1/1	0.88	0.21	85,85,85,85	0
54	MG	1a	1844	1/1	0.88	0.14	61,61,61,61	0
54	MG	1a	1616	1/1	0.88	0.20	80,80,80,80	0
54	MG	1A	3557	1/1	0.88	0.12	59,59,59,59	0
54	MG	2A	3474	1/1	0.88	0.16	67,67,67,67	0
54	MG	2A	3167	1/1	0.88	0.26	61,61,61,61	0
54	MG	2A	3170	1/1	0.88	0.17	62,62,62,62	0
54	MG	2A	3485	1/1	0.88	0.10	63,63,63,63	0
54	MG	1A	3756	1/1	0.88	0.24	61,61,61,61	0
54	MG	1a	1851	1/1	0.88	0.17	71,71,71,71	0
54	MG	1a	1861	1/1	0.88	0.33	73,73,73,73	0
54	MG	2A	3492	1/1	0.88	0.12	71,71,71,71	0
54	MG	2A	3182	1/1	0.88	0.18	73,73,73,73	0
54	MG	2A	3494	1/1	0.88	0.10	69,69,69,69	0
54	MG	2A	3495	1/1	0.88	0.09	65,65,65,65	0
54	MG	1A	3471	1/1	0.88	0.14	59,59,59,59	0
54	MG	1A	3570	1/1	0.88	0.09	44,44,44,44	0
54	MG	2a	3087	1/1	0.88	0.13	73,73,73,73	0
54	MG	1a	1632	1/1	0.88	0.32	79,79,79,79	0
54	MG	2a	3094	1/1	0.88	0.21	74,74,74,74	0
54	MG	1A	3896	1/1	0.88	0.15	64,64,64,64	0
54	MG	1A	3310	1/1	0.88	0.48	49,49,49,49	0
54	MG	2A	3199	1/1	0.88	0.25	71,71,71,71	0
54	MG	1A	3766	1/1	0.88	0.19	62,62,62,62	0
54	MG	1A	3911	1/1	0.88	0.23	41,41,41,41	0
54	MG	2A	3520	1/1	0.88	0.10	34,34,34,34	0
54	MG	1A	3579	1/1	0.88	0.13	64,64,64,64	0
54	MG	1a	1646	1/1	0.88	0.29	61,61,61,61	0
54	MG	1A	3260	1/1	0.88	0.13	66,66,66,66	0
54	MG	2A	3549	1/1	0.88	0.13	41,41,41,41	0
54	MG	1A	3489	1/1	0.88	0.13	64,64,64,64	0
54	MG	1A	3679	1/1	0.88	0.12	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
54	MG	2a	3121	1/1	0.88	0.10	76,76,76,76	0
54	MG	2a	3125	1/1	0.88	0.11	81,81,81,81	0
54	MG	2A	3215	1/1	0.88	0.11	58,58,58,58	0
54	MG	2a	3142	1/1	0.88	0.10	83,83,83,83	0
54	MG	1a	1759	1/1	0.88	0.18	68,68,68,68	0
54	MG	1a	1763	1/1	0.88	0.21	64,64,64,64	0
54	MG	2a	3155	1/1	0.88	0.10	72,72,72,72	0
54	MG	2A	3584	1/1	0.88	0.13	53,53,53,53	0
54	MG	2A	3588	1/1	0.88	0.09	70,70,70,70	0
54	MG	1A	3184	1/1	0.88	0.15	52,52,52,52	0
54	MG	1A	3954	1/1	0.88	0.09	30,30,30,30	0
54	MG	1l	202	1/1	0.88	0.23	79,79,79,79	0
54	MG	1A	3401	1/1	0.88	0.08	75,75,75,75	0
54	MG	2a	3177	1/1	0.88	0.24	80,80,80,80	0
54	MG	1D	311	1/1	0.88	0.21	64,64,64,64	0
54	MG	1D	315	1/1	0.88	0.16	74,74,74,74	0
54	MG	1A	3153	1/1	0.88	0.35	72,72,72,72	0
54	MG	1E	306	1/1	0.88	0.18	53,53,53,53	0
54	MG	1F	315	1/1	0.88	0.60	55,55,55,55	0
54	MG	2A	3639	1/1	0.88	0.12	37,37,37,37	0
54	MG	1A	3597	1/1	0.88	0.20	55,55,55,55	0
54	MG	1A	3128	1/1	0.88	0.22	66,66,66,66	0
57	MPD	1a	1882	8/8	0.88	0.11	54,70,76,81	0
54	MG	2A	3286	1/1	0.88	0.10	42,42,42,42	0
54	MG	1A	3191	1/1	0.88	0.33	65,65,65,65	0
54	MG	1O	201	1/1	0.88	0.14	63,63,63,63	0
54	MG	1A	3833	1/1	0.89	0.08	20,20,20,20	0
54	MG	1A	3642	1/1	0.89	0.21	68,68,68,68	0
54	MG	1O	102	1/1	0.89	0.18	47,47,47,47	0
54	MG	2A	3174	1/1	0.89	0.13	63,63,63,63	0
54	MG	2A	3178	1/1	0.89	0.18	75,75,75,75	0
54	MG	1e	202	1/1	0.89	0.28	63,63,63,63	0
54	MG	1f	201	1/1	0.89	0.25	74,74,74,74	0
54	MG	1f	202	1/1	0.89	0.11	49,49,49,49	0
54	MG	2A	3184	1/1	0.89	0.18	66,66,66,66	0
54	MG	1A	3168	1/1	0.89	0.26	63,63,63,63	0
54	MG	1g	203	1/1	0.89	0.18	69,69,69,69	0
54	MG	1a	1783	1/1	0.89	0.24	77,77,77,77	0
54	MG	1A	3838	1/1	0.89	0.16	68,68,68,68	0
54	MG	1A	3839	1/1	0.89	0.12	59,59,59,59	0
54	MG	1A	3586	1/1	0.89	0.18	61,61,61,61	0
54	MG	1A	3332	1/1	0.89	0.14	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1o	101	1/1	0.89	0.25	58,58,58,58	0
54	MG	17	106	1/1	0.89	0.19	61,61,61,61	0
54	MG	2A	3479	1/1	0.89	0.09	71,71,71,71	0
54	MG	1A	3243	1/1	0.89	0.09	47,47,47,47	0
54	MG	2A	3484	1/1	0.89	0.24	60,60,60,60	0
54	MG	1A	3848	1/1	0.89	0.13	50,50,50,50	0
54	MG	2A	3005	1/1	0.89	0.15	65,65,65,65	0
54	MG	1A	3137	1/1	0.89	0.10	53,53,53,53	0
54	MG	1A	3302	1/1	0.89	0.16	42,42,42,42	0
54	MG	1A	3406	1/1	0.89	0.14	47,47,47,47	0
54	MG	2a	3037	1/1	0.89	0.24	73,73,73,73	0
54	MG	2A	3223	1/1	0.89	0.36	56,56,56,56	0
54	MG	2A	3226	1/1	0.89	0.37	65,65,65,65	0
54	MG	1A	3210	1/1	0.89	0.38	77,77,77,77	0
54	MG	2A	3496	1/1	0.89	0.25	66,66,66,66	0
54	MG	2a	3046	1/1	0.89	0.36	75,75,75,75	0
54	MG	1A	3660	1/1	0.89	0.17	70,70,70,70	0
54	MG	2A	3027	1/1	0.89	0.14	59,59,59,59	0
54	MG	2A	3500	1/1	0.89	0.15	74,74,74,74	0
54	MG	2A	3239	1/1	0.89	0.29	61,61,61,61	0
54	MG	2A	3505	1/1	0.89	0.15	69,69,69,69	0
54	MG	1A	3215	1/1	0.89	0.18	78,78,78,78	0
54	MG	1A	3873	1/1	0.89	0.10	48,48,48,48	0
54	MG	2A	3511	1/1	0.89	0.13	73,73,73,73	0
54	MG	1A	3674	1/1	0.89	0.16	69,69,69,69	0
54	MG	1a	1709	1/1	0.89	0.38	75,75,75,75	0
54	MG	1A	3603	1/1	0.89	0.15	67,67,67,67	0
54	MG	2a	3062	1/1	0.89	0.15	75,75,75,75	0
54	MG	1a	1621	1/1	0.89	0.21	65,65,65,65	0
54	MG	1a	1624	1/1	0.89	0.23	60,60,60,60	0
54	MG	1A	3890	1/1	0.89	0.10	68,68,68,68	0
54	MG	2A	3543	1/1	0.89	0.15	80,80,80,80	0
54	MG	1A	3894	1/1	0.89	0.13	53,53,53,53	0
54	MG	2a	3076	1/1	0.89	0.31	74,74,74,74	0
54	MG	1A	3607	1/1	0.89	0.14	52,52,52,52	0
54	MG	1A	4025	1/1	0.89	0.22	82,82,82,82	0
54	MG	1a	1825	1/1	0.89	0.15	72,72,72,72	0
54	MG	1A	3677	1/1	0.89	0.11	29,29,29,29	0
54	MG	1A	3435	1/1	0.89	0.24	54,54,54,54	0
54	MG	2A	3298	1/1	0.89	0.24	64,64,64,64	0
54	MG	1A	3903	1/1	0.89	0.11	59,59,59,59	0
54	MG	1B	215	1/1	0.89	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
54	MG	1A	3680	1/1	0.89	0.32	37,37,37,37	0
54	MG	2a	3098	1/1	0.89	0.12	66,66,66,66	0
54	MG	1A	3313	1/1	0.89	0.12	62,62,62,62	0
54	MG	1A	3920	1/1	0.89	0.09	45,45,45,45	0
54	MG	2A	3091	1/1	0.89	0.19	58,58,58,58	0
54	MG	2A	3604	1/1	0.89	0.15	41,41,41,41	0
54	MG	2A	3605	1/1	0.89	0.17	48,48,48,48	0
54	MG	2A	3098	1/1	0.89	0.25	62,62,62,62	0
54	MG	1a	1732	1/1	0.89	0.14	61,61,61,61	0
54	MG	2a	3115	1/1	0.89	0.15	71,71,71,71	0
54	MG	2A	3342	1/1	0.89	0.36	71,71,71,71	0
54	MG	1A	3687	1/1	0.89	0.14	60,60,60,60	0
54	MG	1A	3793	1/1	0.89	0.14	43,43,43,43	0
54	MG	1A	3565	1/1	0.89	0.13	47,47,47,47	0
54	MG	2A	3641	1/1	0.89	0.12	49,49,49,49	0
54	MG	2A	3644	1/1	0.89	0.11	79,79,79,79	0
54	MG	1A	3279	1/1	0.89	0.18	65,65,65,65	0
54	MG	2a	3140	1/1	0.89	0.15	77,77,77,77	0
54	MG	1A	3942	1/1	0.89	0.17	63,63,63,63	0
54	MG	2A	3114	1/1	0.89	0.11	54,54,54,54	0
54	MG	2A	3677	1/1	0.89	0.08	57,57,57,57	0
54	MG	2a	3149	1/1	0.89	0.11	54,54,54,54	0
54	MG	1a	1753	1/1	0.89	0.08	53,53,53,53	0
54	MG	2A	3682	1/1	0.89	0.11	64,64,64,64	0
54	MG	2a	3161	1/1	0.89	0.09	68,68,68,68	0
54	MG	2A	3118	1/1	0.89	0.24	47,47,47,47	0
54	MG	1A	3625	1/1	0.89	0.32	39,39,39,39	0
54	MG	1a	1866	1/1	0.89	0.11	57,57,57,57	0
54	MG	2A	3378	1/1	0.89	0.11	65,65,65,65	0
54	MG	2A	3382	1/1	0.89	0.15	73,73,73,73	0
54	MG	1A	3805	1/1	0.89	0.21	63,63,63,63	0
54	MG	1F	317	1/1	0.89	0.16	52,52,52,52	0
54	MG	1a	1760	1/1	0.89	0.16	81,81,81,81	0
54	MG	2A	3402	1/1	0.89	0.14	71,71,71,71	0
54	MG	2A	3135	1/1	0.89	0.17	68,68,68,68	0
54	MG	2A	3138	1/1	0.89	0.11	49,49,49,49	0
54	MG	1A	3697	1/1	0.89	0.10	78,78,78,78	0
54	MG	2t	201	1/1	0.89	0.20	58,58,58,58	0
54	MG	1A	3961	1/1	0.89	0.11	57,57,57,57	0
54	MG	1A	3217	1/1	0.89	0.18	46,46,46,46	0
54	MG	1A	3039	1/1	0.89	0.35	69,69,69,69	0
54	MG	2A	3419	1/1	0.89	0.14	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MPD	2A	3715	8/8	0.89	0.17	68,71,77,78	0
54	MG	1A	3639	1/1	0.89	0.12	66,66,66,66	0
54	MG	1A	3708	1/1	0.89	0.11	53,53,53,53	0
54	MG	2A	3352	1/1	0.90	0.17	57,57,57,57	0
54	MG	1A	3851	1/1	0.90	0.13	53,53,53,53	0
54	MG	1A	3448	1/1	0.90	0.13	44,44,44,44	0
54	MG	1A	3527	1/1	0.90	0.14	58,58,58,58	0
54	MG	1a	1823	1/1	0.90	0.24	74,74,74,74	0
54	MG	2A	3362	1/1	0.90	0.09	69,69,69,69	0
54	MG	1A	3858	1/1	0.90	0.13	42,42,42,42	0
54	MG	2A	3099	1/1	0.90	0.24	55,55,55,55	0
54	MG	2A	3372	1/1	0.90	0.10	57,57,57,57	0
54	MG	18	102	1/1	0.90	0.25	47,47,47,47	0
54	MG	1A	3289	1/1	0.90	0.14	57,57,57,57	0
54	MG	1a	1830	1/1	0.90	0.12	75,75,75,75	0
54	MG	2B	211	1/1	0.90	0.16	74,74,74,74	0
54	MG	1A	3635	1/1	0.90	0.10	24,24,24,24	0
54	MG	2A	3110	1/1	0.90	0.29	67,67,67,67	0
54	MG	1A	3991	1/1	0.90	0.15	46,46,46,46	0
54	MG	2A	3396	1/1	0.90	0.24	73,73,73,73	0
54	MG	2A	3397	1/1	0.90	0.13	51,51,51,51	0
54	MG	1A	3638	1/1	0.90	0.12	42,42,42,42	0
54	MG	2A	3399	1/1	0.90	0.18	67,67,67,67	0
54	MG	2A	3401	1/1	0.90	0.26	69,69,69,69	0
54	MG	1a	1713	1/1	0.90	0.23	72,72,72,72	0
54	MG	1A	3995	1/1	0.90	0.08	89,89,89,89	0
54	MG	1a	1605	1/1	0.90	0.16	63,63,63,63	0
54	MG	1A	3369	1/1	0.90	0.11	47,47,47,47	0
54	MG	1A	3767	1/1	0.90	0.13	44,44,44,44	0
54	MG	2A	3413	1/1	0.90	0.22	86,86,86,86	0
54	MG	25	101	1/1	0.90	0.59	49,49,49,49	0
54	MG	28	102	1/1	0.90	0.25	68,68,68,68	0
54	MG	1A	3773	1/1	0.90	0.17	49,49,49,49	0
54	MG	2a	3003	1/1	0.90	0.42	77,77,77,77	0
54	MG	1A	3881	1/1	0.90	0.18	31,31,31,31	0
54	MG	2A	3128	1/1	0.90	0.18	77,77,77,77	0
54	MG	1A	3190	1/1	0.90	0.12	61,61,61,61	0
54	MG	1A	3889	1/1	0.90	0.08	25,25,25,25	0
54	MG	1A	4014	1/1	0.90	0.13	38,38,38,38	0
54	MG	2A	3144	1/1	0.90	0.23	58,58,58,58	0
54	MG	2A	3148	1/1	0.90	0.28	57,57,57,57	0
54	MG	2A	3433	1/1	0.90	0.16	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3200	1/1	0.90	0.27	53,53,53,53	0
54	MG	1A	3892	1/1	0.90	0.14	53,53,53,53	0
54	MG	1a	1628	1/1	0.90	0.34	70,70,70,70	0
54	MG	2A	3443	1/1	0.90	0.23	60,60,60,60	0
54	MG	1A	3539	1/1	0.90	0.10	26,26,26,26	0
54	MG	1a	1740	1/1	0.90	0.19	58,58,58,58	0
54	MG	1A	3299	1/1	0.90	0.20	50,50,50,50	0
54	MG	2A	3164	1/1	0.90	0.29	56,56,56,56	0
54	MG	1A	3649	1/1	0.90	0.22	59,59,59,59	0
54	MG	2a	3040	1/1	0.90	0.11	84,84,84,84	0
54	MG	1A	3702	1/1	0.90	0.09	71,71,71,71	0
54	MG	2a	3042	1/1	0.90	0.13	66,66,66,66	0
54	MG	2A	3458	1/1	0.90	0.20	75,75,75,75	0
54	MG	2a	3044	1/1	0.90	0.29	80,80,80,80	0
54	MG	2A	3460	1/1	0.90	0.24	74,74,74,74	0
54	MG	2A	3461	1/1	0.90	0.09	71,71,71,71	0
54	MG	1a	1876	1/1	0.90	0.14	76,76,76,76	0
54	MG	1A	4027	1/1	0.90	0.15	69,69,69,69	0
54	MG	1A	3798	1/1	0.90	0.20	63,63,63,63	0
54	MG	1A	3283	1/1	0.90	0.12	41,41,41,41	0
54	MG	1A	3478	1/1	0.90	0.13	44,44,44,44	0
54	MG	1B	220	1/1	0.90	0.25	78,78,78,78	0
54	MG	1A	3912	1/1	0.90	0.09	20,20,20,20	0
54	MG	1a	1651	1/1	0.90	0.29	65,65,65,65	0
54	MG	1a	1761	1/1	0.90	0.27	51,51,51,51	0
54	MG	1A	3916	1/1	0.90	0.10	35,35,35,35	0
54	MG	2A	3189	1/1	0.90	0.32	72,72,72,72	0
54	MG	1a	1764	1/1	0.90	0.28	77,77,77,77	0
54	MG	1A	3709	1/1	0.90	0.29	44,44,44,44	0
54	MG	1A	3711	1/1	0.90	0.11	55,55,55,55	0
54	MG	1A	3928	1/1	0.90	0.08	73,73,73,73	0
54	MG	1a	1772	1/1	0.90	0.17	62,62,62,62	0
54	MG	1n	102	1/1	0.90	0.29	71,71,71,71	0
54	MG	1A	3346	1/1	0.90	0.48	76,76,76,76	0
54	MG	1A	3716	1/1	0.90	0.27	45,45,45,45	0
54	MG	1A	3815	1/1	0.90	0.08	59,59,59,59	0
54	MG	1y	201	1/1	0.90	0.08	72,72,72,72	0
54	MG	2A	3210	1/1	0.90	0.13	59,59,59,59	0
54	MG	2A	3504	1/1	0.90	0.15	59,59,59,59	0
54	MG	1A	3440	1/1	0.90	0.09	28,28,28,28	0
54	MG	2a	3088	1/1	0.90	0.15	76,76,76,76	0
54	MG	1A	3818	1/1	0.90	0.14	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
54	MG	2A	3221	1/1	0.90	0.25	48,48,48,48	0
