Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2025 – 11:40 PM EDT

PDB ID	:	9MTR / pdb_00009mtr
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with mRNA, A-site GGS-mutant Release Factor 1, and P-site fMEAAA KC-peptidyl-tRNAcys at 2.80A resolution
Authors	:	Aleksandrova, E.V.; Syroegin, E.A.; Basu, R.S.; Vassilevski, A.A.; Gagnon, M.G.; Polikanov, Y.S.
Deposited on	:	2025-01-12
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

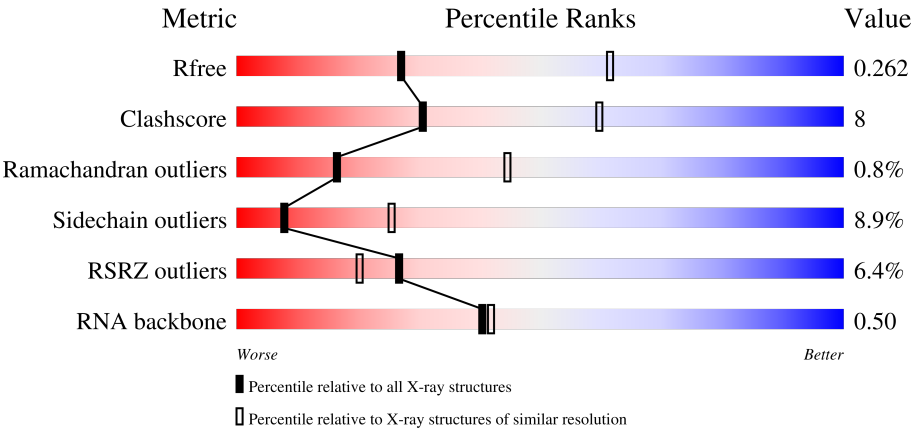
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



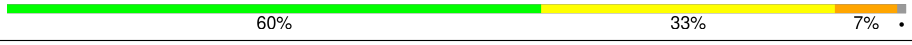
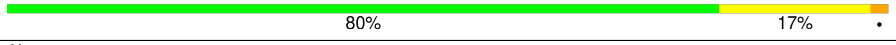
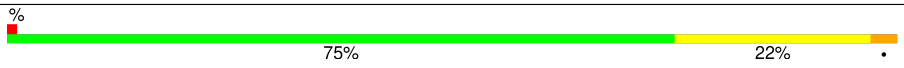
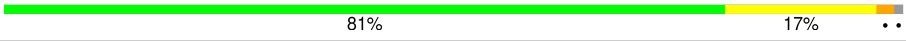
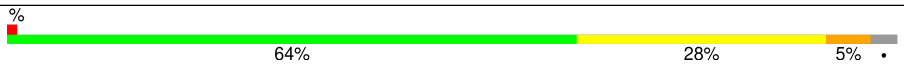
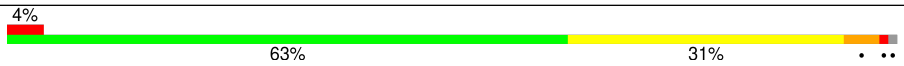
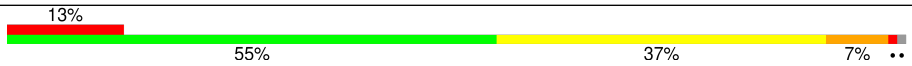
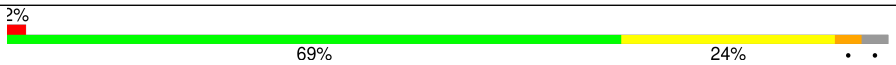
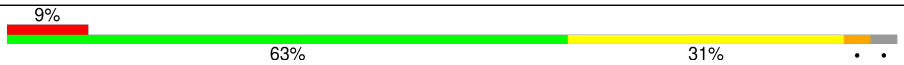
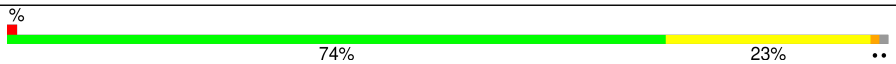
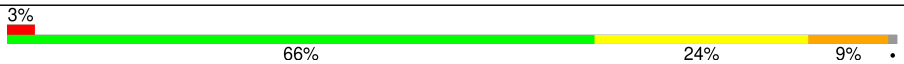
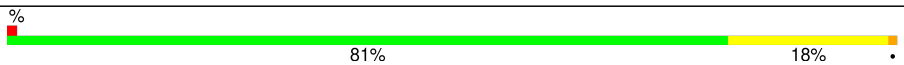
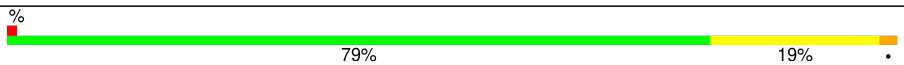
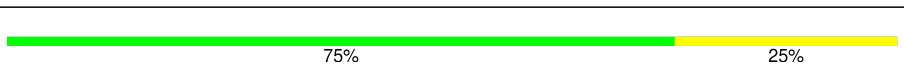
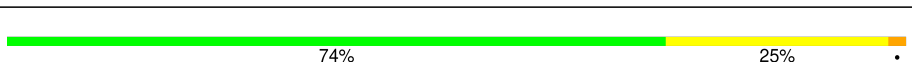
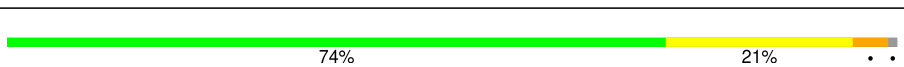
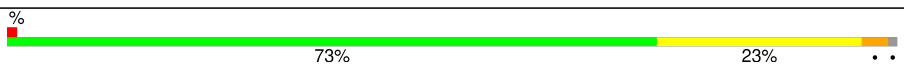
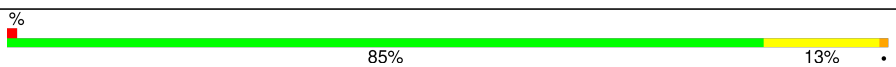
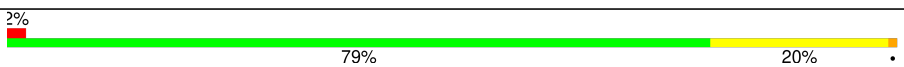
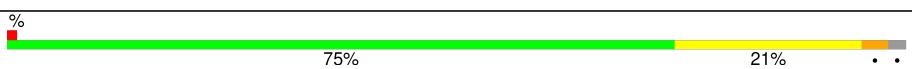
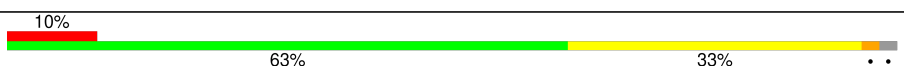
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)
RNA backbone	3690	1037 (3.00-2.60)

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 <=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	6% 65% 28% 6%
1	2A	2915	5% 58% 32% 6%
2	1B	121	75% 20%

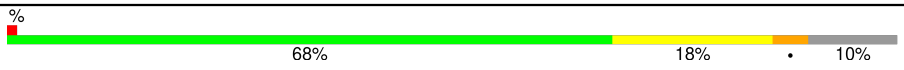
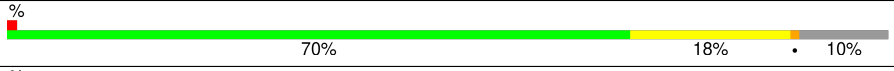
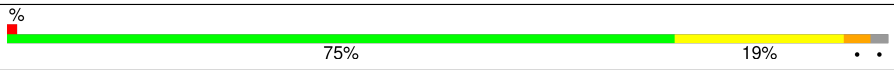
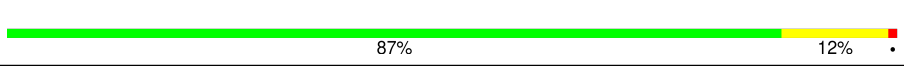
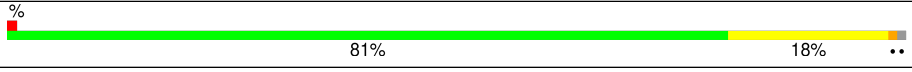
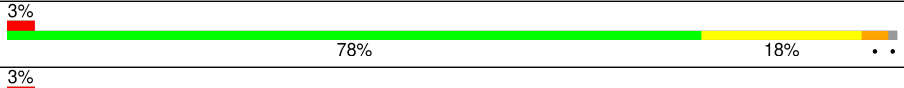
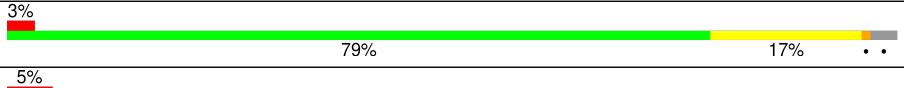
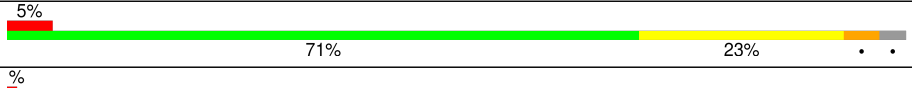
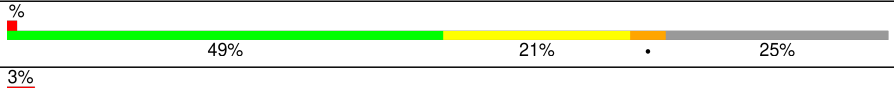
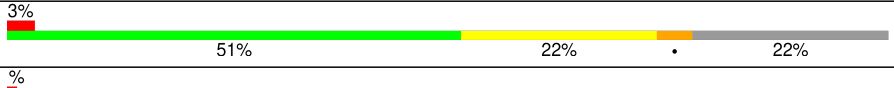
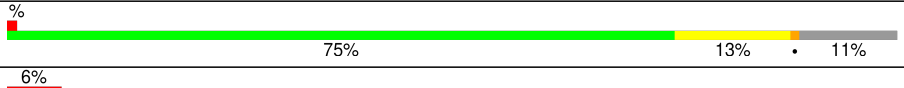
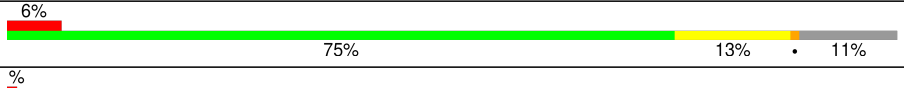
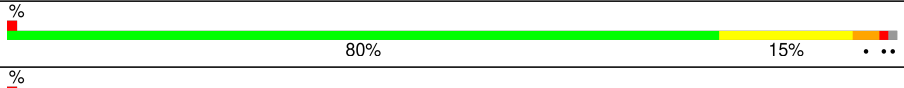
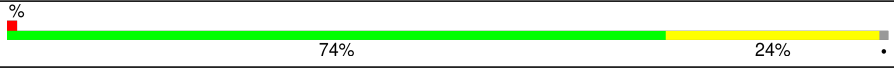
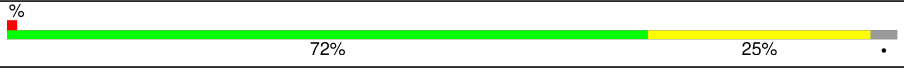
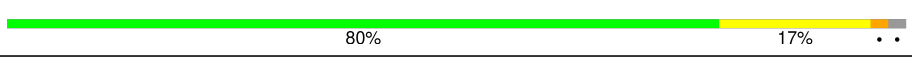
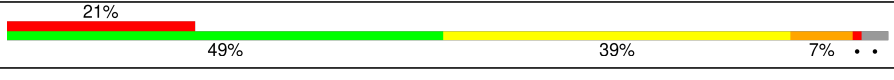
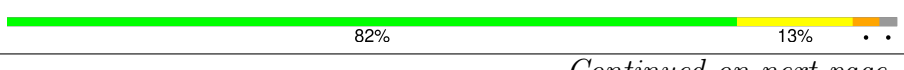
Continued on next page...

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	

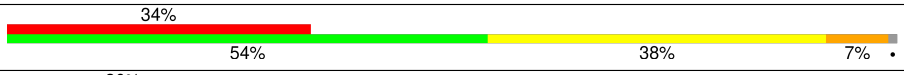
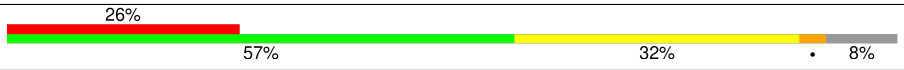
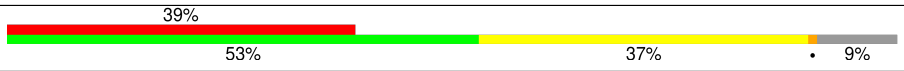
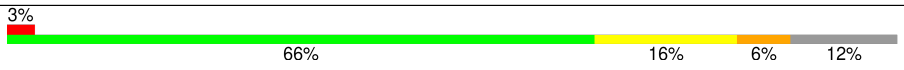
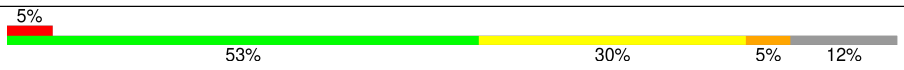
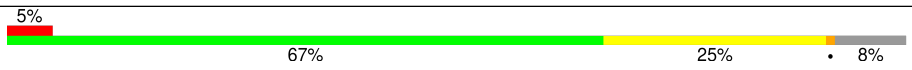
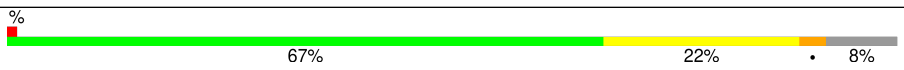
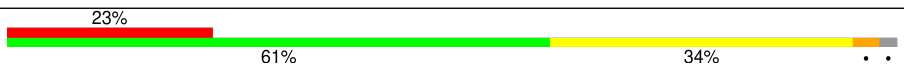
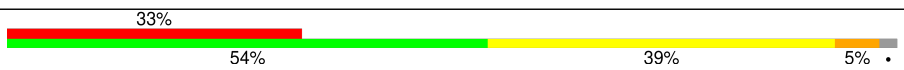
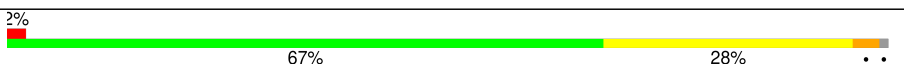
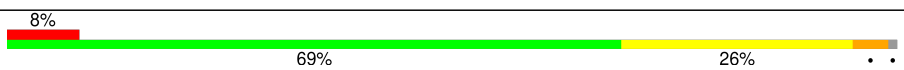
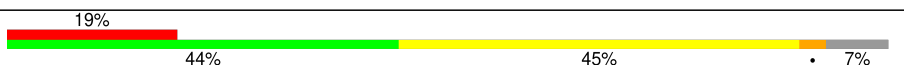
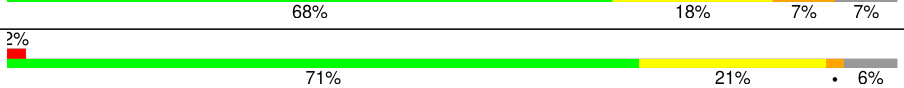
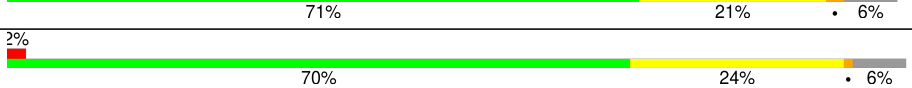
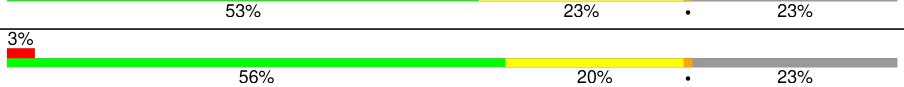
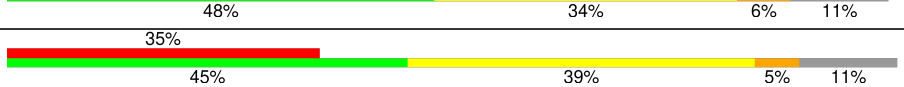
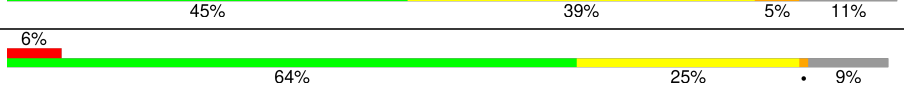
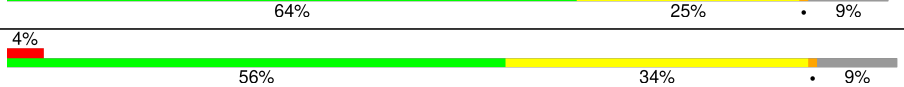
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	25	60	2% 80% 17%
28	16	54	74% 17% 7%
28	26	54	78% 20%
29	17	49	4% 69% 27%
29	27	49	2% 73% 20%
30	18	65	82% 17%
30	28	65	74% 25%
31	19	37	81% 19%
31	29	37	68% 32%
32	1a	1521	8% 52% 38% 9%
32	2a	1521	8% 52% 39% 7%
33	1b	256	14% 51% 34% 5% 10%
33	2b	256	19% 44% 41% 5% 10%
34	1c	239	12% 55% 27% 14%
34	2c	239	13% 51% 34% 14%
35	1d	209	9% 62% 35%
35	2d	209	4% 66% 29%
36	1e	162	% 60% 25% 7% 9%
36	2e	162	4% 51% 36% 9%
37	1f	101	2% 67% 30%
37	2f	101	4% 69% 28%
38	1g	156	9% 74% 24%
38	2g	156	12% 64% 31%
39	1h	138	3% 72% 25%
39	2h	138	68% 28%

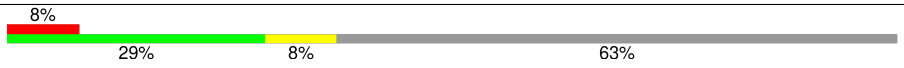
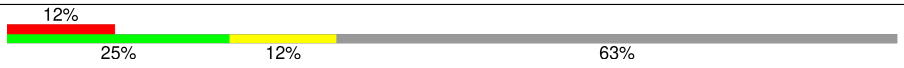
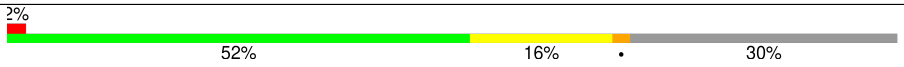
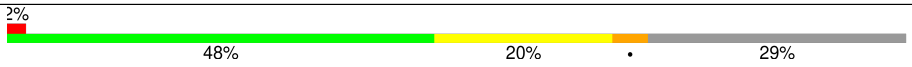
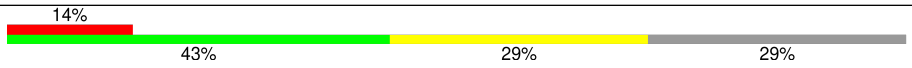
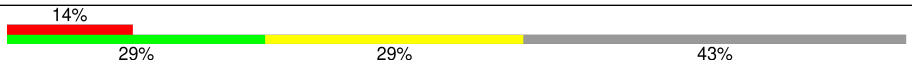
Continued on next page...

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	1v	24	
53	2v	24	
54	1w	354	
54	2w	354	
55	1x	74	
55	2x	74	
56	1z	7	
56	2z	7	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1A	4032	-	-	-	X
57	MG	1U	212	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 296656 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			
22	20	76	Total	C	N	O	S	0	0	0
			604	373	128	102	1			

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			919	566	190	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			907	558	188	159	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called CYS-Stop mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	9	Total	C	N	O	P	0	0	0
			191	86	34	62	9			
53	2v	9	Total	C	N	O	P	0	0	0
			191	86	34	62	9			

- Molecule 54 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	249	Total	C	N	O	S	0	0	0
			1935	1196	359	371	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1953	1207	360	377	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1w	230	SER	GLN	engineered mutation	UNP P96077
2w	230	SER	GLN	engineered mutation	UNP P96077

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	74	Total	C	N	O	P	S	0	0	0
			1577	704	281	517	74	1			
55	2x	74	Total	C	N	O	P	S	0	0	0
			1577	704	281	517	74	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	5	Total	C	N	O	S	0	0	0
			30	18	6	5	1			
56	2z	4	Total	C	N	O	S	0	0	0
			25	15	5	4	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1084	Total	Mg	0	0
			1084	1084		
57	1B	39	Total	Mg	0	0
			39	39		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1D	14	Total Mg 14 14	0	0
57	1E	13	Total Mg 13 13	0	0
57	1F	14	Total Mg 14 14	0	0
57	1G	5	Total Mg 5 5	0	0
57	1H	1	Total Mg 1 1	0	0
57	1I	1	Total Mg 1 1	0	0
57	1N	6	Total Mg 6 6	0	0
57	1O	5	Total Mg 5 5	0	0
57	1P	3	Total Mg 3 3	0	0
57	1Q	6	Total Mg 6 6	0	0
57	1R	5	Total Mg 5 5	0	0
57	1S	3	Total Mg 3 3	0	0
57	1T	3	Total Mg 3 3	0	0
57	1U	12	Total Mg 12 12	0	0
57	1V	8	Total Mg 8 8	0	0
57	1W	5	Total Mg 5 5	0	0
57	1X	6	Total Mg 6 6	0	0
57	1Y	3	Total Mg 3 3	0	0
57	1Z	3	Total Mg 3 3	0	0
57	10	9	Total Mg 9 9	0	0
57	11	3	Total Mg 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	12	2	Total Mg 2 2	0	0
57	13	4	Total Mg 4 4	0	0
57	15	9	Total Mg 9 9	0	0
57	16	3	Total Mg 3 3	0	0
57	17	6	Total Mg 6 6	0	0
57	18	6	Total Mg 6 6	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	221	Total Mg 221 221	0	0
57	1b	2	Total Mg 2 2	0	0
57	1d	1	Total Mg 1 1	0	0
57	1e	1	Total Mg 1 1	0	0
57	1f	2	Total Mg 2 2	0	0
57	1k	1	Total Mg 1 1	0	0
57	1l	1	Total Mg 1 1	0	0
57	1m	1	Total Mg 1 1	0	0
57	1n	1	Total Mg 1 1	0	0
57	1p	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1v	2	Total Mg 2 2	0	0
57	1w	1	Total Mg 1 1	0	0
57	1x	13	Total Mg 13 13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2A	835	Total Mg 835 835	0	0
57	2B	18	Total Mg 18 18	0	0
57	2D	5	Total Mg 5 5	0	0
57	2E	10	Total Mg 10 10	0	0
57	2F	7	Total Mg 7 7	0	0
57	2G	1	Total Mg 1 1	0	0
57	2O	3	Total Mg 3 3	0	0
57	2P	1	Total Mg 1 1	0	0
57	2Q	4	Total Mg 4 4	0	0
57	2R	1	Total Mg 1 1	0	0
57	2T	4	Total Mg 4 4	0	0
57	2U	4	Total Mg 4 4	0	0
57	2V	2	Total Mg 2 2	0	0
57	2W	3	Total Mg 3 3	0	0
57	2Y	1	Total Mg 1 1	0	0
57	2Z	1	Total Mg 1 1	0	0
57	21	2	Total Mg 2 2	0	0
57	23	1	Total Mg 1 1	0	0
57	25	4	Total Mg 4 4	0	0
57	26	1	Total Mg 1 1	0	0
57	27	3	Total Mg 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	28	3	Total Mg 3 3	0	0
57	2a	178	Total Mg 178 178	0	0
57	2d	2	Total Mg 2 2	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	2	Total Mg 2 2	0	0
57	2g	1	Total Mg 1 1	0	0
57	2i	1	Total Mg 1 1	0	0
57	2j	2	Total Mg 2 2	0	0
57	2k	1	Total Mg 1 1	0	0
57	2l	2	Total Mg 2 2	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	2	Total Mg 2 2	0	0
57	2x	8	Total Mg 8 8	0	0

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

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

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

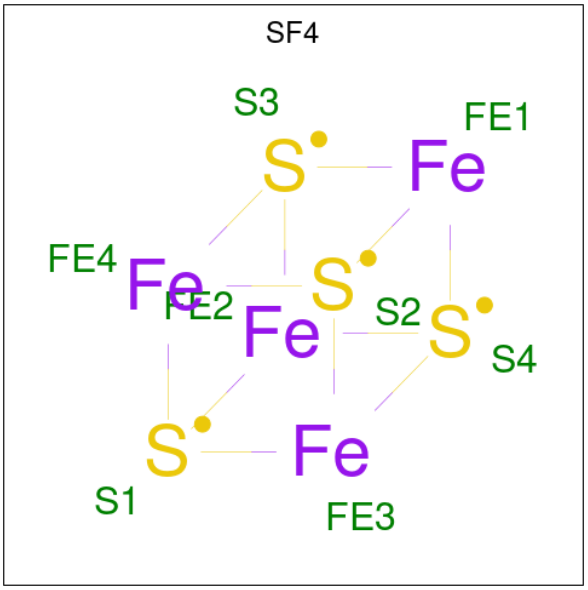
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	14	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	2Y	1	Total Zn 1 1	0	0
59	24	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1897	Total O 1897 1897	0	0
61	1B	61	Total O 61 61	0	0
61	1D	30	Total O 30 30	0	0
61	1E	27	Total O 27 27	0	0
61	1F	18	Total O 18 18	0	0
61	1G	5	Total O 5 5	0	0
61	1H	2	Total O 2 2	0	0
61	1I	1	Total O 1 1	0	0
61	1N	8	Total O 8 8	0	0
61	1O	6	Total O 6 6	0	0
61	1P	23	Total O 23 23	0	0
61	1Q	11	Total O 11 11	0	0
61	1R	11	Total O 11 11	0	0
61	1S	1	Total O 1 1	0	0
61	1T	7	Total O 7 7	0	0
61	1U	13	Total O 13 13	0	0
61	1V	6	Total O 6 6	0	0
61	1W	12	Total O 12 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1X	10	Total O 10 10	0	0
61	1Y	2	Total O 2 2	0	0
61	10	9	Total O 9 9	0	0
61	11	8	Total O 8 8	0	0
61	12	3	Total O 3 3	0	0
61	13	4	Total O 4 4	0	0
61	15	7	Total O 7 7	0	0
61	16	1	Total O 1 1	0	0
61	17	8	Total O 8 8	0	0
61	18	12	Total O 12 12	0	0
61	1a	259	Total O 259 259	0	0
61	1b	1	Total O 1 1	0	0
61	1d	1	Total O 1 1	0	0
61	1f	1	Total O 1 1	0	0
61	1j	1	Total O 1 1	0	0
61	1l	2	Total O 2 2	0	0
61	1n	1	Total O 1 1	0	0
61	1q	4	Total O 4 4	0	0
61	1u	1	Total O 1 1	0	0
61	1v	3	Total O 3 3	0	0
61	1w	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1x	25	Total O 25 25	0	0
61	2A	1003	Total O 1003 1003	0	0
61	2B	14	Total O 14 14	0	0
61	2D	25	Total O 25 25	0	0
61	2E	14	Total O 14 14	0	0
61	2F	12	Total O 12 12	0	0
61	2N	1	Total O 1 1	0	0
61	2O	3	Total O 3 3	0	0
61	2P	7	Total O 7 7	0	0
61	2Q	3	Total O 3 3	0	0
61	2R	4	Total O 4 4	0	0
61	2T	5	Total O 5 5	0	0
61	2U	3	Total O 3 3	0	0
61	2V	1	Total O 1 1	0	0
61	2W	1	Total O 1 1	0	0
61	2X	2	Total O 2 2	0	0
61	20	2	Total O 2 2	0	0
61	21	10	Total O 10 10	0	0
61	25	3	Total O 3 3	0	0
61	27	2	Total O 2 2	0	0
61	28	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

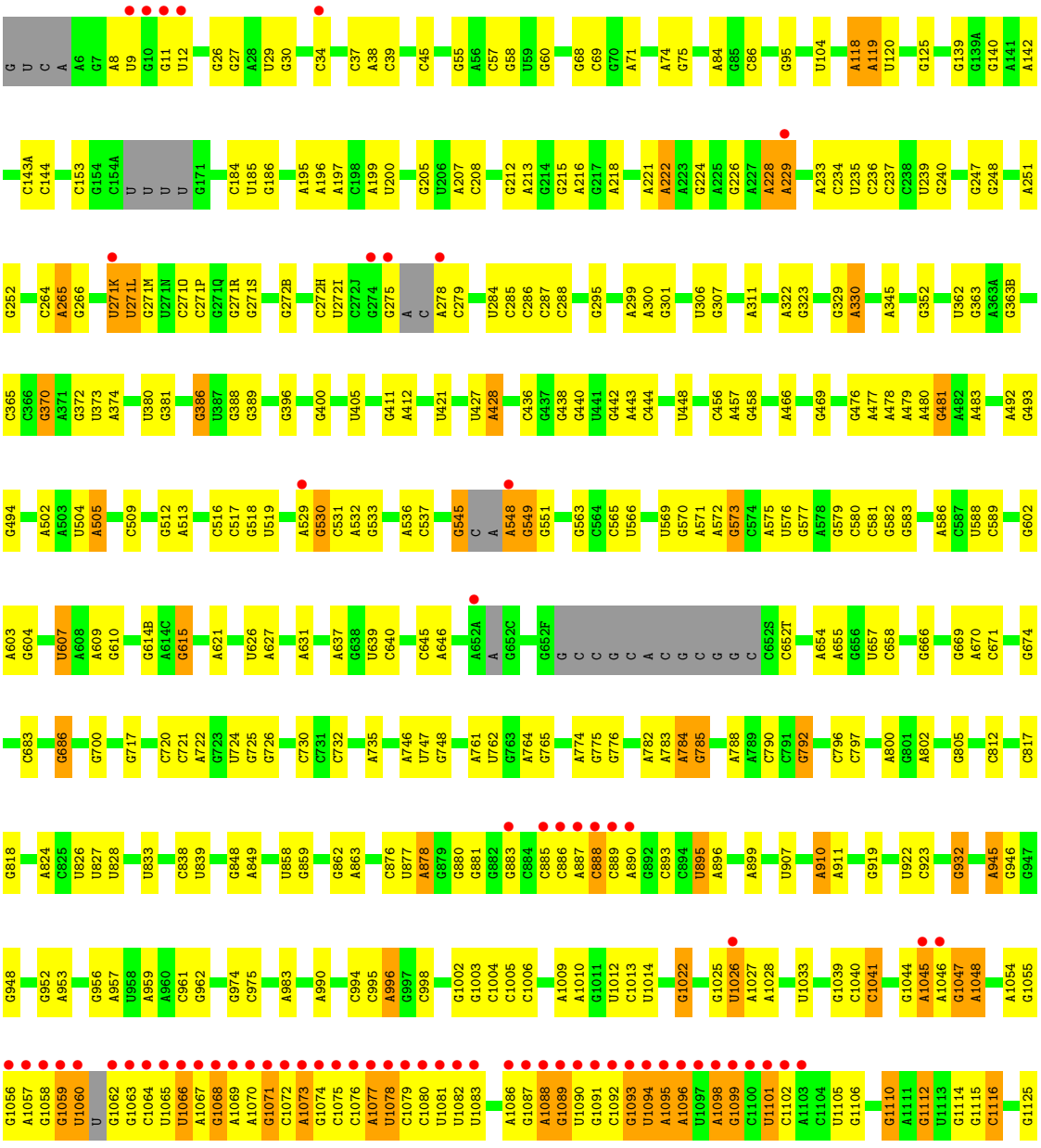
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	29	1	Total O 1 1	0	0
61	2a	130	Total O 130 130	0	0
61	2e	1	Total O 1 1	0	0
61	2i	1	Total O 1 1	0	0
61	2j	2	Total O 2 2	0	0
61	2l	4	Total O 4 4	0	0
61	2n	1	Total O 1 1	0	0
61	2q	2	Total O 2 2	0	0
61	2t	2	Total O 2 2	0	0
61	2v	1	Total O 1 1	0	0
61	2w	1	Total O 1 1	0	0
61	2x	14	Total O 14 14	0	0

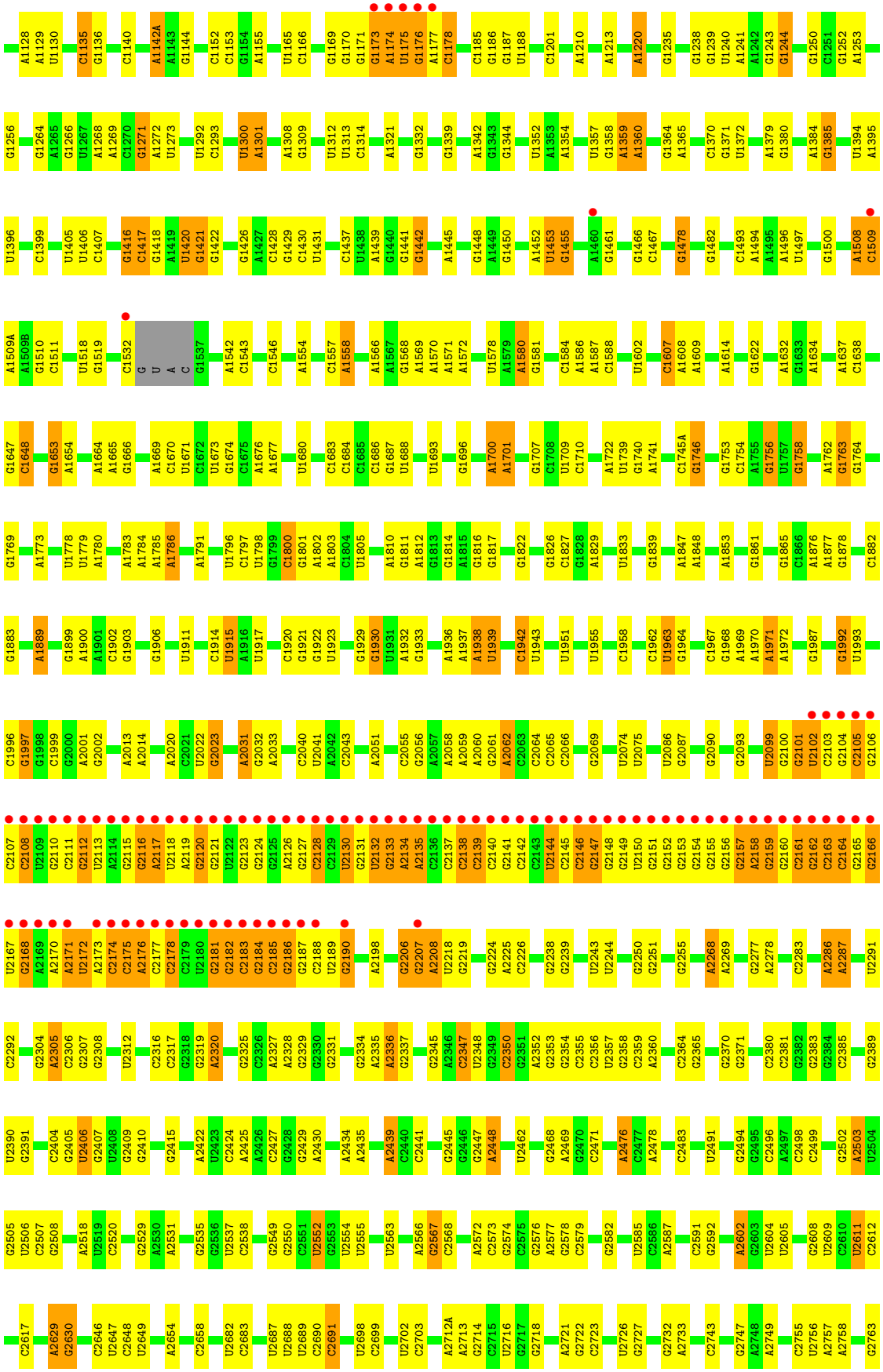
3 Residue-property plots (i)

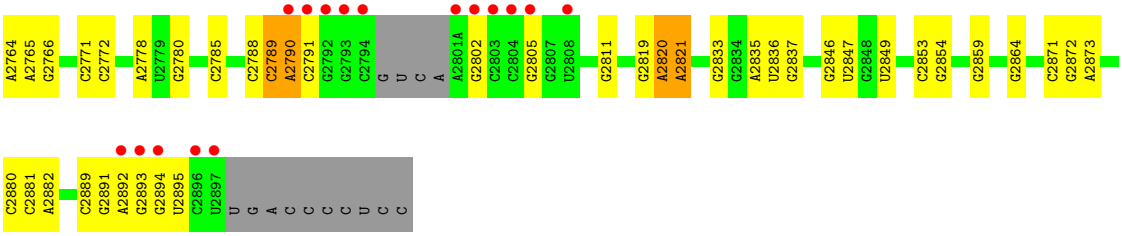
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain 1A:

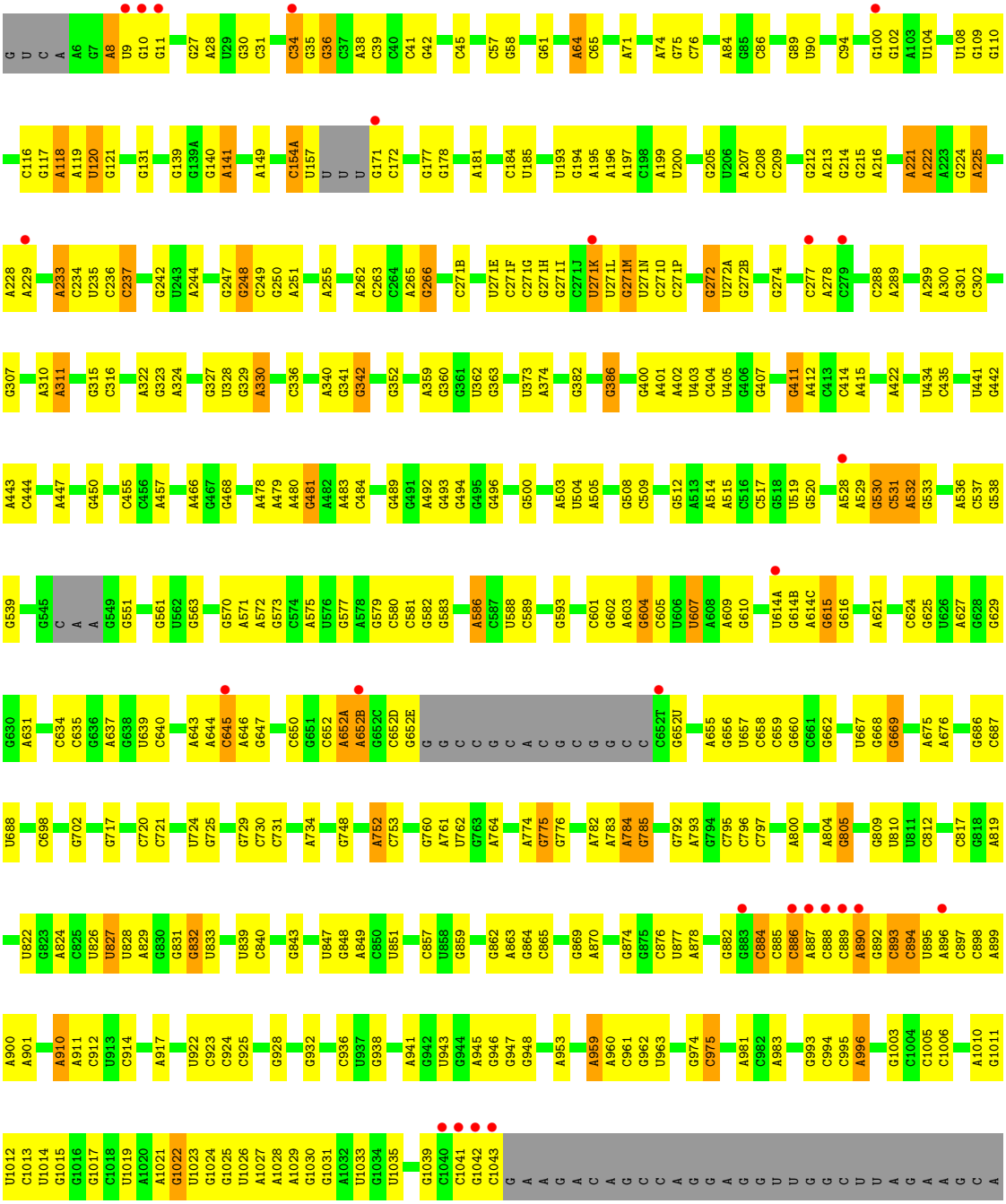


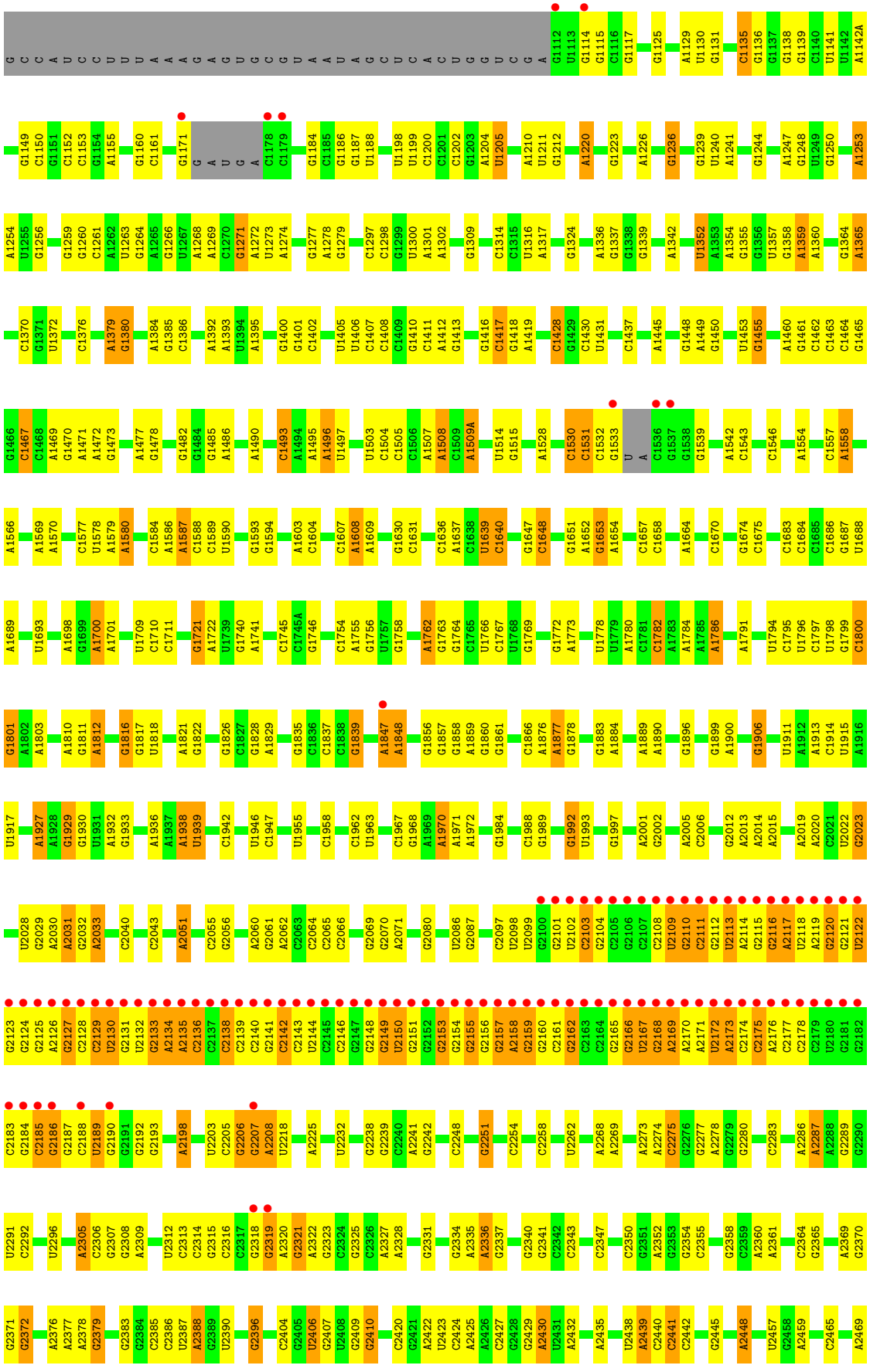

A1128 A1129 U1130 C1135 G1136 C1140 A1142A A1143 G1144 C1152 C1153 G1154 A1155 U1165 C1166 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1185 G1186 G1187 U1188 C1201 A1210 A1213 A1220 G1235 G1238 G1239 U1240 A1241 A1242 G1243 G1244 G1250 C1251 G1252 A1253
G1256 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 U1292 C1293 U1300 A1301 A1308 G1309 U1312 U1313 C1314 A1321 G1332 G1339 A1342 G1343 G1344 U1352 A1353 A1354 U1357 G1358 A1359 A1360 G1364 A1365 C1370 G1371 U1372 A1379 G1380 A1384 G1385 U1394 A1395
U1396 C1399 U1405 U1406 C1407 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1426 A1427 C1428 G1429 C1430 U1431 C1437 U1438 A1439 G1440 G1441 G1442 A1445 G1448 A1449 G1450 A1452 U1453 G1455 A1460 G1461 G1466 C1467 G1478 G1482 C1493 A1494 A1495 A1496 U1497 G1500 A1508 C1509
A1509A A1509B G1510 C1511 U1518 G1519 C1532 G U A C G1537 A1542 C1543 C1546 A1554 C1557 A1558 A1566 A1567 G1568 A1569 A1570 A1571 A1572 U1578 A1579 A1580 G1581 C1584 A1586 A1587 C1588 U1602 C1607 A1608 A1609 A1614 G1622 A1632 G1633 A1634 A1637 C1638
G1647 C1648 G1653 A1654 A1664 A1665 C1666 A1669 C1670 U1671 C1672 U1673 G1674 C1675 A1676 A1677 U1680 C1683 C1684 C1685 C1686 G1687 U1688 U1693 G1696 A1700 A1701 G1707 C1708 U1709 C1710 A1722 U1739 G1740 A1741 C1745A G1746 G1753 C1754 A1755 G1756 U1757 G1758 A1762 G1763 G1764
G1769 A1773 U1778 U1779 A1780 A1783 A1784 A1785 A1786 A1791 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 A1810 G1811 A1812 G1813 G1814 A1815 G1816 G1817 G1822 G1826 C1827 G1828 A1829 U1833 G1839 A1847 A1848 A1853 G1861 G1865 C1866 A1876 A1877 G1878 C1882
G1883 A1889 G1899 A1900 A1901 C1902 G1903 G1906 U1911 C1914 U1915 A1916 U1917 C1920 G1921 G1922 U1923 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 C1942 U1943 U1951 U1955 C1958 C1962 U1963 G1964 C1967 G1968 A1969 A1970 A1971 A1972 G1987 G1992 U1993
C1996 G1997 G1998 C1999 G2000 A2001 G2002 A2013 A2014 A2020 C2021 U2022 G2023 A2031 G2032 A2033 C2040 U2041 A2042 C2043 A2051 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2069 U2074 U2075 U2086 G2087 G2090 G2093 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106
C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 C2124 G2125 A2126 G2127 C2128 C2129 U2130 C2131 U2132 C2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166
U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 A2198 G2206 G2207 A2208 U2218 G2219 G2224 A2225 C2226 G2238 G2239 U2243 U2244 G2250 G2251 G2255 A2268 A2269 G2277 A2278 C2283 A2286 A2287 U2291
C2292 G2304 A2305 C2306 G2307 G2308 U2312 C2316 C2317 G2318 G2319 A2320 G2325 C2326 A2327 A2328 G2329 G2330 G2331 G2334 A2335 A2336 G2337 G2345 A2346 C2347 U2348 G2349 C2350 C2351 A2352 G2353 G2354 C2355 C2356 U2357 G2358 C2359 A2360 C2364 G2365 G2370 G2371 C2380 C2381 G2382 G2383 G2384 C2385 G2389
U2390 G2391 C2404 G2405 U2406 G2407 U2408 G2409 G2410 G2415 A2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 A2434 A2435 A2439 C2440 C2441 G2445 G2446 G2447 A2448 U2462 G2468 A2469 G2470 C2471 A2476 C2477 A2478 C2483 U2491 G2494 G2495 C2496 A2497 C2498 C2499 G2502 A2503 U2504
G2505 U2506 C2507 G2508 A2518 U2519 C2520 G2529 A2530 A2531 G2535 C2536 U2537 C2538 G2549 G2550 C2551 U2552 G2553 U2554 U2555 U2563 A2566 G2567 C2568 A2572 C2573 G2574 C2575 G2576 A2577 G2578 C2579 G2582 U2585 C2586 A2587 C2591 G2592 A2602 G2603 U2604 U2605 G2608 U2609 C2610 U2611 C2612
C2617 A2629 G2630 C2646 U2647 C2648 U2649 A2654 C2658 U2682 C2683 U2687 U2688 U2689 C2690 C2691 U2698 C2699 U2702 C2703 A2712A A2713 G2714 C2715 U2716 G2717 G2718 A2721 G2722 C2723 U2726 G2727 G2732 A2733 C2743 G2747 A2748 A2749 C2755 U2756 A2757 A2758 G2763

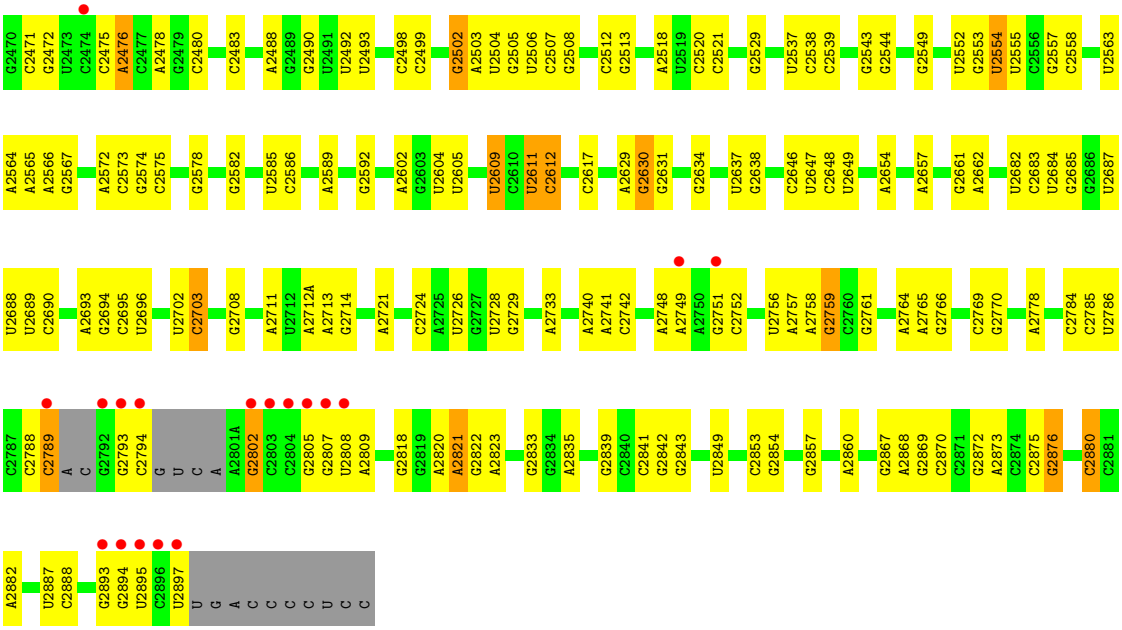


• Molecule 1: 23S Ribosomal RNA

Chain 2A:




G C C A U C C U U U A A A G A G A G U U C G C G U A A A U A G G C U U C G A G1112 U1113 G1114 G1115 C1116 G1117 G1125 A1129 U1130 G1131 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A
G1149 C1150 G1151 C1152 C1153 G1154 A1155 G1160 C1161 G1171 G A A U G A C1178 C1179 G1184 C1185 G1186 G1187 U1188 U1198 U1199 C1200 C1201 C1202 G1203 A1204 U1205 A1210 U1211 G1212 A1220 G1223 A1226 G1236 G1239 U1240 A1241 G1244 A1247 G1248 U1249 G1250 A1253
A1254 U1255 G1256 G1259 G1260 C1261 A1262 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 G1277 A1278 G1279 C1297 C1298 G1299 U1300 A1301 A1302 G1309 C1314 C1315 U1316 A1317 G1324 A1336 G1337 G1338 G1339 A1342 U1352 A1353 A1354 G1355 G1356 U1357 G1358 A1359 A1360 G1364 A1365
C1370 G1371 U1372 C1376 A1379 G1380 A1384 G1385 C1386 A1392 A1393 U1394 A1395 G1400 G1401 C1402 U1405 U1406 C1407 C1408 C1409 G1410 C1411 A1412 G1413 G1416 C1417 G1418 A1419 C1428 G1429 C1430 U1431 C1437 A1445 G1448 A1449 G1450 U1453 G1455 A1460 G1461 C1462 C1463 C1464 G1465
G1466 C1467 C1468 A1469 G1470 A1471 A1472 G1473 A1477 G1478 G1482 G1484 G1485 A1486 A1490 C1493 A1494 A1495 A1496 U1497 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1509A U1514 G1515 A1528 C1530 C1531 C1532 G1533 U A C1536 G1537 G1538 G1539 A1542 C1543 C1546 A1554 C1557 A1558
A1566 A1569 A1570 C1577 U1578 A1579 A1580 C1584 A1586 A1587 C1588 C1589 U1590 G1593 G1594 A1603 C1604 C1607 A1608 A1609 G1630 C1631 C1636 A1637 C1638 U1639 C1640 G1647 C1648 G1651 A1652 G1653 A1654 C1657 C1658 A1664 C1670 G1674 C1675 C1683 C1684 C1685 C1686 G1687 U1688
A1689 U1693 A1698 G1699 A1700 A1701 U1709 C1710 C1711 G1721 A1722 U1739 G1740 A1741 C1745 C1745A G1746 C1754 A1755 G1756 U1757 G1758 A1762 G1763 G1764 C1765 U1766 C1767 U1768 G1769 G1772 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1791 U1794 C1795 U1796 C1797 U1798 G1799 C1800
G1801 A1802 A1803 A1810 G1811 A1812 G1816 G1817 U1818 A1821 G1822 G1826 C1827 G1828 A1829 G1835 C1836 C1837 C1838 G1839 A1847 A1848 G1856 G1857 G1858 A1859 G1860 G1861 C1866 A1876 A1877 G1878 G1883 A1884 A1889 A1890 G1896 G1899 A1900 G1906 U1911 A1912 A1913 C1914 U1915 A1916
U1917 A1927 A1928 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 C1942 U1946 C1947 U1955 C1958 C1962 U1963 C1967 G1968 A1969 A1970 A1971 A1972 G1984 C1988 G1989 G1992 U1993 G1997 A2001 G2002 A2005 C2006 G2012 A2013 A2014 A2015 A2019 A2020 C2021 U2022 G2023
U2028 G2029 A2030 A2031 G2032 A2033 C2040 C2043 A2051 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2069 G2070 A2071 G2080 U2086 G2087 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122
G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 C2182
C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2193 A2198 U2203 C2205 G2206 G2207 A2208 U2218 A2225 U2232 G2238 G2239 C2240 A2241 G2242 C2248 G2251 C2254 C2258 U2262 A2268 A2269 A2273 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2283 A2286 A2287 A2288 G2289 G2290
U2291 C2292 U2296 A2305 C2306 G2307 G2308 A2309 U2312 C2313 C2314 G2315 C2316 C2317 G2318 G2319 A2320 G2321 A2322 G2323 C2324 G2325 C2326 A2327 A2328 G2331 G2334 A2335 A2336 G2337 G2340 G2341 C2342 C2343 C2347 C2350 G2351 A2352 G2353 G2354 C2355 G2358 C2359 A2360 A2361 C2364 G2365 A2369 G2370
G2371 G2372 A2376 A2377 A2378 G2379 G2383 G2384 C2385 C2386 U2387 A2388 G2389 U2390 G2396 C2404 G2405 U2406 G2407 U2408 G2409 G2410 C2420 G2421 A2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2432 A2435 U2438 A2439 C2440 C2441 C2442 G2445 A2448 U2457 G2458 A2459 C2465 A2469

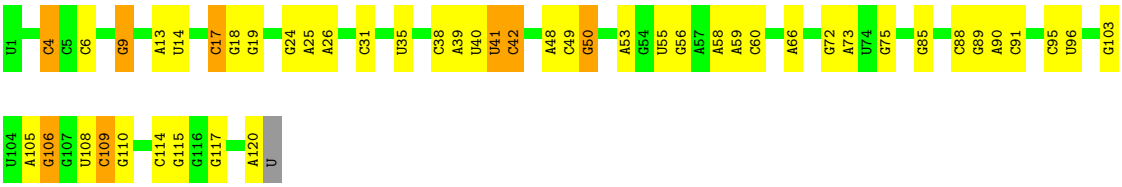


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

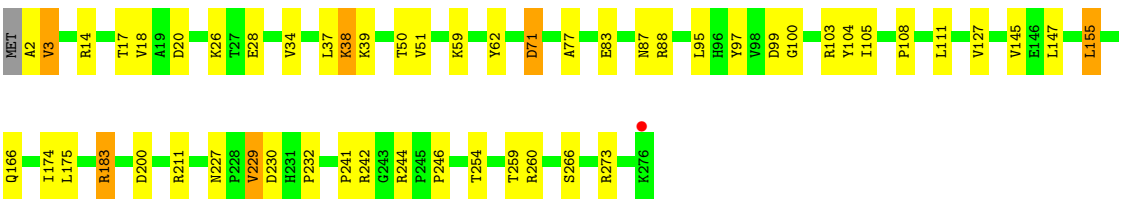
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



• Molecule 3: 50S ribosomal protein L2

Chain 1D:

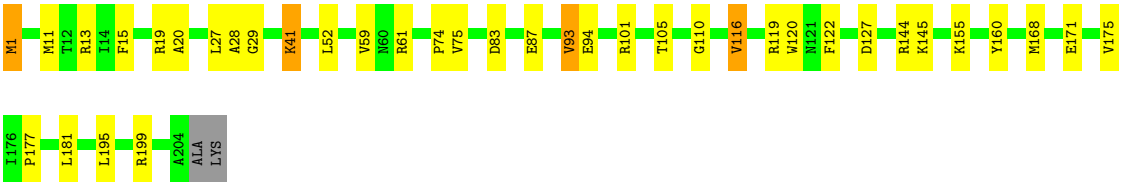


• Molecule 3: 50S ribosomal protein L2

Chain 2D:

• Molecule 4: 50S ribosomal protein L3

Chain 1E:

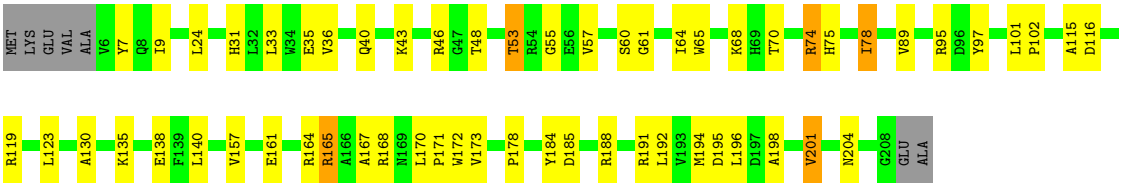


• Molecule 4: 50S ribosomal protein L3

Chain 2E:

• Molecule 5: 50S ribosomal protein L4

Chain 1F:

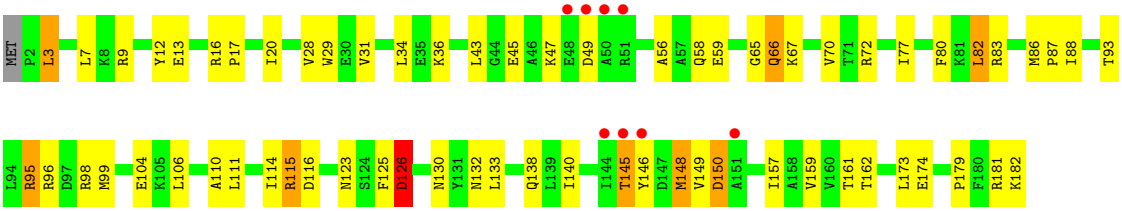


• Molecule 5: 50S ribosomal protein L4

Chain 2F:

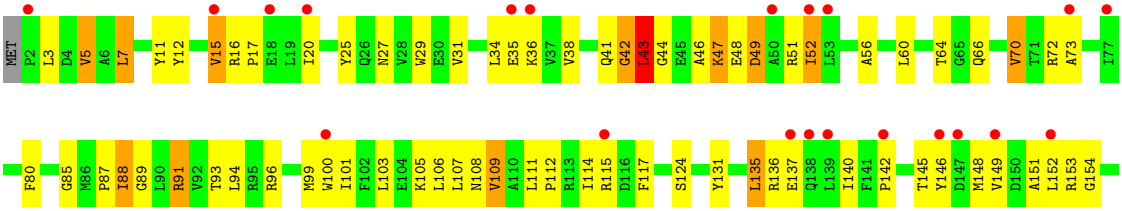
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



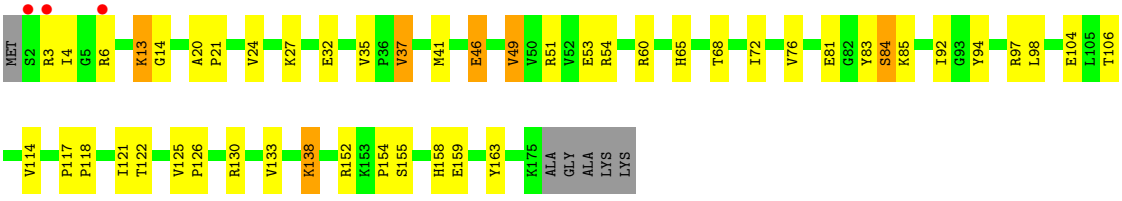
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



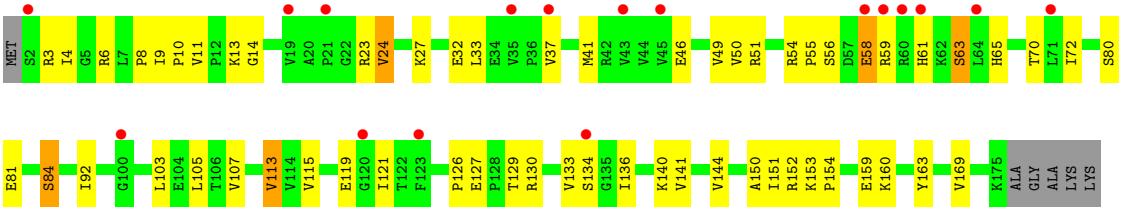
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



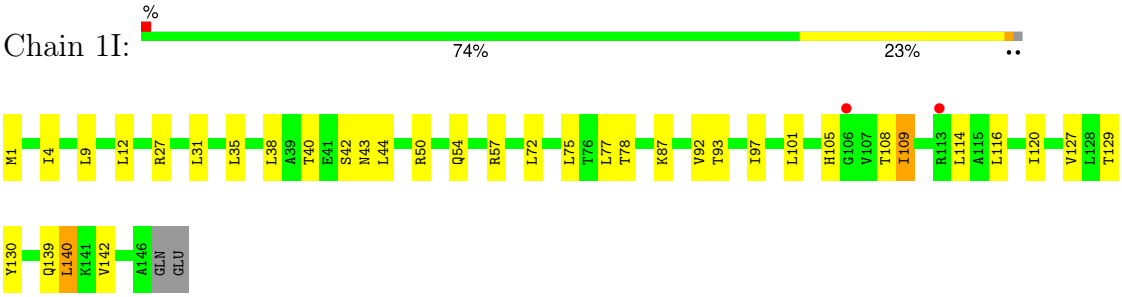
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



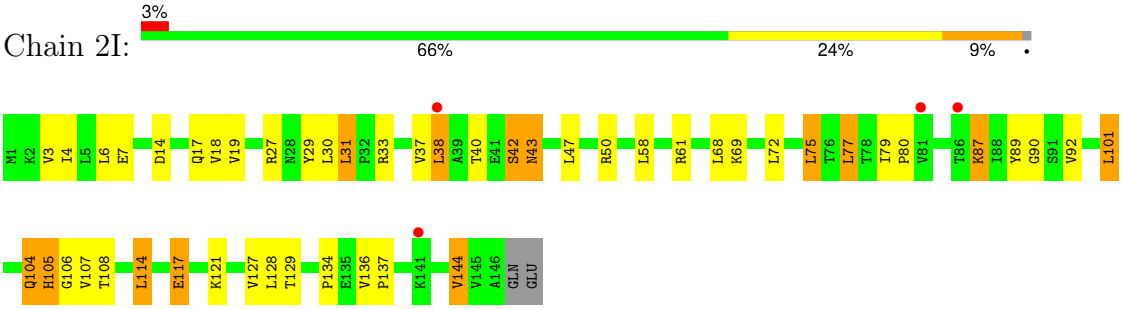
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



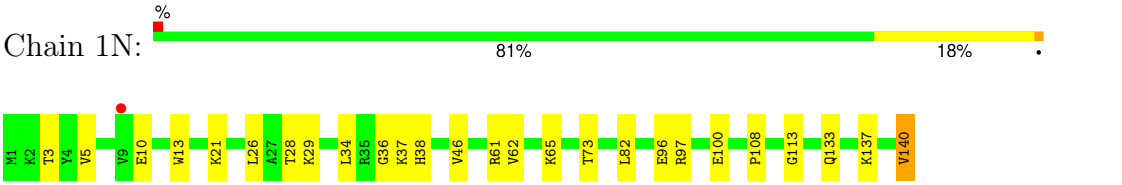
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



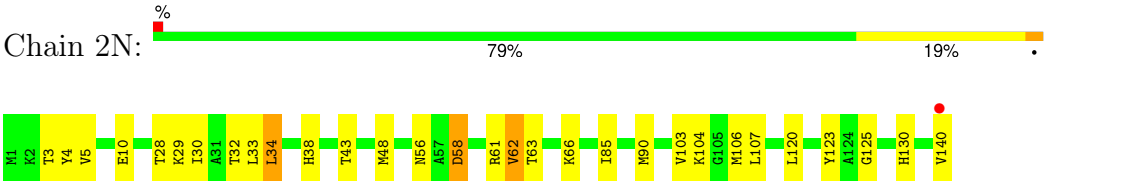
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



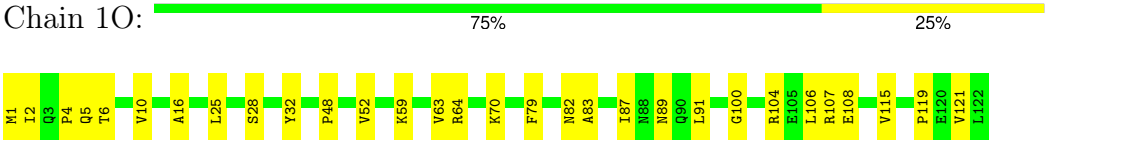
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



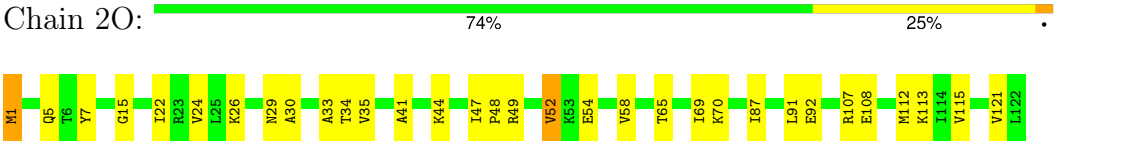
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



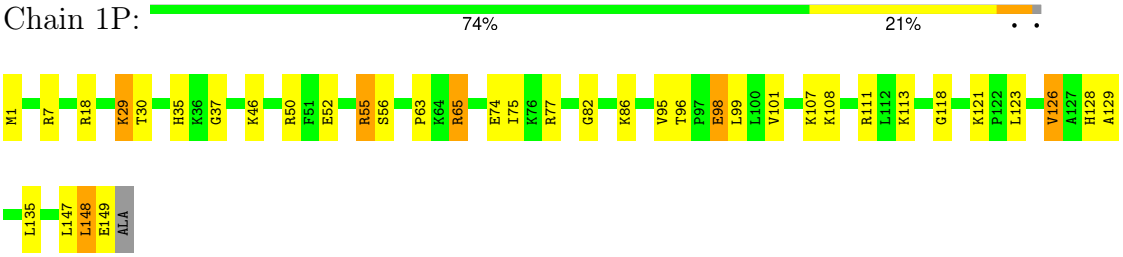
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



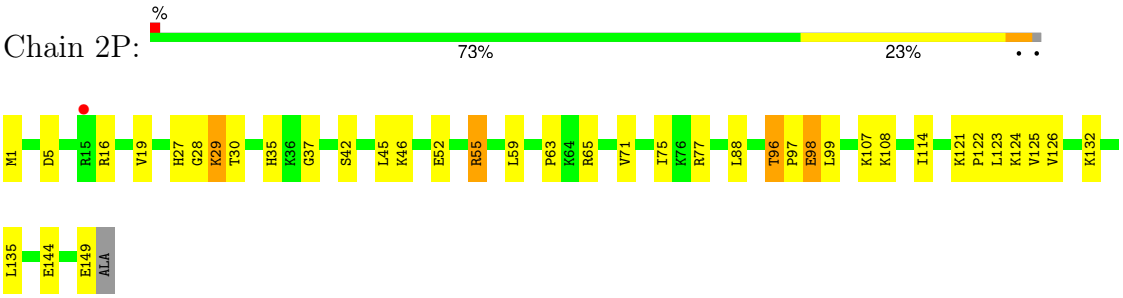
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



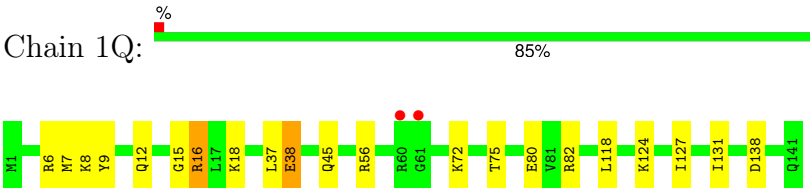
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



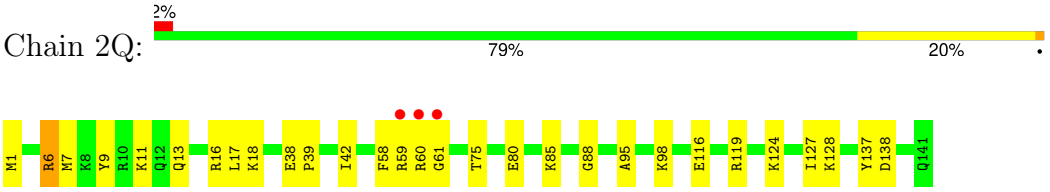
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



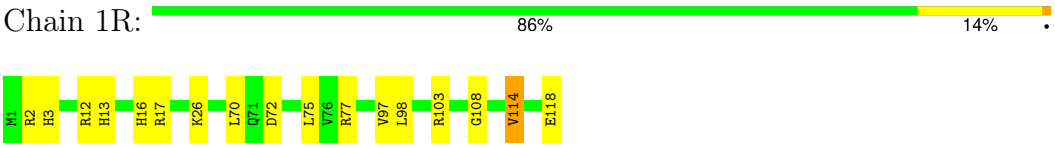
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



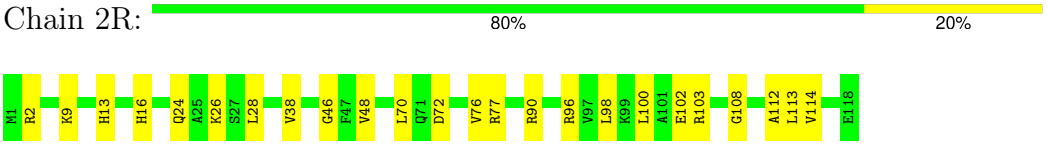
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



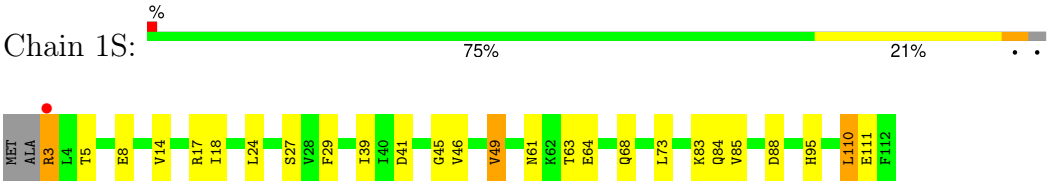
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



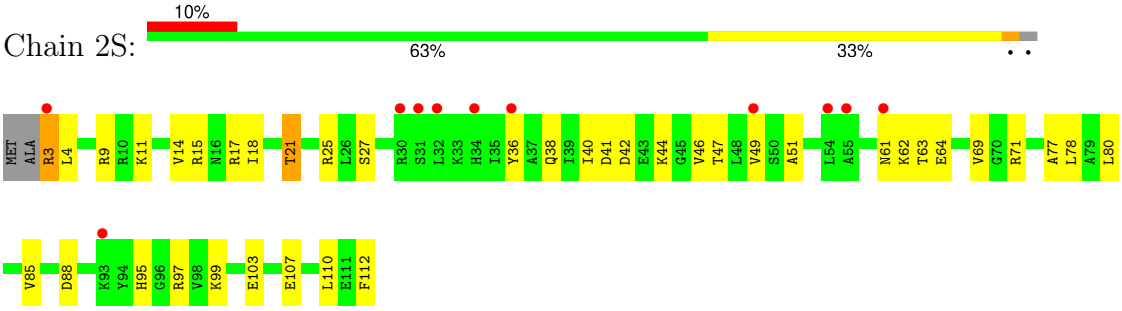
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



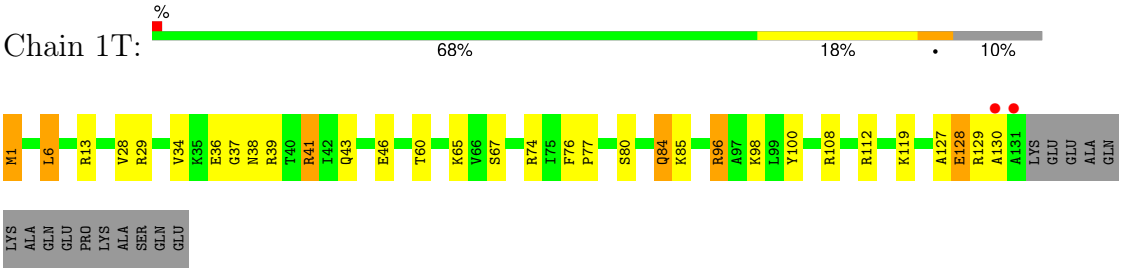
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