54	MG	1A	3441	1/1	0.90	0.11	28,28,28,28	0
54	MG	1F	318	1/1	0.90	0.12	67,67,67,67	0
54	MG	1a	1785	1/1	0.90	0.18	52,52,52,52	0
54	MG	1a	1669	1/1	0.90	0.41	68,68,68,68	0
54	MG	2A	3229	1/1	0.90	0.17	63,63,63,63	0
54	MG	2A	3527	1/1	0.90	0.08	65,65,65,65	0
54	MG	2A	3017	1/1	0.90	0.17	60,60,60,60	0
54	MG	2A	3023	1/1	0.90	0.17	62,62,62,62	0
54	MG	1G	201	1/1	0.90	0.07	79,79,79,79	0
54	MG	2A	3248	1/1	0.90	0.30	48,48,48,48	0
54	MG	1A	3832	1/1	0.90	0.15	66,66,66,66	0
54	MG	1A	3558	1/1	0.90	0.22	58,58,58,58	0
54	MG	2A	3028	1/1	0.90	0.14	44,44,44,44	0
54	MG	1A	3729	1/1	0.90	0.27	41,41,41,41	0
54	MG	1A	3663	1/1	0.90	0.08	49,49,49,49	0
54	MG	2A	3560	1/1	0.90	0.12	54,54,54,54	0
54	MG	1P	203	1/1	0.90	0.24	40,40,40,40	0
54	MG	2A	3037	1/1	0.90	0.25	74,74,74,74	0
54	MG	2A	3279	1/1	0.90	0.12	73,73,73,73	0
54	MG	1P	206	1/1	0.90	0.14	71,71,71,71	0
54	MG	1A	3060	1/1	0.90	0.11	49,49,49,49	0
54	MG	2A	3044	1/1	0.90	0.14	53,53,53,53	0
54	MG	2a	3153	1/1	0.90	0.10	69,69,69,69	0
54	MG	2A	3599	1/1	0.90	0.14	39,39,39,39	0
54	MG	2a	3156	1/1	0.90	0.08	84,84,84,84	0
54	MG	2a	3157	1/1	0.90	0.21	69,69,69,69	0
54	MG	1A	3362	1/1	0.90	0.12	38,38,38,38	0
54	MG	1a	1683	1/1	0.90	0.22	67,67,67,67	0
54	MG	1A	3973	1/1	0.90	0.07	61,61,61,61	0
54	MG	2A	3606	1/1	0.90	0.12	60,60,60,60	0
54	MG	1A	3617	1/1	0.90	0.09	62,62,62,62	0
54	MG	2A	3056	1/1	0.90	0.23	60,60,60,60	0
54	MG	2A	3302	1/1	0.90	0.16	68,68,68,68	0
54	MG	2A	3304	1/1	0.90	0.32	69,69,69,69	0
54	MG	1a	1688	1/1	0.90	0.14	64,64,64,64	0
54	MG	2A	3637	1/1	0.90	0.09	82,82,82,82	0
54	MG	2a	3181	1/1	0.90	0.10	96,96,96,96	0
54	MG	2A	3062	1/1	0.90	0.15	60,60,60,60	0
54	MG	2A	3065	1/1	0.90	0.25	65,65,65,65	0
54	MG	1T	205	1/1	0.90	0.14	73,73,73,73	0
54	MG	1A	3740	1/1	0.90	0.13	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3747	1/1	0.90	0.20	45,45,45,45	0
54	MG	2A	3335	1/1	0.90	0.08	39,39,39,39	0
54	MG	2A	3336	1/1	0.90	0.21	72,72,72,72	0
54	MG	2A	3077	1/1	0.90	0.10	59,59,59,59	0
54	MG	1A	3447	1/1	0.90	0.10	31,31,31,31	0
54	MG	2A	3684	1/1	0.90	0.10	67,67,67,67	0
54	MG	1l	104	1/1	0.90	0.13	55,55,55,55	0
54	MG	1a	1700	1/1	0.90	0.29	78,78,78,78	0
54	MG	1A	3311	1/1	0.91	0.15	59,59,59,59	0
54	MG	1A	3673	1/1	0.91	0.06	29,29,29,29	0
54	MG	1A	3442	1/1	0.91	0.14	27,27,27,27	0
54	MG	2A	3354	1/1	0.91	0.10	71,71,71,71	0
54	MG	1A	3602	1/1	0.91	0.24	58,58,58,58	0
54	MG	2A	3356	1/1	0.91	0.15	64,64,64,64	0
54	MG	1A	3758	1/1	0.91	0.16	63,63,63,63	0
54	MG	1a	1820	1/1	0.91	0.16	71,71,71,71	0
54	MG	2A	3693	1/1	0.91	0.13	80,80,80,80	0
54	MG	2A	3695	1/1	0.91	0.09	74,74,74,74	0
54	MG	2A	3704	1/1	0.91	0.08	49,49,49,49	0
54	MG	1a	1697	1/1	0.91	0.17	67,67,67,67	0
54	MG	1W	203	1/1	0.91	0.09	57,57,57,57	0
54	MG	1A	3053	1/1	0.91	0.24	44,44,44,44	0
54	MG	2A	3368	1/1	0.91	0.13	64,64,64,64	0
54	MG	1a	1701	1/1	0.91	0.22	64,64,64,64	0
54	MG	1A	3860	1/1	0.91	0.10	66,66,66,66	0
54	MG	2A	3374	1/1	0.91	0.14	46,46,46,46	0
54	MG	1A	3125	1/1	0.91	0.23	55,55,55,55	0
54	MG	2A	3111	1/1	0.91	0.15	45,45,45,45	0
54	MG	1A	3987	1/1	0.91	0.11	50,50,50,50	0
54	MG	1a	1833	1/1	0.91	0.20	77,77,77,77	0
54	MG	2A	3386	1/1	0.91	0.09	57,57,57,57	0
54	MG	1A	3678	1/1	0.91	0.12	48,48,48,48	0
54	MG	15	105	1/1	0.91	0.22	36,36,36,36	0
54	MG	2B	216	1/1	0.91	0.07	84,84,84,84	0
54	MG	2B	217	1/1	0.91	0.06	75,75,75,75	0
54	MG	1a	1837	1/1	0.91	0.11	82,82,82,82	0
54	MG	1a	1838	1/1	0.91	0.19	72,72,72,72	0
54	MG	2E	303	1/1	0.91	0.10	32,32,32,32	0
54	MG	1a	1839	1/1	0.91	0.18	52,52,52,52	0
54	MG	1A	3990	1/1	0.91	0.07	22,22,22,22	0
54	MG	1A	3765	1/1	0.91	0.12	60,60,60,60	0
54	MG	1A	3192	1/1	0.91	0.09	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
54	MG	1a	1711	1/1	0.91	0.35	71,71,71,71	0
54	MG	1a	1847	1/1	0.91	0.31	57,57,57,57	0
54	MG	17	107	1/1	0.91	0.12	59,59,59,59	0
54	MG	2T	201	1/1	0.91	0.26	72,72,72,72	0
54	MG	2T	203	1/1	0.91	0.16	61,61,61,61	0
54	MG	1A	3994	1/1	0.91	0.25	43,43,43,43	0
54	MG	19	101	1/1	0.91	0.24	57,57,57,57	0
54	MG	1A	3386	1/1	0.91	0.10	42,42,42,42	0
54	MG	1a	1858	1/1	0.91	0.13	57,57,57,57	0
54	MG	2a	3001	1/1	0.91	0.12	46,46,46,46	0
54	MG	1A	3876	1/1	0.91	0.12	46,46,46,46	0
54	MG	1A	3681	1/1	0.91	0.16	71,71,71,71	0
54	MG	1A	3883	1/1	0.91	0.09	60,60,60,60	0
54	MG	1A	3774	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3391	1/1	0.91	0.19	75,75,75,75	0
54	MG	1a	1607	1/1	0.91	0.08	73,73,73,73	0
54	MG	2A	3169	1/1	0.91	0.08	51,51,51,51	0
54	MG	1A	3285	1/1	0.91	0.18	66,66,66,66	0
54	MG	1A	4011	1/1	0.91	0.21	50,50,50,50	0
54	MG	2a	3023	1/1	0.91	0.16	74,74,74,74	0
54	MG	2A	3173	1/1	0.91	0.28	62,62,62,62	0
54	MG	1A	3620	1/1	0.91	0.07	39,39,39,39	0
54	MG	1a	1613	1/1	0.91	0.17	30,30,30,30	0
54	MG	1a	1730	1/1	0.91	0.24	71,71,71,71	0
54	MG	1A	3329	1/1	0.91	0.06	40,40,40,40	0
54	MG	1A	3195	1/1	0.91	0.25	47,47,47,47	0
54	MG	2A	3183	1/1	0.91	0.20	60,60,60,60	0
54	MG	1b	301	1/1	0.91	0.13	84,84,84,84	0
54	MG	2a	3036	1/1	0.91	0.24	67,67,67,67	0
54	MG	2A	3456	1/1	0.91	0.12	74,74,74,74	0
54	MG	2a	3038	1/1	0.91	0.31	67,67,67,67	0
54	MG	1a	1741	1/1	0.91	0.12	77,77,77,77	0
54	MG	1a	1742	1/1	0.91	0.21	65,65,65,65	0
54	MG	1a	1743	1/1	0.91	0.11	63,63,63,63	0
54	MG	1A	4022	1/1	0.91	0.21	66,66,66,66	0
54	MG	1a	1745	1/1	0.91	0.11	68,68,68,68	0
54	MG	2A	3468	1/1	0.91	0.22	65,65,65,65	0
54	MG	1A	3469	1/1	0.91	0.12	64,64,64,64	0
54	MG	1A	3034	1/1	0.91	0.09	52,52,52,52	0
54	MG	1A	3254	1/1	0.91	0.09	72,72,72,72	0
54	MG	1A	3800	1/1	0.91	0.12	63,63,63,63	0
54	MG	1a	1629	1/1	0.91	0.29	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3481	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3337	1/1	0.91	0.40	68,68,68,68	0
54	MG	2A	3483	1/1	0.91	0.09	61,61,61,61	0
54	MG	1B	202	1/1	0.91	0.19	77,77,77,77	0
54	MG	2A	3207	1/1	0.91	0.33	65,65,65,65	0
54	MG	1A	3568	1/1	0.91	0.17	48,48,48,48	0
54	MG	1B	205	1/1	0.91	0.10	53,53,53,53	0
54	MG	1B	206	1/1	0.91	0.22	67,67,67,67	0
54	MG	1B	208	1/1	0.91	0.09	55,55,55,55	0
54	MG	2A	3216	1/1	0.91	0.20	71,71,71,71	0
54	MG	1u	101	1/1	0.91	0.13	76,76,76,76	0
54	MG	2A	3220	1/1	0.91	0.19	60,60,60,60	0
54	MG	2a	3068	1/1	0.91	0.33	68,68,68,68	0
54	MG	1B	209	1/1	0.91	0.13	61,61,61,61	0
54	MG	1A	3403	1/1	0.91	0.07	37,37,37,37	0
54	MG	2A	3224	1/1	0.91	0.13	74,74,74,74	0
54	MG	1B	211	1/1	0.91	0.09	64,64,64,64	0
54	MG	2a	3079	1/1	0.91	0.35	59,59,59,59	0
54	MG	1B	214	1/1	0.91	0.09	69,69,69,69	0
54	MG	2a	3082	1/1	0.91	0.17	70,70,70,70	0
54	MG	1A	3645	1/1	0.91	0.09	40,40,40,40	0
54	MG	1A	3340	1/1	0.91	0.08	48,48,48,48	0
54	MG	1A	3577	1/1	0.91	0.10	55,55,55,55	0
54	MG	2A	3236	1/1	0.91	0.09	64,64,64,64	0
54	MG	1A	3257	1/1	0.91	0.31	45,45,45,45	0
54	MG	1A	3718	1/1	0.91	0.20	63,63,63,63	0
54	MG	2A	3241	1/1	0.91	0.17	70,70,70,70	0
54	MG	1A	3110	1/1	0.91	0.10	70,70,70,70	0
54	MG	2A	3518	1/1	0.91	0.14	67,67,67,67	0
54	MG	2A	3253	1/1	0.91	0.24	50,50,50,50	0
54	MG	2a	3100	1/1	0.91	0.13	83,83,83,83	0
54	MG	1A	3827	1/1	0.91	0.13	73,73,73,73	0
54	MG	2A	3255	1/1	0.91	0.29	61,61,61,61	0
54	MG	1B	228	1/1	0.91	0.19	71,71,71,71	0
54	MG	2A	3534	1/1	0.91	0.19	58,58,58,58	0
54	MG	2a	3109	1/1	0.91	0.29	75,75,75,75	0
54	MG	2A	3536	1/1	0.91	0.11	60,60,60,60	0
54	MG	1A	3943	1/1	0.91	0.09	51,51,51,51	0
54	MG	2a	3114	1/1	0.91	0.20	75,75,75,75	0
54	MG	2A	3546	1/1	0.91	0.09	73,73,73,73	0
54	MG	2A	3261	1/1	0.91	0.36	74,74,74,74	0
54	MG	1D	314	1/1	0.91	0.08	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
54	MG	1A	3201	1/1	0.91	0.29	62,62,62,62	0
54	MG	1A	3517	1/1	0.91	0.14	35,35,35,35	0
54	MG	1E	304	1/1	0.91	0.10	27,27,27,27	0
54	MG	2a	3123	1/1	0.91	0.11	79,79,79,79	0
54	MG	2A	3040	1/1	0.91	0.24	61,61,61,61	0
54	MG	1A	3955	1/1	0.91	0.10	62,62,62,62	0
54	MG	2A	3562	1/1	0.91	0.13	74,74,74,74	0
54	MG	2A	3563	1/1	0.91	0.09	52,52,52,52	0
54	MG	1F	314	1/1	0.91	0.38	51,51,51,51	0
54	MG	2A	3577	1/1	0.91	0.17	74,74,74,74	0
54	MG	1A	3523	1/1	0.91	0.11	42,42,42,42	0
54	MG	2A	3045	1/1	0.91	0.14	67,67,67,67	0
54	MG	1a	1797	1/1	0.91	0.26	68,68,68,68	0
54	MG	2A	3296	1/1	0.91	0.15	62,62,62,62	0
54	MG	2A	3047	1/1	0.91	0.12	68,68,68,68	0
54	MG	1A	3960	1/1	0.91	0.09	76,76,76,76	0
54	MG	1A	3133	1/1	0.91	0.24	37,37,37,37	0
54	MG	2A	3602	1/1	0.91	0.23	64,64,64,64	0
54	MG	1a	1800	1/1	0.91	0.23	66,66,66,66	0
54	MG	1a	1678	1/1	0.91	0.26	54,54,54,54	0
54	MG	1A	3962	1/1	0.91	0.13	65,65,65,65	0
54	MG	2A	3317	1/1	0.91	0.12	59,59,59,59	0
54	MG	2A	3318	1/1	0.91	0.14	42,42,42,42	0
54	MG	1a	1804	1/1	0.91	0.11	69,69,69,69	0
54	MG	2A	3618	1/1	0.91	0.12	64,64,64,64	0
54	MG	1A	3595	1/1	0.91	0.15	66,66,66,66	0
54	MG	1A	3353	1/1	0.91	0.11	57,57,57,57	0
54	MG	2A	3331	1/1	0.91	0.16	76,76,76,76	0
54	MG	2A	3072	1/1	0.91	0.16	62,62,62,62	0
54	MG	1a	1807	1/1	0.91	0.08	73,73,73,73	0
54	MG	1A	3113	1/1	0.91	0.13	52,52,52,52	0
56	ZIT	2A	3713	52/52	0.91	0.19	43,67,78,85	0
54	MG	1A	3842	1/1	0.91	0.12	53,53,53,53	0
54	MG	2A	3658	1/1	0.91	0.10	52,52,52,52	0
54	MG	2A	3666	1/1	0.91	0.12	44,44,44,44	0
54	MG	2A	3668	1/1	0.91	0.16	69,69,69,69	0
54	MG	2A	3670	1/1	0.91	0.20	73,73,73,73	0
54	MG	1A	3739	1/1	0.91	0.17	46,46,46,46	0
54	MG	1A	3665	1/1	0.91	0.07	42,42,42,42	0
54	MG	1A	3753	1/1	0.92	0.11	58,58,58,58	0
54	MG	2A	3676	1/1	0.92	0.17	70,70,70,70	0
54	MG	1A	3643	1/1	0.92	0.13	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3107	1/1	0.92	0.12	62,62,62,62	0
54	MG	1A	3266	1/1	0.92	0.36	71,71,71,71	0
54	MG	2A	3365	1/1	0.92	0.08	65,65,65,65	0
54	MG	1A	3270	1/1	0.92	0.16	63,63,63,63	0
54	MG	1A	3161	1/1	0.92	0.27	64,64,64,64	0
54	MG	1A	3277	1/1	0.92	0.26	35,35,35,35	0
54	MG	1A	3927	1/1	0.92	0.09	47,47,47,47	0
54	MG	1A	3545	1/1	0.92	0.13	64,64,64,64	0
54	MG	1F	310	1/1	0.92	0.23	59,59,59,59	0
54	MG	2A	3699	1/1	0.92	0.08	49,49,49,49	0
54	MG	2A	3701	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3930	1/1	0.92	0.13	48,48,48,48	0
54	MG	2A	3706	1/1	0.92	0.11	40,40,40,40	0
54	MG	1a	1832	1/1	0.92	0.11	68,68,68,68	0
54	MG	2A	3379	1/1	0.92	0.19	78,78,78,78	0
54	MG	2A	3710	1/1	0.92	0.24	64,64,64,64	0
54	MG	1A	3550	1/1	0.92	0.40	37,37,37,37	0
54	MG	1A	3199	1/1	0.92	0.31	51,51,51,51	0
54	MG	2A	3125	1/1	0.92	0.19	51,51,51,51	0
54	MG	1A	3552	1/1	0.92	0.19	63,63,63,63	0
54	MG	2A	3393	1/1	0.92	0.12	56,56,56,56	0
54	MG	2A	3394	1/1	0.92	0.09	51,51,51,51	0
54	MG	1A	3281	1/1	0.92	0.05	78,78,78,78	0
54	MG	2A	3129	1/1	0.92	0.36	63,63,63,63	0
54	MG	2B	210	1/1	0.92	0.11	71,71,71,71	0
54	MG	1G	202	1/1	0.92	0.07	69,69,69,69	0
54	MG	2A	3133	1/1	0.92	0.20	62,62,62,62	0
54	MG	1A	3780	1/1	0.92	0.19	61,61,61,61	0
54	MG	1A	3134	1/1	0.92	0.06	57,57,57,57	0
54	MG	2A	3140	1/1	0.92	0.33	61,61,61,61	0
54	MG	2A	3405	1/1	0.92	0.24	57,57,57,57	0
54	MG	2D	304	1/1	0.92	0.34	43,43,43,43	0
54	MG	1N	201	1/1	0.92	0.20	49,49,49,49	0