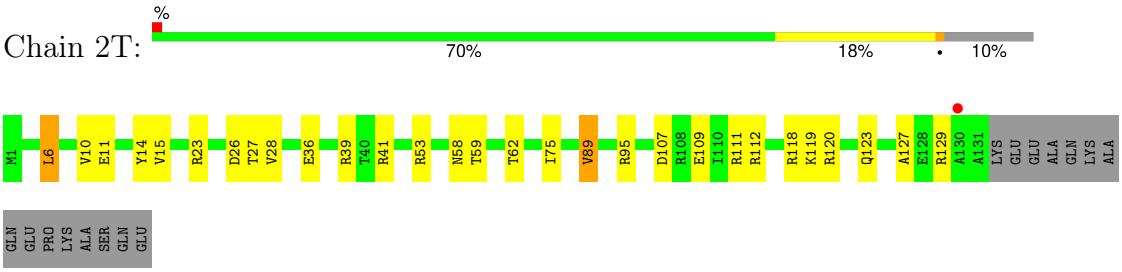
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



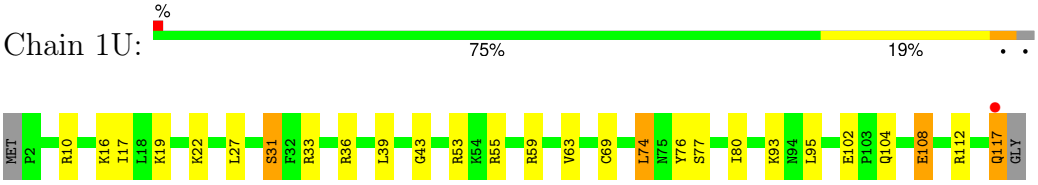
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



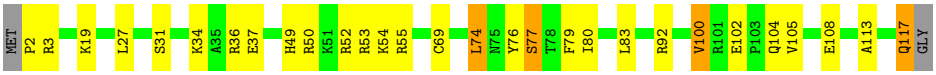
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



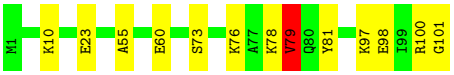
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



• Molecule 17: 50S ribosomal protein L21

Chain 1V:



• Molecule 17: 50S ribosomal protein L21

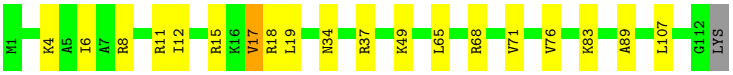
Chain 2V:

• Molecule 18: 50S ribosomal protein L22

Chain 1W:

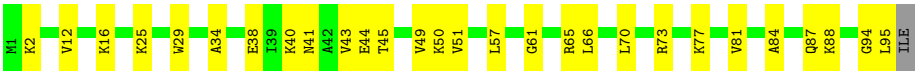
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



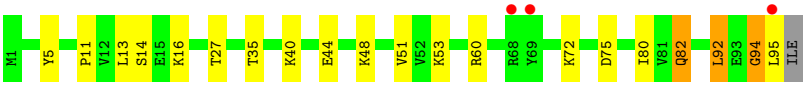
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



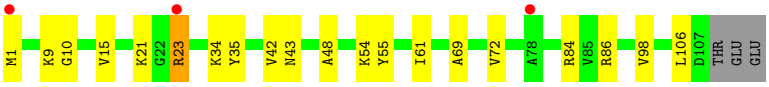
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



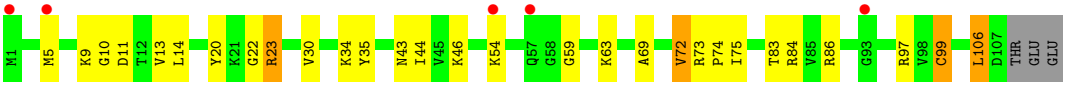
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



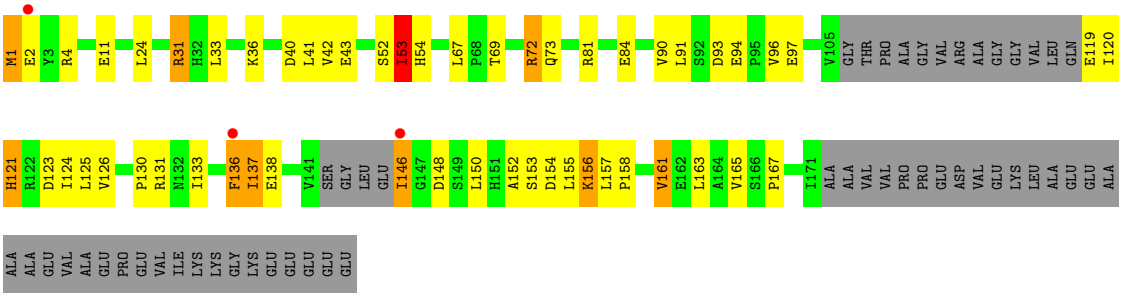
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



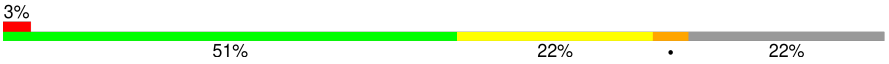
• Molecule 21: 50S ribosomal protein L25

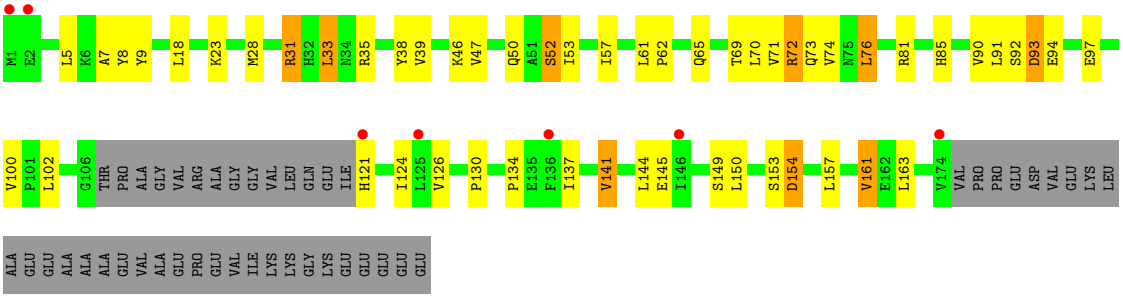
Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

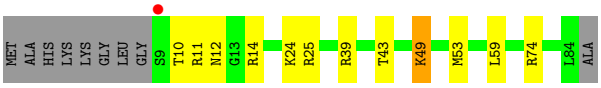
Chain 2Z:





• Molecule 22: 50S ribosomal protein L27

Chain 10:

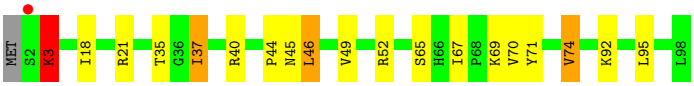


• Molecule 22: 50S ribosomal protein L27

Chain 20:

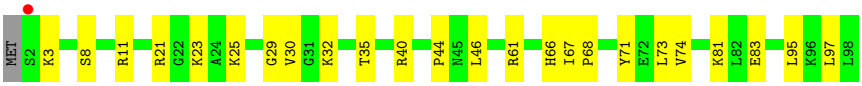
• Molecule 23: 50S ribosomal protein L28

Chain 11:



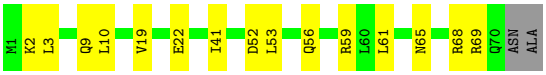
• Molecule 23: 50S ribosomal protein L28

Chain 21:



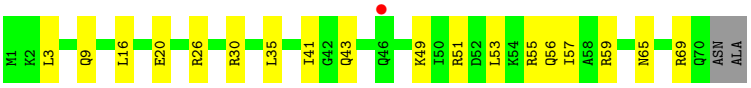
• Molecule 24: 50S ribosomal protein L29

Chain 12:



• Molecule 24: 50S ribosomal protein L29

Chain 22:

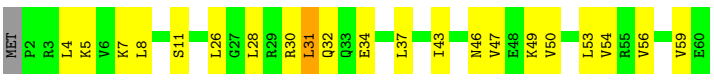


• Molecule 25: 50S ribosomal protein L30

Chain 13:

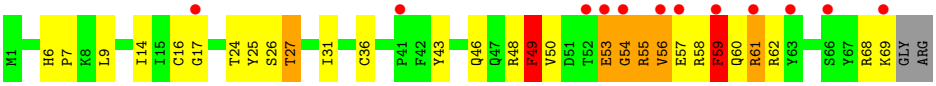
• Molecule 25: 50S ribosomal protein L30

Chain 23:

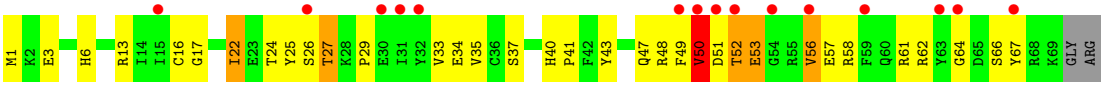


• Molecule 26: 50S ribosomal protein L31

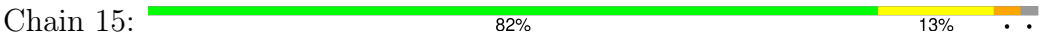
Chain 14:



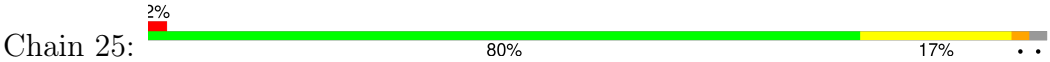
• Molecule 26: 50S ribosomal protein L31



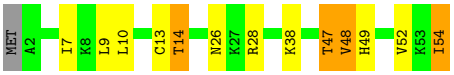
• Molecule 27: 50S ribosomal protein L32



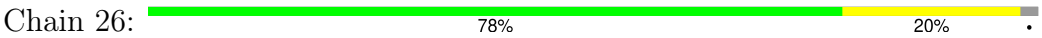
• Molecule 27: 50S ribosomal protein L32



• Molecule 28: 50S ribosomal protein L33

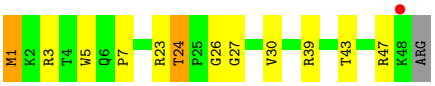


• Molecule 28: 50S ribosomal protein L33



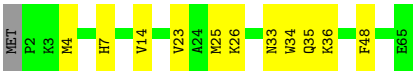
• Molecule 29: 50S ribosomal protein L34

• Molecule 29: 50S ribosomal protein L34



• Molecule 30: 50S ribosomal protein L35

Chain 18:

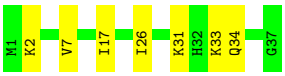


• Molecule 30: 50S ribosomal protein L35

Chain 28:

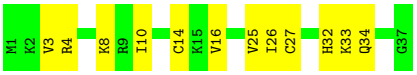
• Molecule 31: 50S ribosomal protein L36

Chain 19:



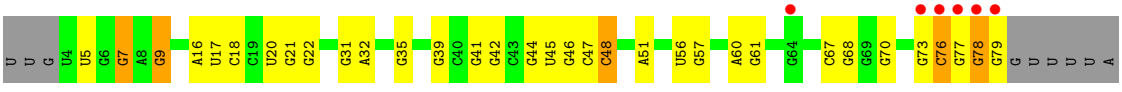
• Molecule 31: 50S ribosomal protein L36

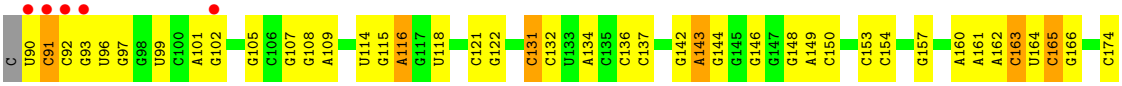
Chain 29:

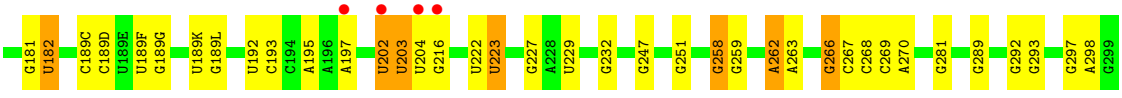


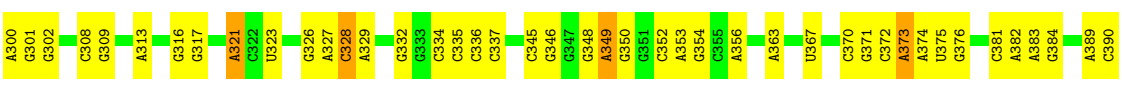
• Molecule 32: 16S Ribosomal RNA

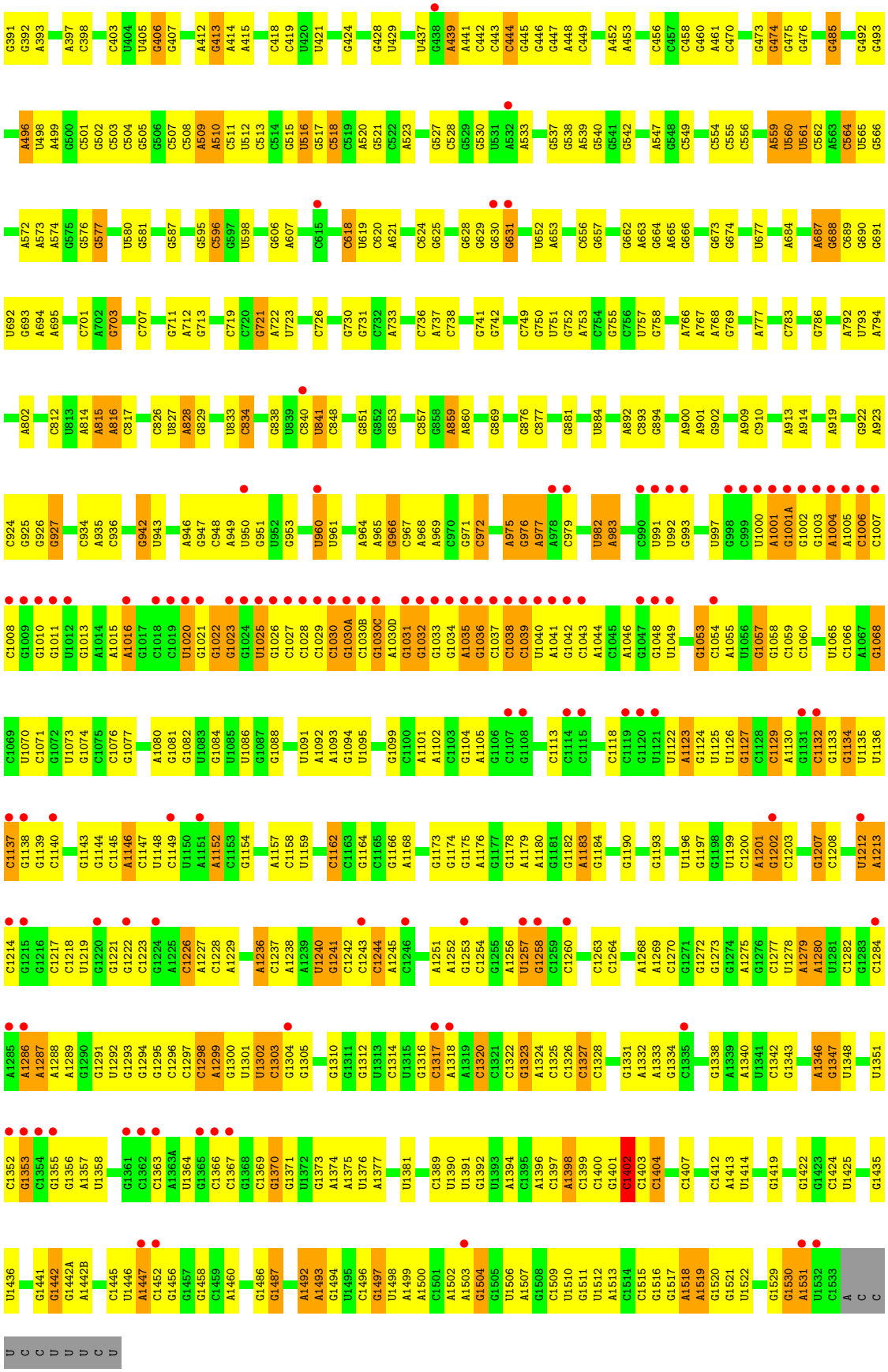
Chain 1a:





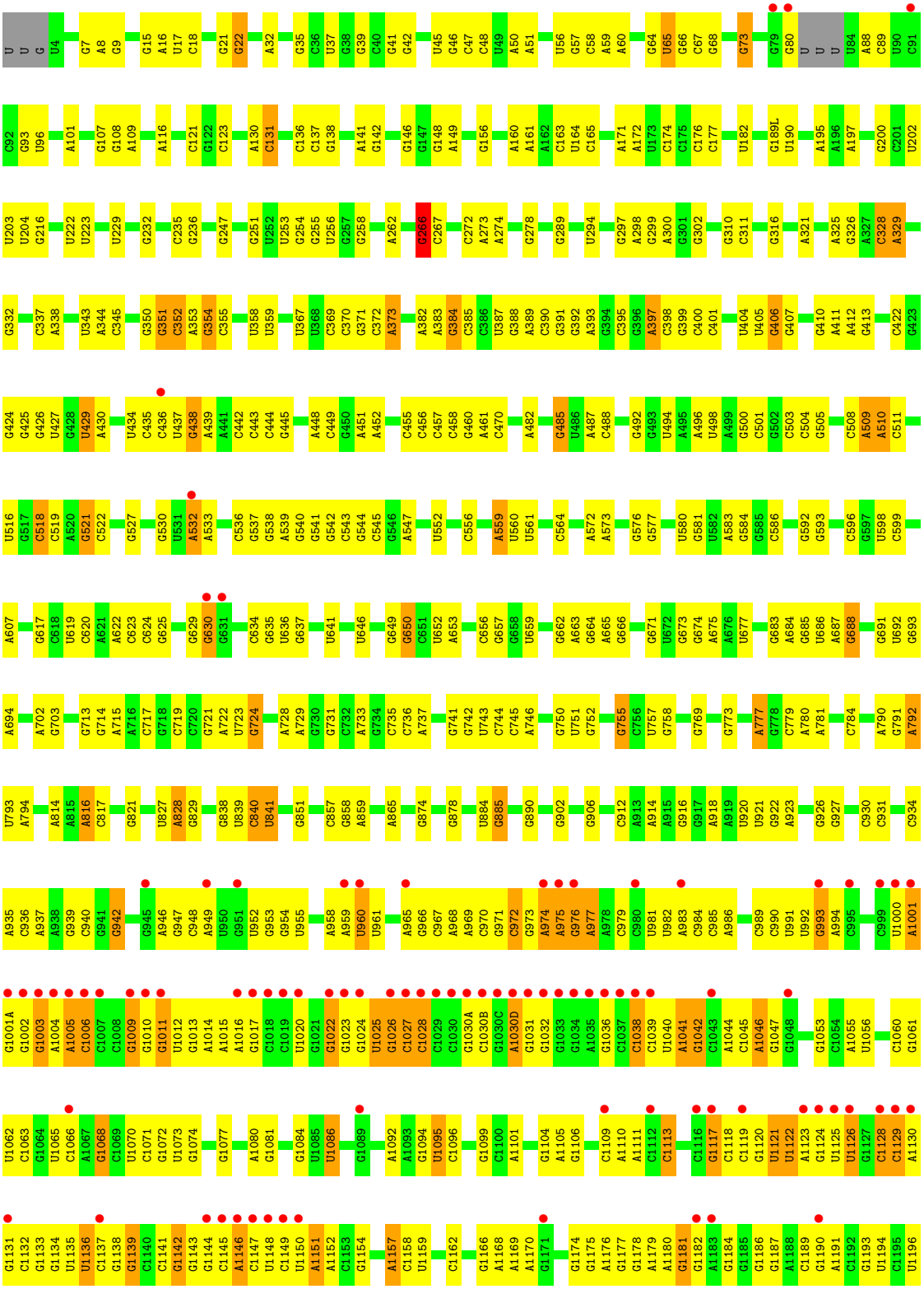


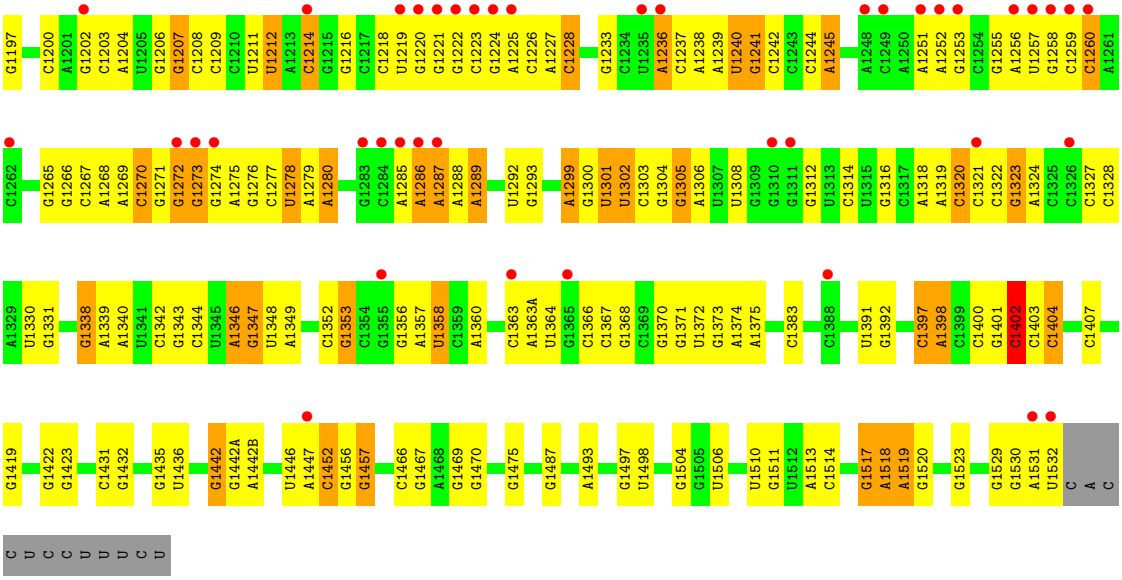



G391 G392 A393 A397 C398 C403 U404 U405 G406 G407 A412 G413 A414 A415 C418 C419 U420 U421 G424 G428 U429 U437 G438 A439 A441 C442 C443 C444 G445 G446 G447 A448 C449 A452 A453 C456 C457 C458 G460 A461 C470 G473 G474 G475 G476 G485 G492 G493
A496 U498 A499 G500 C501 G502 C503 C504 G505 G506 C507 C508 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 C519 A520 G521 C522 A523 G527 C528 G529 G530 U531 A532 A533 G537 G538 A539 G540 G541 G542 A547 G548 C549 C554 C555 C556 A559 U560 U561 C562 A563 C564 U565 G566
A572 A573 A574 G575 G576 G577 U580 G581 G587 G595 C596 G597 U598 G606 A607 C615 C618 U619 C620 A621 C624 G625 G628 G629 G630 G631 U652 A653 C656 G657 G662 A663 G664 A665 G666 G673 G674 U677 A684 A687 G688 C689 G690 G691
U692 G693 A694 A695 C701 A702 G703 C707 G711 A712 G713 C719 C720 G721 A722 U723 C726 G730 G731 C732 A733 C736 A737 C738 G741 G742 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 A766 A767 A768 G769 A777 C783 G786 A792 U793 A794
A802 C812 U813 A814 A815 A816 C817 C826 U827 A828 G829 U833 C834 G838 U839 C840 U841 C848 G851 G852 C853 C857 G858 A859 A860 G869 C876 C877 G881 U884 A892 C893 G894 A900 A901 G902 A909 C910 A913 A914 A919 G922 A923
C924 G925 G926 G927 C934 A935 C936 G942 U943 A946 G947 C948 A949 U950 G951 U952 G953 U960 U961 A964 A965 G966 C967 A968 A969 C970 G971 G972 A975 G976 A977 A978 C979 U982 A983 C990 U991 U992 G993 U997 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007
C1008 G1009 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 A1042 C1043 A1044 C1045 A1046 G1047 G1048 U1049 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 U1065 C1066 A1067 G1068
C1069 U1070 C1071 G1072 U1073 G1074 C1075 C1076 G1077 A1080 G1081 G1082 U1083 G1084 U1085 U1086 G1087 G1088 U1091 A1092 A1093 G1094 U1095 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1113 C1114 C1115 C1118 C1119 G1120 U1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136
C1137 G1138 G1139 C1140 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 A1157 C1158 U1159 C1162 C1163 G1164 C1165 G1166 A1168 G1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1190 G1193 U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 G1207 C1208 U1212 A1213
C1214 G1215 G1216 C1217 C1218 U1219 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 A1236 C1237 A1238 A1239 U1240 G1241 C1242 C1243 C1244 A1245 C1246 A1251 A1252 G1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 C1263 C1264 A1268 A1269 C1270 G1271 G1272 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284
A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 G1295 C1296 C1297 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 G1310 G1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327 C1328 G1331 A1332 A1333 G1334 C1335 G1338 A1339 A1340 U1341 C1342 G1343 A1346 G1347 U1348 U1351
C1352 G1353 C1354 G1355 G1356 A1357 U1358 G1361 C1362 C1363 A1363A U1364 G1365 C1366 C1367 G1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 U1381 C1389 U1390 U1391 G1392 U1393 A1394 C1395 A1396 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 C1407 C1412 A1413 U1414 G1419 G1422 G1423 C1424 U1425 G1435
U1436 G1441 G1442 G1442A A1442B C1445 U1446 A1447 C1452 G1456 G1457 G1458 C1459 A1460 G1486 G1487 A1492 A1493 G1494 U1495 C1496 G1497 U1498 A1499 A1500 C1501 A1502 A1503 G1504 G1505 U1506 A1507 G1508 C1509 U1510 G1511 U1512 A1513 C1514 C1515 G1516 G1517 A1518 A1519 G1520 G1521 U1522 G1529 G1530 A1531 U1532 C1533 A C C
U C C C U U U C U

• Molecule 32: 16S Ribosomal RNA

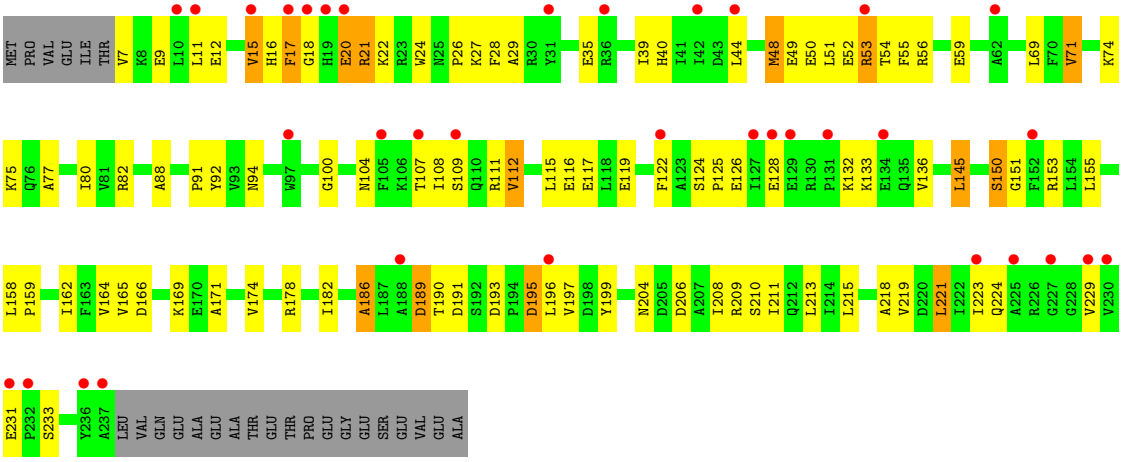
Chain 2a:





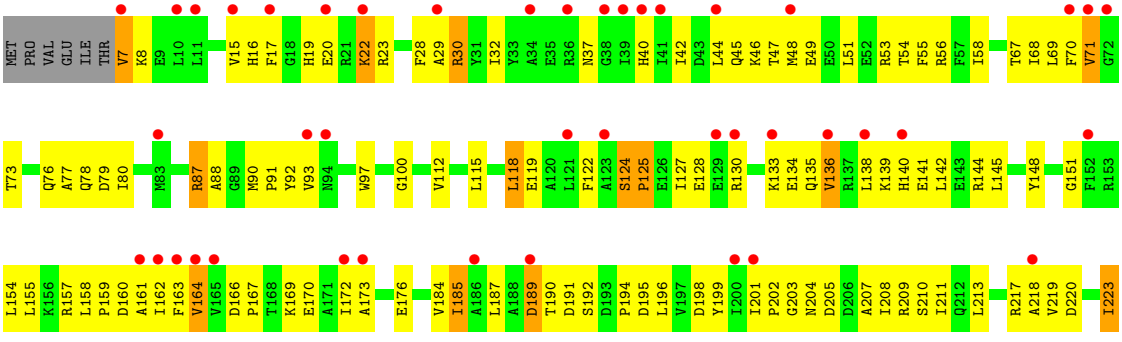
• Molecule 33: 30S ribosomal protein S2

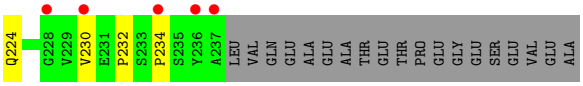
Chain 1b:



• Molecule 33: 30S ribosomal protein S2

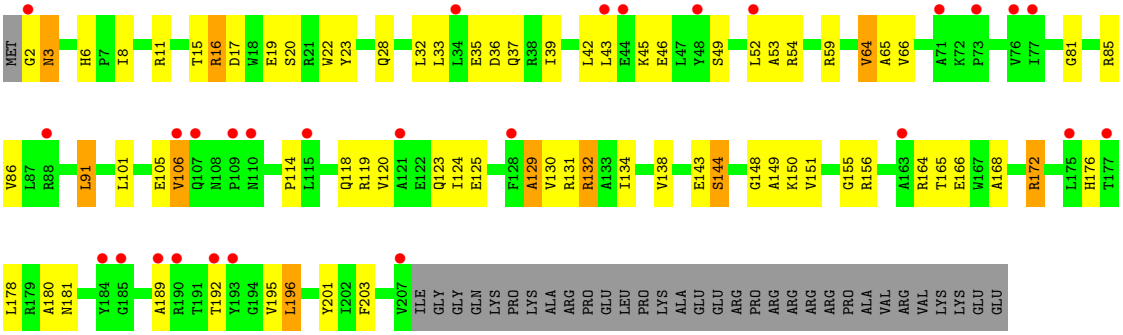
Chain 2b:





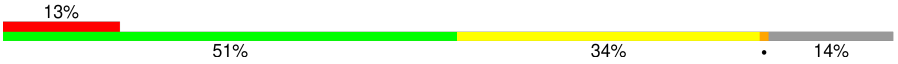
• Molecule 34: 30S ribosomal protein S3

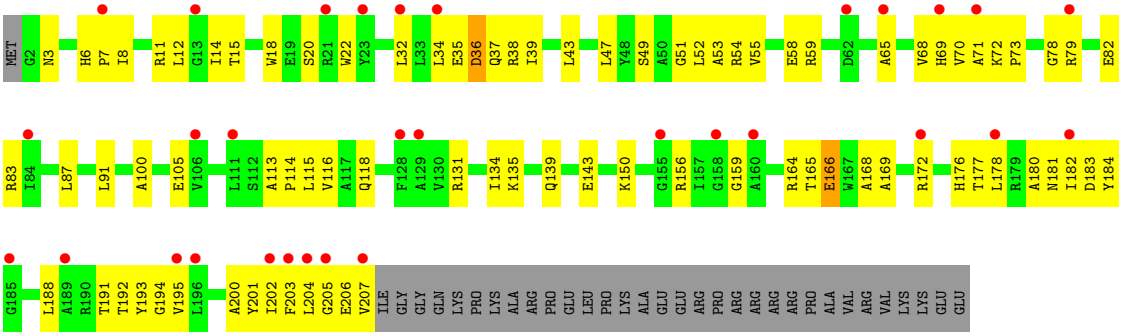
Chain 1c:



• Molecule 34: 30S ribosomal protein S3

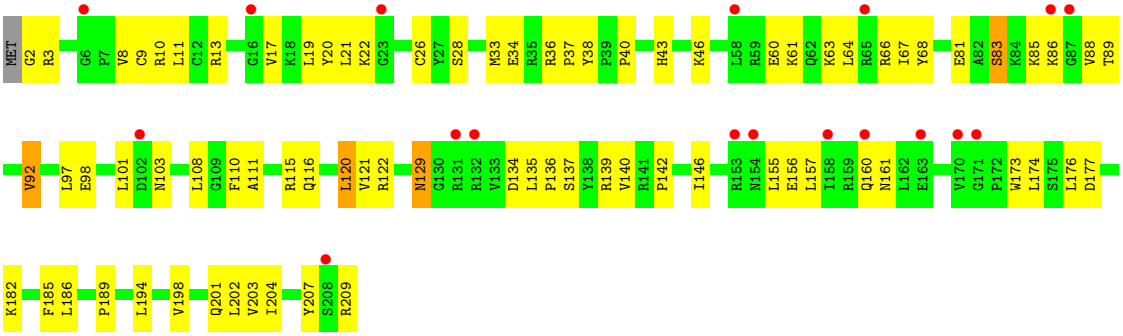
Chain 2c:





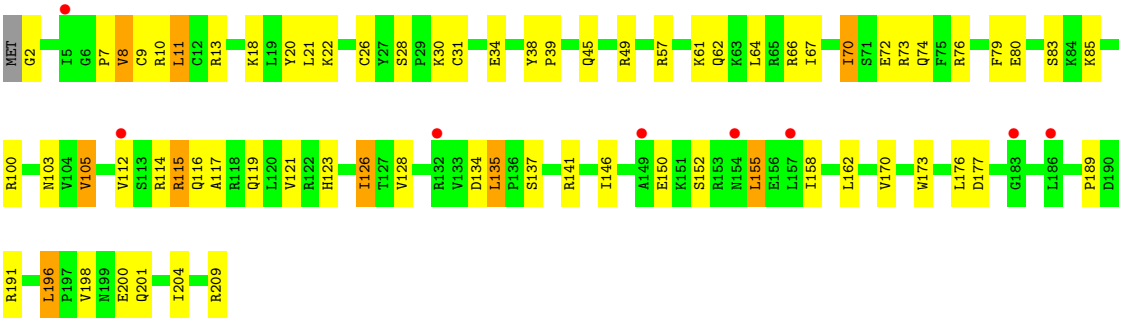
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



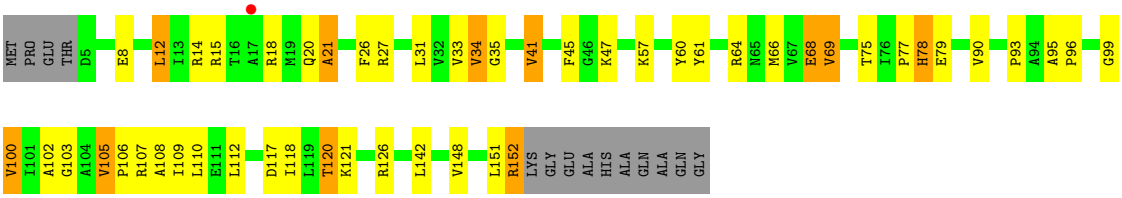
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



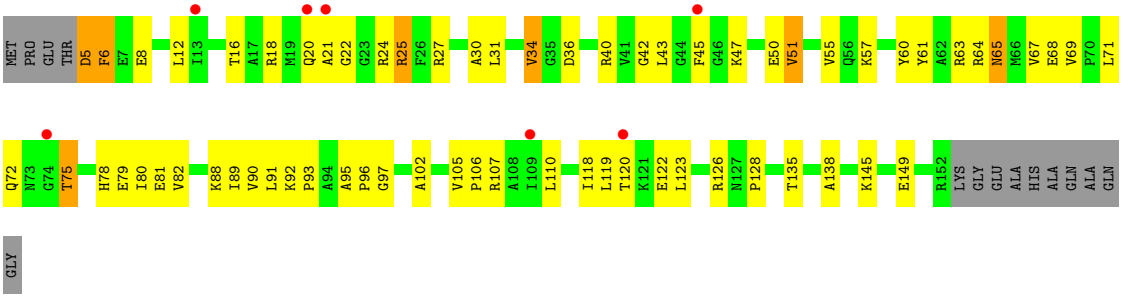
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



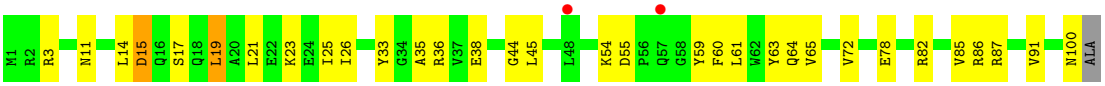
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