54	MG	2A	3407	1/1	0.92	0.12	50,50,50,50	0
54	MG	2E	301	1/1	0.92	0.22	49,49,49,49	0
54	MG	1A	3046	1/1	0.92	0.17	33,33,33,33	0
54	MG	1A	3173	1/1	0.92	0.14	52,52,52,52	0
54	MG	2A	3411	1/1	0.92	0.10	40,40,40,40	0
54	MG	1A	3791	1/1	0.92	0.15	48,48,48,48	0
54	MG	1A	3959	1/1	0.92	0.10	66,66,66,66	0
54	MG	2A	3158	1/1	0.92	0.14	46,46,46,46	0
54	MG	2A	3416	1/1	0.92	0.28	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3175	1/1	0.92	0.14	63,63,63,63	0
54	MG	2R	201	1/1	0.92	0.12	53,53,53,53	0
54	MG	1A	3666	1/1	0.92	0.13	54,54,54,54	0
54	MG	1A	3178	1/1	0.92	0.17	42,42,42,42	0
54	MG	2Y	201	1/1	0.92	0.20	69,69,69,69	0
54	MG	1A	3670	1/1	0.92	0.40	55,55,55,55	0
54	MG	1A	3569	1/1	0.92	0.08	34,34,34,34	0
54	MG	1A	3965	1/1	0.92	0.14	57,57,57,57	0
54	MG	1Z	301	1/1	0.92	0.12	68,68,68,68	0
54	MG	2A	3437	1/1	0.92	0.10	56,56,56,56	0
54	MG	1A	3967	1/1	0.92	0.11	76,76,76,76	0
54	MG	1a	1868	1/1	0.92	0.24	68,68,68,68	0
54	MG	2a	3006	1/1	0.92	0.08	79,79,79,79	0
54	MG	2a	3007	1/1	0.92	0.47	72,72,72,72	0
54	MG	1A	3290	1/1	0.92	0.13	52,52,52,52	0
54	MG	2A	3442	1/1	0.92	0.10	58,58,58,58	0
54	MG	10	104	1/1	0.92	0.08	58,58,58,58	0
54	MG	1A	3291	1/1	0.92	0.14	43,43,43,43	0
54	MG	1A	3216	1/1	0.92	0.18	62,62,62,62	0
54	MG	1A	3370	1/1	0.92	0.10	51,51,51,51	0
54	MG	15	103	1/1	0.92	0.34	46,46,46,46	0
54	MG	1A	3582	1/1	0.92	0.18	62,62,62,62	0
54	MG	2a	3024	1/1	0.92	0.18	66,66,66,66	0
54	MG	2a	3025	1/1	0.92	0.26	67,67,67,67	0
54	MG	1A	3811	1/1	0.92	0.09	39,39,39,39	0
54	MG	1A	3812	1/1	0.92	0.35	40,40,40,40	0
54	MG	1a	1880	1/1	0.92	0.16	67,67,67,67	0
54	MG	2A	3459	1/1	0.92	0.09	63,63,63,63	0
54	MG	2a	3031	1/1	0.92	0.12	46,46,46,46	0
54	MG	2A	3188	1/1	0.92	0.18	48,48,48,48	0
54	MG	17	102	1/1	0.92	0.17	55,55,55,55	0
54	MG	2A	3190	1/1	0.92	0.20	67,67,67,67	0
54	MG	2A	3192	1/1	0.92	0.08	60,60,60,60	0
54	MG	1A	3813	1/1	0.92	0.11	71,71,71,71	0
54	MG	1a	1731	1/1	0.92	0.19	60,60,60,60	0
54	MG	1A	3470	1/1	0.92	0.20	74,74,74,74	0
54	MG	1a	1733	1/1	0.92	0.14	56,56,56,56	0
54	MG	1a	1737	1/1	0.92	0.09	55,55,55,55	0
54	MG	1A	3139	1/1	0.92	0.27	51,51,51,51	0
54	MG	1A	3472	1/1	0.92	0.11	50,50,50,50	0
54	MG	1A	3985	1/1	0.92	0.11	54,54,54,54	0
54	MG	1A	3683	1/1	0.92	0.17	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3588	1/1	0.92	0.22	51,51,51,51	0
54	MG	1A	3686	1/1	0.92	0.10	50,50,50,50	0
54	MG	1a	1746	1/1	0.92	0.18	43,43,43,43	0
54	MG	1A	3589	1/1	0.92	0.09	23,23,23,23	0
54	MG	2a	3050	1/1	0.92	0.28	64,64,64,64	0
54	MG	2A	3490	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3691	1/1	0.92	0.06	55,55,55,55	0
54	MG	2A	3218	1/1	0.92	0.12	65,65,65,65	0
54	MG	1a	1606	1/1	0.92	0.20	58,58,58,58	0
54	MG	1A	3692	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3014	1/1	0.92	0.28	68,68,68,68	0
54	MG	1A	3123	1/1	0.92	0.12	38,38,38,38	0
54	MG	1A	3695	1/1	0.92	0.11	65,65,65,65	0
54	MG	2A	3225	1/1	0.92	0.19	66,66,66,66	0
54	MG	1A	3999	1/1	0.92	0.10	58,58,58,58	0
54	MG	2A	3002	1/1	0.92	0.08	58,58,58,58	0
54	MG	2A	3503	1/1	0.92	0.27	49,49,49,49	0
54	MG	2A	3003	1/1	0.92	0.10	65,65,65,65	0
54	MG	1A	3594	1/1	0.92	0.17	70,70,70,70	0
54	MG	1A	3388	1/1	0.92	0.09	47,47,47,47	0
54	MG	2a	3073	1/1	0.92	0.10	68,68,68,68	0
54	MG	2A	3507	1/1	0.92	0.24	68,68,68,68	0
54	MG	2A	3508	1/1	0.92	0.17	66,66,66,66	0
54	MG	1A	4006	1/1	0.92	0.08	58,58,58,58	0
54	MG	1a	1620	1/1	0.92	0.09	65,65,65,65	0
54	MG	1A	3487	1/1	0.92	0.10	49,49,49,49	0
54	MG	2a	3081	1/1	0.92	0.30	63,63,63,63	0
54	MG	2A	3019	1/1	0.92	0.23	52,52,52,52	0
54	MG	1A	3488	1/1	0.92	0.13	57,57,57,57	0
54	MG	1A	3241	1/1	0.92	0.22	63,63,63,63	0
54	MG	1A	3100	1/1	0.92	0.19	57,57,57,57	0
54	MG	2A	3525	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	4013	1/1	0.92	0.07	36,36,36,36	0
54	MG	2A	3257	1/1	0.92	0.18	55,55,55,55	0
54	MG	1A	3496	1/1	0.92	0.13	55,55,55,55	0
54	MG	2A	3533	1/1	0.92	0.07	88,88,88,88	0
54	MG	1a	1776	1/1	0.92	0.13	73,73,73,73	0
54	MG	1A	4015	1/1	0.92	0.08	28,28,28,28	0
54	MG	2A	3538	1/1	0.92	0.12	44,44,44,44	0
54	MG	1A	4017	1/1	0.92	0.17	71,71,71,71	0
54	MG	1A	4018	1/1	0.92	0.21	63,63,63,63	0
54	MG	1a	1637	1/1	0.92	0.10	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3251	1/1	0.92	0.16	51,51,51,51	0
54	MG	1A	3710	1/1	0.92	0.21	39,39,39,39	0
54	MG	1a	1786	1/1	0.92	0.23	63,63,63,63	0
54	MG	1A	3504	1/1	0.92	0.11	33,33,33,33	0
54	MG	1A	3712	1/1	0.92	0.22	58,58,58,58	0
54	MG	1a	1790	1/1	0.92	0.07	76,76,76,76	0
54	MG	2A	3048	1/1	0.92	0.43	76,76,76,76	0
54	MG	2A	3295	1/1	0.92	0.10	34,34,34,34	0
54	MG	1A	3506	1/1	0.92	0.12	40,40,40,40	0
54	MG	1A	3075	1/1	0.92	0.07	38,38,38,38	0
54	MG	1A	3510	1/1	0.92	0.11	50,50,50,50	0
54	MG	1A	3108	1/1	0.92	0.10	47,47,47,47	0
54	MG	2A	3057	1/1	0.92	0.23	70,70,70,70	0
54	MG	2a	3128	1/1	0.92	0.12	79,79,79,79	0
54	MG	2a	3133	1/1	0.92	0.06	80,80,80,80	0
54	MG	2A	3303	1/1	0.92	0.13	69,69,69,69	0
54	MG	2A	3596	1/1	0.92	0.09	37,37,37,37	0
54	MG	1A	3720	1/1	0.92	0.08	50,50,50,50	0
54	MG	1A	3521	1/1	0.92	0.08	69,69,69,69	0
54	MG	2A	3312	1/1	0.92	0.10	46,46,46,46	0
54	MG	1A	3879	1/1	0.92	0.07	31,31,31,31	0
54	MG	1a	1658	1/1	0.92	0.10	81,81,81,81	0
54	MG	1A	3314	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3323	1/1	0.92	0.16	61,61,61,61	0
54	MG	1A	3622	1/1	0.92	0.10	52,52,52,52	0
54	MG	2A	3608	1/1	0.92	0.11	65,65,65,65	0
54	MG	2A	3611	1/1	0.92	0.16	64,64,64,64	0
54	MG	1A	3624	1/1	0.92	0.16	38,38,38,38	0
54	MG	1A	3012	1/1	0.92	0.17	40,40,40,40	0
54	MG	2A	3081	1/1	0.92	0.62	52,52,52,52	0
54	MG	1A	3160	1/1	0.92	0.32	62,62,62,62	0
54	MG	1A	3321	1/1	0.92	0.12	66,66,66,66	0
54	MG	1a	1667	1/1	0.92	0.07	78,78,78,78	0
54	MG	2A	3638	1/1	0.92	0.10	49,49,49,49	0
54	MG	2a	3179	1/1	0.92	0.14	81,81,81,81	0
54	MG	2A	3337	1/1	0.92	0.11	37,37,37,37	0
54	MG	1A	3633	1/1	0.92	0.17	65,65,65,65	0
54	MG	2A	3643	1/1	0.92	0.07	31,31,31,31	0
54	MG	1B	217	1/1	0.92	0.07	47,47,47,47	0
54	MG	2f	201	1/1	0.92	0.17	57,57,57,57	0
54	MG	2A	3646	1/1	0.92	0.09	78,78,78,78	0
54	MG	1A	3324	1/1	0.92	0.10	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3657	1/1	0.92	0.09	62,62,62,62	0
54	MG	1A	3262	1/1	0.92	0.30	55,55,55,55	0
54	MG	2A	3092	1/1	0.92	0.12	74,74,74,74	0
54	MG	1A	3409	1/1	0.92	0.15	42,42,42,42	0
54	MG	2A	3669	1/1	0.92	0.22	74,74,74,74	0
54	MG	1A	3427	1/1	0.92	0.08	33,33,33,33	0
54	MG	1A	3908	1/1	0.92	0.21	73,73,73,73	0
54	MG	2A	3672	1/1	0.92	0.11	59,59,59,59	0
54	MG	2A	3674	1/1	0.92	0.13	46,46,46,46	0
54	MG	1A	3700	1/1	0.93	0.09	46,46,46,46	0
54	MG	2A	3122	1/1	0.93	0.34	49,49,49,49	0
54	MG	2A	3385	1/1	0.93	0.20	64,64,64,64	0
54	MG	1A	3820	1/1	0.93	0.13	41,41,41,41	0
54	MG	2A	3694	1/1	0.93	0.11	63,63,63,63	0
54	MG	1P	207	1/1	0.93	0.11	64,64,64,64	0
54	MG	2A	3126	1/1	0.93	0.22	67,67,67,67	0
54	MG	1a	1835	1/1	0.93	0.15	63,63,63,63	0
54	MG	1a	1694	1/1	0.93	0.22	75,75,75,75	0
54	MG	1a	1695	1/1	0.93	0.07	82,82,82,82	0
54	MG	1R	203	1/1	0.93	0.21	66,66,66,66	0
54	MG	1A	3238	1/1	0.93	0.27	64,64,64,64	0
54	MG	2A	3134	1/1	0.93	0.09	55,55,55,55	0
54	MG	1A	3091	1/1	0.93	0.09	48,48,48,48	0
54	MG	1T	201	1/1	0.93	0.06	42,42,42,42	0
54	MG	2A	3403	1/1	0.93	0.19	56,56,56,56	0
54	MG	1A	3619	1/1	0.93	0.09	41,41,41,41	0
54	MG	1A	3117	1/1	0.93	0.26	40,40,40,40	0
54	MG	1a	1845	1/1	0.93	0.24	66,66,66,66	0
54	MG	1a	1846	1/1	0.93	0.19	67,67,67,67	0
54	MG	1A	3312	1/1	0.93	0.21	40,40,40,40	0
54	MG	1U	201	1/1	0.93	0.20	44,44,44,44	0
54	MG	2A	3155	1/1	0.93	0.10	73,73,73,73	0
54	MG	2A	3156	1/1	0.93	0.27	48,48,48,48	0
54	MG	1V	203	1/1	0.93	0.12	61,61,61,61	0
54	MG	2A	3159	1/1	0.93	0.16	71,71,71,71	0
54	MG	1A	3247	1/1	0.93	0.12	47,47,47,47	0
54	MG	1W	204	1/1	0.93	0.12	49,49,49,49	0
54	MG	1a	1854	1/1	0.93	0.10	58,58,58,58	0
54	MG	2D	306	1/1	0.93	0.17	55,55,55,55	0
54	MG	1Y	201	1/1	0.93	0.16	68,68,68,68	0
54	MG	2A	3427	1/1	0.93	0.09	66,66,66,66	0
54	MG	2A	3428	1/1	0.93	0.08	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3249	1/1	0.93	0.08	62,62,62,62	0
54	MG	1A	3097	1/1	0.93	0.09	54,54,54,54	0
54	MG	1A	3253	1/1	0.93	0.07	52,52,52,52	0
54	MG	2A	3432	1/1	0.93	0.07	69,69,69,69	0
54	MG	1A	3841	1/1	0.93	0.08	51,51,51,51	0
54	MG	2A	3435	1/1	0.93	0.21	66,66,66,66	0
54	MG	1A	3412	1/1	0.93	0.07	34,34,34,34	0
54	MG	1A	3632	1/1	0.93	0.12	33,33,33,33	0
54	MG	1A	3844	1/1	0.93	0.13	36,36,36,36	0
54	MG	15	101	1/1	0.93	0.17	41,41,41,41	0
54	MG	15	102	1/1	0.93	0.29	33,33,33,33	0
54	MG	2W	202	1/1	0.93	0.28	55,55,55,55	0
54	MG	1A	3532	1/1	0.93	0.12	55,55,55,55	0
54	MG	1A	3413	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3850	1/1	0.93	0.19	54,54,54,54	0
54	MG	2A	3447	1/1	0.93	0.10	57,57,57,57	0
54	MG	15	107	1/1	0.93	0.08	51,51,51,51	0
54	MG	1A	3721	1/1	0.93	0.09	61,61,61,61	0
54	MG	1A	3853	1/1	0.93	0.26	50,50,50,50	0
54	MG	1a	1881	1/1	0.93	0.08	60,60,60,60	0
54	MG	2a	3004	1/1	0.93	0.09	59,59,59,59	0
54	MG	2A	3454	1/1	0.93	0.14	77,77,77,77	0
54	MG	2A	3455	1/1	0.93	0.08	35,35,35,35	0
54	MG	1A	3997	1/1	0.93	0.17	69,69,69,69	0
54	MG	2a	3009	1/1	0.93	0.14	59,59,59,59	0
54	MG	1A	3124	1/1	0.93	0.15	39,39,39,39	0
54	MG	2a	3012	1/1	0.93	0.25	67,67,67,67	0
54	MG	2a	3013	1/1	0.93	0.18	61,61,61,61	0
54	MG	2a	3015	1/1	0.93	0.36	64,64,64,64	0
54	MG	2A	3191	1/1	0.93	0.40	74,74,74,74	0
54	MG	1A	3429	1/1	0.93	0.17	54,54,54,54	0
54	MG	1A	3857	1/1	0.93	0.16	40,40,40,40	0
54	MG	1A	3323	1/1	0.93	0.17	67,67,67,67	0
54	MG	1e	203	1/1	0.93	0.09	66,66,66,66	0
54	MG	2A	3467	1/1	0.93	0.11	43,43,43,43	0
54	MG	2A	3201	1/1	0.93	0.29	74,74,74,74	0
54	MG	1A	4004	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	3067	1/1	0.93	0.22	41,41,41,41	0
54	MG	2A	3472	1/1	0.93	0.11	65,65,65,65	0
54	MG	1A	3157	1/1	0.93	0.36	37,37,37,37	0
54	MG	1A	3439	1/1	0.93	0.10	49,49,49,49	0
54	MG	1A	3865	1/1	0.93	0.13	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
54	MG	1h	202	1/1	0.93	0.19	64,64,64,64	0
54	MG	1A	4010	1/1	0.93	0.13	66,66,66,66	0
54	MG	1A	3044	1/1	0.93	0.12	22,22,22,22	0
54	MG	1A	3867	1/1	0.93	0.10	47,47,47,47	0
54	MG	2A	3212	1/1	0.93	0.13	53,53,53,53	0
54	MG	2A	3213	1/1	0.93	0.21	72,72,72,72	0
54	MG	1A	3106	1/1	0.93	0.17	41,41,41,41	0
54	MG	1A	3164	1/1	0.93	0.07	38,38,38,38	0
54	MG	1A	4016	1/1	0.93	0.07	48,48,48,48	0
54	MG	1A	3741	1/1	0.93	0.12	36,36,36,36	0
54	MG	1a	1754	1/1	0.93	0.13	65,65,65,65	0
54	MG	1A	3334	1/1	0.93	0.08	33,33,33,33	0
54	MG	1A	3748	1/1	0.93	0.10	55,55,55,55	0
54	MG	1A	3065	1/1	0.93	0.10	69,69,69,69	0
54	MG	1A	3653	1/1	0.93	0.28	33,33,33,33	0
54	MG	1A	3271	1/1	0.93	0.10	60,60,60,60	0
54	MG	2a	3048	1/1	0.93	0.23	56,56,56,56	0
54	MG	1a	1762	1/1	0.93	0.07	63,63,63,63	0
54	MG	1a	1625	1/1	0.93	0.26	56,56,56,56	0
54	MG	1A	3085	1/1	0.93	0.39	47,47,47,47	0
54	MG	2A	3231	1/1	0.93	0.11	67,67,67,67	0
54	MG	1a	1627	1/1	0.93	0.10	56,56,56,56	0