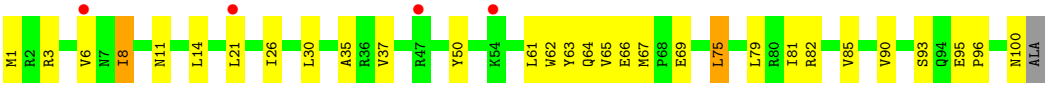
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



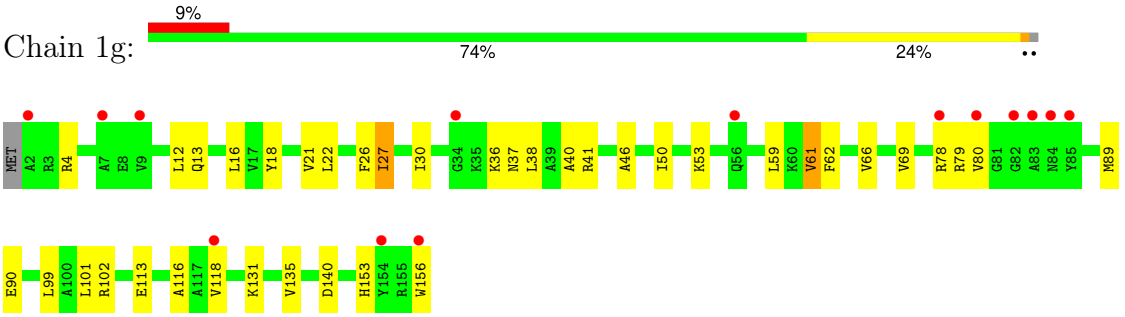
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



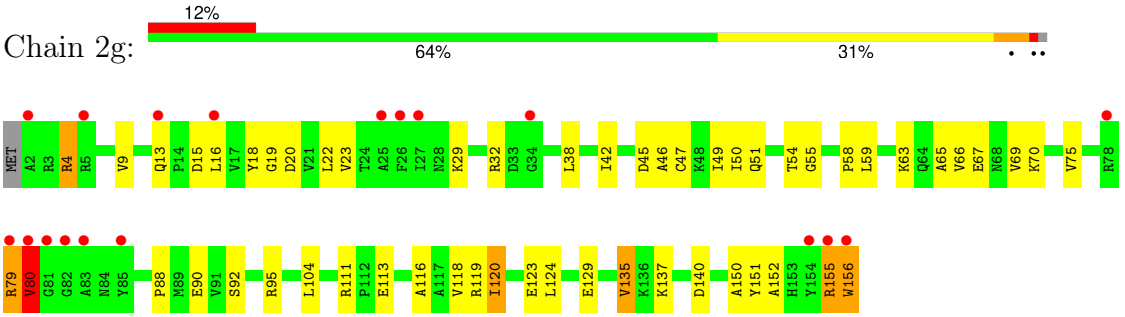
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



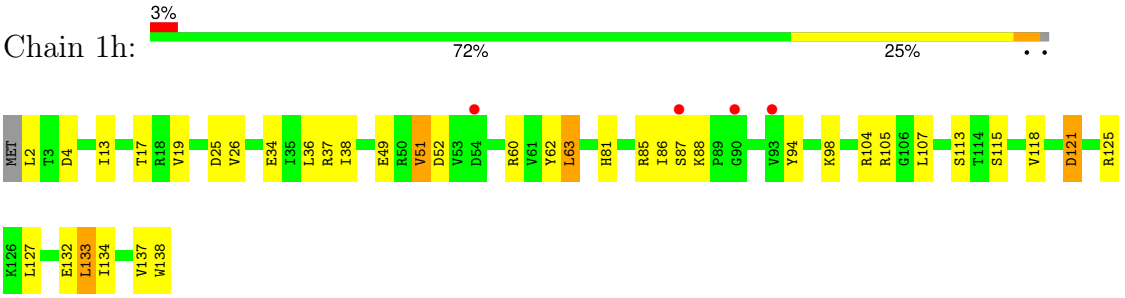
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



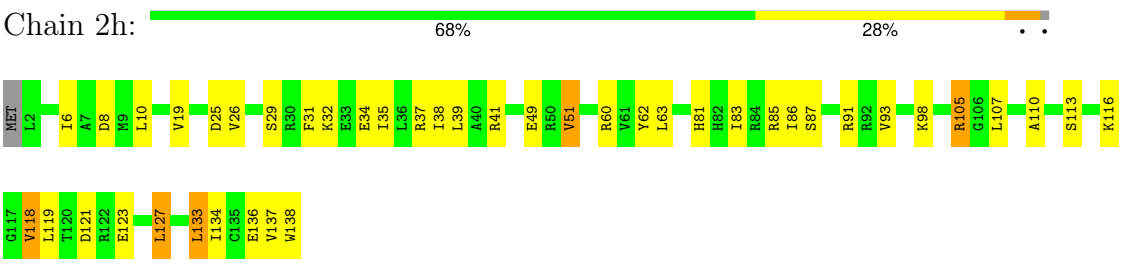
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



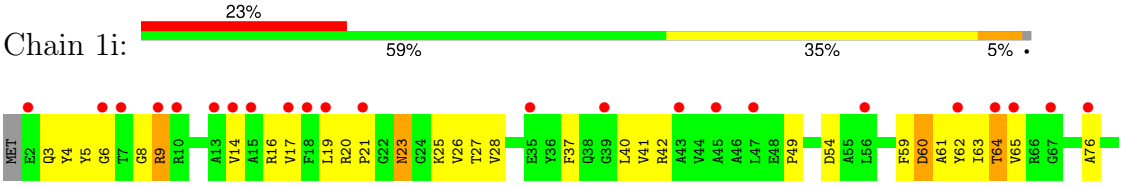
• Molecule 39: 30S ribosomal protein S8

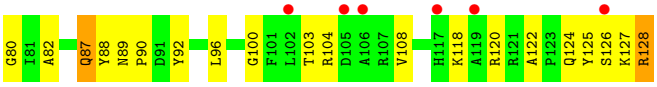
Chain 2h:



• Molecule 40: 30S ribosomal protein S9

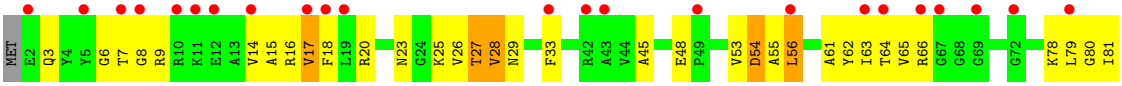
Chain 1i:

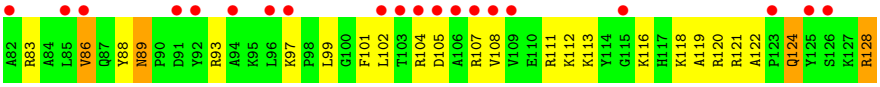




• Molecule 40: 30S ribosomal protein S9

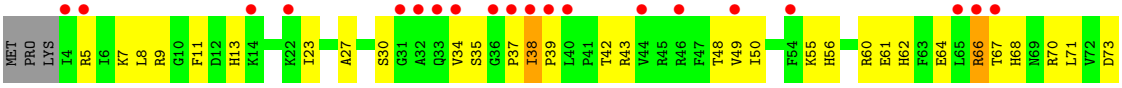
Chain 2i:

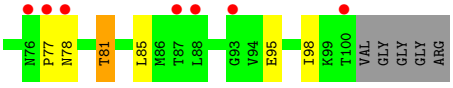




• Molecule 41: 30S ribosomal protein S10

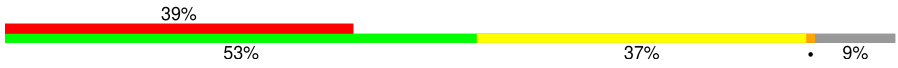
Chain 1j:

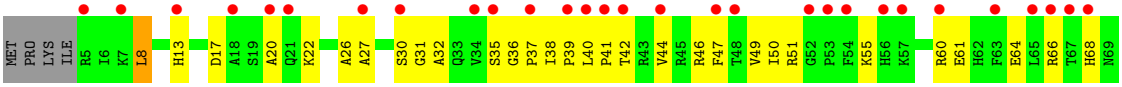


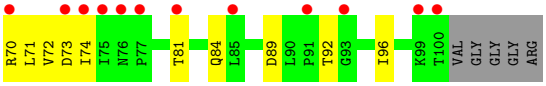


• Molecule 41: 30S ribosomal protein S10

Chain 2j:

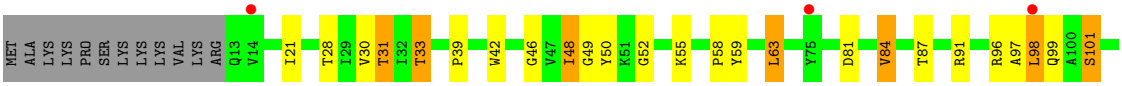


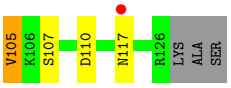




• Molecule 42: 30S ribosomal protein S11

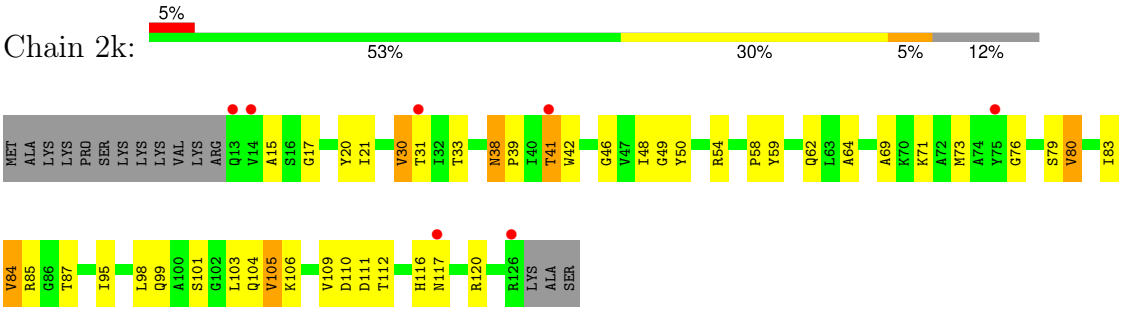
Chain 1k:





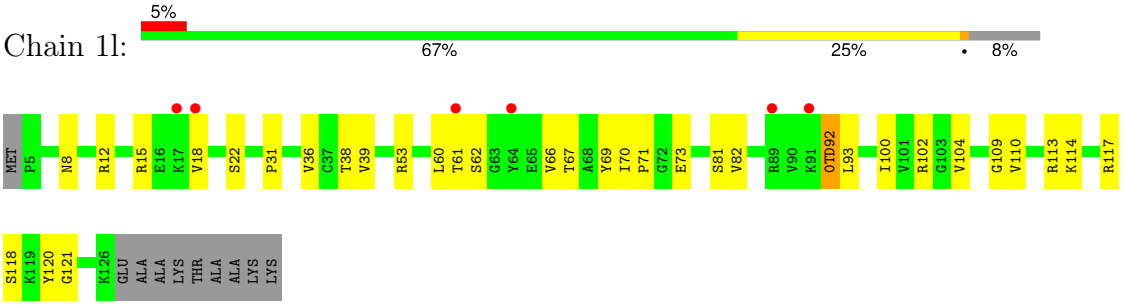
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



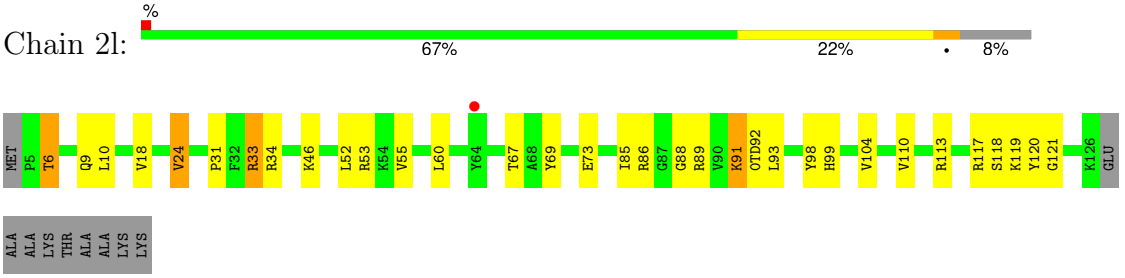
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



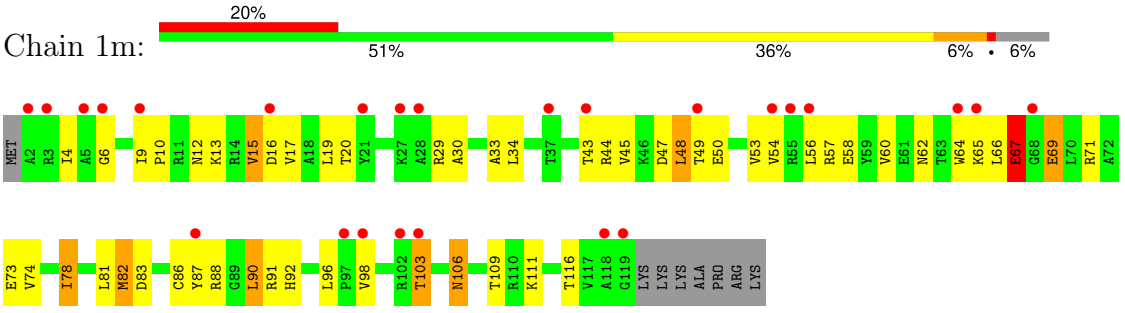
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



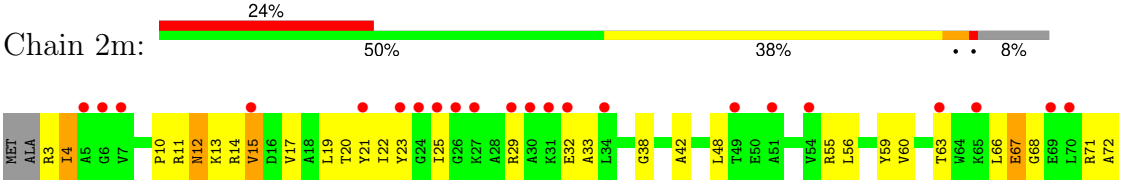
• Molecule 44: 30S ribosomal protein S13

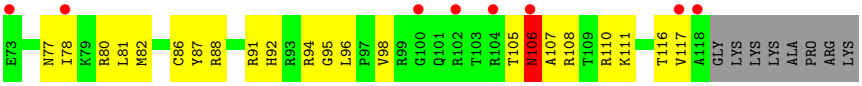
Chain 1m:



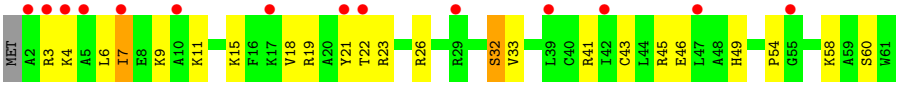
• Molecule 44: 30S ribosomal protein S13

Chain 2m:

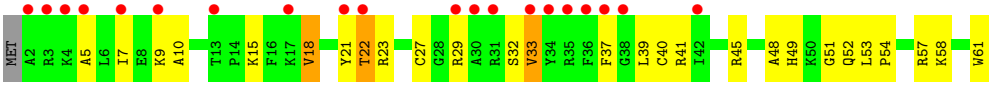




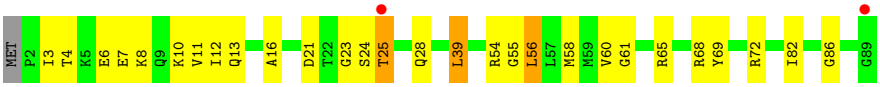
• Molecule 45: 30S ribosomal protein S14 type Z



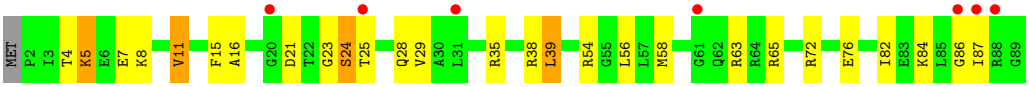
• Molecule 45: 30S ribosomal protein S14 type Z



• Molecule 46: 30S ribosomal protein S15

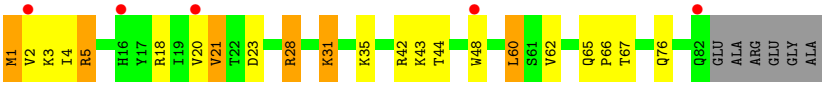


• Molecule 46: 30S ribosomal protein S15



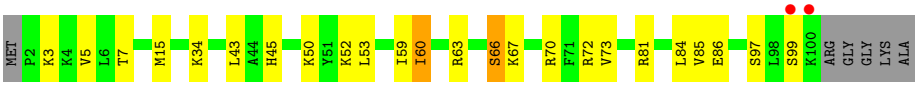
• Molecule 47: 30S ribosomal protein S16

• Molecule 47: 30S ribosomal protein S16



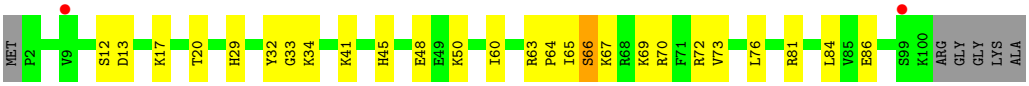
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



• Molecule 48: 30S ribosomal protein S17

Chain 2q:

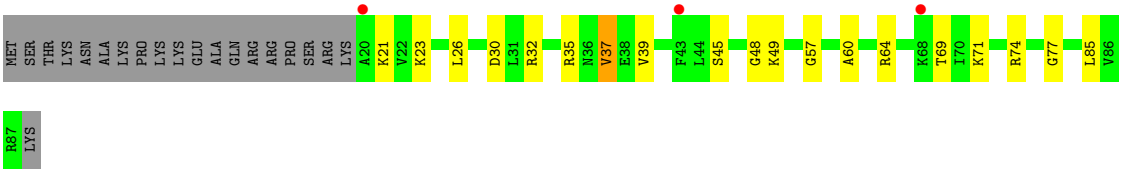


• Molecule 49: 30S ribosomal protein S18

Chain 1r:

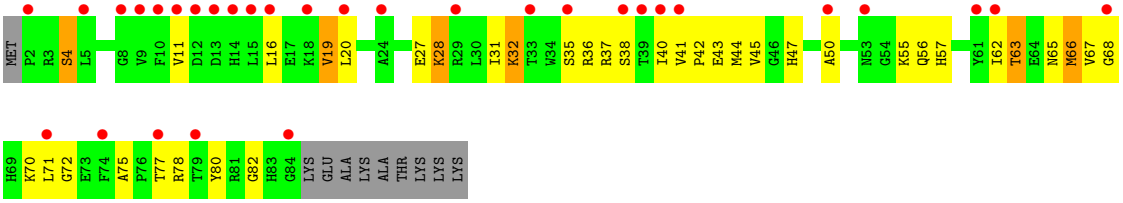
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



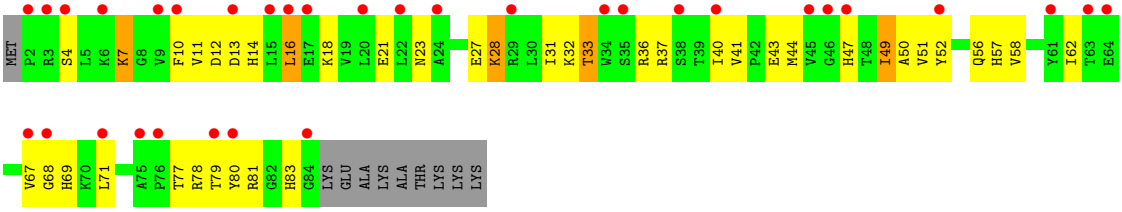
• Molecule 50: 30S ribosomal protein S19

Chain 1s:

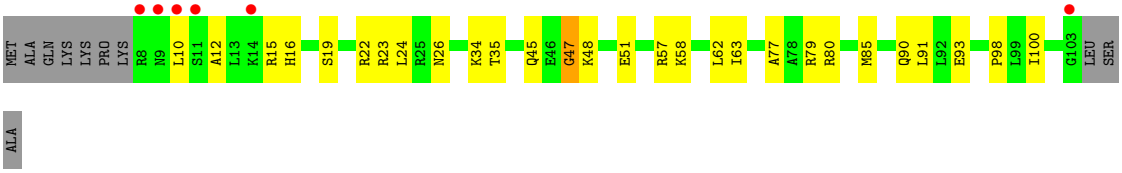


• Molecule 50: 30S ribosomal protein S19

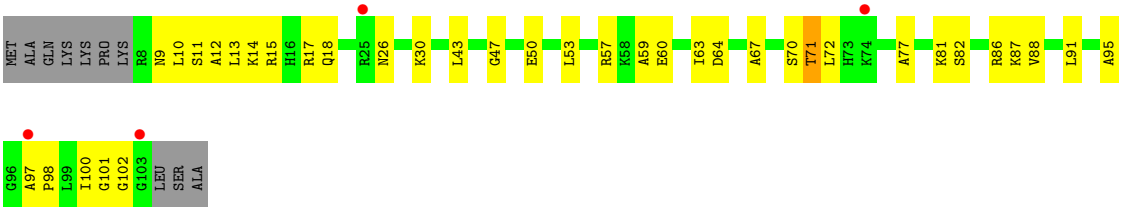
Chain 2s:



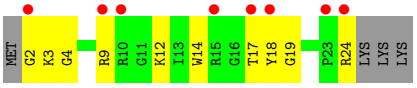
• Molecule 51: 30S ribosomal protein S20



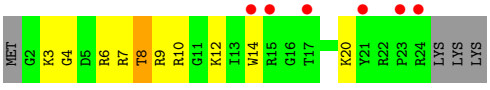
• Molecule 51: 30S ribosomal protein S20



• Molecule 52: 30S ribosomal protein Thx



• Molecule 52: 30S ribosomal protein Thx



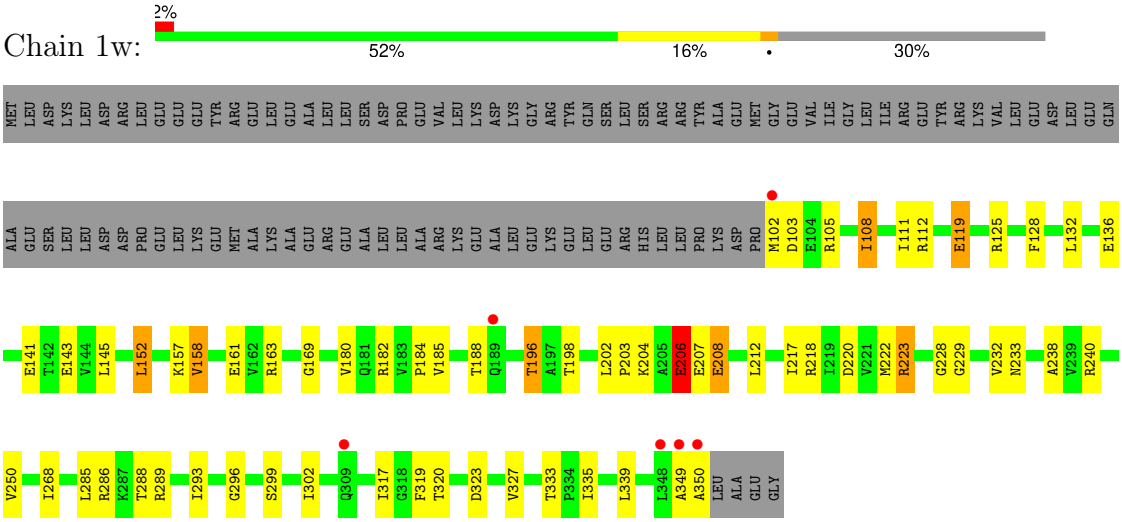
• Molecule 53: CYS-Stop mRNA

• Molecule 53: CYS-Stop mRNA

Chain 2v:

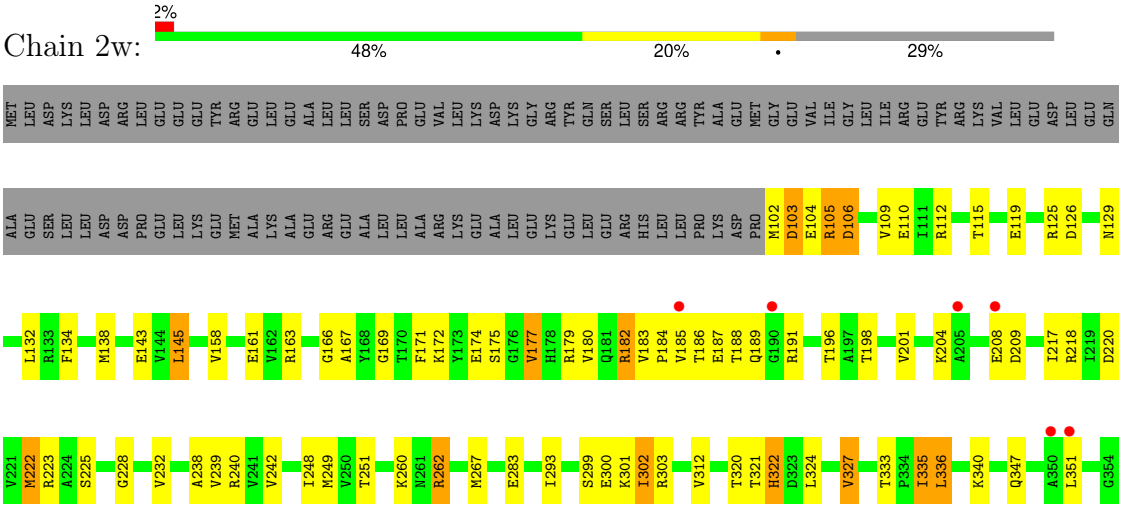
• Molecule 54: Peptide chain release factor 1

Chain 1w:



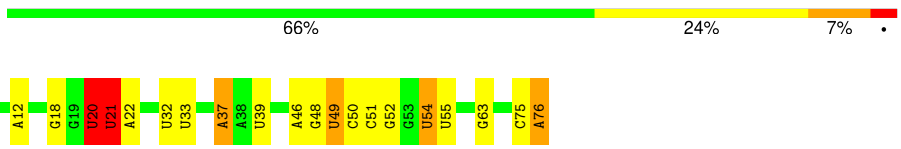
• Molecule 54: Peptide chain release factor 1

Chain 2w:



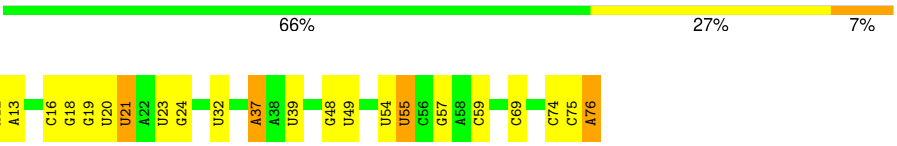
• Molecule 55: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys RNA-part

Chain 1x:



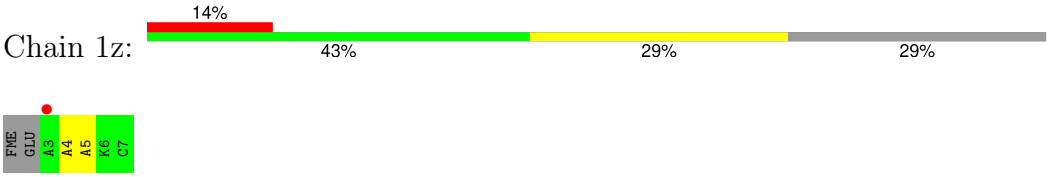
• Molecule 55: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys RNA-part

Chain 2x:



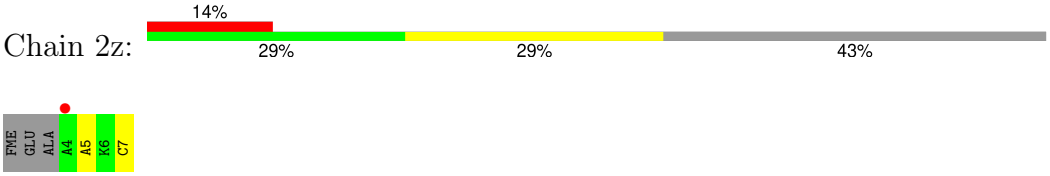
• Molecule 56: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys Peptide-part

Chain 1z:



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

Chain 2z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.01Å 450.19Å 622.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.56 – 2.80 69.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (69.56-2.80) 97.5 (69.56-2.80)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.217 , 0.264 0.216 , 0.262	Depositor DCC
R_{free} test set	71679 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	42.6	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	296656	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 4OC, M2G, 8AN, MIA, 0TD, ZN, UR3, 4SU, 5MU, OMG, SF4, MG, G7M, 2MA, 5MC, PSU, H2U, MA6, OMC, 2MG, K, OMU

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	0.29	0/69011	0.45	1/107720 (0.0%)
1	2A	0.22	0/67295	0.40	1/105042 (0.0%)
2	1B	0.22	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.33	0/4487
3	1D	0.27	0/2186	0.48	0/2944
3	2D	0.24	0/2186	0.47	0/2944
4	1E	0.27	0/1592	0.50	0/2149
4	2E	0.21	0/1592	0.45	0/2149
5	1F	0.27	0/1619	0.50	0/2193
5	2F	0.20	0/1615	0.41	0/2188
6	1G	0.21	0/1448	0.45	0/1957
6	2G	0.19	0/1453	0.42	0/1963
7	1H	0.23	0/1356	0.43	0/1834
7	2H	0.20	0/1356	0.38	0/1834
8	1I	0.21	0/1112	0.42	0/1514
8	2I	0.19	0/1079	0.43	0/1475
9	1N	0.26	0/1144	0.43	0/1543
9	2N	0.19	0/1144	0.38	0/1543
10	1O	0.26	0/943	0.47	0/1269
10	2O	0.22	0/943	0.46	0/1269
11	1P	0.28	0/1152	0.54	0/1533
11	2P	0.21	0/1152	0.44	0/1533
12	1Q	0.26	0/1143	0.48	0/1527
12	2Q	0.21	0/1143	0.42	0/1527
13	1R	0.27	0/982	0.50	0/1312
13	2R	0.21	0/982	0.46	0/1312
14	1S	0.21	0/883	0.44	0/1176
14	2S	0.21	0/880	0.44	0/1172
15	1T	0.25	0/1105	0.49	0/1477
15	2T	0.21	0/1097	0.45	0/1468
16	1U	0.30	0/977	0.48	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	0.27	0/782	0.45	0/1049
17	2V	0.18	0/782	0.38	0/1049
18	1W	0.28	0/897	0.46	0/1205
18	2W	0.23	0/897	0.43	0/1205
19	1X	0.28	0/764	0.55	0/1025
19	2X	0.22	0/764	0.50	2/1025 (0.2%)
20	1Y	0.26	0/819	0.47	0/1095
20	2Y	0.22	0/819	0.47	0/1095
21	1Z	0.22	0/1267	0.49	0/1717
21	2Z	0.22	0/1299	0.47	0/1763
22	10	0.26	0/612	0.51	0/816
22	20	0.19	0/612	0.42	0/816
23	11	0.27	0/762	0.46	0/1014
23	21	0.22	0/762	0.39	0/1014
24	12	0.25	0/590	0.42	0/781
24	22	0.18	0/590	0.37	0/781
25	13	0.28	0/474	0.48	0/635
25	23	0.18	0/469	0.41	0/630
26	14	0.23	0/565	0.61	2/761 (0.3%)
26	24	0.24	0/545	0.49	0/737
27	15	0.28	0/469	0.53	0/635
27	25	0.23	0/469	0.47	0/635
28	16	0.25	0/460	0.49	0/613
28	26	0.21	0/456	0.46	0/608
29	17	0.32	0/426	0.52	0/561
29	27	0.25	0/426	0.49	0/561
30	18	0.26	0/525	0.50	0/691
30	28	0.22	0/525	0.42	0/691
31	19	0.28	0/310	0.47	0/407
31	29	0.22	0/310	0.42	0/407
32	1a	0.21	2/35795 (0.0%)	0.39	0/55864
32	2a	0.20	1/35886 (0.0%)	0.38	2/56005 (0.0%)
33	1b	0.23	0/1881	0.51	0/2542
33	2b	0.24	0/1860	0.49	0/2518
34	1c	0.22	0/1572	0.43	0/2126
34	2c	0.20	0/1566	0.42	0/2119
35	1d	0.20	0/1685	0.43	0/2262
35	2d	0.20	0/1704	0.44	0/2284
36	1e	0.21	0/1145	0.48	0/1543
36	2e	0.22	0/1149	0.47	0/1548
37	1f	0.20	0/823	0.40	0/1115
37	2f	0.21	0/829	0.45	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.21	0/1250	0.40	0/1679
38	2g	0.20	0/1254	0.41	0/1683
39	1h	0.22	0/1108	0.42	0/1494
39	2h	0.18	0/1108	0.45	1/1494 (0.1%)
40	1i	0.21	0/1002	0.48	0/1346
40	2i	0.21	0/997	0.45	0/1343
41	1j	0.22	0/722	0.43	0/982
41	2j	0.22	0/727	0.46	0/988
42	1k	0.19	0/844	0.41	0/1145
42	2k	0.19	0/848	0.39	0/1149
43	1l	0.21	0/937	0.45	0/1260
43	2l	0.20	0/937	0.44	0/1260
44	1m	0.21	0/929	0.46	0/1250
44	2m	0.21	0/917	0.45	0/1234
45	1n	0.20	0/501	0.44	0/664
45	2n	0.21	0/501	0.42	0/664
46	1o	0.21	0/739	0.43	0/985
46	2o	0.19	0/739	0.39	0/985
47	1p	0.20	0/697	0.49	0/939
47	2p	0.19	0/693	0.41	0/935
48	1q	0.20	0/836	0.42	0/1117
48	2q	0.20	0/836	0.46	0/1117
49	1r	0.21	0/560	0.45	0/746
49	2r	0.20	0/560	0.40	0/746
50	1s	0.21	0/667	0.49	0/900
50	2s	0.21	0/661	0.45	0/893
51	1t	0.19	0/730	0.46	0/965
51	2t	0.22	0/729	0.46	0/965
52	1u	0.21	0/203	0.44	0/266
52	2u	0.20	0/203	0.48	0/266
53	1v	0.25	0/213	0.48	0/329
53	2v	0.20	0/213	0.34	0/329
54	1w	0.22	0/1963	0.42	0/2645
54	2w	0.22	0/1981	0.43	0/2668
55	1x	0.25	1/1555 (0.1%)	0.37	0/2419
55	2x	0.23	0/1555	0.36	0/2419
56	1z	0.33	0/29	0.53	0/37
56	2z	0.21	0/24	0.38	0/30
All	All	0.23	4/313618 (0.0%)	0.42	9/468557 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
21	1Z	0	2
33	1b	0	3
33	2b	0	2
56	1z	0	1
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	8	4SU	O3'-P	5.57	1.61	1.56
32	2a	527	G7M	O3'-P	5.28	1.61	1.56
32	1a	1498	UR3	O3'-P	5.16	1.61	1.56
32	1a	527	G7M	O3'-P	5.13	1.61	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1992	G	C2'-C3'-O3'	6.97	119.95	109.50
39	2h	19	VAL	N-CA-C	-6.36	106.32	112.29
1	2A	1992	G	C2'-C3'-O3'	6.34	119.00	109.50
26	14	54	GLY	CA-C-N	5.86	132.72	121.54
26	14	54	GLY	C-N-CA	5.86	132.72	121.54
32	2a	266	G	C2'-C3'-O3'	5.59	117.89	109.50
19	2X	94	GLY	CA-C-N	5.43	131.47	121.70
19	2X	94	GLY	C-N-CA	5.43	131.47	121.70
32	2a	266	G	P-O3'-C3'	5.14	127.91	120.20

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
21	1Z	136	PHE	Peptide
21	1Z	146	ILE	Peptide
33	1b	122	PHE	Peptide
33	1b	186	ALA	Peptide
33	1b	9	GLU	Peptide
56	1z	4	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
11	2P	35	HIS	Peptide
33	2b	124	SER	Peptide
33	2b	22	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	579	0
1	2A	60322	0	30427	655	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	27	0
3	1D	2136	0	2218	42	0
3	2D	2136	0	2218	49	0
4	1E	1559	0	1618	25	0
4	2E	1559	0	1618	26	0
5	1F	1584	0	1625	35	0
5	2F	1580	0	1619	45	0
6	1G	1423	0	1436	36	0
6	2G	1428	0	1438	51	0
7	1H	1330	0	1407	26	0
7	2H	1330	0	1407	37	0
8	1I	1097	0	1140	22	0
8	2I	1064	0	1082	25	0
9	1N	1117	0	1184	10	0
9	2N	1117	0	1184	15	0
10	1O	933	0	996	21	0
10	2O	933	0	996	20	0
11	1P	1135	0	1212	25	0
11	2P	1135	0	1212	26	0
12	1Q	1122	0	1179	13	0
12	2Q	1122	0	1179	16	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	15	0
14	1S	873	0	927	20	0
14	2S	870	0	923	27	0
15	1T	1091	0	1151	20	0
15	2T	1083	0	1136	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	1U	959	0	1019	20	0
16	2U	959	0	1019	22	0
17	1V	771	0	830	8	0
17	2V	771	0	830	12	0
18	1W	886	0	940	13	0
18	2W	886	0	940	10	0
19	1X	750	0	814	17	0
19	2X	750	0	814	13	0
20	1Y	806	0	881	13	0
20	2Y	806	0	881	19	0
21	1Z	1240	0	1240	30	0
21	2Z	1271	0	1273	29	0
22	10	604	0	619	11	0
22	20	604	0	619	11	0
23	11	755	0	826	16	0
23	21	755	0	826	18	0
24	12	588	0	643	6	0
24	22	588	0	643	8	0
25	13	469	0	518	3	0
25	23	464	0	514	13	0
26	14	552	0	533	22	0
26	24	532	0	503	23	0
27	15	455	0	465	9	0
27	25	455	0	465	8	0
28	16	453	0	473	6	0
28	26	449	0	469	8	0
29	17	418	0	467	12	0
29	27	418	0	467	10	0
30	18	517	0	582	8	0
30	28	517	0	582	13	0
31	19	307	0	335	4	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	444	0
32	2a	32327	0	16338	453	0
33	1b	1846	0	1867	54	0
33	2b	1825	0	1828	66	0
34	1c	1548	0	1535	44	0
34	2c	1542	0	1517	64	0
35	1d	1655	0	1672	54	0
35	2d	1674	0	1713	48	0
36	1e	1129	0	1185	38	0
36	2e	1133	0	1191	43	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	1f	810	0	804	18	0
37	2f	816	0	808	21	0
38	1g	1231	0	1238	29	0
38	2g	1235	0	1249	32	0
39	1h	1088	0	1126	21	0
39	2h	1088	0	1126	25	0
40	1i	983	0	986	38	0
40	2i	978	0	966	50	0
41	1j	709	0	650	25	0
41	2j	714	0	672	33	0
42	1k	829	0	825	15	0
42	2k	833	0	836	27	0
43	1l	932	0	981	21	0
43	2l	932	0	981	20	0
44	1m	919	0	951	34	0
44	2m	907	0	934	43	0
45	1n	492	0	529	20	0
45	2n	492	0	529	26	0
46	1o	728	0	760	16	0
46	2o	728	0	760	16	0
47	1p	681	0	697	27	0
47	2p	677	0	686	14	0
48	1q	823	0	891	8	0
48	2q	823	0	891	14	0
49	1r	555	0	618	14	0
49	2r	555	0	618	16	0
50	1s	652	0	662	27	0
50	2s	646	0	644	29	0
51	1t	728	0	798	20	0
51	2t	727	0	796	25	0
52	1u	199	0	208	6	0
52	2u	199	0	208	10	0
53	1v	191	0	97	2	0
53	2v	191	0	97	1	0
54	1w	1935	0	1920	32	0
54	2w	1953	0	1930	43	0
55	1x	1577	0	801	12	0
55	2x	1577	0	801	11	0
56	1z	30	0	32	2	0
56	2z	25	0	27	1	0
57	10	9	0	0	0	0
57	11	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	12	2	0	0	0	0
57	13	4	0	0	0	0
57	15	9	0	0	0	0
57	16	3	0	0	0	0
57	17	6	0	0	0	0
57	18	6	0	0	0	0
57	19	1	0	0	0	0
57	1A	1084	0	0	0	0
57	1B	39	0	0	0	0
57	1D	14	0	0	0	0
57	1E	13	0	0	0	0
57	1F	14	0	0	0	0
57	1G	5	0	0	0	0
57	1H	1	0	0	0	0
57	1I	1	0	0	0	0
57	1N	6	0	0	0	0
57	1O	5	0	0	0	0
57	1P	3	0	0	0	0
57	1Q	6	0	0	0	0
57	1R	5	0	0	0	0
57	1S	3	0	0	0	0
57	1T	3	0	0	0	0
57	1U	12	0	0	0	0
57	1V	8	0	0	0	0
57	1W	5	0	0	0	0
57	1X	6	0	0	0	0
57	1Y	3	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	221	0	0	0	0
57	1b	2	0	0	0	0
57	1d	1	0	0	0	0
57	1e	1	0	0	0	0
57	1f	2	0	0	0	0
57	1k	1	0	0	0	0
57	1l	1	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1p	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	2	0	0	0	0
57	1w	1	0	0	0	0
57	1x	13	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	21	2	0	0	0	0
57	23	1	0	0	0	0
57	25	4	0	0	0	0
57	26	1	0	0	0	0
57	27	3	0	0	0	0
57	28	3	0	0	0	0
57	2A	835	0	0	0	0
57	2B	18	0	0	0	0
57	2D	5	0	0	0	0
57	2E	10	0	0	0	0
57	2F	7	0	0	0	0
57	2G	1	0	0	0	0
57	2O	3	0	0	0	0
57	2P	1	0	0	0	0
57	2Q	4	0	0	0	0
57	2R	1	0	0	0	0
57	2T	4	0	0	0	0
57	2U	4	0	0	0	0
57	2V	2	0	0	0	0
57	2W	3	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	178	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2g	1	0	0	0	0
57	2i	1	0	0	0	0
57	2j	2	0	0	0	0
57	2k	1	0	0	0	0
57	2l	2	0	0	0	0
57	2q	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2x	8	0	0	0	0
58	1A	1	0	0	0	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	9	0	0	0	0
61	11	8	0	0	0	0
61	12	3	0	0	0	0
61	13	4	0	0	0	0
61	15	7	0	0	0	0
61	16	1	0	0	0	0
61	17	8	0	0	1	0
61	18	12	0	0	0	0
61	1A	1897	0	0	67	0
61	1B	61	0	0	2	0
61	1D	30	0	0	1	0
61	1E	27	0	0	3	0
61	1F	18	0	0	1	0
61	1G	5	0	0	3	0
61	1H	2	0	0	0	0
61	1I	1	0	0	0	0
61	1N	8	0	0	0	0
61	1O	6	0	0	0	0
61	1P	23	0	0	0	0
61	1Q	11	0	0	1	0
61	1R	11	0	0	2	0
61	1S	1	0	0	0	0
61	1T	7	0	0	1	0
61	1U	13	0	0	0	0
61	1V	6	0	0	0	0
61	1W	12	0	0	1	0
61	1X	10	0	0	0	0
61	1Y	2	0	0	0	0
61	1a	259	0	0	18	0
61	1b	1	0	0	0	0
61	1d	1	0	0	0	0
61	1f	1	0	0	0	0
61	1j	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1l	2	0	0	0	0
61	1n	1	0	0	0	0
61	1q	4	0	0	0	0
61	1u	1	0	0	0	0
61	1v	3	0	0	0	0
61	1w	3	0	0	0	0
61	1x	25	0	0	3	0
61	20	2	0	0	0	0
61	21	10	0	0	1	0
61	25	3	0	0	0	0
61	27	2	0	0	0	0
61	28	4	0	0	0	0
61	29	1	0	0	0	0
61	2A	1003	0	0	73	0
61	2B	14	0	0	0	0
61	2D	25	0	0	1	0
61	2E	14	0	0	0	0
61	2F	12	0	0	0	0
61	2N	1	0	0	0	0
61	2O	3	0	0	1	0
61	2P	7	0	0	0	0
61	2Q	3	0	0	0	0
61	2R	4	0	0	1	0
61	2T	5	0	0	0	0
61	2U	3	0	0	0	0
61	2V	1	0	0	0	0
61	2W	1	0	0	0	0
61	2X	2	0	0	0	0
61	2a	130	0	0	5	0
61	2e	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	2	0	0	0	0
61	2l	4	0	0	1	0
61	2n	1	0	0	0	0
61	2q	2	0	0	0	0
61	2t	2	0	0	0	0
61	2v	1	0	0	0	0
61	2w	1	0	0	0	0
61	2x	14	0	0	2	0
All	All	296656	0	197040	3915	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 (3915) 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)
1:2A:2129:C:N4	1:2A:2159:G:H1	1.55	1.03
32:1a:1035:A:H2'	32:1a:1036:G:H21	1.24	1.02
1:1A:1082:U:C4	1:1A:1086:A:N1	2.34	0.96
41:2j:30:SER:HB3	41:2j:81:THR:HB	1.46	0.95
1:2A:784:A:OP2	61:2A:3903:HOH:O	1.83	0.94
1:1A:1056:G:H4'	1:1A:1086:A:H8	1.31	0.94
1:1A:1082:U:O4	1:1A:1086:A:N1	2.01	0.93
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.49	0.92
32:2a:664:G:H22	32:2a:741:G:H1	1.18	0.91
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.36	0.91
1:2A:1689:A:H62	1:2A:1698:A:H2	1.16	0.90
1:2A:2589:A:OP1	61:2A:3903:HOH:O	1.91	0.89
15:1T:41:ARG:NH2	32:1a:346:G:OP1	2.07	0.87
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.54	0.86
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.08	0.86
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.56	0.86
1:1A:1332:G:OP1	61:1A:4103:HOH:O	1.93	0.85
1:2A:783:A:OP2	61:2A:3903:HOH:O	1.92	0.85
34:2c:78:GLY:HA3	34:2c:83:ARG:H	1.43	0.84
32:1a:975:A:H4'	32:1a:976:G:H5"	1.58	0.84
29:17:24:THR:HG22	29:17:27:GLY:H	1.43	0.83
1:1A:762:U:OP1	61:1A:4104:HOH:O	1.96	0.83
14:1S:61:ASN:HD22	14:1S:64:GLU:H	1.26	0.82
7:2H:27:LYS:HG2	7:2H:32:GLU:HB3	1.61	0.82
34:2c:34:LEU:HD11	34:2c:38:ARG:HH21	1.44	0.82
22:20:11:ARG:O	22:20:14:ARG:NH2	2.13	0.82
32:2a:677:U:H3	32:2a:713:G:H22	1.26	0.82
32:2a:975:A:H4'	32:2a:976:G:H5"	1.62	0.82
1:1A:2427:C:OP1	61:1A:4105:HOH:O	1.98	0.82
32:1a:964:A:OP1	61:1a:3801:HOH:O	1.98	0.81
1:2A:2129:C:H42	1:2A:2159:G:H1	0.84	0.81
1:2A:2129:C:N3	1:2A:2159:G:N2	2.28	0.81
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.26	0.81
1:1A:1056:G:H4'	1:1A:1086:A:C8	2.16	0.80
1:2A:1031:G:H5"	31:29:8:LYS:HE3	1.63	0.80
1:2A:1271:G:OP2	61:2A:3904:HOH:O	1.99	0.80
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.30	0.80
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.14	0.80
4:1E:127:ASP:OD2	61:1E:401:HOH:O	1.99	0.80
1:1A:833:U:O2	11:1P:55:ARG:NH2	2.15	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:504:C:OP1	61:2a:1801:HOH:O	2.00	0.80
41:2j:38:ILE:HD11	41:2j:71:LEU:HD23	1.65	0.79
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.64	0.79
32:2a:953:G:H5'	32:2a:965:A:H61	1.46	0.79
15:1T:77:PRO:HG2	15:1T:80:SER:HB2	1.63	0.79
5:2F:70:THR:HG22	5:2F:72:ARG:H	1.48	0.79
34:2c:79:ARG:H	34:2c:82:GLU:HB3	1.47	0.79
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.16	0.79
1:2A:1604:C:OP2	61:2A:3907:HOH:O	2.01	0.78
1:1A:1865:G:OP1	61:1A:4106:HOH:O	2.00	0.78
1:2A:752:A:H3'	29:27:1:MET:HE1	1.63	0.78
1:2A:2822:G:OP2	61:2A:3905:HOH:O	2.00	0.78
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.46	0.78
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.66	0.78
1:1A:2022:U:OP1	61:1A:4107:HOH:O	2.02	0.78
26:24:61:ARG:HH12	50:2s:41:VAL:HG12	1.49	0.78
1:2A:1253:A:OP1	61:2A:3906:HOH:O	2.00	0.78
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.65	0.78
1:2A:962:G:OP1	61:2A:3908:HOH:O	2.02	0.78
1:1A:2181:G:H2'	1:1A:2182:G:C8	2.20	0.77
34:1c:35:GLU:OE2	34:1c:59:ARG:NH2	2.18	0.77
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.48	0.77
50:1s:63:THR:H	50:1s:66:MET:HE3	1.48	0.77
32:1a:1401:G:OP1	61:1a:3802:HOH:O	2.03	0.77
1:2A:948:G:OP1	61:2A:3908:HOH:O	2.01	0.77
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.18	0.77
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.18	0.77
1:2A:981:A:OP1	61:2A:3910:HOH:O	2.03	0.77
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.18	0.76
34:2c:32:LEU:HD23	34:2c:59:ARG:HE	1.50	0.76
32:2a:1375:A:H4'	38:2g:29:LYS:HE3	1.67	0.76
1:1A:1082:U:H3	1:1A:1086:A:H61	1.30	0.76
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.18	0.76
1:2A:2807:G:N1	1:2A:2893:G:O6	2.17	0.76
1:2A:2708:G:O6	61:2A:3909:HOH:O	2.02	0.76
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.68	0.76
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.66	0.76
32:1a:1441:G:H5"	32:1a:1442:G:H5'	1.66	0.76
39:1h:17:THR:HG22	39:1h:63:LEU:HG	1.68	0.76
1:1A:1054:A:H61	1:1A:1105:U:H3	1.34	0.75
33:1b:55:PHE:HE1	33:1b:218:ALA:HA	1.52	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:570:G:O6	61:2A:3911:HOH:O	2.04	0.75
32:2a:773:G:N7	61:2a:1805:HOH:O	2.19	0.75
1:2A:468:G:O2'	5:2F:62:ARG:NH2	2.20	0.75
1:2A:2116:G:N7	1:2A:2166:G:N2	2.33	0.75
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.51	0.75
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.69	0.75
29:27:24:THR:HG22	29:27:27:GLY:H	1.51	0.75
50:2s:18:LYS:HA	50:2s:21:GLU:HB2	1.66	0.75
32:2a:1126:U:H3	41:2j:40:LEU:HD11	1.49	0.75
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.20	0.75
1:1A:2185:C:H2'	1:1A:2186:G:H8	1.52	0.75
36:1e:12:LEU:HD11	36:1e:14:ARG:HB3	1.69	0.75
21:1Z:93:ASP:HB2	21:1Z:131:ARG:HH22	1.50	0.74
32:1a:664:G:H22	32:1a:741:G:H1	1.34	0.74
5:1F:89:VAL:O	61:1F:401:HOH:O	2.04	0.74
39:1h:113:SER:HB2	39:1h:134:ILE:HD11	1.70	0.74
1:2A:1670:C:OP1	61:2A:3912:HOH:O	2.05	0.74
50:2s:27:GLU:HB3	50:2s:28:LYS:HB3	1.67	0.74
32:1a:1086:U:H3	32:1a:1099:G:H22	1.34	0.74
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.67	0.74
44:2m:78:ILE:HA	44:2m:81:LEU:HD12	1.69	0.74
35:1d:122:ARG:NH1	35:1d:134:ASP:O	2.21	0.74
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.70	0.74
38:2g:113:GLU:HB2	38:2g:119:ARG:HG2	1.68	0.74
1:2A:2028:U:O4	61:2A:3914:HOH:O	2.06	0.74
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	1.70	0.74
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.52	0.74
34:2c:70:VAL:HG12	34:2c:72:LYS:H	1.51	0.74
1:2A:1022:G:N2	1:2A:1023:U:O4	2.21	0.73
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.53	0.73
2:1B:66:A:H61	2:1B:109:C:H5'	1.52	0.73
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.21	0.73
32:2a:972:C:OP1	61:2a:1802:HOH:O	2.06	0.73
1:1A:1056:G:H5"	1:1A:1057:A:O4'	1.86	0.73
1:1A:2819:G:OP1	61:1A:4110:HOH:O	2.06	0.73
54:1w:119:GLU:HG3	54:1w:184:PRO:HB3	1.70	0.73
32:2a:959:A:HO2'	32:2a:984:C:HO2'	1.33	0.73
1:1A:1648:C:OP1	61:1A:4112:HOH:O	2.07	0.73
32:2a:542:G:OP1	35:2d:10:ARG:NH2	2.21	0.73
1:1A:2350:C:OP2	61:1A:4109:HOH:O	2.06	0.73
32:1a:508:C:OP1	35:1d:209:ARG:NH2	2.22	0.73

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	2.17	0.73
42:2k:110:ASP:HB3	49:2r:85:LEU:HB3	1.71	0.73
1:1A:1453:U:OP1	13:1R:77:ARG:NH1	2.21	0.73
1:2A:2033:A:OP1	61:2A:3914:HOH:O	2.06	0.73
26:24:58:ARG:HH21	50:2s:68:GLY:HA3	1.54	0.73
20:1Y:23:ARG:HG2	20:1Y:42:VAL:HG22	1.70	0.72
33:1b:48:MET:HA	33:1b:51:LEU:HB2	1.70	0.72
55:1x:12:A:OP2	61:1x:201:HOH:O	2.06	0.72
1:1A:2115:G:H1'	1:1A:2171:A:H61	1.54	0.72
1:2A:1782:C:OP1	61:2A:3915:HOH:O	2.07	0.72
1:2A:2207:G:H3'	1:2A:2208:A:H5"	1.70	0.72
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.22	0.72
54:2w:169:GLY:HA2	54:2w:172:LYS:HE3	1.71	0.72
32:1a:407:G:H5"	35:1d:115:ARG:HB3	1.69	0.72
32:2a:942:G:H21	40:2i:124:GLN:HE22	1.37	0.72
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.22	0.72
1:1A:948:G:OP1	61:1A:4115:HOH:O	2.08	0.72
1:2A:2116:G:N2	1:2A:2162:G:OP1	2.23	0.72
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.72	0.72
1:1A:2763:G:OP2	61:1A:4111:HOH:O	2.07	0.72
41:2j:8:LEU:HB3	41:2j:96:ILE:HG23	1.72	0.72
1:1A:1078:U:H3	1:1A:1089:G:H5'	1.54	0.72
1:1A:1269:A:N7	61:1A:4146:HOH:O	2.22	0.72
1:2A:1664:A:OP1	61:2A:3916:HOH:O	2.07	0.72
1:2A:2592:G:OP1	61:2A:3913:HOH:O	2.05	0.72
14:2S:3:ARG:NH1	14:2S:4:LEU:O	2.23	0.72
1:1A:1707:G:N3	61:1A:4151:HOH:O	2.23	0.71
1:1A:2577:A:OP1	61:1A:4108:HOH:O	2.06	0.71
54:2w:240:ARG:HG3	54:2w:251:THR:HG22	1.72	0.71
38:1g:113:GLU:HB3	38:1g:118:VAL:HG13	1.72	0.71
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.71	0.71
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.08	0.71
1:2A:481:G:N7	61:2A:3958:HOH:O	2.24	0.71
5:2F:197:ASP:N	5:2F:197:ASP:OD1	2.21	0.71
1:1A:1041:C:H42	1:1A:1114:G:H1	1.37	0.71
6:1G:123:ASN:O	61:1G:301:HOH:O	2.06	0.71
32:2a:1005:A:OP2	32:2a:1006:C:N4	2.23	0.71
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.73	0.71
1:1A:1185:C:OP2	61:1A:4113:HOH:O	2.07	0.71
17:1V:60:GLU:HB2	17:1V:97:LYS:HE2	1.71	0.71
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:912:C:OP1	43:2l:46:LYS:NZ	2.23	0.71
32:2a:1209:C:O2'	32:2a:1214:C:N4	2.23	0.71
39:2h:81:HIS:ND1	39:2h:138:TRP:OXT	2.19	0.71
54:2w:177:VAL:HG12	54:2w:301:LYS:HA	1.73	0.71
1:1A:2499:C:OP1	61:1A:4114:HOH:O	2.08	0.71
41:1j:5:ARG:HG3	41:1j:71:LEU:HD11	1.72	0.71
6:2G:151:ALA:O	6:2G:153:ARG:NH1	2.24	0.71
39:2h:113:SER:HB2	39:2h:134:ILE:HD11	1.72	0.71
1:1A:2409:G:N7	61:1A:4148:HOH:O	2.22	0.70
6:1G:45:GLU:OE2	61:1G:302:HOH:O	2.09	0.70
32:1a:587:G:N7	61:1a:3815:HOH:O	2.23	0.70
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.73	0.70
1:1A:1342:A:OP2	61:1A:4117:HOH:O	2.09	0.70
32:1a:976:G:H5'	32:1a:1358:U:O2'	1.89	0.70
55:1x:76:8AN:O2P	61:1x:202:HOH:O	2.10	0.70
41:2j:44:VAL:HG12	41:2j:66:ARG:HG2	1.73	0.70
1:2A:833:U:O2	11:2P:55:ARG:NH2	2.24	0.70
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.07	0.70
1:1A:400:G:N7	61:1A:4155:HOH:O	2.23	0.70
1:1A:2337:G:OP1	61:1A:4116:HOH:O	2.08	0.70
1:1A:2790:A:H5'	1:1A:2893:G:H21	1.56	0.70
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.25	0.70
32:2a:972:C:O2'	41:2j:55:LYS:O	2.10	0.70
1:1A:990:A:OP2	61:1A:4118:HOH:O	2.09	0.70
1:1A:2306:C:O2	61:1G:302:HOH:O	2.09	0.70
23:21:32:LYS:O	61:21:201:HOH:O	2.09	0.70
35:2d:7:PRO:HB2	35:2d:10:ARG:HD2	1.74	0.70
6:2G:35:GLU:HB3	6:2G:160:VAL:HG23	1.72	0.70
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.55	0.70
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.73	0.70
44:2m:33:ALA:HB1	44:2m:56:LEU:HD11	1.74	0.69
55:2x:12:A:OP2	61:2x:201:HOH:O	2.10	0.69
1:2A:1970:A:OP1	61:2A:3918:HOH:O	2.10	0.69
32:2a:437:U:H5'	35:2d:155:LEU:HD21	1.72	0.69
1:1A:300:A:OP2	20:1Y:86:ARG:NH2	2.26	0.69
6:2G:44:GLY:N	6:2G:88:ILE:O	2.23	0.69
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.73	0.69
33:2b:118:LEU:HB3	33:2b:142:LEU:HD12	1.75	0.69
1:2A:804:A:OP1	61:2A:3917:HOH:O	2.09	0.69
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.26	0.69
32:1a:504:C:OP1	61:1a:3803:HOH:O	2.10	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.75	0.69
1:1A:1082:U:H3	1:1A:1086:A:N6	1.91	0.69
1:2A:2136:C:C4	1:2A:2155:G:O6	2.46	0.69
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.73	0.69
32:2a:1086:U:H3	32:2a:1099:G:H22	1.38	0.69
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.73	0.69
1:1A:2577:A:OP2	27:15:3:LYS:NZ	2.23	0.69
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.25	0.69
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.24	0.69
28:16:13:CYS:SG	28:16:47:THR:HG21	2.33	0.69
32:1a:79:G:H1	32:1a:90:U:H3	1.39	0.69
1:2A:963:U:OP2	61:2A:3908:HOH:O	2.11	0.69
1:1A:1186:G:OP2	61:1A:4118:HOH:O	2.10	0.69
33:2b:91:PRO:HG2	33:2b:155:LEU:HD13	1.75	0.69
1:1A:469:G:O6	29:17:37:LYS:NZ	2.25	0.69
1:1A:2066:C:OP1	61:1A:4120:HOH:O	2.11	0.69
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.26	0.69
25:13:3:ARG:NH1	25:13:60:GLU:OE2	2.24	0.68
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.74	0.68
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.26	0.68
3:2D:242:ARG:O	61:2D:401:HOH:O	2.09	0.68
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.25	0.68
1:1A:2550:G:OP1	61:1A:4122:HOH:O	2.12	0.68
32:1a:766:A:OP2	61:1a:3804:HOH:O	2.11	0.68
32:2a:1224:G:OP1	61:2a:1803:HOH:O	2.11	0.68
32:2a:1328:C:O2'	44:2m:29:ARG:NH2	2.26	0.68
1:1A:2167:U:H3	1:1A:2171:A:H62	1.42	0.68
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.74	0.68
1:1A:654:A:OP2	61:1A:4119:HOH:O	2.10	0.68
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.23	0.68
13:1R:103:ARG:NH1	13:1R:108:GLY:O	2.27	0.68
1:2A:602:G:HO2'	1:2A:604:G:HO2'	1.36	0.68
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.26	0.68
1:1A:2255:G:OP2	61:1A:4121:HOH:O	2.11	0.68
32:1a:444:C:H2'	32:1a:445:G:H8	1.57	0.68
48:1q:45:HIS:HB3	48:1q:72:ARG:HG2	1.75	0.68
7:2H:3:ARG:HG2	7:2H:6:ARG:HG3	1.76	0.68
6:1G:82:LEU:HD12	6:1G:86:MET:HE3	1.75	0.68
44:1m:60:VAL:HG12	44:1m:66:LEU:HD11	1.74	0.68
1:2A:1812:A:OP2	61:2A:3921:HOH:O	2.12	0.68
32:2a:890:G:O2'	32:2a:906:G:O6	2.11	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:960:U:H5	50:1s:78:ARG:HD3	1.57	0.68
43:1l:70:ILE:HG12	43:1l:100:ILE:HD12	1.75	0.68
54:1w:141:GLU:HB3	54:1w:163:ARG:HB2	1.75	0.68
36:2e:88:LYS:HB3	36:2e:123:LEU:HB2	1.76	0.68
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.75	0.68
47:1p:43:LYS:HA	47:1p:48:TRP:CD1	2.28	0.68
1:1A:2133:G:O2'	1:1A:2134:A:N7	2.26	0.67
32:1a:1351:U:O4	40:1i:118:LYS:NZ	2.26	0.67
38:1g:78:ARG:HE	38:1g:156:TRP:HE3	1.43	0.67
44:2m:91:ARG:HB2	44:2m:98:VAL:HG12	1.76	0.67
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.26	0.67
38:1g:78:ARG:HG2	38:1g:79:ARG:HG3	1.73	0.67
44:2m:94:ARG:HB3	44:2m:96:LEU:HD12	1.75	0.67
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.75	0.67
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.76	0.67
42:1k:99:GLN:HG2	42:1k:105:VAL:HG21	1.75	0.67
1:1A:2499:C:N3	61:1A:4169:HOH:O	2.28	0.67
38:2g:67:GLU:HA	38:2g:70:LYS:HE3	1.77	0.67
1:1A:1082:U:N3	1:1A:1086:A:N6	2.41	0.67
1:2A:1026:U:OP1	61:2A:3919:HOH:O	2.13	0.67
1:1A:2139:C:H42	1:1A:2152:G:H1	1.42	0.67
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.76	0.67
32:1a:17:U:H2'	32:1a:18:C:C6	2.30	0.67
1:2A:652(B):A:N6	1:2A:655:A:N3	2.43	0.67
14:2S:49:VAL:HG11	14:2S:77:ALA:HB2	1.76	0.67
1:1A:2158:A:H4'	1:1A:2159:G:H5'	1.76	0.67
32:1a:1030(D):A:C8	32:1a:1031:G:H1'	2.30	0.67
32:1a:1226:C:H3'	44:1m:96:LEU:HD21	1.75	0.67
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.77	0.67
1:2A:1376:C:OP2	61:2A:3924:HOH:O	2.13	0.67
32:2a:619:U:N3	35:2d:134:ASP:OD1	2.24	0.67
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.59	0.67
44:2m:3:ARG:HG2	44:2m:4:ILE:HG22	1.77	0.67
3:1D:230:ASP:OD1	61:1D:401:HOH:O	2.12	0.66
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	1.77	0.66
1:2A:857:C:OP1	22:20:77:ARG:NH2	2.27	0.66
1:2A:307:G:H21	1:2A:330:A:H62	1.40	0.66
1:2A:2582:G:OP2	61:2A:3922:HOH:O	2.12	0.66
1:2A:2821:A:OP2	61:2R:301:HOH:O	2.13	0.66
1:1A:9:U:H3	1:1A:2629:A:H2	1.41	0.66
32:1a:1396:A:H4'	32:1a:1397:C:H5"	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.29	0.66
21:2Z:93:ASP:HA	21:2Z:130:PRO:HG2	1.76	0.66
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.24	0.66
1:1A:365:C:OP2	61:1A:4123:HOH:O	2.14	0.66
1:2A:2721:A:OP1	61:2A:3923:HOH:O	2.13	0.66
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.29	0.66
1:1A:2119:A:H61	1:1A:2168:G:H8	1.42	0.66
1:2A:1024:G:OP2	61:2A:3919:HOH:O	2.11	0.66
32:2a:519:C:O5'	54:2w:301:LYS:NZ	2.26	0.66
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.75	0.66
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.76	0.66
32:1a:405:U:O4	35:1d:2:GLY:N	2.29	0.66
35:1d:189:PRO:HB2	35:1d:194:LEU:HD21	1.78	0.66
41:1j:50:ILE:HA	41:1j:60:ARG:HG2	1.76	0.66
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.31	0.66
38:2g:46:ALA:HA	38:2g:49:ILE:HD12	1.77	0.66
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.26	0.66
1:2A:848:G:OP1	61:2A:3925:HOH:O	2.14	0.66
32:1a:21:G:OP1	61:1a:3805:HOH:O	2.12	0.66
1:2A:120:U:OP2	61:2A:3920:HOH:O	2.11	0.66
2:2B:105:A:OP1	21:2Z:72:ARG:NH1	2.28	0.66
32:1a:382:A:H2'	32:1a:383:A:C8	2.31	0.66
1:2A:572:A:OP2	17:2V:78:LYS:NZ	2.29	0.66
1:2A:2269:A:OP1	61:2A:3927:HOH:O	2.14	0.66
34:2c:181:ASN:HD21	34:2c:204:LEU:HD12	1.60	0.66
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.60	0.65
34:2c:43:LEU:HB3	34:2c:47:LEU:HD12	1.77	0.65
1:1A:1314:C:OP1	61:1A:4103:HOH:O	2.13	0.65
32:2a:328:C:H4'	32:2a:329:A:H5"	1.77	0.65
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.76	0.65
32:1a:1414:U:H3	32:1a:1486:G:H1	1.43	0.65
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.29	0.65
41:2j:46:ARG:HG2	41:2j:64:GLU:HB3	1.79	0.65
36:1e:8:GLU:HG3	36:1e:34:VAL:HG23	1.77	0.65
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.77	0.65
41:2j:42:THR:HG22	41:2j:68:HIS:HA	1.78	0.65
4:1E:27:LEU:HD22	15:1T:1:MET:HE3	1.78	0.65
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.13	0.65
1:2A:1395:A:OP1	61:2A:3907:HOH:O	2.14	0.65
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.77	0.65
14:2S:38:GLN:HG3	14:2S:40:ILE:HD11	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:230:VAL:HG12	33:2b:232:PRO:HD2	1.79	0.65
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.29	0.65
1:2A:2130:U:O2'	1:2A:2158:A:N6	2.30	0.65
3:2D:147:LEU:HD13	3:2D:155:LEU:HD11	1.77	0.65
32:2a:532:A:N6	32:2a:1206:G:O2'	2.29	0.65
32:2a:1148:U:O2'	40:2i:66:ARG:NH2	2.29	0.65
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.26	0.65
1:2A:2502:G:N7	61:2A:3982:HOH:O	2.29	0.65
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.79	0.65
61:1a:3802:HOH:O	53:1v:19:U:OP1	2.15	0.65
1:2A:382:G:N7	61:2A:3978:HOH:O	2.28	0.65
37:2f:37:VAL:HA	37:2f:65:VAL:HG12	1.79	0.65
42:2k:79:SER:HA	42:2k:104:GLN:HB3	1.77	0.65
1:1A:1271:G:OP2	61:1A:4112:HOH:O	2.15	0.64
1:1A:2859:G:OP1	61:1A:4124:HOH:O	2.15	0.64
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG11	1.79	0.64
1:2A:1721:G:H8	1:2A:1741:A:H62	1.45	0.64
32:1a:991:U:C4	32:1a:1212:U:H1'	2.32	0.64
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.31	0.64
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.79	0.64
11:2P:29:LYS:HD3	11:2P:30:THR:HG23	1.77	0.64
21:1Z:54:HIS:NE2	21:1Z:123:ASP:OD2	2.21	0.64
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.32	0.64
32:1a:1035:A:H2'	32:1a:1036:G:N2	2.06	0.64
1:2A:2133:G:N2	1:2A:2157:G:N7	2.46	0.64
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.78	0.64
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.62	0.64
32:2a:1278:U:H5'	32:2a:1279:A:H5'	1.79	0.64
36:2e:80:ILE:HG22	36:2e:91:LEU:HB2	1.80	0.64
7:1H:27:LYS:HG2	7:1H:32:GLU:HB3	1.79	0.64
1:2A:2114:A:C4	1:2A:2168:G:H1'	2.33	0.64
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.12	0.64
32:1a:192:U:H2'	32:1a:193:C:H6	1.63	0.64
32:2a:953:G:H5'	32:2a:965:A:N6	2.11	0.64
33:2b:204:ASN:HD22	33:2b:207:ALA:H	1.44	0.64
55:2x:4:G:H1	55:2x:69:C:H42	1.42	0.64
1:2A:586:A:OP2	61:2A:3928:HOH:O	2.15	0.64
1:2A:1241:A:OP2	61:2A:3926:HOH:O	2.14	0.64
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.25	0.64
1:1A:2138:C:H42	1:1A:2153:G:H1	1.45	0.64
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:41:G:H2'	32:1a:42:G:C8	2.33	0.64
32:1a:1320:C:O2	50:1s:36:ARG:NH2	2.31	0.64
5:2F:153:SER:HB2	5:2F:190:GLU:H	1.63	0.64
35:1d:8:VAL:HA	35:1d:11:LEU:HD13	1.80	0.64
1:2A:2318:G:H21	14:2S:3:ARG:NE	1.96	0.64
40:2i:28:VAL:HG12	40:2i:63:ILE:HB	1.78	0.64
7:1H:46:GLU:HB2	7:1H:49:VAL:HG23	1.80	0.64
26:14:68:ARG:HH21	26:14:68:ARG:HA	1.61	0.64
32:2a:1272:G:N2	32:2a:1273:G:C5	2.66	0.64
32:1a:445:G:H2'	32:1a:446:G:C8	2.33	0.63
32:1a:1025:U:H3	32:1a:1036:G:H1	1.46	0.63
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.79	0.63
1:2A:2099:U:H3	1:2A:2190:G:H1	1.45	0.63
38:2g:22:LEU:HD23	38:2g:63:LYS:HE3	1.79	0.63
1:1A:476:G:OP1	61:1A:4125:HOH:O	2.15	0.63
1:2A:2499:C:OP2	61:2A:3929:HOH:O	2.15	0.63
24:22:41:ILE:HG13	24:22:43:GLN:HB2	1.81	0.63
34:2c:18:TRP:O	34:2c:54:ARG:NH2	2.31	0.63
1:1A:2336:A:H61	22:10:43:THR:HG22	1.64	0.63
32:1a:1080:A:H5'	36:1e:14:ARG:HH21	1.63	0.63
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.63	0.63
49:1r:40:LEU:HD22	49:1r:70:ILE:HG12	1.79	0.63
32:2a:56:U:H2'	32:2a:57:G:C8	2.33	0.63
33:2b:40:HIS:HB3	33:2b:190:THR:HG21	1.79	0.63
1:1A:2099:U:H3	1:1A:2190:G:H1	1.44	0.63
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.80	0.63
35:2d:100:ARG:NH1	35:2d:137:SER:OG	2.32	0.63
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.30	0.63
1:1A:1607:C:N4	1:1A:1622:G:OP2	2.30	0.63
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.33	0.63
23:11:21:ARG:HD3	23:11:35:THR:HG21	1.81	0.63
32:1a:308:C:H2'	32:1a:309:G:H8	1.64	0.63
32:2a:1162:C:H42	32:2a:1174:G:H1	1.47	0.63
41:2j:8:LEU:HG	41:2j:70:ARG:HB2	1.79	0.63
54:2w:161:GLU:OE2	54:2w:204:LYS:NZ	2.31	0.63
32:2a:1353:G:OP1	52:2u:10:ARG:NH1	2.30	0.63
1:2A:1364:G:OP2	23:21:3:LYS:HG3	1.99	0.63
26:24:16:CYS:SG	26:24:17:GLY:N	2.70	0.63
32:2a:35:G:O2'	43:2l:118:SER:O	2.15	0.63
33:2b:45:GLN:NE2	33:2b:49:GLU:OE2	2.32	0.63
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1U:69:CYS:HB3	16:1U:74:LEU:HD13	1.81	0.63
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.80	0.63
32:2a:316:G:OP2	32:2a:351:G:O2'	2.17	0.63
3:1D:166:GLN:HB2	3:1D:174:ILE:HG22	1.81	0.62
10:2O:107:ARG:HG3	10:2O:112:MET:HE1	1.81	0.62
1:1A:2185:C:H2'	1:1A:2186:G:C8	2.33	0.62
15:1T:108:ARG:HH21	15:1T:112:ARG:HD3	1.63	0.62
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.22	0.62
34:1c:22:TRP:HB3	34:1c:59:ARG:HB2	1.79	0.62
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.63	0.62
32:2a:1271:G:C2	32:2a:1272:G:N7	2.67	0.62
35:1d:111:ALA:HB2	35:1d:120:LEU:HD22	1.80	0.62
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.14	0.62
40:2i:3:GLN:HG2	40:2i:20:ARG:HH21	1.64	0.62
1:1A:1354:A:H5"	3:1D:38:LYS:HD3	1.81	0.62
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.34	0.62
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.32	0.62
1:1A:2602:A:OP1	61:1x:202:HOH:O	2.15	0.62
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.35	0.62
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.25	0.62
1:2A:1352:U:OP2	61:2A:3924:HOH:O	2.16	0.62
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.63	0.62
7:2H:59:ARG:O	7:2H:63:SER:OG	2.18	0.62
33:2b:157:ARG:NH2	33:2b:160:ASP:OD1	2.29	0.62
1:1A:607:U:OP1	5:1F:102:PRO:HA	1.99	0.62
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.14	0.62
1:2A:2115:G:H2'	1:2A:2116:G:H3'	1.81	0.62
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.33	0.62
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.28	0.62
15:2T:36:GLU:OE2	15:2T:41:ARG:NH2	2.31	0.62
32:2a:1055:A:N3	34:2c:156:ARG:NH1	2.47	0.62
1:1A:1671:U:O4	61:1A:4122:HOH:O	2.16	0.62
32:1a:1129:C:H42	32:1a:1143:G:H1	1.47	0.62
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.31	0.62
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.81	0.62
1:1A:1673:U:OP1	61:1A:4127:HOH:O	2.16	0.62
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.26	0.62
22:10:24:LYS:O	22:10:25:ARG:NH1	2.33	0.62
33:1b:15:VAL:HB	33:1b:209:ARG:HG2	1.81	0.62
44:1m:58:GLU:O	44:1m:62:ASN:ND2	2.24	0.62
1:1A:2134:A:H2'	1:1A:2135:A:C8	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.15	0.62
34:2c:73:PRO:HD3	34:2c:105:GLU:HG3	1.82	0.62
51:2t:57:ARG:HH22	51:2t:100:ILE:HD12	1.65	0.62
54:2w:145:LEU:HD21	54:2w:161:GLU:HB2	1.82	0.62
55:2x:7:U:O2'	55:2x:49:U:OP2	2.15	0.62
7:2H:33:LEU:HD21	7:2H:136:ILE:HG13	1.82	0.62
33:2b:93:VAL:HG21	33:2b:97:TRP:HD1	1.65	0.62
1:1A:1056:G:N2	1:1A:1102:C:OP2	2.30	0.61
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.35	0.61
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.32	0.61
1:2A:531:C:OP1	1:2A:561:G:N1	2.32	0.61
36:2e:5:ASP:N	36:2e:5:ASP:OD1	2.33	0.61
15:1T:98:LYS:NZ	61:1T:301:HOH:O	2.12	0.61
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.81	0.61
34:1c:43:LEU:HD11	34:1c:91:LEU:HD11	1.82	0.61
40:1i:4:TYR:HD1	40:1i:87:GLN:HE21	1.46	0.61
54:1w:196:THR:HG21	54:1w:296:GLY:O	2.01	0.61
1:2A:593:G:H4'	30:28:63:PRO:HB3	1.81	0.61
1:2A:1648:C:OP1	61:2A:3904:HOH:O	2.16	0.61
41:2j:20:ALA:HB1	41:2j:37:PRO:HB3	1.83	0.61
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.83	0.61
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.32	0.61
7:2H:3:ARG:NH1	7:2H:4:ILE:H	1.98	0.61
33:2b:100:GLY:N	33:2b:176:GLU:OE2	2.31	0.61
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.81	0.61
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.82	0.61
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.82	0.61
40:1i:88:TYR:HD2	40:1i:89:ASN:HD22	1.48	0.61
51:1t:58:LYS:HE3	51:1t:62:LEU:HD11	1.82	0.61
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.31	0.61
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.34	0.61
41:2j:50:ILE:HA	41:2j:60:ARG:HG2	1.82	0.61
32:1a:1055:A:H2'	34:1c:156:ARG:HD2	1.82	0.61
1:2A:193:U:OP2	61:2A:3930:HOH:O	2.15	0.61
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.35	0.61
1:2A:2396:G:OP1	23:21:25:LYS:NZ	2.27	0.61
2:2B:106:G:H5'	21:2Z:31:ARG:HG3	1.83	0.61
32:2a:444:C:H2'	32:2a:445:G:H8	1.66	0.61
36:2e:8:GLU:OE2	36:2e:63:ARG:NH2	2.29	0.61
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.31	0.61
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.82	0.61
1:1A:2592:G:OP1	61:1A:4128:HOH:O	2.16	0.61
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.36	0.61
40:1i:16:ARG:HB2	40:1i:64:THR:HG23	1.81	0.61
7:2H:80:SER:OG	7:2H:81:GLU:N	2.32	0.61
8:2I:4:ILE:HG12	8:2I:18:VAL:HG12	1.82	0.61
1:2A:761:A:OP2	61:2A:3933:HOH:O	2.16	0.61
25:23:8:LEU:HB2	25:23:28:LEU:HD13	1.83	0.61
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.36	0.61
37:1f:35:ALA:HB1	37:1f:65:VAL:HG11	1.82	0.61
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.17	0.61
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.66	0.61
32:1a:972:C:O2'	41:1j:55:LYS:O	2.18	0.60
54:1w:206:GLU:HB2	54:1w:208:GLU:HG2	1.83	0.60
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.82	0.60
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.83	0.60
32:1a:877:C:OP1	39:1h:88:LYS:NZ	2.26	0.60
1:2A:2005:A:OP1	61:2A:3931:HOH:O	2.16	0.60
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.35	0.60
32:2a:952:U:H2'	32:2a:953:G:H8	1.65	0.60
32:2a:1348:U:H2'	32:2a:1349:A:H8	1.66	0.60
36:2e:102:ALA:HB1	36:2e:106:PRO:HG2	1.83	0.60
1:1A:1637:A:OP2	61:1A:4129:HOH:O	2.16	0.60
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.36	0.60
15:1T:127:ALA:C	15:1T:129:ARG:H	2.09	0.60
33:1b:77:ALA:HB2	33:1b:211:ILE:HG21	1.83	0.60
15:2T:39:ARG:NH2	32:2a:345:C:OP2	2.33	0.60
32:2a:673:G:H2'	32:2a:674:G:C8	2.36	0.60
1:1A:881:G:H1	1:1A:895:U:H3	1.50	0.60
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.19	0.60
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.36	0.60
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	1.84	0.60
32:1a:35:G:O2'	43:1l:118:SER:O	2.18	0.60
32:1a:1118:C:OP1	40:1i:9:ARG:NH1	2.34	0.60
45:1n:21:TYR:OH	45:1n:23:ARG:NH2	2.34	0.60
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.36	0.60
6:2G:11:TYR:HA	6:2G:15:VAL:HG22	1.83	0.60
31:19:2:LYS:NZ	31:19:31:LYS:O	2.33	0.60
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.35	0.60
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.83	0.60
32:2a:1145:C:H4'	32:2a:1146:A:H5'	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.66	0.60
32:1a:390:C:O3'	47:1p:28:ARG:NH2	2.32	0.60
32:1a:966:M2G:HM11	40:1i:127:LYS:HD2	1.84	0.60
32:1a:1326:C:H2'	32:1a:1327:C:C6	2.36	0.60
1:2A:644:A:H4'	1:2A:645:C:C4	2.37	0.60
1:2A:848:G:H2'	1:2A:849:A:C8	2.36	0.60
1:2A:1011:G:OP1	16:2U:77:SER:OG	2.18	0.60
38:2g:151:TYR:OH	42:2k:54:ARG:NH1	2.35	0.60
2:1B:95:C:OP2	61:1B:301:HOH:O	2.16	0.60
32:1a:1004:A:H62	32:1a:1036:G:N2	1.99	0.60
44:1m:19:LEU:HD11	44:1m:56:LEU:HD21	1.83	0.60
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.64	0.60
32:2a:1211:U:H4'	32:2a:1212:U:H5'	1.83	0.60
1:1A:962:G:OP1	61:1A:4115:HOH:O	2.16	0.60
32:1a:444:C:H2'	32:1a:445:G:C8	2.37	0.60
33:1b:50:GLU:OE1	33:1b:53:ARG:NH1	2.35	0.60
35:2d:196:LEU:HB2	35:2d:198:VAL:HG22	1.84	0.60
1:2A:222:A:OP1	61:2A:3934:HOH:O	2.17	0.60
1:2A:2169:A:H2'	1:2A:2170:A:C8	2.37	0.60
32:2a:1193:G:O2'	36:2e:25:ARG:NH2	2.35	0.60
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.48	0.59
32:1a:574:A:OP2	61:1a:3806:HOH:O	2.16	0.59
32:2a:108:G:N1	51:2t:15:ARG:HG2	2.18	0.59
36:2e:89:ILE:HG12	36:2e:135:THR:HG22	1.82	0.59
40:2i:97:LYS:HA	40:2i:102:LEU:HD22	1.84	0.59
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	1.82	0.59
1:1A:1671:U:OP2	61:1A:4126:HOH:O	2.15	0.59
33:1b:21:ARG:HA	33:1b:39:ILE:HA	1.83	0.59
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.03	0.59
32:1a:975:A:HO2'	45:1n:32:SER:HG	1.48	0.59
33:1b:16:HIS:CD2	33:1b:18:GLY:H	2.20	0.59
1:2A:943:U:OP2	61:2A:3932:HOH:O	2.16	0.59
32:2a:1022:G:H2'	32:2a:1023:G:C8	2.37	0.59
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.18	0.59
32:1a:1129:C:H5"	40:1i:16:ARG:HH12	1.67	0.59
32:1a:1446:U:H4'	32:1a:1447:A:C6	2.38	0.59
33:1b:50:GLU:O	33:1b:54:THR:N	2.25	0.59
44:1m:88:ARG:O	44:1m:92:HIS:ND1	2.36	0.59
50:1s:19:VAL:HG21	50:1s:44:MET:HG2	1.84	0.59
1:2A:307:G:N7	61:2A:4000:HOH:O	2.31	0.59
1:2A:1464:C:H2'	1:2A:1465:G:C8	2.37	0.59