54	MG	1A	3453	1/1	0.93	0.07	36,36,36,36	0
54	MG	2A	3238	1/1	0.93	0.10	60,60,60,60	0
54	MG	2A	3018	1/1	0.93	0.30	52,52,52,52	0
54	MG	1A	3206	1/1	0.93	0.25	54,54,54,54	0
54	MG	1a	1771	1/1	0.93	0.15	82,82,82,82	0
54	MG	2A	3243	1/1	0.93	0.13	63,63,63,63	0
54	MG	2A	3513	1/1	0.93	0.12	67,67,67,67	0
54	MG	1A	3278	1/1	0.93	0.38	47,47,47,47	0
54	MG	2A	3516	1/1	0.93	0.14	75,75,75,75	0
54	MG	2A	3249	1/1	0.93	0.15	48,48,48,48	0
54	MG	1A	3086	1/1	0.93	0.50	49,49,49,49	0
54	MG	1A	3211	1/1	0.93	0.38	46,46,46,46	0
54	MG	1B	204	1/1	0.93	0.08	51,51,51,51	0
54	MG	2A	3256	1/1	0.93	0.29	66,66,66,66	0
54	MG	1a	1636	1/1	0.93	0.33	67,67,67,67	0
54	MG	2A	3033	1/1	0.93	0.29	57,57,57,57	0
54	MG	1a	1778	1/1	0.93	0.12	72,72,72,72	0
54	MG	1A	3465	1/1	0.93	0.09	52,52,52,52	0
54	MG	1A	3899	1/1	0.93	0.10	58,58,58,58	0
54	MG	2A	3265	1/1	0.93	0.16	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3083	1/1	0.93	0.10	71,71,71,71	0
54	MG	1a	1781	1/1	0.93	0.33	63,63,63,63	0
54	MG	1a	1639	1/1	0.93	0.30	82,82,82,82	0
54	MG	1A	3578	1/1	0.93	0.10	39,39,39,39	0
54	MG	2A	3278	1/1	0.93	0.09	56,56,56,56	0
54	MG	1A	3672	1/1	0.93	0.06	45,45,45,45	0
54	MG	1A	3213	1/1	0.93	0.14	32,32,32,32	0
54	MG	1a	1787	1/1	0.93	0.08	71,71,71,71	0
54	MG	2A	3289	1/1	0.93	0.09	42,42,42,42	0
54	MG	1a	1645	1/1	0.93	0.19	53,53,53,53	0
54	MG	1A	3777	1/1	0.93	0.07	53,53,53,53	0
54	MG	1A	3354	1/1	0.93	0.08	27,27,27,27	0
54	MG	1A	3913	1/1	0.93	0.11	26,26,26,26	0
54	MG	1A	3111	1/1	0.93	0.37	33,33,33,33	0
54	MG	2A	3582	1/1	0.93	0.10	64,64,64,64	0
54	MG	1B	219	1/1	0.93	0.20	43,43,43,43	0
54	MG	2A	3586	1/1	0.93	0.08	79,79,79,79	0
54	MG	1A	3584	1/1	0.93	0.21	62,62,62,62	0
54	MG	1A	3144	1/1	0.93	0.09	40,40,40,40	0
54	MG	1A	3042	1/1	0.93	0.12	60,60,60,60	0
54	MG	2A	3064	1/1	0.93	0.19	62,62,62,62	0
54	MG	1A	3219	1/1	0.93	0.37	44,44,44,44	0
54	MG	2A	3067	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3069	1/1	0.93	0.20	52,52,52,52	0
54	MG	1A	3373	1/1	0.93	0.13	54,54,54,54	0
54	MG	2a	3120	1/1	0.93	0.10	77,77,77,77	0
54	MG	2A	3071	1/1	0.93	0.24	53,53,53,53	0
54	MG	1A	3483	1/1	0.93	0.11	27,27,27,27	0
54	MG	1A	3484	1/1	0.93	0.15	58,58,58,58	0
54	MG	1a	1802	1/1	0.93	0.12	58,58,58,58	0
54	MG	2a	3132	1/1	0.93	0.11	75,75,75,75	0
54	MG	1B	229	1/1	0.93	0.16	60,60,60,60	0
54	MG	2A	3079	1/1	0.93	0.41	67,67,67,67	0
54	MG	2a	3137	1/1	0.93	0.07	46,46,46,46	0
54	MG	1A	3934	1/1	0.93	0.11	42,42,42,42	0
54	MG	1A	3936	1/1	0.93	0.13	64,64,64,64	0
54	MG	2A	3616	1/1	0.93	0.08	59,59,59,59	0
54	MG	2a	3144	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3374	1/1	0.93	0.09	56,56,56,56	0
54	MG	2A	3627	1/1	0.93	0.10	88,88,88,88	0
54	MG	2a	3152	1/1	0.93	0.09	79,79,79,79	0
54	MG	1A	3221	1/1	0.93	0.27	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
54	MG	1A	3223	1/1	0.93	0.56	44,44,44,44	0
54	MG	2A	3339	1/1	0.93	0.08	36,36,36,36	0
54	MG	1A	3804	1/1	0.93	0.17	60,60,60,60	0
54	MG	2A	3341	1/1	0.93	0.12	77,77,77,77	0
54	MG	1a	1672	1/1	0.93	0.10	62,62,62,62	0
54	MG	1E	308	1/1	0.93	0.12	63,63,63,63	0
54	MG	1A	3950	1/1	0.93	0.06	45,45,45,45	0
54	MG	1A	3688	1/1	0.93	0.25	41,41,41,41	0
54	MG	2A	3648	1/1	0.93	0.07	71,71,71,71	0
54	MG	2A	3651	1/1	0.93	0.08	59,59,59,59	0
54	MG	1a	1677	1/1	0.93	0.17	58,58,58,58	0
54	MG	1A	3806	1/1	0.93	0.06	77,77,77,77	0
54	MG	1A	3293	1/1	0.93	0.22	50,50,50,50	0
54	MG	2A	3659	1/1	0.93	0.13	74,74,74,74	0
54	MG	2A	3105	1/1	0.93	0.12	58,58,58,58	0
54	MG	2a	3182	1/1	0.93	0.08	75,75,75,75	0
54	MG	1A	3227	1/1	0.93	0.17	61,61,61,61	0
54	MG	1A	3500	1/1	0.93	0.08	24,24,24,24	0
54	MG	1A	3501	1/1	0.93	0.08	36,36,36,36	0
54	MG	2A	3109	1/1	0.93	0.22	67,67,67,67	0
54	MG	1a	1824	1/1	0.93	0.20	63,63,63,63	0
54	MG	1A	3232	1/1	0.93	0.42	47,47,47,47	0
56	ZIT	1A	4033	52/52	0.93	0.13	35,56,72,82	0
54	MG	1a	1826	1/1	0.93	0.12	63,63,63,63	0
54	MG	1A	3234	1/1	0.93	0.15	39,39,39,39	0
54	MG	2A	3373	1/1	0.93	0.07	49,49,49,49	0
54	MG	2A	3678	1/1	0.93	0.08	65,65,65,65	0
54	MG	1a	1828	1/1	0.93	0.10	71,71,71,71	0
54	MG	1A	3182	1/1	0.93	0.20	42,42,42,42	0
54	MG	1A	3816	1/1	0.93	0.26	49,49,49,49	0
54	MG	1A	3146	1/1	0.93	0.08	34,34,34,34	0
59	ZN	24	501	1/1	0.93	0.16	146,146,146,146	0
54	MG	1A	3885	1/1	0.94	0.14	43,43,43,43	0
54	MG	1B	207	1/1	0.94	0.34	65,65,65,65	0
54	MG	1a	1648	1/1	0.94	0.26	61,61,61,61	0
54	MG	1a	1649	1/1	0.94	0.19	48,48,48,48	0
54	MG	1A	3529	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3421	1/1	0.94	0.16	43,43,43,43	0
54	MG	2A	3363	1/1	0.94	0.12	66,66,66,66	0
54	MG	1A	3228	1/1	0.94	0.21	36,36,36,36	0
54	MG	2A	3366	1/1	0.94	0.10	38,38,38,38	0
54	MG	2A	3683	1/1	0.94	0.15	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3891	1/1	0.94	0.07	38,38,38,38	0
54	MG	2A	3685	1/1	0.94	0.14	57,57,57,57	0
54	MG	1A	3333	1/1	0.94	0.12	48,48,48,48	0
54	MG	2A	3687	1/1	0.94	0.09	62,62,62,62	0
54	MG	2A	3370	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3114	1/1	0.94	0.28	45,45,45,45	0
54	MG	1A	3432	1/1	0.94	0.18	71,71,71,71	0
54	MG	1a	1815	1/1	0.94	0.19	70,70,70,70	0
54	MG	1A	3233	1/1	0.94	0.24	42,42,42,42	0
54	MG	1a	1817	1/1	0.94	0.10	61,61,61,61	0
54	MG	1a	1818	1/1	0.94	0.12	72,72,72,72	0
54	MG	1a	1661	1/1	0.94	0.30	68,68,68,68	0
54	MG	2A	3702	1/1	0.94	0.14	69,69,69,69	0
54	MG	1A	3196	1/1	0.94	0.10	57,57,57,57	0
54	MG	2A	3115	1/1	0.94	0.31	57,57,57,57	0
54	MG	2A	3383	1/1	0.94	0.18	55,55,55,55	0
54	MG	2A	3384	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3339	1/1	0.94	0.11	53,53,53,53	0
54	MG	1a	1664	1/1	0.94	0.11	67,67,67,67	0
54	MG	1A	3197	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3391	1/1	0.94	0.10	41,41,41,41	0
54	MG	1A	3547	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3288	1/1	0.94	0.25	49,49,49,49	0
54	MG	1A	3655	1/1	0.94	0.19	42,42,42,42	0
54	MG	1A	3769	1/1	0.94	0.08	50,50,50,50	0
54	MG	1A	3343	1/1	0.94	0.13	33,33,33,33	0
54	MG	1A	3056	1/1	0.94	0.09	51,51,51,51	0
54	MG	1D	312	1/1	0.94	0.16	30,30,30,30	0
54	MG	1A	3918	1/1	0.94	0.11	25,25,25,25	0
54	MG	1A	3919	1/1	0.94	0.12	26,26,26,26	0
54	MG	1A	3775	1/1	0.94	0.12	50,50,50,50	0
54	MG	1A	3923	1/1	0.94	0.34	46,46,46,46	0
54	MG	1A	3776	1/1	0.94	0.13	65,65,65,65	0
54	MG	2D	303	1/1	0.94	0.42	48,48,48,48	0
54	MG	1A	3658	1/1	0.94	0.12	58,58,58,58	0
54	MG	1E	309	1/1	0.94	0.10	32,32,32,32	0
54	MG	1F	305	1/1	0.94	0.12	43,43,43,43	0
54	MG	2A	3145	1/1	0.94	0.09	48,48,48,48	0
54	MG	1A	3555	1/1	0.94	0.09	61,61,61,61	0
54	MG	1A	3781	1/1	0.94	0.07	32,32,32,32	0
54	MG	1A	3084	1/1	0.94	0.34	44,44,44,44	0
54	MG	2F	301	1/1	0.94	0.26	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
54	MG	1F	316	1/1	0.94	0.13	63,63,63,63	0
54	MG	1a	1686	1/1	0.94	0.17	65,65,65,65	0
54	MG	1A	3349	1/1	0.94	0.12	40,40,40,40	0
54	MG	1A	3789	1/1	0.94	0.15	44,44,44,44	0
54	MG	1A	3170	1/1	0.94	0.15	39,39,39,39	0
54	MG	1a	1691	1/1	0.94	0.16	45,45,45,45	0
54	MG	2Q	202	1/1	0.94	0.08	65,65,65,65	0
54	MG	1A	3938	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	3940	1/1	0.94	0.07	63,63,63,63	0
54	MG	1A	3171	1/1	0.94	0.18	51,51,51,51	0
54	MG	2V	203	1/1	0.94	0.10	71,71,71,71	0
54	MG	1A	3244	1/1	0.94	0.16	46,46,46,46	0
54	MG	1A	3669	1/1	0.94	0.14	56,56,56,56	0
54	MG	1a	1863	1/1	0.94	0.09	64,64,64,64	0
54	MG	1A	3795	1/1	0.94	0.12	54,54,54,54	0
54	MG	23	101	1/1	0.94	0.14	57,57,57,57	0
54	MG	1a	1699	1/1	0.94	0.25	70,70,70,70	0
54	MG	1A	3948	1/1	0.94	0.12	56,56,56,56	0
54	MG	1P	205	1/1	0.94	0.13	54,54,54,54	0
54	MG	2A	3440	1/1	0.94	0.10	39,39,39,39	0
54	MG	1A	3355	1/1	0.94	0.14	27,27,27,27	0
54	MG	1A	3952	1/1	0.94	0.07	31,31,31,31	0
54	MG	1Q	205	1/1	0.94	0.08	56,56,56,56	0
54	MG	1A	3356	1/1	0.94	0.13	49,49,49,49	0
54	MG	1A	3246	1/1	0.94	0.13	45,45,45,45	0
54	MG	1A	3571	1/1	0.94	0.13	40,40,40,40	0
54	MG	1A	3573	1/1	0.94	0.25	60,60,60,60	0
54	MG	1A	3120	1/1	0.94	0.31	35,35,35,35	0
54	MG	1a	1878	1/1	0.94	0.25	68,68,68,68	0
54	MG	1A	3468	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3103	1/1	0.94	0.08	57,57,57,57	0
54	MG	1T	206	1/1	0.94	0.17	57,57,57,57	0
54	MG	2a	3019	1/1	0.94	0.07	54,54,54,54	0
54	MG	1A	3807	1/1	0.94	0.07	48,48,48,48	0
54	MG	2A	3457	1/1	0.94	0.09	63,63,63,63	0
54	MG	1V	201	1/1	0.94	0.34	34,34,34,34	0
54	MG	1A	3301	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3198	1/1	0.94	0.22	52,52,52,52	0
54	MG	1V	204	1/1	0.94	0.15	59,59,59,59	0
54	MG	2A	3200	1/1	0.94	0.34	64,64,64,64	0
54	MG	1W	201	1/1	0.94	0.14	51,51,51,51	0
54	MG	1A	3207	1/1	0.94	0.13	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
54	MG	1A	3303	1/1	0.94	0.27	38,38,38,38	0
54	MG	1A	3968	1/1	0.94	0.17	58,58,58,58	0
54	MG	1g	201	1/1	0.94	0.32	69,69,69,69	0
54	MG	1A	3473	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3473	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3971	1/1	0.94	0.06	32,32,32,32	0
54	MG	1A	3376	1/1	0.94	0.09	43,43,43,43	0
54	MG	1A	3209	1/1	0.94	0.38	48,48,48,48	0
54	MG	10	105	1/1	0.94	0.12	55,55,55,55	0
54	MG	2A	3211	1/1	0.94	0.32	70,70,70,70	0
54	MG	11	101	1/1	0.94	0.14	48,48,48,48	0
54	MG	1A	3378	1/1	0.94	0.07	37,37,37,37	0
54	MG	1A	3480	1/1	0.94	0.08	63,63,63,63	0
54	MG	1a	1736	1/1	0.94	0.16	74,74,74,74	0
54	MG	2A	3488	1/1	0.94	0.09	64,64,64,64	0
54	MG	1A	3689	1/1	0.94	0.08	68,68,68,68	0
54	MG	1A	3380	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3819	1/1	0.94	0.14	50,50,50,50	0
54	MG	1A	3383	1/1	0.94	0.07	26,26,26,26	0
54	MG	1A	3384	1/1	0.94	0.08	48,48,48,48	0
54	MG	1A	3826	1/1	0.94	0.12	51,51,51,51	0
54	MG	2A	3001	1/1	0.94	0.28	61,61,61,61	0
54	MG	1A	3058	1/1	0.94	0.20	59,59,59,59	0
54	MG	1A	3828	1/1	0.94	0.15	28,28,28,28	0
54	MG	1A	3051	1/1	0.94	0.24	51,51,51,51	0
54	MG	1A	3212	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3501	1/1	0.94	0.07	43,43,43,43	0
54	MG	2A	3007	1/1	0.94	0.06	45,45,45,45	0
54	MG	2A	3233	1/1	0.94	0.30	44,44,44,44	0
54	MG	2A	3009	1/1	0.94	0.12	40,40,40,40	0
54	MG	1A	3126	1/1	0.94	0.28	53,53,53,53	0
54	MG	2a	3063	1/1	0.94	0.24	70,70,70,70	0
54	MG	2a	3064	1/1	0.94	0.09	69,69,69,69	0
54	MG	2A	3237	1/1	0.94	0.11	56,56,56,56	0
54	MG	18	101	1/1	0.94	0.19	58,58,58,58	0
54	MG	1A	3835	1/1	0.94	0.08	32,32,32,32	0
54	MG	2A	3509	1/1	0.94	0.06	60,60,60,60	0
54	MG	2a	3070	1/1	0.94	0.22	61,61,61,61	0
54	MG	2a	3071	1/1	0.94	0.14	65,65,65,65	0
54	MG	1A	3836	1/1	0.94	0.07	26,26,26,26	0
54	MG	19	102	1/1	0.94	0.10	65,65,65,65	0
54	MG	2A	3242	1/1	0.94	0.23	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3075	1/1	0.94	0.11	57,57,57,57	0
54	MG	2A	3020	1/1	0.94	0.18	47,47,47,47	0
54	MG	2a	3077	1/1	0.94	0.38	61,61,61,61	0
54	MG	2A	3022	1/1	0.94	0.18	57,57,57,57	0
54	MG	1A	3498	1/1	0.94	0.09	23,23,23,23	0
54	MG	2A	3250	1/1	0.94	0.14	37,37,37,37	0
54	MG	2A	3251	1/1	0.94	0.12	58,58,58,58	0
54	MG	1A	3068	1/1	0.94	0.17	45,45,45,45	0
54	MG	2A	3524	1/1	0.94	0.10	58,58,58,58	0
54	MG	1A	3316	1/1	0.94	0.16	61,61,61,61	0
54	MG	1A	3605	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3703	1/1	0.94	0.15	50,50,50,50	0
54	MG	2A	3030	1/1	0.94	0.18	36,36,36,36	0
54	MG	1A	3704	1/1	0.94	0.12	57,57,57,57	0
54	MG	2a	3090	1/1	0.94	0.14	82,82,82,82	0
54	MG	2A	3032	1/1	0.94	0.22	60,60,60,60	0
54	MG	1A	3606	1/1	0.94	0.10	54,54,54,54	0
54	MG	2A	3262	1/1	0.94	0.08	63,63,63,63	0
54	MG	1A	4002	1/1	0.94	0.13	18,18,18,18	0
54	MG	2A	3544	1/1	0.94	0.08	64,64,64,64	0
54	MG	2A	3035	1/1	0.94	0.23	65,65,65,65	0
54	MG	2A	3266	1/1	0.94	0.10	49,49,49,49	0
54	MG	1a	1608	1/1	0.94	0.09	72,72,72,72	0
54	MG	1A	3020	1/1	0.94	0.26	43,43,43,43	0
54	MG	2A	3038	1/1	0.94	0.17	56,56,56,56	0
54	MG	2a	3106	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3555	1/1	0.94	0.06	58,58,58,58	0
54	MG	2A	3270	1/1	0.94	0.15	60,60,60,60	0
54	MG	2A	3275	1/1	0.94	0.15	49,49,49,49	0
54	MG	1A	3609	1/1	0.94	0.11	58,58,58,58	0
54	MG	1A	3267	1/1	0.94	0.22	55,55,55,55	0
54	MG	2A	3280	1/1	0.94	0.09	43,43,43,43	0
54	MG	2A	3281	1/1	0.94	0.21	52,52,52,52	0
54	MG	2A	3573	1/1	0.94	0.07	46,46,46,46	0
54	MG	2A	3575	1/1	0.94	0.08	63,63,63,63	0
54	MG	1A	3611	1/1	0.94	0.19	60,60,60,60	0
54	MG	2A	3578	1/1	0.94	0.09	61,61,61,61	0
54	MG	2A	3283	1/1	0.94	0.12	57,57,57,57	0
54	MG	1A	3188	1/1	0.94	0.31	53,53,53,53	0
54	MG	1A	3507	1/1	0.94	0.09	32,32,32,32	0
54	MG	2A	3290	1/1	0.94	0.14	64,64,64,64	0
54	MG	2A	3590	1/1	0.94	0.07	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
54	MG	1a	1617	1/1	0.94	0.09	75,75,75,75	0
54	MG	1A	3322	1/1	0.94	0.20	60,60,60,60	0
54	MG	1a	1619	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3294	1/1	0.94	0.13	47,47,47,47	0
54	MG	2A	3598	1/1	0.94	0.11	61,61,61,61	0
54	MG	2A	3050	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3618	1/1	0.94	0.09	49,49,49,49	0
54	MG	1A	3132	1/1	0.94	0.15	45,45,45,45	0
54	MG	2a	3151	1/1	0.94	0.07	84,84,84,84	0
54	MG	1a	1623	1/1	0.94	0.07	56,56,56,56	0
54	MG	2A	3054	1/1	0.94	0.26	64,64,64,64	0
54	MG	1A	3511	1/1	0.94	0.10	27,27,27,27	0
54	MG	1a	1784	1/1	0.94	0.10	61,61,61,61	0
54	MG	1A	3513	1/1	0.94	0.08	44,44,44,44	0
54	MG	2A	3609	1/1	0.94	0.07	55,55,55,55	0
54	MG	2A	3610	1/1	0.94	0.06	78,78,78,78	0
54	MG	2a	3163	1/1	0.94	0.08	83,83,83,83	0
54	MG	2A	3061	1/1	0.94	0.07	46,46,46,46	0
54	MG	2a	3165	1/1	0.94	0.08	68,68,68,68	0
54	MG	1A	3404	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3063	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3519	1/1	0.94	0.12	53,53,53,53	0
54	MG	1A	3728	1/1	0.94	0.09	67,67,67,67	0
54	MG	2A	3626	1/1	0.94	0.07	59,59,59,59	0
54	MG	1A	3158	1/1	0.94	0.22	42,42,42,42	0
54	MG	1A	3093	1/1	0.94	0.32	39,39,39,39	0
54	MG	2A	3327	1/1	0.94	0.07	57,57,57,57	0
54	MG	1A	3627	1/1	0.94	0.20	42,42,42,42	0
54	MG	1a	1792	1/1	0.94	0.13	73,73,73,73	0
54	MG	1A	3630	1/1	0.94	0.19	38,38,38,38	0
54	MG	1A	3327	1/1	0.94	0.13	51,51,51,51	0
54	MG	2A	3075	1/1	0.94	0.13	63,63,63,63	0
54	MG	1A	3328	1/1	0.94	0.23	49,49,49,49	0
54	MG	1A	3878	1/1	0.94	0.11	74,74,74,74	0
54	MG	2A	3338	1/1	0.94	0.06	45,45,45,45	0
54	MG	1A	4030	1/1	0.94	0.13	64,64,64,64	0
54	MG	2A	3652	1/1	0.94	0.08	72,72,72,72	0
54	MG	1B	201	1/1	0.94	0.14	54,54,54,54	0
54	MG	1a	1640	1/1	0.94	0.17	74,74,74,74	0
54	MG	1A	3224	1/1	0.94	0.53	42,42,42,42	0
54	MG	1A	3880	1/1	0.94	0.12	50,50,50,50	0
54	MG	2A	3086	1/1	0.94	0.13	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
54	MG	1A	3076	1/1	0.94	0.23	47,47,47,47	0
58	ARG	1B	230	12/12	0.94	0.10	33,49,59,61	0
54	MG	2A	3353	1/1	0.94	0.12	66,66,66,66	0
54	MG	1A	3745	1/1	0.94	0.12	63,63,63,63	0
54	MG	1A	3010	1/1	0.95	0.14	62,62,62,62	0
54	MG	2A	3010	1/1	0.95	0.11	73,73,73,73	0
54	MG	1A	3537	1/1	0.95	0.06	38,38,38,38	0
54	MG	2A	3015	1/1	0.95	0.21	41,41,41,41	0
54	MG	1A	3229	1/1	0.95	0.21	39,39,39,39	0
54	MG	1A	3154	1/1	0.95	0.20	47,47,47,47	0
54	MG	1A	3348	1/1	0.95	0.07	39,39,39,39	0
54	MG	1a	1768	1/1	0.95	0.12	67,67,67,67	0
54	MG	2B	215	1/1	0.95	0.10	66,66,66,66	0
54	MG	1A	3893	1/1	0.95	0.06	49,49,49,49	0
54	MG	1A	3760	1/1	0.95	0.15	56,56,56,56	0
54	MG	2A	3450	1/1	0.95	0.12	69,69,69,69	0
54	MG	1a	1622	1/1	0.95	0.06	55,55,55,55	0
54	MG	2D	305	1/1	0.95	0.12	49,49,49,49	0
54	MG	1A	3069	1/1	0.95	0.24	41,41,41,41	0
54	MG	1A	3127	1/1	0.95	0.09	52,52,52,52	0
54	MG	1A	3544	1/1	0.95	0.16	43,43,43,43	0
54	MG	1a	1775	1/1	0.95	0.11	68,68,68,68	0
54	MG	1A	3650	1/1	0.95	0.14	50,50,50,50	0
54	MG	1A	3444	1/1	0.95	0.09	28,28,28,28	0
54	MG	1A	3193	1/1	0.95	0.21	55,55,55,55	0
54	MG	2F	303	1/1	0.95	0.16	52,52,52,52	0
54	MG	1A	3072	1/1	0.95	0.06	45,45,45,45	0
54	MG	1A	3654	1/1	0.95	0.21	52,52,52,52	0
54	MG	1A	3296	1/1	0.95	0.14	40,40,40,40	0
54	MG	1A	3449	1/1	0.95	0.11	29,29,29,29	0
54	MG	2A	3466	1/1	0.95	0.12	33,33,33,33	0
54	MG	1B	216	1/1	0.95	0.06	61,61,61,61	0
54	MG	1A	3452	1/1	0.95	0.10	19,19,19,19	0
54	MG	2A	3039	1/1	0.95	0.19	64,64,64,64	0
54	MG	1A	3129	1/1	0.95	0.10	67,67,67,67	0
54	MG	2T	202	1/1	0.95	0.11	70,70,70,70	0
54	MG	1A	3360	1/1	0.95	0.09	15,15,15,15	0
54	MG	2V	201	1/1	0.95	0.12	70,70,70,70	0
54	MG	1A	3782	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3922	1/1	0.95	0.06	45,45,45,45	0
54	MG	1A	3054	1/1	0.95	0.17	38,38,38,38	0
54	MG	1A	3661	1/1	0.95	0.15	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
54	MG	1a	1643	1/1	0.95	0.07	62,62,62,62	0
54	MG	1A	3662	1/1	0.95	0.09	39,39,39,39	0
54	MG	1A	3559	1/1	0.95	0.08	58,58,58,58	0
54	MG	28	101	1/1	0.95	0.10	63,63,63,63	0
54	MG	1A	3561	1/1	0.95	0.14	59,59,59,59	0
54	MG	2A	3252	1/1	0.95	0.29	54,54,54,54	0
54	MG	1D	301	1/1	0.95	0.18	57,57,57,57	0
54	MG	1D	305	1/1	0.95	0.08	44,44,44,44	0
54	MG	1D	310	1/1	0.95	0.16	44,44,44,44	0
54	MG	2a	3005	1/1	0.95	0.31	61,61,61,61	0
54	MG	2A	3055	1/1	0.95	0.09	41,41,41,41	0
54	MG	1A	3163	1/1	0.95	0.11	50,50,50,50	0
54	MG	1A	3459	1/1	0.95	0.11	53,53,53,53	0
54	MG	1D	313	1/1	0.95	0.21	49,49,49,49	0
54	MG	2A	3060	1/1	0.95	0.07	52,52,52,52	0
54	MG	1a	1655	1/1	0.95	0.18	58,58,58,58	0
54	MG	1A	3460	1/1	0.95	0.06	61,61,61,61	0
54	MG	1A	3935	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3365	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3462	1/1	0.95	0.06	19,19,19,19	0
54	MG	2A	3066	1/1	0.95	0.29	46,46,46,46	0
54	MG	1A	3939	1/1	0.95	0.10	57,57,57,57	0
54	MG	2A	3068	1/1	0.95	0.14	33,33,33,33	0
54	MG	2A	3272	1/1	0.95	0.07	51,51,51,51	0
54	MG	1A	3464	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3055	1/1	0.95	0.46	36,36,36,36	0
54	MG	1F	303	1/1	0.95	0.25	38,38,38,38	0
54	MG	1A	3801	1/1	0.95	0.07	40,40,40,40	0
54	MG	1A	3245	1/1	0.95	0.36	49,49,49,49	0
54	MG	2A	3074	1/1	0.95	0.06	47,47,47,47	0
54	MG	1F	312	1/1	0.95	0.14	50,50,50,50	0
54	MG	2A	3284	1/1	0.95	0.07	58,58,58,58	0
54	MG	1F	313	1/1	0.95	0.09	33,33,33,33	0
54	MG	2A	3514	1/1	0.95	0.18	63,63,63,63	0
54	MG	1A	3944	1/1	0.95	0.07	68,68,68,68	0
54	MG	1A	3946	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3109	1/1	0.95	0.09	43,43,43,43	0
54	MG	1A	3166	1/1	0.95	0.26	36,36,36,36	0
54	MG	1A	3203	1/1	0.95	0.28	47,47,47,47	0
54	MG	1A	3951	1/1	0.95	0.08	74,74,74,74	0
54	MG	1A	3580	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3309	1/1	0.95	0.33	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3250	1/1	0.95	0.30	68,68,68,68	0
54	MG	2A	3530	1/1	0.95	0.06	68,68,68,68	0
54	MG	1A	3167	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3957	1/1	0.95	0.11	50,50,50,50	0
54	MG	1N	204	1/1	0.95	0.23	60,60,60,60	0
54	MG	2A	3535	1/1	0.95	0.07	63,63,63,63	0
54	MG	2A	3093	1/1	0.95	0.10	64,64,64,64	0
54	MG	2A	3096	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	3585	1/1	0.95	0.09	68,68,68,68	0
54	MG	2A	3309	1/1	0.95	0.10	38,38,38,38	0
54	MG	1A	3477	1/1	0.95	0.06	65,65,65,65	0
54	MG	2A	3547	1/1	0.95	0.08	59,59,59,59	0
54	MG	2A	3313	1/1	0.95	0.12	47,47,47,47	0
54	MG	1A	3038	1/1	0.95	0.14	51,51,51,51	0
54	MG	2A	3550	1/1	0.95	0.07	64,64,64,64	0
54	MG	1A	3169	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3255	1/1	0.95	0.10	54,54,54,54	0
54	MG	2A	3321	1/1	0.95	0.10	35,35,35,35	0
54	MG	1A	3690	1/1	0.95	0.07	59,59,59,59	0
54	MG	1A	3482	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3208	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3328	1/1	0.95	0.16	69,69,69,69	0
54	MG	2A	3329	1/1	0.95	0.08	44,44,44,44	0
54	MG	2A	3564	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3570	1/1	0.95	0.10	47,47,47,47	0
54	MG	1A	3593	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3969	1/1	0.95	0.11	57,57,57,57	0
54	MG	2A	3332	1/1	0.95	0.11	53,53,53,53	0
54	MG	1A	3387	1/1	0.95	0.06	15,15,15,15	0
54	MG	1T	203	1/1	0.95	0.06	57,57,57,57	0
54	MG	1A	3317	1/1	0.95	0.21	47,47,47,47	0
54	MG	1A	3057	1/1	0.95	0.14	56,56,56,56	0
54	MG	1a	1696	1/1	0.95	0.20	55,55,55,55	0
54	MG	1a	1842	1/1	0.95	0.20	78,78,78,78	0
54	MG	2A	3117	1/1	0.95	0.19	57,57,57,57	0
54	MG	1A	3138	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3829	1/1	0.95	0.24	43,43,43,43	0
54	MG	1U	202	1/1	0.95	0.13	36,36,36,36	0
54	MG	2A	3343	1/1	0.95	0.09	59,59,59,59	0
54	MG	1U	204	1/1	0.95	0.10	48,48,48,48	0
54	MG	1U	207	1/1	0.95	0.21	45,45,45,45	0
54	MG	2A	3600	1/1	0.95	0.08	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
54	MG	2A	3351	1/1	0.95	0.21	52,52,52,52	0
54	MG	1a	1702	1/1	0.95	0.35	71,71,71,71	0
54	MG	2A	3603	1/1	0.95	0.07	89,89,89,89	0
54	MG	2a	3091	1/1	0.95	0.07	41,41,41,41	0
54	MG	1A	3598	1/1	0.95	0.09	32,32,32,32	0
54	MG	2a	3093	1/1	0.95	0.12	70,70,70,70	0
54	MG	1A	3599	1/1	0.95	0.16	47,47,47,47	0
54	MG	1A	3393	1/1	0.95	0.08	35,35,35,35	0
54	MG	1A	3495	1/1	0.95	0.12	61,61,61,61	0
54	MG	1a	1855	1/1	0.95	0.20	74,74,74,74	0
54	MG	2A	3132	1/1	0.95	0.12	69,69,69,69	0
54	MG	1A	3320	1/1	0.95	0.09	45,45,45,45	0
54	MG	1a	1859	1/1	0.95	0.12	57,57,57,57	0
54	MG	1A	3002	1/1	0.95	0.09	55,55,55,55	0
54	MG	2A	3136	1/1	0.95	0.13	47,47,47,47	0
54	MG	1A	3265	1/1	0.95	0.19	67,67,67,67	0
54	MG	1A	3028	1/1	0.95	0.29	38,38,38,38	0
54	MG	1A	3176	1/1	0.95	0.24	41,41,41,41	0
54	MG	2A	3369	1/1	0.95	0.16	70,70,70,70	0
54	MG	1A	3608	1/1	0.95	0.09	55,55,55,55	0
54	MG	2A	3147	1/1	0.95	0.26	55,55,55,55	0
54	MG	2A	3635	1/1	0.95	0.06	55,55,55,55	0
54	MG	2A	3636	1/1	0.95	0.10	59,59,59,59	0
54	MG	1A	3269	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3151	1/1	0.95	0.16	64,64,64,64	0
54	MG	1A	3029	1/1	0.95	0.17	40,40,40,40	0
54	MG	2A	3640	1/1	0.95	0.09	33,33,33,33	0
54	MG	10	106	1/1	0.95	0.10	65,65,65,65	0
54	MG	1A	3064	1/1	0.95	0.12	34,34,34,34	0
54	MG	2a	3127	1/1	0.95	0.10	74,74,74,74	0
54	MG	1a	1718	1/1	0.95	0.08	72,72,72,72	0