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:62:GLN:NE2	2.34	0.59
36:2e:6:PHE:HB3	36:2e:34:VAL:HG22	1.84	0.59
37:2f:8:ILE:HD13	37:2f:26:ILE:HD13	1.83	0.59
1:1A:1077:A:H2'	1:1A:1078:U:H4'	1.84	0.59
1:1A:2508:G:OP1	54:1w:223:ARG:NH2	2.35	0.59
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.66	0.59
8:1I:92:VAL:HB	8:1I:120:ILE:HB	1.83	0.59
32:1a:1226:C:H2'	44:1m:103:THR:HB	1.85	0.59
1:2A:2136:C:C2	1:2A:2155:G:N1	2.70	0.59
7:2H:24:VAL:HG21	7:2H:72:ILE:HG12	1.85	0.59
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.68	0.59
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.38	0.59
42:2k:41:THR:HG21	42:2k:71:LYS:HB3	1.82	0.59
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.02	0.59
1:2A:1639:U:H2'	1:2A:1640:C:H5"	1.84	0.59
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.03	0.59
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.35	0.59
1:2A:2612:C:OP2	27:25:2:ALA:N	2.36	0.59
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.85	0.59
32:2a:620:C:C2	35:2d:135:LEU:HG	2.38	0.59
32:2a:1240:U:OP2	38:2g:116:ALA:N	2.36	0.59
50:2s:33:THR:HG22	50:2s:51:VAL:HA	1.85	0.59
1:1A:1500:G:N2	3:1D:99:ASP:O	2.35	0.59
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.11	0.59
32:1a:1286:A:N6	32:1a:1355:G:OP1	2.34	0.59
33:1b:80:ILE:HD11	33:1b:211:ILE:HB	1.85	0.59
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.84	0.59
26:24:34:GLU:HG2	26:24:35:VAL:HG23	1.84	0.59
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.35	0.59
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.12	0.59
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.35	0.59
38:2g:69:VAL:HG22	38:2g:135:VAL:HG12	1.85	0.59
1:1A:2110:G:H5"	1:1A:2111:C:H5	1.68	0.59
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.85	0.59
3:2D:71:ASP:OD2	3:2D:103:ARG:NH2	2.35	0.59
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.84	0.59
32:2a:1150:U:H4'	41:2j:41:PRO:HG3	1.84	0.59
11:1P:86:LYS:HB3	11:1P:118:GLY:HA3	1.85	0.59
32:1a:445:G:H2'	32:1a:446:G:H8	1.66	0.59
50:1s:36:ARG:HB3	50:1s:72:GLY:HA3	1.85	0.59
37:2f:62:TRP:CH2	37:2f:64:GLN:HB2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:912:C:OP1	12:2Q:9:TYR:OH	2.15	0.58
7:2H:105:LEU:HB2	7:2H:113:VAL:HG12	1.85	0.58
32:2a:959:A:O2'	32:2a:984:C:O2'	2.08	0.58
1:1A:1072:C:N4	1:1A:1098:A:OP1	2.35	0.58
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.36	0.58
32:1a:946:A:H2'	32:1a:947:G:C8	2.38	0.58
39:1h:121:ASP:OD1	39:1h:121:ASP:N	2.36	0.58
2:2B:9:G:P	14:2S:25:ARG:HH22	2.26	0.58
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.33	0.58
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.39	0.58
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.85	0.58
32:1a:979:C:OP1	32:1a:1223:C:N4	2.37	0.58
36:1e:78:HIS:HE1	36:1e:142:LEU:HA	1.68	0.58
1:2A:2121:G:H1	1:2A:2177:C:H42	1.51	0.58
26:24:40:HIS:HB3	26:24:43:TYR:HD2	1.69	0.58
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.38	0.58
4:1E:29:GLY:HA3	61:1E:403:HOH:O	2.03	0.58
34:1c:150:LYS:HB3	34:1c:201:TYR:HB2	1.85	0.58
42:1k:81:ASP:OD1	42:1k:107:SER:OG	2.20	0.58
44:1m:67:GLU:HG3	44:1m:71:ARG:HH21	1.67	0.58
32:2a:64:G:H4'	32:2a:65:U:H3'	1.84	0.58
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.39	0.58
1:1A:2304:G:H22	1:1A:2312:U:H3	1.51	0.58
7:1H:97:ARG:NH1	7:1H:104:GLU:OE1	2.36	0.58
32:1a:414:A:H2'	32:1a:415:A:H8	1.67	0.58
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.21	0.58
44:1m:4:ILE:HD12	44:1m:57:ARG:HB2	1.85	0.58
1:2A:2508:G:OP1	54:2w:223:ARG:NH1	2.29	0.58
44:2m:19:LEU:HD11	44:2m:56:LEU:HD21	1.85	0.58
44:2m:88:ARG:O	44:2m:92:HIS:ND1	2.35	0.58
32:1a:1373:G:H5"	38:1g:36:LYS:HE2	1.86	0.58
32:2a:222:U:H2'	32:2a:223:U:C6	2.39	0.58
35:2d:18:LYS:NZ	35:2d:31:CYS:SG	2.74	0.58
47:2p:5:ARG:NH2	47:2p:28:ARG:HA	2.18	0.58
1:1A:1072:C:H42	1:1A:1098:A:P	2.26	0.58
1:1A:1987:G:OP2	61:1A:4130:HOH:O	2.16	0.58
26:24:24:THR:OG1	26:24:25:TYR:N	2.32	0.58
43:2l:60:LEU:HD21	43:2l:85:ILE:HD11	1.84	0.58
32:1a:757:U:H2'	32:1a:758:G:O4'	2.03	0.58
1:2A:1647:G:OP1	61:2A:3904:HOH:O	2.17	0.58
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:124:SER:HB3	33:2b:125:PRO:CD	2.34	0.58
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.68	0.58
32:1a:308:C:H2'	32:1a:309:G:C8	2.38	0.58
32:1a:309:G:O2'	32:1a:607:A:N1	2.36	0.58
32:1a:894:G:N7	61:1a:3833:HOH:O	2.32	0.58
32:2a:503:C:O2'	32:2a:510:A:N1	2.34	0.58
32:2a:1106:G:H5"	34:2c:172:ARG:HG2	1.85	0.58
33:2b:93:VAL:HG21	33:2b:97:TRP:CD1	2.39	0.58
40:2i:26:VAL:HG23	40:2i:33:PHE:HB2	1.85	0.58
40:2i:86:VAL:HG11	40:2i:93:ARG:HE	1.68	0.58
1:1A:218:A:C2	1:1A:235:U:H4'	2.39	0.58
8:1I:31:LEU:HD21	8:1I:38:LEU:HG	1.85	0.58
32:1a:41:G:H2'	32:1a:42:G:H8	1.69	0.58
32:1a:953:G:H5'	32:1a:965:A:H61	1.69	0.58
54:1w:220:ASP:HB2	54:1w:240:ARG:HB3	1.86	0.58
1:1A:2163:C:H2'	1:1A:2164:C:H5'	1.86	0.57
1:1A:2353:G:N7	61:1A:4198:HOH:O	2.31	0.57
3:2D:260:ARG:HH22	3:2D:266:SER:HB2	1.68	0.57
32:2a:1275:A:H2'	32:2a:1276:G:O4'	2.04	0.57
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.22	0.57
15:1T:39:ARG:NH2	32:1a:345:C:OP2	2.31	0.57
26:14:53:GLU:HB2	26:14:55:ARG:H	1.68	0.57
32:1a:812:C:O2	61:1a:3807:HOH:O	2.16	0.57
1:2A:302:C:OP2	20:2Y:73:ARG:NH1	2.34	0.57
20:2Y:23:ARG:CZ	20:2Y:23:ARG:HA	2.35	0.57
32:2a:424:G:H2'	32:2a:425:G:H8	1.69	0.57
32:2a:1265:G:C4	32:2a:1271:G:N2	2.72	0.57
41:2j:27:ALA:HA	41:2j:81:THR:OG1	2.03	0.57
38:1g:78:ARG:HG3	38:1g:156:TRP:HZ3	1.68	0.57
1:2A:2572:A:C8	4:2E:144:ARG:HD3	2.39	0.57
32:2a:406:G:N2	35:2d:119:GLN:OE1	2.29	0.57
32:2a:952:U:H2'	32:2a:953:G:C8	2.40	0.57
32:2a:1285:A:H5'	32:2a:1286:A:C2	2.39	0.57
34:1c:42:LEU:HA	34:1c:45:LYS:HB3	1.86	0.57
41:1j:64:GLU:OE2	41:1j:66:ARG:NH1	2.37	0.57
47:1p:34:GLU:OE1	47:1p:59:TRP:NE1	2.35	0.57
32:2a:45:U:H2'	32:2a:46:G:C8	2.40	0.57
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.22	0.57
32:2a:1092:A:H5"	38:2g:4:ARG:CZ	2.34	0.57
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.86	0.57
14:1S:39:ILE:HB	14:1S:49:VAL:HG13	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.34	0.57
21:1Z:146:ILE:N	21:1Z:148:ASP:H	2.03	0.57
32:1a:56:U:H2'	32:1a:57:G:C8	2.40	0.57
32:1a:1030(D):A:H8	32:1a:1031:G:H1'	1.67	0.57
41:1j:5:ARG:NH1	41:1j:73:ASP:OD1	2.37	0.57
32:2a:123:C:OP1	32:2a:311:C:O2'	2.20	0.57
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.05	0.57
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.86	0.57
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.39	0.57
40:1i:20:ARG:O	40:1i:60:ASP:N	2.38	0.57
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.38	0.57
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.37	0.57
26:24:48:ARG:O	26:24:50:VAL:N	2.35	0.57
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.37	0.57
32:1a:950:U:H2'	32:1a:951:G:C8	2.39	0.57
32:1a:1030:C:C4	32:1a:1030(A):G:H1'	2.39	0.57
38:1g:89:MET:HE3	38:1g:90:GLU:H	1.69	0.57
34:2c:87:LEU:O	34:2c:91:LEU:N	2.37	0.57
34:2c:181:ASN:HD22	34:2c:204:LEU:HB2	1.70	0.57
39:2h:110:ALA:HB1	39:2h:133:LEU:HD21	1.85	0.57
32:1a:950:U:H2'	32:1a:951:G:H8	1.70	0.57
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.21	0.57
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.40	0.57
33:1b:115:LEU:C	33:1b:117:GLU:H	2.12	0.57
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.38	0.57
34:2c:65:ALA:HA	34:2c:100:ALA:HB3	1.87	0.57
40:2i:29:ASN:HD21	40:2i:65:VAL:H	1.52	0.57
1:1A:2100:G:H2'	1:1A:2101:G:O4'	2.05	0.57
20:1Y:23:ARG:HG2	20:1Y:42:VAL:CG2	2.35	0.57
32:1a:656:C:O2'	46:1o:28:GLN:OE1	2.23	0.57
1:2A:184:C:H2'	1:2A:185:U:C6	2.39	0.57
1:2A:1762:A:N1	61:2A:4001:HOH:O	2.31	0.57
10:2O:87:ILE:HD12	10:2O:91:LEU:HA	1.87	0.57
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.04	0.57
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	1.87	0.57
23:21:21:ARG:HD3	23:21:35:THR:HG21	1.86	0.57
1:1A:1054:A:N6	1:1A:1105:U:H3	2.00	0.57
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.40	0.57
15:1T:36:GLU:O	15:1T:38:ASN:N	2.34	0.57
32:1a:1269:A:HO2'	32:1a:1325:C:HO2'	1.52	0.57
1:2A:323:G:O2'	1:2A:1205:U:N3	2.29	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:643:A:N1	1:2A:2369:A:O2'	2.37	0.57
3:2D:136:ILE:O	3:2D:168:ARG:NH2	2.38	0.57
14:2S:38:GLN:OE1	14:2S:47:THR:OG1	2.16	0.57
33:2b:185:ILE:HG23	33:2b:199:TYR:HB2	1.85	0.57
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.40	0.56
1:1A:1420:U:O2'	1:1A:1421:G:OP1	2.23	0.56
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.22	0.56
32:1a:814:A:H2'	32:1a:816:A:H5"	1.87	0.56
5:2F:120:GLU:HB3	5:2F:122:LYS:HG2	1.86	0.56
21:2Z:157:LEU:HD23	21:2Z:161:VAL:HG23	1.86	0.56
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.86	0.56
32:1a:1182:G:H4'	32:1a:1183:A:H5"	1.87	0.56
33:1b:100:GLY:O	33:1b:104:ASN:N	2.35	0.56
1:2A:248:G:OP1	61:2A:3936:HOH:O	2.17	0.56
1:2A:2657:A:O3'	7:2H:160:LYS:NZ	2.37	0.56
1:2A:2682:U:O2'	15:2T:58:ASN:ND2	2.38	0.56
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.88	0.56
42:2k:48:ILE:O	42:2k:50:TYR:N	2.36	0.56
1:1A:1082:U:O4	1:1A:1086:A:C6	2.59	0.56
1:1A:2115:G:H1'	1:1A:2171:A:N6	2.20	0.56
4:1E:110:GLY:O	61:1R:301:HOH:O	2.18	0.56
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	1.86	0.56
10:1O:64:ARG:HG2	10:1O:79:PHE:CG	2.40	0.56
24:12:10:LEU:HD21	24:12:59:ARG:HG2	1.87	0.56
32:1a:736:C:H2'	32:1a:737:A:C8	2.40	0.56
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.87	0.56
48:1q:66:SER:OG	48:1q:67:LYS:O	2.24	0.56
1:2A:1035:U:H5"	7:2H:59:ARG:HD3	1.86	0.56
11:2P:19:VAL:HG12	11:2P:27:HIS:HB3	1.87	0.56
32:2a:624:C:H2'	32:2a:625:G:H8	1.70	0.56
32:2a:946:A:H2'	32:2a:947:G:C8	2.40	0.56
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.86	0.56
33:2b:30:ARG:NH2	33:2b:195:ASP:OD1	2.39	0.56
39:2h:51:VAL:HG11	39:2h:60:ARG:HH12	1.71	0.56
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.87	0.56
6:1G:59:GLU:OE2	6:1G:138:GLN:NE2	2.37	0.56
27:15:16:ARG:HG3	27:15:17:ASP:N	2.20	0.56
32:1a:1310:G:OP2	44:1m:88:ARG:NH2	2.38	0.56
36:1e:100:VAL:HG13	36:1e:107:ARG:HH12	1.71	0.56
1:2A:468:G:N7	29:27:39:ARG:NH2	2.50	0.56
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.87	0.56
15:2T:107:ASP:OD2	15:2T:111:ARG:NH1	2.38	0.56
18:2W:65:LEU:HD12	18:2W:68:ARG:NH2	2.21	0.56
33:2b:128:GLU:OE1	33:2b:135:GLN:NE2	2.32	0.56
55:2x:74:C:OP1	61:2x:202:HOH:O	2.18	0.56
1:1A:1466:G:HO2'	1:1A:1546:C:HO2'	1.52	0.56
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.05	0.56
12:1Q:38:GLU:HG3	12:1Q:127:ILE:HB	1.88	0.56
32:1a:673:G:H2'	32:1a:674:G:C8	2.39	0.56
51:1t:90:GLN:HA	51:1t:93:GLU:HG3	1.88	0.56
20:2Y:13:VAL:HB	20:2Y:72:VAL:HG22	1.88	0.56
8:1I:75:LEU:HD22	8:1I:105:HIS:HD2	1.70	0.56
1:2A:1772:G:OP1	61:2A:3938:HOH:O	2.18	0.56
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	1.88	0.56
32:2a:444:C:H2'	32:2a:445:G:C8	2.40	0.56
32:2a:1327:C:H2'	32:2a:1328:C:C6	2.41	0.56
34:2c:52:LEU:HD11	34:2c:55:VAL:HG23	1.86	0.56
54:2w:103:ASP:OD2	54:2w:172:LYS:NZ	2.27	0.56
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.32	0.56
32:1a:56:U:H2'	32:1a:57:G:H8	1.70	0.56
32:1a:1456:G:N1	51:1t:51:GLU:OE2	2.35	0.56
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.87	0.56
1:2A:2314:C:H2'	1:2A:2315:G:H8	1.71	0.56
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.88	0.56
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.88	0.56
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.41	0.56
33:2b:73:THR:OG1	33:2b:170:GLU:OE2	2.20	0.56
1:1A:2155:G:H3'	1:1A:2156:G:C8	2.41	0.56
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.39	0.56
3:1D:95:LEU:HD11	3:1D:105:ILE:HD13	1.87	0.56
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.37	0.56
39:1h:49:GLU:OE2	39:1h:62:TYR:OH	2.24	0.56
1:2A:479:A:N3	1:2A:481:G:H5"	2.21	0.56
1:2A:1354:A:H2'	1:2A:1355:G:O4'	2.06	0.56
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.87	0.56
1:1A:184:C:H2'	1:1A:185:U:C6	2.41	0.56
61:1A:4338:HOH:O	11:1P:37:GLY:HA3	2.05	0.56
32:1a:560:U:O2'	32:1a:561:U:OP2	2.23	0.56
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.21	0.56
33:2b:155:LEU:HD21	33:2b:159:PRO:HD3	1.88	0.56
37:2f:100:ASN:HD21	49:2r:23:LYS:HE3	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:588:U:H2'	1:1A:589:C:C6	2.41	0.56
1:2A:494:G:OP1	18:2W:8:ARG:NH1	2.38	0.56
1:2A:589:C:P	11:2P:16:ARG:HH12	2.29	0.56
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.21	0.56
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.41	0.55
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.41	0.55
2:1B:91:C:H5'	12:1Q:18:LYS:HA	1.88	0.55
4:1E:59:VAL:HG21	4:1E:74:PRO:HB3	1.87	0.55
9:1N:29:LYS:HD3	9:1N:140:VAL:HB	1.88	0.55
29:17:5:TRP:NE1	29:17:7:PRO:HG3	2.21	0.55
32:1a:1277:C:H1'	32:1a:1282:C:O2	2.06	0.55
46:1o:6:GLU:OE2	46:1o:6:GLU:N	2.39	0.55
54:1w:222:MET:HG2	54:1w:238:ALA:HB3	1.87	0.55
1:2A:154(A):C:H42	1:2A:171:G:H1	1.54	0.55
1:2A:911:A:OP1	61:2A:3939:HOH:O	2.18	0.55
32:2a:518:C:P	54:2w:179:ARG:HH12	2.28	0.55
33:2b:28:PHE:CD1	33:2b:194:PRO:HG3	2.41	0.55
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.21	0.55
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.87	0.55
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.39	0.55
5:1F:9:ILE:HD13	5:1F:123:LEU:HD23	1.88	0.55
15:1T:128:GLU:C	15:1T:130:ALA:H	2.14	0.55
32:1a:1030(C):G:N7	32:1a:1031:G:N2	2.53	0.55
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.42	0.55
33:1b:223:ILE:HD12	33:1b:229:VAL:HA	1.89	0.55
50:2s:43:GLU:N	50:2s:43:GLU:OE1	2.39	0.55
34:1c:59:ARG:HG2	34:1c:64:VAL:HB	1.89	0.55
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.53	0.55
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.41	0.55
2:2B:75:G:O2'	21:2Z:85:HIS:NE2	2.28	0.55
35:2d:61:LYS:NZ	35:2d:72:GLU:OE1	2.37	0.55
1:1A:1252:G:N7	16:1U:36:ARG:NH1	2.53	0.55
2:1B:106:G:H5'	21:1Z:31:ARG:HB3	1.89	0.55
33:1b:158:LEU:HG	33:1b:182:ILE:HD11	1.87	0.55
34:1c:19:GLU:HG2	34:1c:54:ARG:HE	1.72	0.55
35:1d:140:VAL:HG11	35:1d:146:ILE:HD11	1.88	0.55
1:2A:869:G:O3'	12:2Q:6:ARG:NH1	2.39	0.55
38:2g:156:TRP:CD1	38:2g:156:TRP:H	2.24	0.55
55:2x:23:U:H2'	55:2x:24:G:C8	2.41	0.55
1:1A:671:C:N4	61:1A:4257:HOH:O	2.40	0.55
18:1W:11:ARG:HD3	18:1W:82:LEU:HD12	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1497:G:N7	61:1a:3836:HOH:O	2.33	0.55
34:1c:52:LEU:HD22	34:1c:53:ALA:H	1.71	0.55
1:2A:668:G:H5'	1:2A:669:G:OP2	2.06	0.55
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.40	0.55
6:2G:103:LEU:HD23	6:2G:106:LEU:HD23	1.88	0.55
32:2a:448:A:P	32:2a:485:G:H22	2.29	0.55
34:2c:12:LEU:HD11	45:2n:51:GLY:HA2	1.88	0.55
36:2e:93:PRO:HG2	39:2h:105:ARG:CZ	2.37	0.55
37:2f:35:ALA:HA	37:2f:67:MET:HB3	1.88	0.55
54:2w:187:GLU:HG2	54:2w:191:ARG:H	1.71	0.55
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.41	0.55
32:1a:881:G:P	43:1l:12:ARG:HH22	2.29	0.55
35:1d:20:TYR:HD1	35:1d:26:CYS:HB3	1.71	0.55
1:2A:994:C:OP2	16:2U:54:LYS:NZ	2.37	0.55
32:2a:17:U:H2'	32:2a:18:C:C6	2.42	0.55
32:2a:1404:5MC:O2	32:2a:1519:MA6:O2'	2.20	0.55
1:1A:1416:G:O2'	1:1A:1417:C:OP2	2.18	0.55
1:1A:2120:G:H2'	1:1A:2121:G:H8	1.72	0.55
11:1P:126:VAL:HG12	11:1P:148:LEU:HD13	1.87	0.55
1:2A:1029:A:N1	1:2A:2465:C:O2'	2.38	0.55
1:2A:1309:G:H4'	29:27:7:PRO:HB2	1.88	0.55
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.41	0.55
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.06	0.55
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.42	0.55
21:1Z:1:MET:H2	21:1Z:2:GLU:HA	1.69	0.55
32:1a:263:A:OP1	51:1t:79:ARG:NH1	2.40	0.55
32:1a:943:U:H1'	40:1i:124:GLN:HE22	1.71	0.55
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.88	0.55
38:1g:50:ILE:HG21	38:1g:61:VAL:HG11	1.89	0.55
1:2A:1021:A:H62	1:2A:1141:U:H3	1.53	0.55
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.06	0.55
32:2a:1175:G:H2'	32:2a:1176:A:C8	2.42	0.55
33:2b:15:VAL:HG13	33:2b:209:ARG:HG2	1.89	0.55
49:2r:26:LEU:HD21	49:2r:39:VAL:HG13	1.88	0.55
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.88	0.55
26:14:24:THR:OG1	26:14:25:TYR:N	2.34	0.55
32:1a:263:A:P	51:1t:79:ARG:HH12	2.30	0.55
44:1m:81:LEU:HD22	44:1m:88:ARG:HB2	1.88	0.55
47:1p:58:TYR:O	47:1p:61:SER:OG	2.22	0.55
1:2A:336:C:O2'	20:2Y:35:TYR:OH	2.25	0.55
1:2A:884:C:H3'	1:2A:885:C:C6	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.39	0.55
32:2a:1130:A:H2'	32:2a:1131:G:C8	2.42	0.55
54:2w:321:THR:OG1	54:2w:322:HIS:N	2.40	0.55
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.40	0.55
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.07	0.55
41:1j:9:ARG:NH2	41:1j:95:GLU:OE2	2.39	0.55
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.38	0.55
1:2A:1496:A:N3	1:2A:1577:C:O2'	2.38	0.55
1:2A:2313:C:H4'	6:2G:91:ARG:HG3	1.88	0.55
13:2R:100:LEU:HD21	13:2R:113:LEU:HD23	1.88	0.55
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.89	0.55
1:1A:774:A:N3	1:1A:774:A:H2'	2.22	0.54
1:1A:1073:A:H2'	1:1A:1074:G:H8	1.71	0.54
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.42	0.54
1:1A:2469:A:O2'	12:1Q:56:ARG:NE	2.40	0.54
38:1g:153:HIS:CE1	42:1k:58:PRO:HD2	2.41	0.54
50:1s:28:LYS:HB3	50:1s:47:HIS:HD2	1.71	0.54
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.40	0.54
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.42	0.54
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.89	0.54
32:2a:56:U:H2'	32:2a:57:G:H8	1.72	0.54
45:2n:21:TYR:OH	45:2n:23:ARG:NH2	2.40	0.54
6:1G:12:TYR:HA	6:1G:16:ARG:HG3	1.87	0.54
26:14:56:VAL:O	26:14:60:GLN:HB2	2.07	0.54
32:1a:414:A:H2'	32:1a:415:A:C8	2.42	0.54
33:1b:12:GLU:HB3	33:1b:213:LEU:HD21	1.90	0.54
1:2A:900:A:H2'	1:2A:901:A:H8	1.72	0.54
10:2O:49:ARG:NH2	32:2a:1423:G:OP1	2.32	0.54
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.88	0.54
32:2a:373:A:O2'	32:2a:451:A:N7	2.40	0.54
33:2b:184:VAL:HG13	33:2b:198:ASP:H	1.71	0.54
34:2c:37:GLN:HE22	45:2n:52:GLN:HB3	1.73	0.54
35:2d:76:ARG:NH2	35:2d:80:GLU:OE2	2.37	0.54
1:1A:1753:G:N1	1:1A:1756:G:OP2	2.39	0.54
21:1Z:40:ASP:HB3	21:1Z:43:GLU:HB2	1.90	0.54
33:1b:189:ASP:OD1	33:1b:189:ASP:N	2.37	0.54
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.90	0.54
9:2N:104:LYS:HA	9:2N:107:LEU:HD12	1.90	0.54
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.89	0.54
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.06	0.54
22:20:18:ALA:O	22:20:20:ARG:NH1	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:536:A:H2'	1:1A:537:C:C6	2.41	0.54
54:1w:161:GLU:OE2	54:1w:204:LYS:NZ	2.26	0.54
1:2A:288:C:H2'	1:2A:289:A:C8	2.43	0.54
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.42	0.54
1:2A:2331:G:O2'	22:20:43:THR:HG22	2.08	0.54
15:2T:27:THR:HB	15:2T:89:VAL:HG22	1.89	0.54
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.30	0.54
1:1A:1364:G:P	23:11:3:LYS:HG3	2.47	0.54
1:1A:1971:A:OP1	61:1A:4131:HOH:O	2.17	0.54
42:1k:84:VAL:HG23	42:1k:110:ASP:HA	1.89	0.54
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.42	0.54
1:2A:2340:G:H2'	1:2A:2341:G:H8	1.72	0.54
7:2H:121:ILE:HG13	7:2H:144:VAL:HG21	1.88	0.54
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	1.90	0.54
32:1a:142:G:H2'	32:1a:143:A:C8	2.42	0.54
32:1a:892:A:H2'	32:1a:893:C:C6	2.42	0.54
32:1a:1038:C:H2'	32:1a:1039:C:C6	2.42	0.54
32:1a:1303:C:OP1	61:1a:3809:HOH:O	2.18	0.54
1:2A:2504:U:OP2	61:2A:3937:HOH:O	2.18	0.54
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.43	0.54
6:2G:47:LYS:NZ	6:2G:80:PHE:O	2.31	0.54
1:1A:1951:U:O4	61:1A:4134:HOH:O	2.19	0.54
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.41	0.54
19:1X:50:LYS:HB3	19:1X:84:ALA:HB2	1.90	0.54
32:1a:473:G:OP2	47:1p:75:ARG:HD3	2.07	0.54
39:1h:86:ILE:HG21	39:1h:133:LEU:HD13	1.90	0.54
44:1m:50:GLU:HA	44:1m:53:VAL:HB	1.89	0.54
27:25:41:PRO:O	27:25:44:THR:OG1	2.23	0.54
32:2a:1009:G:H1	32:2a:1020:U:H3	1.56	0.54
3:1D:37:LEU:HD22	3:1D:87:ASN:ND2	2.23	0.54
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.07	0.54
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.43	0.54
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.42	0.54
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.08	0.54
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.40	0.54
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.72	0.54
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.89	0.54
39:2h:35:ILE:O	39:2h:39:LEU:HD12	2.07	0.54
50:2s:11:VAL:HG11	50:2s:16:LEU:HG	1.89	0.54
1:1A:1068:G:H1'	1:1A:1096:A:N3	2.22	0.54
6:1G:36:LYS:HD3	6:1G:95:ARG:HH12	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1W:71:VAL:HA	18:1W:107:LEU:HD23	1.90	0.54
32:1a:229:U:H5”	47:1p:33:ILE:HD13	1.90	0.54
32:1a:1291:G:H5”	38:1g:41:ARG:HH21	1.72	0.54
34:1c:17:ASP:O	34:1c:54:ARG:NH2	2.41	0.54
36:1e:78:HIS:CE1	36:1e:142:LEU:HD23	2.43	0.54
1:2A:141:A:H8	1:2A:1408:C:HO2’	1.54	0.54
1:2A:1532:C:H3’	1:2A:1533:G:H8	1.73	0.54
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.39	0.54
1:2A:2749:A:H1’	7:2H:63:SER:HB3	1.90	0.54
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.90	0.54
32:2a:1273:G:H3’	32:2a:1274:G:H8	1.72	0.54
32:2a:1330:U:H4’	44:2m:23:TYR:CE1	2.41	0.54
34:2c:113:ALA:HB2	34:2c:183:ASP:HB3	1.88	0.54
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.38	0.54
1:1A:2161:C:O2’	1:1A:2162:G:H8	1.90	0.54
32:1a:376:G:H4’	47:1p:5:ARG:HH11	1.72	0.54
32:1a:390:C:H2’	32:1a:391:G:C8	2.43	0.54
32:1a:1132:C:H2’	32:1a:1133:G:H8	1.72	0.54
33:1b:16:HIS:HD2	33:1b:18:GLY:H	1.56	0.54
36:1e:102:ALA:HB1	36:1e:106:PRO:HB2	1.88	0.54
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.22	0.54
1:2A:1266:G:O2’	1:2A:2012:G:O6	2.24	0.54
32:2a:297:G:N2	32:2a:300:A:OP2	2.40	0.54
32:2a:677:U:O2	32:2a:777:A:O2’	2.24	0.54
35:2d:11:LEU:HG	35:2d:66:ARG:HG2	1.89	0.54
51:2t:14:LYS:HG2	51:2t:18:GLN:HE21	1.72	0.54
32:1a:922:G:H4’	36:1e:20:GLN:HA	1.90	0.53
32:1a:1347:G:N2	32:1a:1373:G:H2’	2.23	0.53
1:2A:588:U:H2’	1:2A:589:C:C6	2.43	0.53
1:2A:2125:G:H1’	1:2A:2173:A:H61	1.73	0.53
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.40	0.53
32:2a:1239:A:H62	32:2a:1299:A:H62	1.56	0.53
33:2b:15:VAL:HG21	33:2b:213:LEU:HD22	1.90	0.53
33:2b:115:LEU:HD13	33:2b:145:LEU:HB2	1.89	0.53
34:2c:58:GLU:HB2	34:2c:65:ALA:HB3	1.90	0.53
34:2c:180:ALA:HB1	34:2c:203:PHE:CE1	2.44	0.53
38:2g:20:ASP:HB3	38:2g:23:VAL:HG22	1.90	0.53
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.89	0.53
51:2t:57:ARG:NH2	51:2t:100:ILE:HD12	2.22	0.53
6:1G:16:ARG:HB2	6:1G:17:PRO:HD3	1.89	0.53
7:1H:72:ILE:O	7:1H:76:VAL:HG23	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:22:LYS:HG2	60:1d:302:SF4:S4	2.48	0.53
36:1e:27:ARG:NH1	36:1e:27:ARG:HB2	2.24	0.53
44:1m:92:HIS:CE1	44:1m:98:VAL:HG21	2.43	0.53
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.07	0.53
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.90	0.53
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.41	0.53
15:2T:127:ALA:C	15:2T:129:ARG:H	2.16	0.53
32:2a:545:C:H5'	35:2d:72:GLU:HB2	1.89	0.53
32:2a:948:C:H2'	32:2a:949:A:H8	1.72	0.53
32:2a:977:A:O2'	32:2a:981:U:N3	2.41	0.53
32:2a:1110:A:OP2	61:2a:1804:HOH:O	2.19	0.53
32:2a:1292:U:H2'	32:2a:1293:G:C8	2.43	0.53
1:1A:2785:C:OP1	4:1E:41:LYS:HE3	2.08	0.53
32:1a:1073:U:H2'	32:1a:1074:G:H8	1.73	0.53
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.22	0.53
36:1e:90:VAL:O	36:1e:120:THR:HA	2.09	0.53
54:1w:198:THR:HB	54:1w:293:ILE:HG12	1.89	0.53
11:2P:88:LEU:HD11	11:2P:114:ILE:HD12	1.90	0.53
21:2Z:153:SER:OG	21:2Z:154:ASP:N	2.39	0.53
32:2a:1025:U:H1'	32:2a:1026:G:N7	2.23	0.53
45:2n:32:SER:O	45:2n:40:CYS:HA	2.08	0.53
1:1A:732:C:OP1	61:1A:4135:HOH:O	2.19	0.53
1:1A:1066:U:O2'	1:1A:1069:A:N6	2.37	0.53
1:1A:1670:C:OP1	61:1A:4126:HOH:O	2.19	0.53