54	MG	1A	3613	1/1	0.95	0.14	51,51,51,51	0
54	MG	2A	3157	1/1	0.95	0.27	57,57,57,57	0
54	MG	1A	3508	1/1	0.95	0.08	33,33,33,33	0
54	MG	2a	3136	1/1	0.95	0.07	73,73,73,73	0
54	MG	1A	3181	1/1	0.95	0.31	50,50,50,50	0
54	MG	2A	3655	1/1	0.95	0.07	37,37,37,37	0
54	MG	1A	3996	1/1	0.95	0.07	55,55,55,55	0
54	MG	1A	3273	1/1	0.95	0.28	39,39,39,39	0
54	MG	1A	3275	1/1	0.95	0.14	59,59,59,59	0
54	MG	2A	3163	1/1	0.95	0.19	62,62,62,62	0
54	MG	2a	3148	1/1	0.95	0.09	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3663	1/1	0.95	0.09	75,75,75,75	0
54	MG	2A	3665	1/1	0.95	0.08	83,83,83,83	0
54	MG	1a	1725	1/1	0.95	0.17	71,71,71,71	0
54	MG	1a	1726	1/1	0.95	0.18	73,73,73,73	0
54	MG	2a	3154	1/1	0.95	0.11	71,71,71,71	0
54	MG	1A	3722	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3724	1/1	0.95	0.13	39,39,39,39	0
54	MG	1A	3147	1/1	0.95	0.38	42,42,42,42	0
54	MG	2A	3172	1/1	0.95	0.08	49,49,49,49	0
54	MG	1A	3220	1/1	0.95	0.08	48,48,48,48	0
54	MG	2a	3162	1/1	0.95	0.14	56,56,56,56	0
54	MG	17	101	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	4003	1/1	0.95	0.06	58,58,58,58	0
54	MG	1A	3518	1/1	0.95	0.07	54,54,54,54	0
54	MG	1a	1734	1/1	0.95	0.08	34,34,34,34	0
54	MG	2a	3168	1/1	0.95	0.13	69,69,69,69	0
54	MG	1a	1735	1/1	0.95	0.15	49,49,49,49	0
54	MG	2a	3172	1/1	0.95	0.10	79,79,79,79	0
54	MG	1A	3417	1/1	0.95	0.08	28,28,28,28	0
54	MG	1A	3045	1/1	0.95	0.18	34,34,34,34	0
54	MG	1a	1739	1/1	0.95	0.09	74,74,74,74	0
54	MG	1A	3732	1/1	0.95	0.07	32,32,32,32	0
54	MG	1A	3425	1/1	0.95	0.12	30,30,30,30	0
54	MG	1A	3734	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3426	1/1	0.95	0.06	24,24,24,24	0
54	MG	1A	3871	1/1	0.95	0.07	60,60,60,60	0
54	MG	1A	3280	1/1	0.95	0.18	52,52,52,52	0
54	MG	2A	3418	1/1	0.95	0.08	67,67,67,67	0
54	MG	1A	3874	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3526	1/1	0.95	0.13	54,54,54,54	0
54	MG	2l	201	1/1	0.95	0.13	68,68,68,68	0
54	MG	1A	3001	1/1	0.95	0.05	41,41,41,41	0
54	MG	2A	3425	1/1	0.95	0.06	58,58,58,58	0
55	HGR	2A	3712	36/36	0.95	0.12	38,43,49,51	0
54	MG	2A	3197	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3186	1/1	0.95	0.27	41,41,41,41	0
54	MG	1A	3016	1/1	0.95	0.34	40,40,40,40	0
54	MG	1A	3433	1/1	0.95	0.07	25,25,25,25	0
54	MG	1A	4021	1/1	0.95	0.09	60,60,60,60	0
54	MG	1a	1755	1/1	0.95	0.12	61,61,61,61	0
54	MG	1A	3636	1/1	0.95	0.07	29,29,29,29	0
54	MG	2A	3434	1/1	0.95	0.09	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
54	MG	1A	3342	1/1	0.95	0.09	56,56,56,56	0
54	MG	1A	3750	1/1	0.95	0.07	39,39,39,39	0
59	ZN	14	501	1/1	0.95	0.16	140,140,140,140	0
54	MG	1a	1614	1/1	0.95	0.07	60,60,60,60	0
54	MG	1A	3494	1/1	0.96	0.05	35,35,35,35	0
54	MG	1A	3415	1/1	0.96	0.06	33,33,33,33	0
54	MG	1A	3258	1/1	0.96	0.26	40,40,40,40	0
54	MG	2A	3008	1/1	0.96	0.08	43,43,43,43	0
54	MG	1A	3671	1/1	0.96	0.12	41,41,41,41	0
54	MG	2V	202	1/1	0.96	0.14	56,56,56,56	0
54	MG	1A	3877	1/1	0.96	0.05	38,38,38,38	0
54	MG	2W	201	1/1	0.96	0.42	51,51,51,51	0
54	MG	2A	3011	1/1	0.96	0.06	40,40,40,40	0
54	MG	1A	3768	1/1	0.96	0.07	55,55,55,55	0
54	MG	2A	3522	1/1	0.96	0.11	37,37,37,37	0
54	MG	2A	3013	1/1	0.96	0.05	26,26,26,26	0
54	MG	1A	3497	1/1	0.96	0.12	59,59,59,59	0
54	MG	2A	3526	1/1	0.96	0.05	83,83,83,83	0
54	MG	2A	3166	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3770	1/1	0.96	0.08	58,58,58,58	0
54	MG	1A	3771	1/1	0.96	0.09	46,46,46,46	0
54	MG	1a	1675	1/1	0.96	0.25	53,53,53,53	0
54	MG	2A	3532	1/1	0.96	0.09	67,67,67,67	0
54	MG	1A	3772	1/1	0.96	0.20	43,43,43,43	0
54	MG	1U	205	1/1	0.96	0.30	36,36,36,36	0
54	MG	1U	206	1/1	0.96	0.23	42,42,42,42	0
54	MG	1A	4005	1/1	0.96	0.04	41,41,41,41	0
54	MG	2A	3175	1/1	0.96	0.10	52,52,52,52	0
54	MG	2A	3541	1/1	0.96	0.07	61,61,61,61	0
54	MG	2A	3177	1/1	0.96	0.30	70,70,70,70	0
54	MG	1A	3418	1/1	0.96	0.07	25,25,25,25	0
54	MG	2A	3545	1/1	0.96	0.07	65,65,65,65	0
54	MG	1A	3886	1/1	0.96	0.10	28,28,28,28	0
54	MG	2A	3026	1/1	0.96	0.08	55,55,55,55	0
54	MG	2a	3017	1/1	0.96	0.09	57,57,57,57	0
54	MG	2A	3181	1/1	0.96	0.08	54,54,54,54	0
54	MG	1A	3092	1/1	0.96	0.26	36,36,36,36	0
54	MG	1A	3424	1/1	0.96	0.07	21,21,21,21	0
54	MG	1A	3306	1/1	0.96	0.16	40,40,40,40	0
54	MG	1A	3307	1/1	0.96	0.33	43,43,43,43	0
54	MG	2A	3554	1/1	0.96	0.09	35,35,35,35	0
54	MG	1A	3778	1/1	0.96	0.08	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
54	MG	1a	1687	1/1	0.96	0.09	55,55,55,55	0
54	MG	2a	3026	1/1	0.96	0.22	60,60,60,60	0
54	MG	1A	3779	1/1	0.96	0.19	64,64,64,64	0
54	MG	1A	3308	1/1	0.96	0.20	49,49,49,49	0
54	MG	1A	3183	1/1	0.96	0.06	62,62,62,62	0
54	MG	1A	3218	1/1	0.96	0.11	51,51,51,51	0
54	MG	1A	3358	1/1	0.96	0.08	24,24,24,24	0
54	MG	2A	3565	1/1	0.96	0.16	49,49,49,49	0
54	MG	2A	3567	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	3784	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3901	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	3682	1/1	0.96	0.06	50,50,50,50	0
54	MG	2A	3042	1/1	0.96	0.08	29,29,29,29	0
54	MG	2A	3576	1/1	0.96	0.09	73,73,73,73	0
54	MG	1A	3904	1/1	0.96	0.10	48,48,48,48	0
54	MG	11	105	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3788	1/1	0.96	0.07	54,54,54,54	0
54	MG	2A	3380	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3381	1/1	0.96	0.06	35,35,35,35	0
54	MG	13	103	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3018	1/1	0.96	0.23	32,32,32,32	0
54	MG	1A	3040	1/1	0.96	0.10	53,53,53,53	0
54	MG	1A	3512	1/1	0.96	0.07	27,27,27,27	0
54	MG	1a	1822	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3071	1/1	0.96	0.20	38,38,38,38	0
54	MG	2A	3389	1/1	0.96	0.09	60,60,60,60	0
54	MG	2a	3051	1/1	0.96	0.09	83,83,83,83	0
54	MG	2A	3390	1/1	0.96	0.13	74,74,74,74	0
54	MG	1A	4029	1/1	0.96	0.09	61,61,61,61	0
54	MG	1A	3156	1/1	0.96	0.24	38,38,38,38	0
54	MG	1A	3367	1/1	0.96	0.09	33,33,33,33	0
54	MG	1A	3315	1/1	0.96	0.17	62,62,62,62	0
54	MG	2A	3395	1/1	0.96	0.05	37,37,37,37	0
54	MG	1A	3099	1/1	0.96	0.14	38,38,38,38	0
54	MG	17	103	1/1	0.96	0.07	41,41,41,41	0
54	MG	17	104	1/1	0.96	0.26	45,45,45,45	0
54	MG	1A	3225	1/1	0.96	0.14	34,34,34,34	0
54	MG	2A	3217	1/1	0.96	0.08	52,52,52,52	0
54	MG	1A	3226	1/1	0.96	0.33	37,37,37,37	0
54	MG	1A	3011	1/1	0.96	0.25	64,64,64,64	0
54	MG	1A	3802	1/1	0.96	0.08	73,73,73,73	0
54	MG	1a	1715	1/1	0.96	0.11	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
54	MG	1A	3101	1/1	0.96	0.21	47,47,47,47	0
54	MG	2a	3069	1/1	0.96	0.31	50,50,50,50	0
54	MG	1A	3130	1/1	0.96	0.06	37,37,37,37	0
54	MG	1A	3162	1/1	0.96	0.09	38,38,38,38	0
54	MG	1A	3698	1/1	0.96	0.08	58,58,58,58	0
54	MG	2A	3629	1/1	0.96	0.06	57,57,57,57	0
54	MG	2A	3410	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3451	1/1	0.96	0.08	29,29,29,29	0
54	MG	1A	3808	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3381	1/1	0.96	0.05	20,20,20,20	0
54	MG	1A	3033	1/1	0.96	0.20	58,58,58,58	0
54	MG	2A	3232	1/1	0.96	0.50	47,47,47,47	0
54	MG	1A	3535	1/1	0.96	0.08	24,24,24,24	0
54	MG	1A	3022	1/1	0.96	0.05	45,45,45,45	0
54	MG	2A	3421	1/1	0.96	0.06	63,63,63,63	0
54	MG	1A	3077	1/1	0.96	0.29	37,37,37,37	0
54	MG	1B	223	1/1	0.96	0.08	68,68,68,68	0
54	MG	2A	3078	1/1	0.96	0.15	56,56,56,56	0
54	MG	2A	3647	1/1	0.96	0.07	69,69,69,69	0
54	MG	2A	3426	1/1	0.96	0.04	55,55,55,55	0
54	MG	1A	3326	1/1	0.96	0.27	38,38,38,38	0
54	MG	2A	3080	1/1	0.96	0.11	47,47,47,47	0
54	MG	2A	3654	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3458	1/1	0.96	0.09	49,49,49,49	0
54	MG	1A	3623	1/1	0.96	0.11	58,58,58,58	0
54	MG	1A	3023	1/1	0.96	0.15	36,36,36,36	0
54	MG	2A	3244	1/1	0.96	0.22	46,46,46,46	0
54	MG	2a	3097	1/1	0.96	0.11	58,58,58,58	0
54	MG	2A	3245	1/1	0.96	0.12	46,46,46,46	0
54	MG	2A	3660	1/1	0.96	0.06	68,68,68,68	0
54	MG	2A	3661	1/1	0.96	0.06	59,59,59,59	0
54	MG	2A	3246	1/1	0.96	0.15	60,60,60,60	0
54	MG	2A	3664	1/1	0.96	0.06	82,82,82,82	0
54	MG	1A	3541	1/1	0.96	0.06	53,53,53,53	0
54	MG	2A	3436	1/1	0.96	0.12	44,44,44,44	0
54	MG	2a	3105	1/1	0.96	0.09	71,71,71,71	0
54	MG	2A	3667	1/1	0.96	0.06	46,46,46,46	0
54	MG	1A	3080	1/1	0.96	0.24	45,45,45,45	0
54	MG	1A	3389	1/1	0.96	0.09	21,21,21,21	0
54	MG	1A	3081	1/1	0.96	0.12	49,49,49,49	0
54	MG	1a	1860	1/1	0.96	0.15	56,56,56,56	0
54	MG	1A	3463	1/1	0.96	0.19	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1862	1/1	0.96	0.12	44,44,44,44	0
54	MG	1A	3063	1/1	0.96	0.05	40,40,40,40	0
54	MG	1A	3140	1/1	0.96	0.08	36,36,36,36	0
54	MG	2A	3097	1/1	0.96	0.31	63,63,63,63	0
54	MG	2A	3258	1/1	0.96	0.28	51,51,51,51	0
54	MG	1A	3394	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3395	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3048	1/1	0.96	0.22	56,56,56,56	0
54	MG	2a	3126	1/1	0.96	0.05	71,71,71,71	0
54	MG	1A	3397	1/1	0.96	0.12	53,53,53,53	0
54	MG	2A	3104	1/1	0.96	0.09	56,56,56,56	0
54	MG	2a	3129	1/1	0.96	0.05	61,61,61,61	0
54	MG	2a	3131	1/1	0.96	0.08	83,83,83,83	0
54	MG	2A	3453	1/1	0.96	0.07	65,65,65,65	0
54	MG	1E	301	1/1	0.96	0.17	38,38,38,38	0
54	MG	1A	3172	1/1	0.96	0.22	38,38,38,38	0
54	MG	1E	305	1/1	0.96	0.05	39,39,39,39	0
54	MG	1A	3335	1/1	0.96	0.14	50,50,50,50	0
54	MG	1A	3026	1/1	0.96	0.28	37,37,37,37	0
54	MG	2a	3141	1/1	0.96	0.08	72,72,72,72	0
54	MG	1A	3730	1/1	0.96	0.19	41,41,41,41	0
54	MG	2A	3271	1/1	0.96	0.05	39,39,39,39	0
54	MG	2A	3698	1/1	0.96	0.15	73,73,73,73	0
54	MG	1A	3560	1/1	0.96	0.14	60,60,60,60	0
54	MG	2a	3146	1/1	0.96	0.12	78,78,78,78	0
54	MG	2A	3700	1/1	0.96	0.06	63,63,63,63	0
54	MG	1A	3174	1/1	0.96	0.15	34,34,34,34	0
54	MG	2A	3277	1/1	0.96	0.10	51,51,51,51	0
54	MG	1F	307	1/1	0.96	0.07	43,43,43,43	0
54	MG	2A	3705	1/1	0.96	0.12	46,46,46,46	0
54	MG	1A	3115	1/1	0.96	0.13	36,36,36,36	0
54	MG	1A	3037	1/1	0.96	0.08	40,40,40,40	0
54	MG	1A	3567	1/1	0.96	0.09	38,38,38,38	0
54	MG	1a	1758	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3252	1/1	0.96	0.28	33,33,33,33	0
54	MG	2a	3160	1/1	0.96	0.08	78,78,78,78	0
54	MG	2A	3119	1/1	0.96	0.05	42,42,42,42	0
54	MG	1A	3481	1/1	0.96	0.10	50,50,50,50	0
54	MG	2A	3288	1/1	0.96	0.09	37,37,37,37	0
54	MG	1A	3089	1/1	0.96	0.05	41,41,41,41	0
54	MG	1A	3407	1/1	0.96	0.21	57,57,57,57	0
54	MG	2B	207	1/1	0.96	0.09	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
54	MG	1A	3572	1/1	0.96	0.07	56,56,56,56	0
54	MG	1A	3179	1/1	0.96	0.39	42,42,42,42	0
54	MG	1A	3485	1/1	0.96	0.09	63,63,63,63	0
54	MG	1a	1766	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3980	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3575	1/1	0.96	0.09	36,36,36,36	0
54	MG	1A	3486	1/1	0.96	0.07	58,58,58,58	0
54	MG	1A	3004	1/1	0.96	0.10	44,44,44,44	0
54	MG	1A	3752	1/1	0.96	0.11	26,26,26,26	0
54	MG	1m	201	1/1	0.96	0.04	81,81,81,81	0
54	MG	1A	3411	1/1	0.96	0.08	34,34,34,34	0
54	MG	1A	3754	1/1	0.96	0.10	53,53,53,53	0
54	MG	2A	3137	1/1	0.96	0.10	58,58,58,58	0
54	MG	1A	3345	1/1	0.96	0.17	43,43,43,43	0
54	MG	2D	307	1/1	0.96	0.10	63,63,63,63	0
54	MG	2A	3310	1/1	0.96	0.10	52,52,52,52	0
54	MG	1A	3581	1/1	0.96	0.08	48,48,48,48	0
54	MG	1A	3664	1/1	0.96	0.09	60,60,60,60	0
54	MG	2A	3314	1/1	0.96	0.12	37,37,37,37	0
54	MG	1Q	201	1/1	0.96	0.10	43,43,43,43	0
54	MG	1Q	204	1/1	0.96	0.20	56,56,56,56	0
54	MG	1A	3869	1/1	0.96	0.10	45,45,45,45	0
54	MG	2A	3320	1/1	0.96	0.10	50,50,50,50	0
57	MPD	18	103	8/8	0.96	0.11	32,41,48,49	0
54	MG	2A	3150	1/1	0.96	0.17	61,61,61,61	0
54	MG	2A	3322	1/1	0.96	0.07	39,39,39,39	0
54	MG	1R	202	1/1	0.96	0.11	45,45,45,45	0
54	MG	2O	201	1/1	0.96	0.16	68,68,68,68	0
54	MG	1A	3151	1/1	0.96	0.10	58,58,58,58	0
54	MG	1R	204	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3492	1/1	0.96	0.05	56,56,56,56	0
54	MG	2Q	203	1/1	0.96	0.06	75,75,75,75	0
54	MG	1A	3862	1/1	0.97	0.10	26,26,26,26	0
54	MG	2A	3350	1/1	0.97	0.06	62,62,62,62	0
54	MG	1a	1654	1/1	0.97	0.07	47,47,47,47	0
54	MG	2W	203	1/1	0.97	0.12	73,73,73,73	0
54	MG	2A	3537	1/1	0.97	0.07	79,79,79,79	0
54	MG	2A	3021	1/1	0.97	0.05	44,44,44,44	0
54	MG	2A	3540	1/1	0.97	0.05	27,27,27,27	0
54	MG	1G	204	1/1	0.97	0.11	56,56,56,56	0
54	MG	2A	3542	1/1	0.97	0.08	65,65,65,65	0
54	MG	27	101	1/1	0.97	0.19	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
54	MG	1A	3159	1/1	0.97	0.12	40,40,40,40	0
54	MG	1A	3009	1/1	0.97	0.07	39,39,39,39	0
54	MG	1N	202	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3450	1/1	0.97	0.06	30,30,30,30	0
54	MG	2A	3358	1/1	0.97	0.07	65,65,65,65	0
54	MG	1A	3520	1/1	0.97	0.13	30,30,30,30	0
54	MG	1A	3231	1/1	0.97	0.19	35,35,35,35	0
54	MG	2A	3029	1/1	0.97	0.08	47,47,47,47	0
54	MG	1P	202	1/1	0.97	0.28	36,36,36,36	0
54	MG	1A	3522	1/1	0.97	0.08	43,43,43,43	0
54	MG	1P	204	1/1	0.97	0.10	67,67,67,67	0
54	MG	1A	3019	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3989	1/1	0.97	0.04	57,57,57,57	0
54	MG	1A	3015	1/1	0.97	0.11	38,38,38,38	0
54	MG	1A	3390	1/1	0.97	0.07	19,19,19,19	0
54	MG	2A	3561	1/1	0.97	0.06	50,50,50,50	0
54	MG	2A	3193	1/1	0.97	0.06	49,49,49,49	0
54	MG	1Q	202	1/1	0.97	0.09	45,45,45,45	0
54	MG	1Q	203	1/1	0.97	0.06	41,41,41,41	0
54	MG	2A	3196	1/1	0.97	0.09	51,51,51,51	0
54	MG	1A	3021	1/1	0.97	0.21	45,45,45,45	0
54	MG	1A	3456	1/1	0.97	0.05	32,32,32,32	0
54	MG	1R	201	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3235	1/1	0.97	0.12	31,31,31,31	0
54	MG	1A	3102	1/1	0.97	0.26	38,38,38,38	0
54	MG	1A	3041	1/1	0.97	0.17	47,47,47,47	0
54	MG	1A	3531	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3104	1/1	0.97	0.20	26,26,26,26	0
54	MG	2A	3581	1/1	0.97	0.07	41,41,41,41	0
54	MG	1A	3105	1/1	0.97	0.25	35,35,35,35	0
54	MG	2A	3583	1/1	0.97	0.06	38,38,38,38	0
54	MG	1A	3136	1/1	0.97	0.36	33,33,33,33	0
54	MG	1A	3202	1/1	0.97	0.19	39,39,39,39	0
54	MG	2A	3587	1/1	0.97	0.06	71,71,71,71	0
54	MG	1A	3292	1/1	0.97	0.08	49,49,49,49	0
54	MG	1A	3785	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3059	1/1	0.97	0.12	21,21,21,21	0
54	MG	1A	3615	1/1	0.97	0.04	37,37,37,37	0
54	MG	2A	3595	1/1	0.97	0.08	57,57,57,57	0
54	MG	1A	3294	1/1	0.97	0.14	47,47,47,47	0
54	MG	1A	3030	1/1	0.97	0.05	39,39,39,39	0
54	MG	1A	3205	1/1	0.97	0.23	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
54	MG	2A	3058	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3248	1/1	0.97	0.10	54,54,54,54	0
54	MG	1A	3043	1/1	0.97	0.09	36,36,36,36	0
54	MG	1A	3897	1/1	0.97	0.18	39,39,39,39	0
54	MG	1V	202	1/1	0.97	0.21	38,38,38,38	0
54	MG	1A	3794	1/1	0.97	0.07	49,49,49,49	0
54	MG	2A	3222	1/1	0.97	0.14	53,53,53,53	0
54	MG	1A	3083	1/1	0.97	0.28	38,38,38,38	0
54	MG	1A	3546	1/1	0.97	0.12	26,26,26,26	0
54	MG	1W	202	1/1	0.97	0.15	39,39,39,39	0
54	MG	1A	3902	1/1	0.97	0.13	49,49,49,49	0
54	MG	1A	3143	1/1	0.97	0.07	31,31,31,31	0
54	MG	1A	3062	1/1	0.97	0.18	34,34,34,34	0
54	MG	1A	3907	1/1	0.97	0.08	65,65,65,65	0
54	MG	2A	3230	1/1	0.97	0.11	43,43,43,43	0
54	MG	2A	3614	1/1	0.97	0.09	73,73,73,73	0
54	MG	1A	3031	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3706	1/1	0.97	0.22	55,55,55,55	0
54	MG	1A	3112	1/1	0.97	0.32	37,37,37,37	0
54	MG	1A	3553	1/1	0.97	0.08	32,32,32,32	0
54	MG	2A	3235	1/1	0.97	0.21	47,47,47,47	0
54	MG	1A	3628	1/1	0.97	0.22	40,40,40,40	0
54	MG	1A	3914	1/1	0.97	0.05	39,39,39,39	0
54	MG	2A	3634	1/1	0.97	0.06	54,54,54,54	0
54	MG	2A	3420	1/1	0.97	0.11	44,44,44,44	0
54	MG	1A	3629	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	4028	1/1	0.97	0.20	63,63,63,63	0
54	MG	1A	3917	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3554	1/1	0.97	0.09	57,57,57,57	0
54	MG	1A	4031	1/1	0.97	0.05	57,57,57,57	0
54	MG	1A	3177	1/1	0.97	0.12	32,32,32,32	0
54	MG	2A	3083	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3414	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3714	1/1	0.97	0.20	46,46,46,46	0
54	MG	1A	3715	1/1	0.97	0.08	57,57,57,57	0
54	MG	2A	3087	1/1	0.97	0.17	55,55,55,55	0
54	MG	1A	3925	1/1	0.97	0.09	51,51,51,51	0
54	MG	1A	3032	1/1	0.97	0.05	24,24,24,24	0
54	MG	1A	3634	1/1	0.97	0.05	44,44,44,44	0
54	MG	1A	3416	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3214	1/1	0.97	0.24	34,34,34,34	0
54	MG	1a	1856	1/1	0.97	0.06	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3094	1/1	0.97	0.12	55,55,55,55	0
54	MG	1A	3259	1/1	0.97	0.07	34,34,34,34	0
54	MG	1A	3419	1/1	0.97	0.13	34,34,34,34	0
54	MG	1A	3640	1/1	0.97	0.12	55,55,55,55	0
54	MG	2A	3662	1/1	0.97	0.09	46,46,46,46	0
54	MG	1A	3641	1/1	0.97	0.09	25,25,25,25	0
54	MG	2A	3444	1/1	0.97	0.07	69,69,69,69	0
54	MG	1A	3420	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3563	1/1	0.97	0.09	26,26,26,26	0
54	MG	2A	3263	1/1	0.97	0.06	72,72,72,72	0
54	MG	1a	1864	1/1	0.97	0.07	59,59,59,59	0
54	MG	1B	218	1/1	0.97	0.10	35,35,35,35	0
54	MG	1A	3564	1/1	0.97	0.04	33,33,33,33	0
54	MG	1A	3824	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	3825	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3005	1/1	0.97	0.09	22,22,22,22	0
54	MG	1A	3149	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3364	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3945	1/1	0.97	0.05	75,75,75,75	0
54	MG	2a	3107	1/1	0.97	0.06	74,74,74,74	0
54	MG	2A	3273	1/1	0.97	0.12	20,20,20,20	0
54	MG	2A	3679	1/1	0.97	0.07	69,69,69,69	0
54	MG	2a	3112	1/1	0.97	0.07	71,71,71,71	0
54	MG	1a	1873	1/1	0.97	0.06	54,54,54,54	0
54	MG	2A	3681	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3088	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3831	1/1	0.97	0.21	42,42,42,42	0
54	MG	1A	3264	1/1	0.97	0.34	37,37,37,37	0
54	MG	1a	1738	1/1	0.97	0.12	47,47,47,47	0
54	MG	1a	1609	1/1	0.97	0.05	64,64,64,64	0
54	MG	1A	3017	1/1	0.97	0.31	39,39,39,39	0
54	MG	1D	302	1/1	0.97	0.09	60,60,60,60	0
54	MG	2a	3122	1/1	0.97	0.14	56,56,56,56	0
54	MG	1D	304	1/1	0.97	0.12	40,40,40,40	0
54	MG	1A	3090	1/1	0.97	0.08	43,43,43,43	0
54	MG	1D	306	1/1	0.97	0.16	44,44,44,44	0
54	MG	1D	308	1/1	0.97	0.06	46,46,46,46	0
54	MG	1A	3738	1/1	0.97	0.08	52,52,52,52	0
54	MG	2A	3696	1/1	0.97	0.06	55,55,55,55	0
54	MG	2a	3130	1/1	0.97	0.05	80,80,80,80	0
54	MG	2A	3697	1/1	0.97	0.09	35,35,35,35	0
54	MG	1A	3953	1/1	0.97	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
54	MG	2A	3475	1/1	0.97	0.12	57,57,57,57	0
54	MG	2A	3476	1/1	0.97	0.06	74,74,74,74	0
54	MG	2a	3135	1/1	0.97	0.05	72,72,72,72	0
54	MG	1A	3431	1/1	0.97	0.10	31,31,31,31	0
54	MG	2A	3478	1/1	0.97	0.05	30,30,30,30	0
54	MG	2a	3139	1/1	0.97	0.06	78,78,78,78	0
54	MG	2A	3703	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3372	1/1	0.97	0.07	31,31,31,31	0
54	MG	2A	3130	1/1	0.97	0.05	36,36,36,36	0
54	MG	1a	1751	1/1	0.97	0.11	59,59,59,59	0
54	MG	1A	3118	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3743	1/1	0.97	0.05	35,35,35,35	0
54	MG	2A	3709	1/1	0.97	0.11	64,64,64,64	0
54	MG	2a	3147	1/1	0.97	0.06	76,76,76,76	0
54	MG	1D	316	1/1	0.97	0.09	63,63,63,63	0
54	MG	2A	3711	1/1	0.97	0.05	55,55,55,55	0
54	MG	2A	3299	1/1	0.97	0.14	42,42,42,42	0
54	MG	1D	317	1/1	0.97	0.06	47,47,47,47	0
54	MG	2A	3301	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3958	1/1	0.97	0.05	58,58,58,58	0
54	MG	1A	3576	1/1	0.97	0.09	62,62,62,62	0
54	MG	1l	201	1/1	0.97	0.13	62,62,62,62	0
54	MG	2A	3305	1/1	0.97	0.07	46,46,46,46	0
54	MG	2A	3306	1/1	0.97	0.06	48,48,48,48	0
54	MG	1E	302	1/1	0.97	0.20	44,44,44,44	0
54	MG	2A	3142	1/1	0.97	0.17	42,42,42,42	0
54	MG	2A	3143	1/1	0.97	0.10	42,42,42,42	0
54	MG	2A	3311	1/1	0.97	0.08	62,62,62,62	0
54	MG	1A	3268	1/1	0.97	0.13	43,43,43,43	0
54	MG	1A	3375	1/1	0.97	0.06	36,36,36,36	0
54	MG	2A	3146	1/1	0.97	0.18	76,76,76,76	0
54	MG	1A	3050	1/1	0.97	0.18	55,55,55,55	0
54	MG	2a	3169	1/1	0.97	0.08	79,79,79,79	0
54	MG	2a	3170	1/1	0.97	0.06	71,71,71,71	0
54	MG	1E	307	1/1	0.97	0.09	25,25,25,25	0
54	MG	2A	3149	1/1	0.97	0.10	35,35,35,35	0
54	MG	1A	3505	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3024	1/1	0.97	0.08	24,24,24,24	0
54	MG	2a	3176	1/1	0.97	0.06	67,67,67,67	0
54	MG	1a	1633	1/1	0.97	0.12	41,41,41,41	0
54	MG	1a	1634	1/1	0.97	0.09	48,48,48,48	0
54	MG	1E	310	1/1	0.97	0.09	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3325	1/1	0.97	0.09	32,32,32,32	0
54	MG	1A	3846	1/1	0.97	0.12	51,51,51,51	0
54	MG	1F	304	1/1	0.97	0.23	40,40,40,40	0
54	MG	1A	3187	1/1	0.97	0.21	42,42,42,42	0
54	MG	1F	306	1/1	0.97	0.12	35,35,35,35	0
54	MG	2F	302	1/1	0.97	0.05	47,47,47,47	0
54	MG	1A	3379	1/1	0.97	0.06	24,24,24,24	0
54	MG	2F	304	1/1	0.97	0.23	50,50,50,50	0
54	MG	1A	3025	1/1	0.97	0.26	48,48,48,48	0
54	MG	1F	311	1/1	0.97	0.06	40,40,40,40	0
55	HGR	1A	4032	36/36	0.97	0.08	25,29,35,40	0
54	MG	2A	3519	1/1	0.97	0.07	59,59,59,59	0
54	MG	1A	3095	1/1	0.97	0.17	43,43,43,43	0
54	MG	1A	3757	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3855	1/1	0.97	0.04	51,51,51,51	0
54	MG	1A	3274	1/1	0.97	0.05	44,44,44,44	0
54	MG	2Q	201	1/1	0.97	0.07	63,63,63,63	0
54	MG	1A	3446	1/1	0.97	0.10	31,31,31,31	0
54	MG	2A	3168	1/1	0.97	0.06	55,55,55,55	0
54	MG	2A	3528	1/1	0.97	0.07	66,66,66,66	0
54	MG	1A	3070	1/1	0.97	0.25	37,37,37,37	0
54	MG	1A	3514	1/1	0.97	0.07	72,72,72,72	0
54	MG	1a	1650	1/1	0.97	0.11	55,55,55,55	0
54	MG	1A	3515	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3861	1/1	0.97	0.11	45,45,45,45	0
59	ZN	2n	3102	1/1	0.97	0.07	103,103,103,103	0
54	MG	2A	3165	1/1	0.98	0.20	46,46,46,46	0
54	MG	1A	3735	1/1	0.98	0.05	46,46,46,46	0
54	MG	2A	3673	1/1	0.98	0.03	53,53,53,53	0
54	MG	1A	3796	1/1	0.98	0.07	40,40,40,40	0
54	MG	1A	3533	1/1	0.98	0.07	25,25,25,25	0
54	MG	1A	3864	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3276	1/1	0.98	0.08	32,32,32,32	0
54	MG	2a	3053	1/1	0.98	0.05	64,64,64,64	0
54	MG	2A	3276	1/1	0.98	0.07	42,42,42,42	0
54	MG	2A	3521	1/1	0.98	0.09	48,48,48,48	0