1:1A:2146:C:H5"	1:1A:2147:G:C2	2.44	0.53
32:1a:1221:G:OP1	32:1a:1320:C:N4	2.32	0.53
1:2A:1339:G:H5"	19:2X:16:LYS:HD3	1.90	0.53
1:2A:1859:A:N6	1:2A:1883:G:O2'	2.41	0.53
1:2A:1968:G:OP1	61:2A:3913:HOH:O	2.19	0.53
1:2A:2113:U:N3	1:2A:2114:A:N7	2.56	0.53
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.44	0.53
19:2X:5:TYR:CZ	24:22:30:ARG:HB2	2.43	0.53
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.08	0.53
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD21	1.88	0.53
1:1A:1754:C:OP1	15:1T:96:ARG:NH1	2.39	0.53
33:1b:178:ARG:NH1	33:1b:196:LEU:O	2.42	0.53
54:1w:202:LEU:HD13	54:1w:285:LEU:HD11	1.89	0.53
1:2A:480:A:O2'	20:2Y:46:LYS:O	2.24	0.53
6:2G:5:VAL:HG21	6:2G:100:TRP:HB3	1.89	0.53
7:2H:3:ARG:NH2	7:2H:65:HIS:HB3	2.23	0.53
32:2a:1004:A:H5"	32:2a:1024:G:N2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:116:LYS:HD3	39:2h:127:LEU:HD13	1.90	0.53
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.08	0.53
5:1F:7:TYR:CD2	5:1F:24:LEU:HB2	2.44	0.53
21:1Z:125:LEU:HB3	21:1Z:165:VAL:HG13	1.90	0.53
42:1k:59:TYR:CZ	42:1k:63:LEU:HD21	2.43	0.53
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.07	0.53
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.22	0.53
6:2G:73:ALA:HB3	6:2G:85:GLY:H	1.73	0.53
26:24:48:ARG:HG3	26:24:52:THR:HG23	1.89	0.53
32:2a:15:G:H21	36:2e:18:ARG:HA	1.73	0.53
32:2a:728:A:H2'	32:2a:729:A:C8	2.43	0.53
32:2a:1175:G:H2'	32:2a:1176:A:H8	1.74	0.53
32:2a:1191:A:OP2	34:2c:3:ASN:ND2	2.42	0.53
56:2z:5:ALA:HB1	56:2z:7:CYS:SG	2.48	0.53
1:1A:919:G:N2	1:1A:2269:A:OP2	2.38	0.53
1:1A:1250:G:N7	11:1P:18:ARG:NH2	2.57	0.53
11:1P:29:LYS:HD3	11:1P:30:THR:HG23	1.89	0.53
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.90	0.53
32:2a:176:C:H2'	32:2a:177:C:C6	2.44	0.53
32:1a:1199:U:OP1	61:1a:3801:HOH:O	2.18	0.53
6:2G:38:VAL:HG22	6:2G:93:THR:HG22	1.91	0.53
23:21:44:PRO:HB2	23:21:46:LEU:HD13	1.91	0.53
32:2a:443:C:H2'	32:2a:444:C:H6	1.73	0.53
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.41	0.53
32:2a:1221:G:OP1	32:2a:1320:C:N4	2.42	0.53
33:2b:46:LYS:HA	33:2b:49:GLU:HG3	1.89	0.53
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.91	0.53
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	1.89	0.53
1:1A:800:A:H8	1:1A:800:A:OP1	1.92	0.53
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.44	0.53
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	1.91	0.53
1:2A:2254:C:OP2	61:2A:3941:HOH:O	2.19	0.53
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.23	0.53
32:2a:936:C:H2'	32:2a:937:A:O4'	2.08	0.53
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.74	0.53
10:1O:10:VAL:HG11	10:1O:16:ALA:HB3	1.91	0.53
32:1a:67:C:H2'	32:1a:68:G:C8	2.44	0.53
32:1a:684:A:N6	61:1a:3851:HOH:O	2.42	0.53
34:1c:134:ILE:HG23	34:1c:151:VAL:HB	1.91	0.53
45:1n:6:LEU:HB3	45:1n:23:ARG:NH2	2.23	0.53
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:998:C:OP1	61:1A:4132:HOH:O	2.18	0.52
1:1A:1068:G:H2'	1:1A:1096:A:O2'	2.09	0.52
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.45	0.52
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.43	0.52
44:1m:74:VAL:O	44:1m:78:ILE:HG12	2.09	0.52
46:1o:4:THR:HG1	46:1o:7:GLU:HG3	1.74	0.52
3:2D:121:PRO:HB3	3:2D:135:PHE:CE2	2.44	0.52
8:2I:38:LEU:HB2	8:2I:40:THR:HG23	1.91	0.52
41:2j:37:PRO:HA	41:2j:72:VAL:HG22	1.91	0.52
44:2m:80:ARG:HH12	50:2s:69:HIS:HE1	1.57	0.52
54:2w:174:GLU:OE1	54:2w:303:ARG:NH1	2.40	0.52
1:1A:883:G:H22	1:1A:893:C:H42	1.57	0.52
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.73	0.52
1:1A:2821:A:OP2	61:1R:301:HOH:O	2.19	0.52
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.39	0.52
32:1a:507:C:OP2	32:1a:508:C:O2'	2.19	0.52
1:2A:41:C:H2'	1:2A:42:G:C8	2.44	0.52
1:2A:884:C:H3'	1:2A:885:C:H6	1.74	0.52
1:2A:1204:A:H2	1:2A:1241:A:H62	1.56	0.52
1:2A:2563:U:O2	1:2A:2565:A:H8	1.93	0.52
7:2H:150:ALA:HA	7:2H:153:LYS:HG2	1.90	0.52
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.90	0.52
32:2a:67:C:H2'	32:2a:68:G:C8	2.45	0.52
32:2a:683:G:H2'	32:2a:684:A:C8	2.45	0.52
32:2a:1327:C:H5"	52:2u:20:LYS:HB3	1.91	0.52
1:1A:1093:G:H3'	1:1A:1094:U:C5'	2.40	0.52
8:1I:54:GLN:HG3	8:1I:57:ARG:NH1	2.25	0.52
8:1I:93:THR:O	8:1I:97:ILE:HG13	2.09	0.52
9:1N:73:THR:HB	9:1N:82:LEU:HD11	1.91	0.52
32:1a:1257:U:H5'	32:1a:1258:G:H5'	1.91	0.52
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.44	0.52
11:2P:59:LEU:HD11	30:28:10:ALA:HA	1.92	0.52
17:2V:1:MET:HE2	17:2V:43:GLU:HB2	1.92	0.52
34:2c:6:HIS:HD2	34:2c:7:PRO:HD2	1.74	0.52
42:2k:48:ILE:HD13	42:2k:64:ALA:HA	1.91	0.52
1:1A:2727:G:O2'	10:1O:70:LYS:NZ	2.42	0.52
7:1H:97:ARG:HD3	7:1H:104:GLU:OE2	2.10	0.52
32:1a:31:G:O2'	32:1a:48:C:N4	2.42	0.52
32:1a:162:A:C5	32:1a:163:C:H1'	2.44	0.52
39:1h:81:HIS:N	39:1h:138:TRP:O	2.40	0.52
1:2A:265:A:C8	1:2A:266:G:H1'	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.44	0.52
1:2A:1607:C:H5"	1:2A:1608:A:H5'	1.91	0.52
6:2G:20:ILE:HA	6:2G:25:TYR:HD2	1.74	0.52
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.44	0.52
33:2b:47:THR:HG22	33:2b:202:PRO:HG2	1.91	0.52
33:2b:134:GLU:O	33:2b:138:LEU:HG	2.09	0.52
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.44	0.52
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.43	0.52
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.44	0.52
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.42	0.52
19:1X:65:ARG:HE	19:1X:70:LEU:HD11	1.75	0.52
29:17:24:THR:O	29:17:28:ARG:HG3	2.10	0.52
1:2A:271(H):G:H4'	23:21:81:LYS:HG2	1.90	0.52
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.70	0.52
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.36	0.52
32:2a:1053:G:N7	32:2a:1200:C:H5"	2.24	0.52
39:2h:34:GLU:HB3	39:2h:118:VAL:HG11	1.91	0.52
39:2h:87:SER:HB2	39:2h:93:VAL:HB	1.92	0.52
42:2k:85:ARG:HE	42:2k:111:ASP:HB3	1.75	0.52
1:1A:1466:G:O2'	1:1A:1546:C:O2'	2.26	0.52
32:1a:711:G:H2'	32:1a:712:A:C8	2.45	0.52
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.92	0.52
35:1d:201:GLN:HA	35:1d:204:ILE:HD12	1.92	0.52
37:1f:36:ARG:NH2	37:1f:38:GLU:OE2	2.43	0.52
1:2A:2336:A:H61	22:20:43:THR:HG22	1.75	0.52
3:2D:20:ASP:OD1	3:2D:20:ASP:N	2.42	0.52
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.39	0.52
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	1.90	0.52
6:2G:173:LEU:HD22	6:2G:178:PHE:CE1	2.44	0.52
32:2a:1000:U:O4	32:2a:1001:A:N6	2.43	0.52
32:2a:1060:C:H5"	41:2j:51:ARG:HG2	1.91	0.52
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.24	0.52
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.25	0.52
1:1A:1114:G:H2'	1:1A:1115:G:C8	2.45	0.52
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.44	0.52
1:1A:2743:C:OP1	31:19:33:LYS:NZ	2.40	0.52
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.45	0.52
22:10:11:ARG:O	22:10:14:ARG:NH2	2.42	0.52
29:17:9:ARG:CZ	29:17:47:ARG:HG3	2.39	0.52
32:1a:975:A:N1	41:1j:48:THR:HB	2.24	0.52
32:1a:1366:C:O2'	41:1j:60:ARG:NH1	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1664:A:H2	10:2O:1:MET:HE1	1.74	0.52
5:2F:165:ARG:HG2	5:2F:168:ARG:HH21	1.73	0.52
8:2I:79:ILE:HD13	8:2I:92:VAL:HG21	1.92	0.52
32:2a:136:C:O2'	47:2p:65:GLN:NE2	2.27	0.52
32:2a:487:A:H2'	32:2a:488:C:O4'	2.09	0.52
32:2a:920:U:H2'	32:2a:921:U:C6	2.45	0.52
32:2a:1072:G:H2'	32:2a:1073:U:C6	2.44	0.52
34:2c:52:LEU:HD13	34:2c:68:VAL:HG13	1.91	0.52
32:1a:737:A:H2'	32:1a:738:C:C6	2.45	0.52
32:1a:1346:A:N1	32:1a:1374:A:H5"	2.25	0.52
36:1e:18:ARG:HH11	36:1e:27:ARG:HH12	1.58	0.52
44:1m:13:LYS:HA	44:1m:44:ARG:HH11	1.74	0.52
48:1q:81:ARG:HB3	48:1q:84:LEU:HD12	1.92	0.52
1:2A:2371:G:O2'	28:26:46:HIS:ND1	2.28	0.52
32:2a:109:A:H2'	32:2a:326:G:N2	2.25	0.52
33:2b:54:THR:HG22	33:2b:199:TYR:HB3	1.92	0.52
1:1A:1508:A:O2'	1:1A:1509:C:OP1	2.26	0.52
32:1a:1137:C:H4'	32:1a:1138:G:C2	2.44	0.52
37:1f:38:GLU:HB2	37:1f:64:GLN:HG2	1.90	0.52
1:2A:2112:G:C5	1:2A:2113:U:H1'	2.45	0.52
1:2A:2748:A:O2'	7:2H:63:SER:O	2.25	0.52
1:2A:2788:C:O2'	1:2A:2809:A:N3	2.43	0.52
32:2a:1121:U:H2'	32:2a:1122:U:C6	2.44	0.52
37:2f:3:ARG:HB3	37:2f:93:SER:HB2	1.92	0.52
1:1A:566:U:OP1	11:1P:29:LYS:HE3	2.09	0.52
32:1a:652:U:O4	32:1a:752:G:O2'	2.21	0.52
33:1b:171:ALA:HA	33:1b:174:VAL:HG22	1.92	0.52
34:1c:22:TRP:CE2	45:1n:54:PRO:HG2	2.45	0.52
38:1g:78:ARG:HH21	38:1g:156:TRP:HB3	1.75	0.52
1:2A:890:A:H2'	1:2A:892:G:C8	2.44	0.52
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.44	0.52
21:2Z:8:TYR:HB2	21:2Z:38:TYR:CE2	2.44	0.52
32:2a:1346:A:N1	32:2a:1374:A:H5"	2.25	0.52
37:2f:26:ILE:O	37:2f:30:LEU:HG	2.10	0.52
51:2t:43:LEU:O	51:2t:47:GLY:N	2.43	0.52
1:1A:185:U:H4'	1:1A:218:A:H4'	1.92	0.51
1:1A:666:G:H1'	30:18:4:MET:HE3	1.92	0.51
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.10	0.51
1:1A:1602:U:O4	61:1A:4117:HOH:O	2.18	0.51
2:1B:12:C:N3	22:10:74:ARG:NH2	2.58	0.51
2:1B:58:A:OP2	61:1B:302:HOH:O	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:26:LYS:HB3	3:1D:83:GLU:HG2	1.92	0.51
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.92	0.51
32:1a:828:A:H2'	32:1a:829:G:O4'	2.10	0.51
32:1a:1202:G:H2'	32:1a:1203:C:O4'	2.10	0.51
33:1b:69:LEU:HD13	33:1b:91:PRO:HB2	1.92	0.51
47:1p:75:ARG:O	47:1p:78:GLY:N	2.41	0.51
1:2A:27:G:N2	1:2A:512:G:H1'	2.25	0.51
1:2A:1355:G:O6	61:2A:3944:HOH:O	2.19	0.51
1:2A:2794:C:N4	1:2A:2802:G:O6	2.42	0.51
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.90	0.51
54:2w:103:ASP:HB3	54:2w:169:GLY:HA3	1.91	0.51
1:1A:228:A:H3'	1:1A:229:A:C5'	2.40	0.51
1:1A:1778:U:O2	61:1A:4136:HOH:O	2.19	0.51
1:1A:2134:A:H1'	1:1A:2159:G:O2'	2.10	0.51
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.10	0.51
2:1B:13:A:N1	2:1B:69:G:O2'	2.40	0.51
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.11	0.51
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.93	0.51
32:1a:1226:C:O2'	44:1m:111:LYS:NZ	2.43	0.51
35:1d:43:HIS:HB3	35:1d:46:LYS:HD2	1.91	0.51
1:2A:139:G:H2'	1:2A:140:G:N7	2.25	0.51
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.45	0.51
21:2Z:18:LEU:HG	21:2Z:23:LYS:HB2	1.91	0.51
32:2a:1030(D):A:H8	32:2a:1031:G:C8	2.28	0.51
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.92	0.51
40:2i:45:ALA:HA	40:2i:48:GLU:HG2	1.91	0.51
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.46	0.51
32:1a:60:A:N1	32:1a:107:G:O2'	2.38	0.51
32:1a:118:U:O4	61:1a:3810:HOH:O	2.19	0.51
32:1a:1244:C:H2'	32:1a:1245:A:C8	2.46	0.51
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.93	0.51
34:1c:11:ARG:HB3	34:1c:15:THR:HB	1.92	0.51
37:1f:60:PHE:CE2	49:1r:78:LEU:HD21	2.45	0.51
38:1g:27:ILE:HD13	38:1g:40:ALA:HA	1.92	0.51
1:2A:624:C:OP1	61:2A:3943:HOH:O	2.19	0.51
1:2A:1200:C:H1'	16:2U:2:PRO:HG3	1.91	0.51
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.10	0.51
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.43	0.51
16:2U:113:ALA:O	16:2U:117:GLN:NE2	2.43	0.51
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.45	0.51
40:2i:6:GLY:HA3	40:2i:80:GLY:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.42	0.51
1:1A:583:G:OP2	16:1U:10:ARG:NH1	2.37	0.51
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.42	0.51
1:1A:2390:U:P	30:18:35:GLN:HE22	2.33	0.51
32:1a:719:C:N4	49:1r:71:LYS:HE2	2.25	0.51
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.45	0.51
32:1a:1162:C:H42	32:1a:1174:G:H1	1.59	0.51
50:1s:20:LEU:HD21	50:1s:43:GLU:HG2	1.91	0.51
1:2A:307:G:N1	1:2A:310:A:OP2	2.41	0.51
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.26	0.51
32:2a:624:C:H2'	32:2a:625:G:C8	2.45	0.51
32:2a:629:G:H2'	32:2a:630:G:O4'	2.11	0.51
32:2a:1244:C:H2'	32:2a:1245:A:C8	2.46	0.51
54:2w:228:GLY:HA3	54:2w:232:VAL:HB	1.91	0.51
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.29	0.51
1:1A:1452:A:OP2	61:1A:4138:HOH:O	2.19	0.51
1:1A:1557:C:H5"	1:1A:1558:A:OP2	2.11	0.51
1:1A:2065:C:H2'	1:1A:2066:C:H6	1.75	0.51
1:1A:2648:C:H2'	1:1A:2649:U:C6	2.46	0.51
32:1a:1016:A:HO2'	32:1a:1217:C:HO2'	1.48	0.51
32:1a:1207:2MG:H2'	32:1a:1208:C:C6	2.45	0.51
1:2A:839:U:H2'	1:2A:840:C:C6	2.44	0.51
1:2A:1906:G:OP2	1:2A:1929:G:O2'	2.29	0.51
1:2A:2185:C:H2'	1:2A:2186:G:O4'	2.11	0.51
10:2O:22:ILE:HG23	10:2O:41:ALA:HA	1.93	0.51
32:2a:1005:A:H1'	32:2a:1036:G:H1	1.75	0.51
32:2a:1070:U:H2'	32:2a:1071:C:C6	2.45	0.51
38:2g:75:VAL:HG12	38:2g:88:PRO:HA	1.92	0.51
39:2h:37:ARG:HH21	39:2h:38:ILE:HD11	1.75	0.51
45:2n:22:THR:HG22	45:2n:33:VAL:HB	1.92	0.51
48:2q:32:TYR:O	48:2q:34:LYS:N	2.37	0.51
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.46	0.51
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.11	0.51
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.11	0.51
1:1A:1971:A:OP2	3:1D:242:ARG:NH2	2.43	0.51
18:1W:10:VAL:HG21	18:1W:103:ILE:HD12	1.93	0.51
37:1f:44:GLY:HA2	37:1f:59:TYR:CZ	2.45	0.51
1:2A:975:C:OP1	61:2A:3942:HOH:O	2.19	0.51
1:2A:1297:C:O2'	1:2A:1302:A:N1	2.44	0.51
2:2B:66:A:H61	2:2B:109:C:H5'	1.76	0.51
6:2G:41:GLN:O	6:2G:43:LEU:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.92	0.51
35:2d:103:ASN:OD1	35:2d:114:ARG:NH2	2.40	0.51
54:2w:110:GLU:OE1	54:2w:112:ARG:NH1	2.42	0.51
1:1A:518:G:H2'	1:1A:519:U:C6	2.46	0.51
1:1A:2090:G:N2	23:11:45:ASN:OD1	2.30	0.51
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.93	0.51
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.93	0.51
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.42	0.51
1:2A:1653:G:C6	13:2R:9:LYS:HB2	2.46	0.51
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.75	0.51
33:2b:204:ASN:ND2	33:2b:207:ALA:H	2.08	0.51
35:2d:20:TYR:HD1	35:2d:26:CYS:HB3	1.76	0.51
1:1A:295:G:H4'	20:1Y:1:MET:HE3	1.93	0.51
1:1A:372:G:OP2	23:11:69:LYS:NZ	2.37	0.51
1:1A:721:C:H2'	1:1A:722:A:C8	2.46	0.51
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.91	0.51
32:1a:192:U:H2'	32:1a:193:C:C6	2.44	0.51
35:1d:9:CYS:O	35:1d:13:ARG:HG3	2.10	0.51
36:1e:77:PRO:HD2	36:1e:142:LEU:HD22	1.93	0.51
9:2N:103:VAL:HG11	9:2N:120:LEU:HD22	1.93	0.51
32:2a:973:G:H3'	32:2a:974:A:H5"	1.91	0.51
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.75	0.51
1:1A:1060:U:H3	1:1A:1088:A:H8	1.58	0.51
2:1B:42:C:O2	6:1G:93:THR:N	2.25	0.51
32:1a:577:G:OP1	61:1a:3811:HOH:O	2.19	0.51
45:1n:45:ARG:O	45:1n:49:HIS:HD2	1.93	0.51
50:1s:28:LYS:HB3	50:1s:47:HIS:CD2	2.45	0.51
50:1s:42:PRO:HA	50:1s:45:VAL:HG23	1.91	0.51
1:2A:271(K):U:O2	8:2I:50:ARG:HD3	2.11	0.51
1:2A:271(P):C:O3'	8:2I:42:SER:OG	2.28	0.51
1:2A:1653:G:H3'	13:2R:2:ARG:HD3	1.92	0.51
1:2A:2307:G:N1	6:2G:43:LEU:O	2.40	0.51
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.43	0.51
20:2Y:5:MET:HG2	20:2Y:30:VAL:HG11	1.93	0.51
32:2a:298:A:H8	32:2a:298:A:OP1	1.94	0.51
36:2e:43:LEU:H	36:2e:65:ASN:HD22	1.59	0.51
42:2k:84:VAL:HG21	42:2k:95:ILE:HD11	1.92	0.51
46:2o:15:PHE:CE1	46:2o:84:LYS:HD3	2.46	0.51
52:2u:3:LYS:HD3	52:2u:14:TRP:CD1	2.46	0.51
1:1A:284:U:H2'	1:1A:285:C:C6	2.46	0.51
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.24	0.51
32:1a:533:A:OP1	61:1a:3808:HOH:O	2.18	0.51
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.28	0.51
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.59	0.51
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.46	0.51
32:2a:979:C:OP1	32:2a:1223:C:N4	2.43	0.51
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.44	0.51
1:1A:1418:G:OP2	61:1A:4137:HOH:O	2.19	0.50
1:1A:1669:A:OP2	61:1A:4122:HOH:O	2.18	0.50
1:1A:2062:A:H2	56:1z:5:ALA:HB1	1.76	0.50
1:1A:2131:G:C2	1:1A:2157:G:H1'	2.45	0.50
1:1A:2552:OMU:OP2	61:1A:4127:HOH:O	2.20	0.50
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.75	0.50
32:1a:73:G:H1	32:1a:96:U:H3	1.59	0.50
32:1a:1369:C:H2'	32:1a:1370:G:C8	2.46	0.50
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.46	0.50
1:2A:760:G:OP1	61:2A:3940:HOH:O	2.18	0.50
2:2B:38:C:H2'	2:2B:39:A:C8	2.46	0.50
25:23:46:ASN:O	25:23:50:VAL:HG22	2.10	0.50
32:2a:1004:A:H5"	32:2a:1024:G:H22	1.75	0.50
32:2a:1179:A:H5"	40:2i:102:LEU:HD12	1.93	0.50
32:2a:1289:A:OP1	52:2u:10:ARG:NH2	2.44	0.50
55:2x:4:G:H1	55:2x:69:C:N4	2.09	0.50
1:1A:1922:G:H2'	1:1A:1923:U:C6	2.46	0.50
1:1A:2149:G:H2'	1:1A:2150:U:O4'	2.11	0.50
32:1a:443:C:H2'	32:1a:444:C:C6	2.47	0.50
35:1d:98:GLU:OE2	35:1d:103:ASN:ND2	2.35	0.50
41:1j:61:GLU:OE1	45:1n:45:ARG:NE	2.43	0.50
1:2A:1223:G:N2	1:2A:1226:A:OP2	2.38	0.50
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.42	0.50
4:2E:54:GLN:HB2	4:2E:76:ARG:HG3	1.93	0.50
24:22:9:GLN:HE22	24:22:56:GLN:HB3	1.76	0.50
30:28:28:GLY:O	30:28:36:LYS:NZ	2.32	0.50
32:2a:58:C:O2'	32:2a:388:G:N7	2.37	0.50
1:1A:995:C:O2	9:1N:3:THR:OG1	2.29	0.50
7:1H:98:LEU:HG	7:1H:125:VAL:HG23	1.92	0.50
14:1S:61:ASN:ND2	14:1S:64:GLU:HG3	2.26	0.50
33:1b:133:LYS:O	33:1b:136:VAL:HG22	2.11	0.50
34:1c:144:SER:O	34:1c:144:SER:OG	2.20	0.50
41:1j:7:LYS:HB3	41:1j:71:LEU:HD13	1.93	0.50
42:1k:21:ILE:HG12	42:1k:30:VAL:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.46	0.50
51:1t:34:LYS:HZ2	51:1t:80:ARG:HH12	1.58	0.50
1:2A:2841:C:H2'	1:2A:2842:G:C8	2.46	0.50
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.92	0.50
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.11	0.50
52:2u:9:ARG:HH12	52:2u:10:ARG:HH21	1.59	0.50
1:1A:748:G:O6	18:1W:90:ARG:NH1	2.43	0.50
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.45	0.50
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	1.93	0.50
32:1a:389:A:C6	32:1a:390:C:H1'	2.47	0.50
32:1a:1049:U:C6	32:1a:1201:A:H5'	2.47	0.50
46:1o:68:ARG:O	46:1o:72:ARG:HG3	2.10	0.50
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.46	0.50
21:2Z:28:MET:O	21:2Z:35:ARG:N	2.35	0.50
43:2l:89:ARG:HE	43:2l:91:LYS:HA	1.76	0.50
1:1A:236:C:H2'	1:1A:237:C:C6	2.46	0.50
1:1A:1091:G:H2'	1:1A:1092:C:C6	2.47	0.50
1:1A:1441:G:H2'	1:1A:1442:G:H8	1.77	0.50
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.94	0.50
34:1c:134:ILE:HG22	34:1c:168:ALA:HB3	1.93	0.50
38:1g:46:ALA:O	38:1g:50:ILE:HG12	2.12	0.50
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.75	0.50
1:2A:822:U:OP2	61:2A:3945:HOH:O	2.19	0.50
1:2A:1364:G:P	23:21:3:LYS:HG3	2.52	0.50
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.10	0.50
3:2D:71:ASP:HB3	3:2D:103:ARG:HH12	1.77	0.50
7:2H:3:ARG:HE	7:2H:54:ARG:HH12	1.59	0.50
32:2a:1226:C:O2'	44:2m:111:LYS:NZ	2.26	0.50
44:2m:92:HIS:CE1	44:2m:98:VAL:HG11	2.46	0.50
47:2p:1:MET:HE3	47:2p:3:LYS:HD2	1.92	0.50
1:1A:264:C:O2'	1:1A:265:A:H2'	2.12	0.50
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.11	0.50
1:1A:2177:C:H2'	1:1A:2178:C:O4'	2.11	0.50
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.47	0.50
26:14:59:PHE:HD1	26:14:60:GLN:HG2	1.75	0.50
32:1a:881:G:OP2	43:1l:12:ARG:NH2	2.45	0.50
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.95	0.50
32:1a:1272:G:H2'	32:1a:1273:G:O4'	2.12	0.50
35:1d:33:MET:HE3	35:1d:37:PRO:HA	1.92	0.50
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.92	0.50
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.12	0.50
1:2A:1670:C:OP1	61:2A:3947:HOH:O	2.20	0.50
1:2A:2135:A:C4	1:2A:2136:C:H5	2.30	0.50
1:2A:2887:U:H2'	1:2A:2888:C:C6	2.47	0.50
6:2G:42:GLY:HA2	6:2G:89:GLY:HA3	1.93	0.50
32:2a:663:A:O3'	49:2r:64:ARG:NH2	2.43	0.50
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.41	0.50
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.75	0.50
1:1A:1062:G:C2	1:1A:1088:A:H2'	2.46	0.50
1:1A:1082:U:C4	1:1A:1086:A:C6	2.99	0.50
1:1A:2120:G:H2'	1:1A:2121:G:C8	2.47	0.50
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.47	0.50
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.92	0.50
47:1p:52:ASP:CG	47:1p:55:ARG:HG2	2.36	0.50
1:2A:615:G:OP1	5:2F:40:GLN:NE2	2.37	0.50
1:2A:959:A:N3	1:2A:2457:U:O2'	2.41	0.50
1:2A:2887:U:H2'	1:2A:2888:C:H6	1.77	0.50
5:2F:153:SER:HB2	5:2F:189:THR:HA	1.93	0.50
6:2G:41:GLN:O	6:2G:43:LEU:HD22	2.11	0.50
32:2a:1327:C:OP1	52:2u:12:LYS:NZ	2.43	0.50
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.11	0.50
36:2e:72:GLN:O	36:2e:75:THR:HG22	2.12	0.50
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.93	0.50
1:1A:876:C:H2'	1:1A:877:U:O4'	2.12	0.50
1:1A:2062:A:C2	56:1z:5:ALA:HB1	2.47	0.50
5:1F:170:LEU:HD13	5:1F:172:TRP:CZ2	2.47	0.50
26:14:46:GLN:HB3	26:14:48:ARG:HG2	1.93	0.50
33:1b:174:VAL:O	33:1b:178:ARG:HG3	2.12	0.50
1:2A:580:C:H2'	1:2A:581:C:C6	2.47	0.50
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.47	0.50
26:24:48:ARG:HD2	26:24:51:ASP:O	2.11	0.50
31:29:10:ILE:HD12	31:29:32:HIS:HA	1.92	0.50
32:2a:1005:A:H1'	32:2a:1036:G:N1	2.27	0.50
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.47	0.50
32:2a:1095:U:H5"	32:2a:1109:C:O2	2.10	0.50
36:2e:27:ARG:HD3	36:2e:47:LYS:HB3	1.93	0.50
1:1A:1920:OMC:HM22	1:1A:1921:G:O4'	2.12	0.50
7:1H:41:MET:HE2	7:1H:65:HIS:HA	1.94	0.50
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.47	0.50
33:1b:119:GLU:OE2	33:1b:153:ARG:NH1	2.45	0.50
33:1b:132:LYS:O	33:1b:136:VAL:HG13	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:10:PRO:HB2	44:1m:13:LYS:HD2	1.94	0.50
1:2A:586:A:N1	1:2A:809:G:O2'	2.41	0.50
1:2A:2853:C:H2'	1:2A:2854:G:C8	2.47	0.50
6:2G:35:GLU:HG3	6:2G:36:LYS:HG2	1.93	0.50
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.93	0.50
32:2a:1292:U:H2'	32:2a:1293:G:H8	1.77	0.50
50:2s:49:ILE:HD13	50:2s:71:LEU:HD21	1.94	0.50
1:1A:1081:U:H6	1:1A:1081:U:H3'	1.77	0.49
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.47	0.49
1:1A:2250:G:O2'	1:1A:2496:C:OP1	2.26	0.49
1:1A:2336:A:H61	22:10:43:THR:CG2	2.24	0.49
19:1X:2:LYS:HZ1	19:1X:38:GLU:CD	2.19	0.49
32:1a:149:A:H2'	32:1a:150:C:C6	2.46	0.49
32:1a:1049:U:OP1	45:1n:3:ARG:HB2	2.11	0.49
36:1e:152:ARG:NH2	39:1h:107:LEU:O	2.45	0.49
40:1i:8:GLY:C	40:1i:76:ALA:HB1	2.37	0.49
1:2A:829:A:N7	1:2A:2248:C:H5'	2.27	0.49
1:2A:1261:C:OP2	18:2W:83:LYS:NZ	2.37	0.49
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.11	0.49
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.96	0.49
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.12	0.49
32:2a:942:G:H21	40:2i:124:GLN:NE2	2.08	0.49
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	1.94	0.49
4:1E:15:PHE:HA	4:1E:19:ARG:O	2.11	0.49
32:1a:115:G:H4'	32:1a:116:A:O5'	2.12	0.49
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.46	0.49
1:2A:247:G:H4'	1:2A:386:G:C5	2.47	0.49
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.27	0.49
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.27	0.49
1:2A:2232:U:P	23:21:40:ARG:HH12	2.35	0.49
3:2D:75:ILE:HG21	3:2D:99:ASP:HB2	1.95	0.49
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.12	0.49
8:2I:77:LEU:HD13	8:2I:101:LEU:HB2	1.94	0.49
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.47	0.49
37:2f:8:ILE:HD11	37:2f:79:LEU:HD13	1.94	0.49
1:1A:1783:A:N7	61:1A:4222:HOH:O	2.35	0.49
1:1A:2439:A:H5'	1:1A:2439:A:C8	2.46	0.49
4:1E:181:LEU:HD11	15:1T:6:LEU:HD12	1.94	0.49
8:1I:87:LYS:HD3	8:1I:87:LYS:H	1.78	0.49
21:1Z:130:PRO:HA	21:1Z:133:ILE:HD11	1.94	0.49
32:1a:925:G:H1'	32:1a:1502:A:C4	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:64:LEU:HD13	35:1d:198:VAL:HG21	1.94	0.49
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.30	0.49
12:2Q:138:ASP:OD2	21:2Z:81:ARG:NH1	2.45	0.49
20:2Y:23:ARG:HA	20:2Y:23:ARG:NE	2.27	0.49
32:2a:73:G:H1	32:2a:96:U:H3	1.60	0.49
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.26	0.49
44:2m:80:ARG:HH12	50:2s:69:HIS:CE1	2.29	0.49
1:1A:370:G:H8	1:1A:370:G:OP2	1.95	0.49
1:1A:2648:C:H2'	1:1A:2649:U:H6	1.76	0.49
3:1D:108:PRO:HD2	3:1D:111:LEU:HD22	1.95	0.49
18:1W:31:GLU:OE1	61:1W:301:HOH:O	2.19	0.49
21:1Z:119:GLU:O	21:1Z:121:HIS:N	2.45	0.49
32:1a:7:G:H5'	32:1a:298:A:O4'	2.13	0.49
32:1a:449:C:N3	47:1p:42:ARG:NH1	2.59	0.49
32:1a:1326:C:OP1	52:1u:12:LYS:HE2	2.12	0.49
36:1e:105:VAL:HG22	36:1e:106:PRO:HD3	1.93	0.49