54	MG	1A	3135	1/1	0.98	0.17	35,35,35,35	0
54	MG	2A	3523	1/1	0.98	0.13	34,34,34,34	0
54	MG	1A	3684	1/1	0.98	0.16	48,48,48,48	0
54	MG	1A	3366	1/1	0.98	0.04	32,32,32,32	0
54	MG	1A	3949	1/1	0.98	0.05	51,51,51,51	0
54	MG	2A	3400	1/1	0.98	0.05	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
54	MG	1A	3230	1/1	0.98	0.19	44,44,44,44	0
54	MG	2A	3176	1/1	0.98	0.06	71,71,71,71	0
54	MG	1H	202	1/1	0.98	0.06	58,58,58,58	0
54	MG	2A	3690	1/1	0.98	0.04	85,85,85,85	0
54	MG	1A	3742	1/1	0.98	0.04	56,56,56,56	0
54	MG	2A	3285	1/1	0.98	0.04	42,42,42,42	0
54	MG	1A	3872	1/1	0.98	0.08	32,32,32,32	0
54	MG	2A	3287	1/1	0.98	0.07	38,38,38,38	0
54	MG	1A	3368	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3744	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3119	1/1	0.98	0.13	34,34,34,34	0
54	MG	1P	201	1/1	0.98	0.30	39,39,39,39	0
54	MG	2A	3539	1/1	0.98	0.05	76,76,76,76	0
54	MG	2A	3412	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3746	1/1	0.98	0.04	49,49,49,49	0
54	MG	1A	3082	1/1	0.98	0.17	34,34,34,34	0
54	MG	1A	3371	1/1	0.98	0.09	58,58,58,58	0
54	MG	1A	3256	1/1	0.98	0.06	41,41,41,41	0
54	MG	2A	3417	1/1	0.98	0.05	42,42,42,42	0
54	MG	1A	3121	1/1	0.98	0.10	27,27,27,27	0
54	MG	1A	3410	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3338	1/1	0.98	0.09	41,41,41,41	0
54	MG	1A	3644	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3422	1/1	0.98	0.05	48,48,48,48	0
54	MG	1A	3502	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3755	1/1	0.98	0.09	46,46,46,46	0
54	MG	2A	3553	1/1	0.98	0.08	60,60,60,60	0
54	MG	2a	3089	1/1	0.98	0.05	77,77,77,77	0
54	MG	1B	212	1/1	0.98	0.08	47,47,47,47	0
54	MG	1A	3548	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3194	1/1	0.98	0.14	39,39,39,39	0
54	MG	1A	3122	1/1	0.98	0.06	29,29,29,29	0
54	MG	2A	3559	1/1	0.98	0.14	58,58,58,58	0
54	MG	2a	3095	1/1	0.98	0.07	53,53,53,53	0
54	MG	2A	3095	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3094	1/1	0.98	0.06	40,40,40,40	0
54	MG	1A	3821	1/1	0.98	0.09	55,55,55,55	0
54	MG	1A	3287	1/1	0.98	0.10	17,17,17,17	0
54	MG	1A	3823	1/1	0.98	0.05	42,42,42,42	0
54	MG	2A	3004	1/1	0.98	0.06	43,43,43,43	0
54	MG	2A	3566	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3761	1/1	0.98	0.07	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
54	MG	2A	3568	1/1	0.98	0.04	71,71,71,71	0
54	MG	2A	3102	1/1	0.98	0.06	33,33,33,33	0
54	MG	2B	218	1/1	0.98	0.09	66,66,66,66	0
54	MG	2D	301	1/1	0.98	0.19	49,49,49,49	0
54	MG	2a	3108	1/1	0.98	0.16	61,61,61,61	0
54	MG	2D	302	1/1	0.98	0.08	52,52,52,52	0
54	MG	2a	3110	1/1	0.98	0.06	75,75,75,75	0
54	MG	2A	3315	1/1	0.98	0.07	32,32,32,32	0
54	MG	2A	3316	1/1	0.98	0.11	32,32,32,32	0
54	MG	1B	222	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3142	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3013	1/1	0.98	0.08	29,29,29,29	0
54	MG	1A	3239	1/1	0.98	0.28	39,39,39,39	0
54	MG	2A	3579	1/1	0.98	0.05	70,70,70,70	0
54	MG	1A	3705	1/1	0.98	0.05	58,58,58,58	0
54	MG	2E	302	1/1	0.98	0.14	45,45,45,45	0
54	MG	1A	3604	1/1	0.98	0.08	43,43,43,43	0
54	MG	2E	304	1/1	0.98	0.10	30,30,30,30	0
54	MG	1U	203	1/1	0.98	0.38	43,43,43,43	0
54	MG	1A	3830	1/1	0.98	0.25	44,44,44,44	0
54	MG	2A	3214	1/1	0.98	0.06	67,67,67,67	0
54	MG	2A	3326	1/1	0.98	0.05	33,33,33,33	0
54	MG	2A	3014	1/1	0.98	0.06	51,51,51,51	0
54	MG	1A	3382	1/1	0.98	0.13	33,33,33,33	0
54	MG	1A	3905	1/1	0.98	0.06	29,29,29,29	0
54	MG	2A	3592	1/1	0.98	0.07	65,65,65,65	0
54	MG	1A	3240	1/1	0.98	0.18	36,36,36,36	0
54	MG	2A	3594	1/1	0.98	0.04	48,48,48,48	0
54	MG	1D	303	1/1	0.98	0.09	40,40,40,40	0
54	MG	1A	3096	1/1	0.98	0.09	24,24,24,24	0
54	MG	1A	3909	1/1	0.98	0.03	52,52,52,52	0
54	MG	1A	3423	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3466	1/1	0.98	0.11	57,57,57,57	0
54	MG	1D	309	1/1	0.98	0.13	36,36,36,36	0
54	MG	1A	3073	1/1	0.98	0.06	41,41,41,41	0
54	MG	2A	3123	1/1	0.98	0.19	44,44,44,44	0
54	MG	1A	3516	1/1	0.98	0.07	28,28,28,28	0
54	MG	1X	101	1/1	0.98	0.11	43,43,43,43	0
54	MG	2A	3464	1/1	0.98	0.07	66,66,66,66	0
54	MG	1A	3612	1/1	0.98	0.09	27,27,27,27	0
54	MG	1A	3993	1/1	0.98	0.09	63,63,63,63	0
54	MG	10	101	1/1	0.98	0.09	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3350	1/1	0.98	0.08	54,54,54,54	0
54	MG	2A	3346	1/1	0.98	0.08	57,57,57,57	0
54	MG	2a	3150	1/1	0.98	0.10	54,54,54,54	0
54	MG	1A	3074	1/1	0.98	0.06	36,36,36,36	0
54	MG	2A	3349	1/1	0.98	0.09	44,44,44,44	0
54	MG	1A	3566	1/1	0.98	0.05	36,36,36,36	0
54	MG	1A	3352	1/1	0.98	0.09	25,25,25,25	0
54	MG	2A	3615	1/1	0.98	0.04	82,82,82,82	0
54	MG	1A	3428	1/1	0.98	0.05	27,27,27,27	0
54	MG	2A	3617	1/1	0.98	0.06	64,64,64,64	0
54	MG	1A	3921	1/1	0.98	0.05	21,21,21,21	0
54	MG	2A	3619	1/1	0.98	0.05	53,53,53,53	0
54	MG	2A	3620	1/1	0.98	0.04	71,71,71,71	0
54	MG	1A	3295	1/1	0.98	0.06	48,48,48,48	0
54	MG	1E	303	1/1	0.98	0.09	43,43,43,43	0
54	MG	2A	3628	1/1	0.98	0.05	48,48,48,48	0
54	MG	1A	3052	1/1	0.98	0.26	44,44,44,44	0
54	MG	2a	3166	1/1	0.98	0.11	55,55,55,55	0
54	MG	2A	3480	1/1	0.98	0.05	42,42,42,42	0
54	MG	13	101	1/1	0.98	0.12	33,33,33,33	0
54	MG	2a	3010	1/1	0.98	0.05	54,54,54,54	0
54	MG	2A	3139	1/1	0.98	0.06	42,42,42,42	0
54	MG	1A	3007	1/1	0.98	0.04	44,44,44,44	0
54	MG	2A	3360	1/1	0.98	0.08	48,48,48,48	0
54	MG	2a	3014	1/1	0.98	0.03	61,61,61,61	0
54	MG	2a	3174	1/1	0.98	0.05	64,64,64,64	0
54	MG	2A	3141	1/1	0.98	0.09	59,59,59,59	0
54	MG	1A	3047	1/1	0.98	0.12	16,16,16,16	0
54	MG	2A	3487	1/1	0.98	0.11	43,43,43,43	0
54	MG	1A	3849	1/1	0.98	0.05	41,41,41,41	0
54	MG	2A	3247	1/1	0.98	0.09	23,23,23,23	0
54	MG	2A	3642	1/1	0.98	0.04	42,42,42,42	0
54	MG	1A	3726	1/1	0.98	0.07	49,49,49,49	0
54	MG	1a	1857	1/1	0.98	0.09	72,72,72,72	0
54	MG	1A	3929	1/1	0.98	0.05	59,59,59,59	0
54	MG	15	104	1/1	0.98	0.17	29,29,29,29	0
54	MG	1A	3786	1/1	0.98	0.05	36,36,36,36	0
54	MG	2A	3649	1/1	0.98	0.04	60,60,60,60	0
54	MG	1a	1767	1/1	0.98	0.07	53,53,53,53	0
54	MG	2A	3049	1/1	0.98	0.16	52,52,52,52	0
54	MG	2A	3497	1/1	0.98	0.06	62,62,62,62	0
54	MG	1F	301	1/1	0.98	0.07	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1F	302	1/1	0.98	0.13	40,40,40,40	0
54	MG	1A	3357	1/1	0.98	0.07	25,25,25,25	0
54	MG	1A	3078	1/1	0.98	0.15	45,45,45,45	0
54	MG	2A	3377	1/1	0.98	0.10	39,39,39,39	0
54	MG	1A	3359	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3438	1/1	0.98	0.05	36,36,36,36	0
54	MG	1A	3003	1/1	0.98	0.04	27,27,27,27	0
54	MG	17	105	1/1	0.98	0.17	42,42,42,42	0
54	MG	1F	308	1/1	0.98	0.20	30,30,30,30	0
54	MG	1F	309	1/1	0.98	0.16	35,35,35,35	0
54	MG	1A	3937	1/1	0.98	0.12	47,47,47,47	0
54	MG	1A	3049	1/1	0.98	0.03	27,27,27,27	0
54	MG	1A	3006	1/1	0.98	0.03	29,29,29,29	0
59	ZN	1n	104	1/1	0.98	0.04	74,74,74,74	0
59	ZN	2Y	202	1/1	0.98	0.04	93,93,93,93	0
54	MG	2A	3387	1/1	0.98	0.11	36,36,36,36	0
54	MG	1A	3399	1/1	0.98	0.05	29,29,29,29	0
60	SF4	1d	303	8/8	0.98	0.05	60,65,70,78	0
60	SF4	2d	501	8/8	0.98	0.05	67,82,83,88	0
54	MG	2A	3653	1/1	0.99	0.04	70,70,70,70	0
54	MG	2A	3589	1/1	0.99	0.09	44,44,44,44	0
54	MG	1A	3493	1/1	0.99	0.06	32,32,32,32	0
54	MG	1B	213	1/1	0.99	0.04	42,42,42,42	0
54	MG	2A	3344	1/1	0.99	0.03	36,36,36,36	0
54	MG	1A	3884	1/1	0.99	0.06	43,43,43,43	0
54	MG	1A	3976	1/1	0.99	0.06	26,26,26,26	0
54	MG	1A	3977	1/1	0.99	0.05	35,35,35,35	0
54	MG	2A	3348	1/1	0.99	0.02	38,38,38,38	0
54	MG	1A	4012	1/1	0.99	0.03	63,63,63,63	0
54	MG	1A	3263	1/1	0.99	0.17	34,34,34,34	0
54	MG	1A	3590	1/1	0.99	0.07	50,50,50,50	0
54	MG	1A	3915	1/1	0.99	0.03	55,55,55,55	0
54	MG	1A	3242	1/1	0.99	0.30	34,34,34,34	0
54	MG	2A	3308	1/1	0.99	0.09	50,50,50,50	0
54	MG	1A	3888	1/1	0.99	0.07	43,43,43,43	0
54	MG	1A	3434	1/1	0.99	0.05	42,42,42,42	0
54	MG	2a	3159	1/1	0.99	0.04	64,64,64,64	0
54	MG	1A	3305	1/1	0.99	0.13	25,25,25,25	0
54	MG	1A	3717	1/1	0.99	0.04	44,44,44,44	0
54	MG	11	103	1/1	0.99	0.06	53,53,53,53	0
54	MG	1A	3436	1/1	0.99	0.02	30,30,30,30	0
54	MG	2A	3103	1/1	0.99	0.06	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3330	1/1	0.99	0.09	21,21,21,21	0
54	MG	1A	3222	1/1	0.99	0.03	41,41,41,41	0
54	MG	2A	3364	1/1	0.99	0.03	62,62,62,62	0
54	MG	2A	3557	1/1	0.99	0.04	49,49,49,49	0
54	MG	2A	3274	1/1	0.99	0.06	51,51,51,51	0
54	MG	1A	3924	1/1	0.99	0.03	42,42,42,42	0
54	MG	1A	3868	1/1	0.99	0.06	54,54,54,54	0
54	MG	1A	3286	1/1	0.99	0.10	22,22,22,22	0
54	MG	2A	3463	1/1	0.99	0.06	37,37,37,37	0
54	MG	1A	3762	1/1	0.99	0.11	38,38,38,38	0
54	MG	1a	1852	1/1	0.99	0.03	47,47,47,47	0
54	MG	2A	3622	1/1	0.99	0.03	66,66,66,66	0
54	MG	2A	3623	1/1	0.99	0.06	35,35,35,35	0
54	MG	2A	3688	1/1	0.99	0.04	52,52,52,52	0
54	MG	2A	3624	1/1	0.99	0.05	40,40,40,40	0
54	MG	2A	3625	1/1	0.99	0.04	60,60,60,60	0
54	MG	1a	1853	1/1	0.99	0.05	61,61,61,61	0
54	MG	1A	3847	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3549	1/1	0.99	0.06	33,33,33,33	0
54	MG	2A	3469	1/1	0.99	0.03	50,50,50,50	0
54	MG	2A	3630	1/1	0.99	0.11	57,57,57,57	0
54	MG	2A	3569	1/1	0.99	0.03	53,53,53,53	0
54	MG	2k	201	1/1	0.99	0.10	57,57,57,57	0
54	MG	1A	3900	1/1	0.99	0.03	27,27,27,27	0
54	MG	2A	3633	1/1	0.99	0.03	58,58,58,58	0
54	MG	2A	3571	1/1	0.99	0.05	42,42,42,42	0
54	MG	1D	307	1/1	0.99	0.03	19,19,19,19	0
54	MG	1A	3723	1/1	0.99	0.03	36,36,36,36	0
54	MG	2A	3574	1/1	0.99	0.04	41,41,41,41	0
54	MG	2X	101	1/1	0.99	0.07	63,63,63,63	0
54	MG	1A	3932	1/1	0.99	0.06	54,54,54,54	0
54	MG	1A	3668	1/1	0.99	0.04	50,50,50,50	0
54	MG	1A	3474	1/1	0.99	0.04	27,27,27,27	0
54	MG	1A	3966	1/1	0.99	0.03	49,49,49,49	0
54	MG	1A	3852	1/1	0.99	0.06	23,23,23,23	0
54	MG	2A	3580	1/1	0.99	0.06	47,47,47,47	0
54	MG	1A	3475	1/1	0.99	0.06	32,32,32,32	0
54	MG	2A	3645	1/1	0.99	0.03	47,47,47,47	0
54	MG	1A	3906	1/1	0.99	0.05	42,42,42,42	0
59	ZN	1Y	202	1/1	0.99	0.02	62,62,62,62	0
54	MG	1A	3347	1/1	0.99	0.08	30,30,30,30	0
59	ZN	15	109	1/1	0.99	0.02	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
59	ZN	16	501	1/1	0.99	0.05	47,47,47,47	0
54	MG	1a	1748	1/1	0.99	0.11	42,42,42,42	0
54	MG	1A	3490	1/1	0.99	0.03	49,49,49,49	0
54	MG	2a	3138	1/1	0.99	0.07	52,52,52,52	0
59	ZN	25	102	1/1	0.99	0.03	68,68,68,68	0
59	ZN	29	501	1/1	0.99	0.03	73,73,73,73	0
54	MG	2A	3650	1/1	0.99	0.04	44,44,44,44	0
54	MG	1A	3141	1/1	0.99	0.13	26,26,26,26	0
54	MG	1A	3422	1/1	0.99	0.08	23,23,23,23	0
54	MG	2A	3621	1/1	1.00	0.02	66,66,66,66	0
59	ZN	19	104	1/1	1.00	0.10	65,65,65,65	0
54	MG	1A	3534	1/1	1.00	0.07	31,31,31,31	0
54	MG	1A	3361	1/1	1.00	0.05	36,36,36,36	0
54	MG	1A	3499	1/1	1.00	0.07	49,49,49,49	0
54	MG	1A	3882	1/1	1.00	0.07	33,33,33,33	0
59	ZN	26	501	1/1	1.00	0.02	65,65,65,65	0
54	MG	1A	3637	1/1	1.00	0.06	32,32,32,32	0
54	MG	1A	3467	1/1	1.00	0.02	27,27,27,27	0
54	MG	2a	3124	1/1	1.00	0.03	60,60,60,60	0
54	MG	2A	3585	1/1	1.00	0.03	43,43,43,43	0

6.5 Other polymers

There are no such residues in this entry.