1:2A:41:C:H2'	1:2A:42:G:H8	1.77	0.49
1:2A:652(D):C:H2'	1:2A:652(E):G:O4'	2.12	0.49
1:2A:1324:G:N7	61:2A:4023:HOH:O	2.34	0.49
32:2a:302:G:O2'	32:2a:556:C:H5"	2.13	0.49
32:2a:974:A:P	45:2n:41:ARG:HH21	2.35	0.49
32:2a:1216:G:H5"	45:2n:5:ALA:HB2	1.94	0.49
35:2d:105:VAL:HG21	35:2d:126:ILE:HD13	1.95	0.49
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.12	0.49
1:1A:2167:U:H3	1:1A:2171:A:N6	2.07	0.49
6:1G:115:ARG:NH1	44:1m:6:GLY:O	2.45	0.49
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.30	0.49
42:1k:48:ILE:O	42:1k:50:TYR:N	2.42	0.49
48:1q:3:LYS:HD2	48:1q:60:ILE:HD11	1.95	0.49
50:1s:36:ARG:HH12	50:1s:75:ALA:HB3	1.77	0.49
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.13	0.49
1:2A:1637:A:H4'	1:2A:2711:A:O2'	2.12	0.49
1:2A:2882:A:OP1	13:2R:96:ARG:NE	2.40	0.49
32:2a:21:G:H2'	32:2a:22:G:C8	2.48	0.49
32:2a:443:C:H2'	32:2a:444:C:C6	2.48	0.49
32:2a:583:A:H2'	32:2a:584:G:O4'	2.12	0.49
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.47	0.49
1:1A:29:U:H2'	1:1A:30:G:C8	2.48	0.49
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.12	0.49
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.94	0.49
1:2A:212:G:H2'	1:2A:213:A:O4'	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:655:A:H8	1:2A:656:G:O4'	1.96	0.49
1:2A:1014:U:H2'	1:2A:1015:G:H8	1.78	0.49
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.37	0.49
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	1.94	0.49
40:2i:23:ASN:OD1	40:2i:23:ASN:N	2.45	0.49
44:2m:11:ARG:O	44:2m:13:LYS:N	2.45	0.49
54:2w:184:PRO:C	54:2w:186:THR:H	2.20	0.49
1:1A:2116:G:H3'	1:1A:2117:A:C8	2.47	0.49
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.13	0.49
3:1D:18:VAL:HG12	3:1D:211:ARG:NH2	2.28	0.49
10:1O:87:ILE:HD12	10:1O:91:LEU:HA	1.94	0.49
33:1b:12:GLU:HA	33:1b:15:VAL:HG13	1.94	0.49
1:2A:774:A:H2'	1:2A:774:A:N3	2.28	0.49
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.12	0.49
1:2A:2448:A:OP1	61:2A:3911:HOH:O	2.19	0.49
5:2F:36:VAL:O	5:2F:40:GLN:HG3	2.12	0.49
32:2a:405:U:O4	35:2d:2:GLY:N	2.45	0.49
32:2a:1320:C:O2	50:2s:36:ARG:NH2	2.41	0.49
34:2c:181:ASN:ND2	34:2c:204:LEU:HD12	2.25	0.49
38:2g:47:CYS:O	38:2g:50:ILE:HG22	2.13	0.49
42:2k:17:GLY:O	42:2k:80:VAL:HA	2.13	0.49
44:2m:11:ARG:C	44:2m:13:LYS:H	2.20	0.49
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.24	0.49
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.13	0.49
10:1O:64:ARG:HB2	10:1O:83:ALA:HB3	1.94	0.49
32:1a:392:G:H2'	32:1a:393:A:C8	2.47	0.49
32:1a:515:G:H2'	32:1a:516:PSU:O4'	2.13	0.49
32:1a:677:U:H3	32:1a:713:G:H22	1.60	0.49
42:1k:33:THR:HA	42:1k:39:PRO:HA	1.95	0.49
1:2A:441:U:H2'	1:2A:442:G:C8	2.48	0.49
1:2A:828:U:H4'	1:2A:831:G:N1	2.27	0.49
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.26	0.49
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.12	0.49
1:2A:2807:G:C2	1:2A:2808:U:H1'	2.47	0.49
4:2E:2:LYS:HB2	4:2E:95:ILE:HD12	1.95	0.49
32:2a:438:G:O2'	32:2a:494:U:O4	2.28	0.49
32:2a:537:G:H5"	43:2l:113:ARG:NH1	2.27	0.49
32:2a:1130:A:OP1	40:2i:16:ARG:NH2	2.44	0.49
32:2a:1206:G:O2'	34:2c:193:TYR:HA	2.13	0.49
33:2b:55:PHE:HA	33:2b:58:ILE:HD12	1.95	0.49
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:67:LYS:C	48:2q:69:LYS:H	2.21	0.49
1:1A:2563:U:H4'	10:1O:28:SER:HA	1.95	0.49
3:1D:37:LEU:HD13	3:1D:62:TYR:HB2	1.94	0.49
32:1a:181:G:N2	32:1a:182:U:O4	2.28	0.49
35:1d:61:LYS:HG3	35:1d:203:VAL:HG13	1.95	0.49
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.94	0.49
1:2A:288:C:H2'	1:2A:289:A:H8	1.76	0.49
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.60	0.49
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.37	0.49
3:2D:25:THR:HG21	3:2D:113:VAL:HG21	1.95	0.49
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.95	0.49
32:2a:176:C:H2'	32:2a:177:C:H6	1.77	0.49
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.13	0.49
48:2q:81:ARG:HB3	48:2q:84:LEU:HD12	1.95	0.49
1:1A:1014:U:OP2	61:1A:4139:HOH:O	2.20	0.49
1:1A:1653:G:H3'	13:1R:2:ARG:HD3	1.94	0.49
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.45	0.49
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.47	0.49
32:1a:258:G:H2'	32:1a:259:G:H8	1.78	0.49
32:1a:1073:U:H2'	32:1a:1074:G:C8	2.47	0.49
32:1a:1292:U:P	38:1g:41:ARG:HH22	2.35	0.49
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.48	0.49
37:1f:61:LEU:HB3	37:1f:63:TYR:HE2	1.77	0.49
39:1h:13:ILE:O	39:1h:17:THR:HG23	2.13	0.49
1:2A:359:A:H2'	1:2A:360:G:O4'	2.13	0.49
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.27	0.49
1:2A:800:A:H8	1:2A:800:A:OP1	1.96	0.49
1:2A:2175:C:H2'	1:2A:2176:A:C8	2.48	0.49
32:2a:662:G:H2'	32:2a:663:A:C8	2.48	0.49
32:2a:674:G:H21	42:2k:116:HIS:HB2	1.78	0.49
32:2a:1225:A:H2'	32:2a:1225:A:N3	2.27	0.49
34:2c:35:GLU:O	34:2c:39:ILE:HG12	2.13	0.49
50:2s:50:ALA:HA	50:2s:58:VAL:O	2.13	0.49
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.21	0.48
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.46	0.48
2:1B:66:A:N6	2:1B:109:C:H5'	2.26	0.48
28:16:10:LEU:HG	28:16:54:ILE:HG13	1.95	0.48
32:1a:923:A:OP1	36:1e:21:ALA:HB2	2.13	0.48
33:1b:215:LEU:O	33:1b:219:VAL:HG12	2.13	0.48
41:1j:23:ILE:O	41:1j:27:ALA:N	2.44	0.48
51:1t:58:LYS:O	51:1t:62:LEU:HD12	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:10:G:H2'	1:2A:11:G:C8	2.47	0.48
1:2A:109:G:H2'	1:2A:110:G:O4'	2.13	0.48
1:2A:810:U:C4	11:2P:29:LYS:O	2.66	0.48
7:2H:3:ARG:HH11	7:2H:4:ILE:H	1.60	0.48
9:2N:29:LYS:HD3	9:2N:140:VAL:HB	1.95	0.48
32:2a:352:C:O2'	32:2a:354:G:OP1	2.28	0.48
32:2a:449:C:O2	47:2p:42:ARG:NH1	2.46	0.48
32:2a:593:G:H1	32:2a:646:U:H3	1.61	0.48
32:2a:1130:A:H4'	40:2i:3:GLN:HE22	1.78	0.48
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.13	0.48
1:1A:1068:G:O2'	1:1A:1070:A:N7	2.42	0.48
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.95	0.48
32:1a:537:G:H5"	43:1l:113:ARG:NH1	2.28	0.48
32:1a:826:C:H2'	32:1a:827:U:C6	2.49	0.48
32:1a:1301:U:O2'	32:1a:1302:U:H3'	2.13	0.48
1:2A:1359:A:H2	1:2A:1372:U:O4	1.97	0.48
1:2A:1821:A:H2'	1:2A:1822:G:H8	1.78	0.48
2:2B:48:A:H4'	14:2S:95:HIS:CD2	2.48	0.48
1:1A:476:G:H4'	1:1A:502:A:N1	2.29	0.48
1:1A:2175:C:H2'	1:1A:2176:A:C8	2.49	0.48
14:1S:24:LEU:HB2	14:1S:85:VAL:HG12	1.95	0.48
32:1a:750:G:N3	46:1o:23:GLY:HA3	2.27	0.48
32:1a:924:C:O2'	32:1a:1502:A:N1	2.43	0.48
34:1c:20:SER:HB3	45:1n:54:PRO:HG3	1.95	0.48
42:1k:31:THR:HA	42:1k:42:TRP:HA	1.94	0.48
49:1r:44:LEU:HD21	49:1r:70:ILE:HG21	1.96	0.48
55:1x:75:C:H2'	55:1x:76:8AN:H1'	1.95	0.48
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.13	0.48
1:2A:1782:C:H1'	1:2A:2609:U:H5"	1.94	0.48
1:2A:2684:U:OP1	15:2T:53:ARG:HD3	2.12	0.48
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.13	0.48
9:2N:30:ILE:HG22	9:2N:34:LEU:HD22	1.95	0.48
18:2W:19:LEU:HB3	27:25:25:LEU:HG	1.96	0.48
29:27:26:GLY:O	29:27:30:VAL:HG23	2.13	0.48
35:2d:70:ILE:HG13	35:2d:74:GLN:HB2	1.94	0.48
38:2g:155:ARG:O	38:2g:155:ARG:HG2	2.13	0.48
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.95	0.48
44:2m:106:ASN:OD1	44:2m:106:ASN:N	2.44	0.48
1:1A:373:U:H2'	1:1A:374:A:H8	1.79	0.48
1:1A:1359:A:H61	1:1A:1372:U:H3	1.61	0.48
32:1a:520:A:O2'	43:1l:73:GLU:OE2	2.24	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:927:G:O2'	32:1a:1503:A:N7	2.42	0.48
35:1d:157:LEU:O	35:1d:161:ASN:ND2	2.46	0.48
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.48	0.48
1:2A:2136:C:N3	1:2A:2155:G:C6	2.81	0.48
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.48	0.48
6:2G:114:ILE:HB	6:2G:117:PHE:HB2	1.95	0.48
14:2S:99:LYS:NZ	14:2S:103:GLU:OE2	2.30	0.48
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.96	0.48
35:2d:112:VAL:H	35:2d:116:GLN:NE2	2.12	0.48
38:2g:49:ILE:HD13	38:2g:118:VAL:HG12	1.95	0.48
42:2k:58:PRO:O	42:2k:62:GLN:N	2.45	0.48
1:1A:1010:A:N3	1:1A:1153:C:H1'	2.29	0.48
1:1A:2130:U:H5'	1:1A:2132:U:O2'	2.13	0.48
1:1A:2146:C:H4'	1:1A:2147:G:H5"	1.95	0.48
7:1H:3:ARG:NH1	7:1H:4:ILE:H	2.12	0.48
32:1a:1004:A:N7	32:1a:1036:G:N1	2.61	0.48
32:1a:1251:A:H2'	32:1a:1252:A:C8	2.48	0.48
35:1d:20:TYR:CD1	35:1d:26:CYS:HB3	2.48	0.48
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.95	0.48
5:2F:135:LYS:HB2	5:2F:138:GLU:HG3	1.96	0.48
32:2a:1187:G:H5'	40:2i:113:LYS:NZ	2.27	0.48
38:2g:92:SER:O	38:2g:95:ARG:N	2.47	0.48
39:2h:49:GLU:OE2	39:2h:62:TYR:OH	2.19	0.48
44:2m:11:ARG:HB2	44:2m:12:ASN:HD22	1.77	0.48
1:1A:2139:C:N4	1:1A:2152:G:H1	2.08	0.48
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.28	0.48
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.60	0.48
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.13	0.48
32:1a:136:C:H1'	47:1p:1:MET:HG3	1.95	0.48
32:1a:160:A:H2'	32:1a:161:A:O4'	2.13	0.48
33:1b:150:SER:OG	33:1b:151:GLY:N	2.46	0.48
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.79	0.48
1:2A:1810:A:H2'	1:2A:1811:G:O4'	2.13	0.48
1:2A:2103:C:H42	1:2A:2186:G:H1	1.61	0.48
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.12	0.48
26:24:64:GLY:C	26:24:66:SER:H	2.21	0.48
32:2a:634:C:H2'	32:2a:635:G:H8	1.79	0.48
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.48	0.48
32:2a:1270:C:H2'	32:2a:1271:G:C8	2.48	0.48
37:2f:96:PRO:HB3	49:2r:30:ASP:CG	2.38	0.48
49:2r:21:LYS:HD3	49:2r:57:GLY:HA3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1394:U:H2'	1:1A:1395:A:O4'	2.14	0.48
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.47	0.48
1:1A:1915:5MU:H1'	54:1w:286:ARG:HD2	1.95	0.48
1:1A:2138:C:N4	1:1A:2153:G:H1	2.11	0.48
32:1a:437:U:H5'	35:1d:155:LEU:HD11	1.95	0.48
32:1a:691:G:H2'	32:1a:692:U:C6	2.49	0.48
32:1a:1071:C:OP1	36:1e:27:ARG:NH2	2.46	0.48
32:1a:1130:A:OP2	40:1i:62:TYR:OH	2.26	0.48
1:2A:184:C:H2'	1:2A:185:U:H6	1.78	0.48
1:2A:478:A:N1	1:2A:500:G:H4'	2.29	0.48
1:2A:2103:C:H2'	1:2A:2104:G:O4'	2.14	0.48
20:2Y:83:THR:HG21	20:2Y:99:CYS:HB2	1.94	0.48
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.27	0.48
43:2l:86:ARG:NH1	61:2l:301:HOH:O	2.47	0.48
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.13	0.48
1:1A:2131:G:N1	1:1A:2157:G:H1'	2.29	0.48
1:1A:2189:U:H2'	1:1A:2190:G:C8	2.49	0.48
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.96	0.48
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.49	0.48
38:1g:78:ARG:HG3	38:1g:156:TRP:CZ3	2.47	0.48
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.95	0.48
44:1m:29:ARG:HD3	44:1m:64:TRP:CE2	2.48	0.48
47:1p:23:ASP:OD2	47:1p:25:ARG:NH2	2.46	0.48
1:2A:34:C:N4	1:2A:447:A:H61	2.10	0.48
1:2A:629:G:H5"	1:2A:650:C:O2'	2.13	0.48
1:2A:922:U:H2'	1:2A:923:C:C6	2.48	0.48
1:2A:2140:C:N3	1:2A:2151:G:O6	2.47	0.48
5:2F:127:GLU:HA	5:2F:196:LEU:HD11	1.95	0.48
32:2a:272:C:H2'	32:2a:273:A:H8	1.79	0.48
32:2a:1135:U:H4'	32:2a:1136:U:C5	2.48	0.48
54:2w:126:ASP:OD2	54:2w:182:ARG:NH2	2.47	0.48
1:1A:247:G:H4'	1:1A:386:G:C5	2.48	0.48
1:1A:551:G:O2'	1:1A:1220:A:N3	2.32	0.48
1:1A:581:C:H2'	1:1A:582:G:C8	2.48	0.48
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.79	0.48
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.36	0.48
1:1A:1176:G:H21	1:1A:1178:C:P	2.37	0.48
1:1A:1779:U:H2'	61:1A:4222:HOH:O	2.13	0.48
1:1A:2128:C:H42	1:1A:2160:G:H1	1.60	0.48
1:1A:2494:G:O2'	12:1Q:80:GLU:HA	2.14	0.48
32:1a:370:C:H2'	32:1a:371:G:C8	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:473:G:H2'	32:1a:474:G:H8	1.78	0.48
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.47	0.48
32:1a:1070:U:H2'	32:1a:1071:C:H6	1.78	0.48
33:1b:115:LEU:HB2	33:1b:145:LEU:HD22	1.96	0.48
35:1d:129:ASN:N	35:1d:129:ASN:OD1	2.47	0.48
37:1f:15:ASP:OD1	37:1f:17:SER:N	2.39	0.48
54:1w:218:ARG:NH1	54:1w:220:ASP:OD2	2.47	0.48
1:2A:1297:C:H2'	1:2A:1298:C:H6	1.78	0.48
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.13	0.48
1:2A:2117:A:O2'	1:2A:2118:U:H5"	2.14	0.48
3:2D:71:ASP:CG	3:2D:103:ARG:HH22	2.20	0.48
8:2I:14:ASP:O	8:2I:17:GLN:HB3	2.14	0.48
11:2P:121:LYS:O	11:2P:123:LEU:N	2.46	0.48
28:26:12:GLU:OE1	28:26:19:ARG:NH1	2.47	0.48
32:2a:370:C:H2'	32:2a:371:G:H8	1.78	0.48
32:2a:521:G:H4'	43:2l:73:GLU:HG2	1.94	0.48
32:2a:1356:G:H2'	32:2a:1357:A:C8	2.49	0.48
34:2c:113:ALA:O	34:2c:116:VAL:HG22	2.14	0.48
54:2w:106:ASP:HA	54:2w:167:ALA:HB3	1.94	0.48
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.29	0.48
1:1A:1922:G:H2'	1:1A:1923:U:H6	1.79	0.48
8:1I:27:ARG:HD3	23:11:71:TYR:CE2	2.49	0.48
9:1N:21:LYS:HD3	9:1N:26:LEU:HD13	1.96	0.48
28:16:38:LYS:HB2	28:16:49:HIS:CE1	2.48	0.48
32:1a:624:C:H2'	32:1a:625:G:C8	2.48	0.48
32:1a:983:A:H1'	32:1a:1049:U:O2	2.14	0.48
33:1b:59:GLU:HB3	33:1b:221:LEU:HD11	1.96	0.48
35:1d:156:GLU:HB3	35:1d:160:GLN:HE21	1.79	0.48
36:1e:45:PHE:CD2	36:1e:47:LYS:HE2	2.48	0.48
47:1p:75:ARG:HG3	47:1p:80:PHE:HD2	1.79	0.48
1:2A:224:G:H2'	1:2A:225:A:O4'	2.14	0.48
1:2A:1453:U:O2'	1:2A:1455:G:N7	2.44	0.48
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.49	0.48
1:2A:2724:C:OP1	4:2E:118:LYS:NZ	2.46	0.48
3:2D:166:GLN:HB2	3:2D:174:ILE:HG22	1.95	0.48
16:2U:79:PHE:CZ	16:2U:83:LEU:HD11	2.49	0.48
32:2a:1003:G:H4'	32:2a:1003:G:OP1	2.12	0.48
32:2a:1397:C:H5"	32:2a:1398:A:C8	2.49	0.48
33:2b:68:ILE:HG12	33:2b:161:ALA:HB3	1.94	0.48
36:2e:6:PHE:HE1	36:2e:36:ASP:HB3	1.78	0.48
41:2j:81:THR:HA	41:2j:84:GLN:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:848:G:H2'	1:1A:849:A:C8	2.49	0.47
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.49	0.47
4:1E:93:VAL:HG22	61:1E:403:HOH:O	2.14	0.47
6:1G:36:LYS:HD3	6:1G:95:ARG:NH1	2.28	0.47
20:1Y:86:ARG:HB3	20:1Y:98:VAL:HG23	1.96	0.47
26:14:58:ARG:HE	50:1s:68:GLY:H	1.62	0.47
32:1a:108:G:C6	51:1t:15:ARG:HG2	2.48	0.47
32:1a:370:C:H2'	32:1a:371:G:H8	1.79	0.47
32:1a:1037:C:H2'	32:1a:1038:C:C6	2.48	0.47
1:2A:1278:A:H2'	1:2A:1279:G:C8	2.48	0.47
1:2A:2575:C:OP2	61:2A:3948:HOH:O	2.20	0.47
21:2Z:100:VAL:HG11	21:2Z:134:PRO:HG2	1.96	0.47
32:2a:1015:A:H1'	32:2a:1219:U:H5'	1.95	0.47
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.79	0.47
32:2a:1267:C:O2	32:2a:1327:C:H4'	2.14	0.47
32:2a:1452:C:H5'	32:2a:1457:G:C4	2.49	0.47
34:2c:131:ARG:HH21	34:2c:135:LYS:HE3	1.79	0.47
50:2s:4:SER:HB3	50:2s:7:LYS:HD2	1.95	0.47
1:1A:1745(A):C:H5'	1:1A:1746:G:OP2	2.14	0.47
1:1A:1802:A:N1	1:1A:1822:G:H1'	2.29	0.47
1:1A:2166:G:H2'	1:1A:2167:U:C6	2.49	0.47
1:1A:2531:A:N3	1:1A:2658:C:O2'	2.47	0.47
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.30	0.47
21:1Z:152:ALA:HB3	21:1Z:167:PRO:HA	1.96	0.47
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.45	0.47
32:1a:269:C:H2'	32:1a:270:A:C8	2.49	0.47
32:1a:501:C:H2'	32:1a:502:G:C8	2.49	0.47
32:1a:512:U:H2'	32:1a:513:C:C6	2.49	0.47
32:1a:530:G:H22	32:1a:1492:A:H61	1.61	0.47
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	1.96	0.47
39:1h:34:GLU:HB3	39:1h:118:VAL:HG11	1.96	0.47
40:1i:28:VAL:HG22	40:1i:63:ILE:HD13	1.96	0.47
1:2A:2109:U:C2'	1:2A:2110:G:H5'	2.44	0.47
1:2A:2275:C:H6	1:2A:2275:C:H5'	1.79	0.47
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.49	0.47
1:2A:2685:G:O6	61:2A:3935:HOH:O	2.17	0.47
24:22:16:LEU:HD13	24:22:20:GLU:HB3	1.96	0.47
25:23:26:LEU:HD21	25:23:46:ASN:HB2	1.95	0.47
32:2a:7:G:H2'	36:2e:119:LEU:HD22	1.96	0.47
32:2a:1046:A:H3'	32:2a:1047:G:H8	1.79	0.47
50:2s:40:ILE:HB	50:2s:67:VAL:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:226:G:H21	1:1A:228:A:H62	1.61	0.47
1:1A:579:G:H2'	1:1A:580:C:C6	2.49	0.47
1:1A:2059:A:H2'	1:1A:2503:2MA:HM23	1.96	0.47
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.14	0.47
1:1A:2355:C:H1'	22:10:39:ARG:HH21	1.78	0.47
35:1d:83:SER:HA	35:1d:89:THR:HG21	1.97	0.47
47:1p:45:THR:HG23	47:1p:47:ASP:H	1.78	0.47
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.40	0.47
54:1w:317:ILE:HD13	54:1w:339:LEU:HG	1.95	0.47
1:2A:1639:U:C2'	1:2A:1640:C:H5"	2.45	0.47
3:2D:101:GLU:OE2	3:2D:103:ARG:NE	2.39	0.47
10:2O:35:VAL:HG13	10:2O:65:THR:HG23	1.96	0.47
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.40	0.47
34:2c:164:ARG:HG2	34:2c:165:THR:H	1.79	0.47
51:2t:57:ARG:NH1	51:2t:101:GLY:O	2.42	0.47
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.14	0.47
1:1A:2189:U:H2'	1:1A:2190:G:H8	1.78	0.47
32:1a:392:G:H2'	32:1a:393:A:H8	1.80	0.47
32:1a:562:C:H1'	43:1l:15:ARG:HB3	1.96	0.47
32:1a:859:A:OP2	32:1a:869:G:N2	2.44	0.47
32:1a:977:A:H1'	32:1a:982:U:O4	2.13	0.47
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.79	0.47
6:2G:109:VAL:HG23	26:24:33:VAL:HG21	1.95	0.47
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.95	0.47
14:2S:62:LYS:HB3	14:2S:97:ARG:NE	2.28	0.47
32:2a:384:G:H2'	32:2a:385:C:C6	2.49	0.47
32:2a:1216:G:H5"	45:2n:5:ALA:CB	2.43	0.47
33:2b:167:PRO:HG2	33:2b:192:SER:HB3	1.96	0.47
35:2d:117:ALA:O	35:2d:121:VAL:HG23	2.14	0.47
37:2f:82:ARG:HB2	37:2f:85:VAL:HG23	1.97	0.47
44:2m:14:ARG:NE	44:2m:42:ALA:HA	2.29	0.47
44:2m:68:GLY:H	44:2m:71:ARG:HB2	1.79	0.47
46:2o:4:THR:HG1	46:2o:7:GLU:HG3	1.79	0.47
54:2w:222:MET:HG2	54:2w:238:ALA:HB3	1.95	0.47
55:2x:12:A:H2'	55:2x:13:A:O4'	2.15	0.47
1:1A:1800:C:OP2	3:1D:266:SER:OG	2.27	0.47
8:1I:77:LEU:HB3	8:1I:142:VAL:HG22	1.95	0.47
32:1a:565:U:H3'	32:1a:566:G:H2'	1.96	0.47
32:1a:783:C:OP1	32:1a:1515:C:O2'	2.30	0.47
39:1h:51:VAL:HG11	39:1h:60:ARG:HH12	1.79	0.47
44:1m:67:GLU:HG3	44:1m:71:ARG:NH2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:492:A:H2'	1:2A:493:G:O4'	2.15	0.47
1:2A:827:U:OP1	61:2A:3949:HOH:O	2.20	0.47
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.49	0.47
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.49	0.47
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.48	0.47
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.45	0.47
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.29	0.47
33:2b:97:TRP:CH2	33:2b:173:ALA:HA	2.49	0.47
34:2c:20:SER:OG	34:2c:36:ASP:OD2	2.22	0.47
39:2h:86:ILE:HD11	39:2h:136:GLU:HG2	1.94	0.47
44:2m:68:GLY:O	44:2m:72:ALA:N	2.47	0.47
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.97	0.47
1:1A:1889:A:H1'	1:1A:2087:G:O4'	2.15	0.47
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.49	0.47
8:1I:9:LEU:HD21	8:1I:35:LEU:HD13	1.96	0.47
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.14	0.47
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.15	0.47
32:1a:9:G:OP2	36:1e:121:LYS:NZ	2.45	0.47
32:1a:92:C:H2'	32:1a:93:G:C8	2.49	0.47
32:1a:1091:U:O2'	32:1a:1093:A:N7	2.45	0.47
35:1d:156:GLU:O	35:1d:160:GLN:HG3	2.14	0.47
45:1n:3:ARG:O	45:1n:7:ILE:N	2.38	0.47
47:1p:39:TYR:CZ	47:1p:41:PRO:HB3	2.50	0.47
1:2A:536:A:H2'	1:2A:537:C:C6	2.50	0.47
1:2A:1200:C:H5'	61:2A:4061:HOH:O	2.13	0.47
2:2B:38:C:H2'	2:2B:39:A:H8	1.79	0.47
32:2a:7:G:H5'	32:2a:298:A:O4'	2.15	0.47
32:2a:109:A:C6	32:2a:326:G:C6	3.03	0.47
32:2a:688:G:H5'	42:2k:46:GLY:C	2.40	0.47
33:2b:42:ILE:HG21	33:2b:202:PRO:O	2.14	0.47
33:2b:87:ARG:HD2	33:2b:234:PRO:HD2	1.96	0.47
36:2e:105:VAL:HG21	36:2e:128:PRO:HB3	1.95	0.47
54:2w:312:VAL:HG23	54:2w:324:LEU:HG	1.96	0.47
1:1A:300:A:P	20:1Y:86:ARG:HH22	2.37	0.47
1:1A:858:U:O2	1:1A:2268:A:H2'	2.14	0.47
1:1A:1155:A:OP1	16:1U:55:ARG:HD3	2.15	0.47
1:1A:1942:5MC:OP2	1:1A:1943:U:O2'	2.25	0.47
2:1B:24:G:N7	2:1B:56:G:H2'	2.29	0.47
5:1F:24:LEU:HD13	5:1F:115:ALA:HA	1.96	0.47
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.15	0.47
20:1Y:21:LYS:HE2	20:1Y:21:LYS:HB3	1.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:72:ARG:HD3	21:1Z:72:ARG:HA	1.68	0.47
32:1a:45:U:H2'	32:1a:46:G:C8	2.50	0.47
32:1a:109:A:C6	32:1a:326:G:C6	3.02	0.47
32:1a:153:C:H2'	32:1a:154:C:C6	2.49	0.47
32:1a:413:G:N2	32:1a:428:G:H1'	2.29	0.47
32:1a:447:G:O6	32:1a:485:G:O2'	2.30	0.47
32:1a:580:U:H2'	32:1a:581:G:O4'	2.15	0.47
32:1a:1145:C:H4'	32:1a:1146:A:H8	1.79	0.47
32:1a:1236:A:H2'	32:1a:1237:C:C6	2.50	0.47
33:1b:24:TRP:HZ3	33:1b:29:ALA:HB2	1.80	0.47
36:1e:110:LEU:HD13	36:1e:118:ILE:HD13	1.96	0.47
41:1j:30:SER:HB3	41:1j:81:THR:HG23	1.96	0.47
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.79	0.47
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.49	0.47
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.14	0.47
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.47	0.47
1:2A:2110:G:C2	1:2A:2120:G:H1'	2.50	0.47
1:2A:2122:U:H2'	1:2A:2123:G:C8	2.50	0.47
1:2A:2242:G:OP1	61:2A:3950:HOH:O	2.20	0.47
1:2A:2564:A:OP1	1:2A:2648:C:H4'	2.15	0.47
4:2E:28:ALA:HB3	4:2E:93:VAL:HG13	1.96	0.47
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.48	0.47
15:2T:53:ARG:O	15:2T:59:THR:HG23	2.14	0.47
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.96	0.47
32:2a:343:U:O2'	32:2a:344:A:H2'	2.15	0.47
32:2a:960:U:H2'	32:2a:960:U:O2	2.15	0.47
34:2c:68:VAL:HG12	34:2c:70:VAL:HG23	1.97	0.47
38:2g:152:ALA:O	38:2g:155:ARG:HD3	2.15	0.47
1:1A:1071:G:H1'	1:1A:1089:G:C2	2.50	0.47
1:1A:1670:C:OP2	61:1A:4122:HOH:O	2.21	0.47
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.97	0.47
1:1A:1865:G:N2	1:1A:1877:A:OP2	2.45	0.47
1:1A:2462:U:H1'	1:1A:2491:U:O4	2.15	0.47
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.14	0.47
21:1Z:52:SER:O	21:1Z:53:ILE:HG12	2.15	0.47
32:1a:1048:G:OP1	45:1n:3:ARG:HB3	2.15	0.47
32:1a:1132:C:H2'	32:1a:1133:G:C8	2.49	0.47
32:1a:1175:G:H2'	32:1a:1176:A:H8	1.79	0.47
35:1d:108:LEU:HB3	35:1d:110:PHE:CE1	2.49	0.47
40:1i:3:GLN:HG2	40:1i:20:ARG:NH2	2.30	0.47
1:2A:817:C:O2'	1:2A:839:U:OP1	2.25	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:826:U:H4'	11:2P:55:ARG:HB3	1.97	0.47
1:2A:862:G:H2'	1:2A:863:A:O4'	2.14	0.47
1:2A:2065:C:H4'	1:2A:2251:OMG:HM22	1.95	0.47
21:2Z:102:LEU:HD23	21:2Z:137:ILE:HB	1.97	0.47
32:2a:382:A:H2'	32:2a:383:A:C8	2.50	0.47
35:2d:176:LEU:HD12	35:2d:177:ASP:H	1.80	0.47
36:2e:78:HIS:HB3	39:2h:107:LEU:HD12	1.96	0.47
47:2p:60:LEU:HD12	47:2p:60:LEU:HA	1.74	0.47
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.50	0.47
6:1G:181:ARG:HG2	6:1G:182:LYS:H	1.80	0.47
9:1N:36:GLY:HA2	9:1N:38:HIS:CE1	2.50	0.47
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.50	0.47
32:1a:618:C:H5'	32:1a:619:U:H5"	1.97	0.47
32:1a:1212:U:H4'	32:1a:1213:A:C8	2.50	0.47
36:1e:60:TYR:CE1	36:1e:64:ARG:HD2	2.49	0.47
38:1g:99:LEU:HD23	38:1g:102:ARG:HH12	1.80	0.47
1:2A:515:A:H1'	1:2A:581:C:H1'	1.97	0.47
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.80	0.47
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.50	0.47
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.50	0.47
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.30	0.47
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.79	0.47
35:2d:64:LEU:HB2	35:2d:198:VAL:HG11	1.97	0.47
36:2e:60:TYR:CE1	36:2e:64:ARG:HD2	2.49	0.47
1:1A:657:U:H2'	1:1A:658:C:C6	2.49	0.47
1:1A:2698:U:O4	61:1A:4141:HOH:O	2.20	0.47
6:1G:149:VAL:HG22	6:1G:150:ASP:H	1.80	0.47
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.50	0.47
41:1j:13:HIS:HB3	41:1j:68:HIS:CD2	2.50	0.47
1:2A:403:U:H4'	1:2A:404:C:H5'	1.96	0.47
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.14	0.47
2:2B:14:U:H1'	2:2B:108:U:O2'	2.15	0.47
3:2D:71:ASP:CB	3:2D:103:ARG:HH12	2.28	0.47
3:2D:183:ARG:HD2	3:2D:185:VAL:HG22	1.97	0.47
14:2S:71:ARG:NH1	14:2S:107:GLU:OE2	2.48	0.47
32:2a:253:U:H2'	32:2a:254:G:C8	2.50	0.47
32:2a:1015:A:N3	32:2a:1218:C:O2'	2.44	0.47
32:2a:1124:G:H5'	41:2j:38:ILE:HG23	1.96	0.47
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.50	0.47
1:1A:582:G:H2'	1:1A:583:G:C8	2.50	0.46
1:1A:1665:A:H2'	1:1A:1666:G:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.30	0.46
1:1A:2112:G:H2'	1:1A:2112:G:N3	2.30	0.46
1:1A:2188:C:H2'	1:1A:2189:U:O4'	2.15	0.46
14:1S:3:ARG:HD3	14:1S:3:ARG:HA	1.60	0.46
14:1S:61:ASN:ND2	14:1S:64:GLU:H	2.04	0.46
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.13	0.46
32:1a:859:A:H2'	32:1a:860:A:O4'	2.14	0.46
37:1f:11:ASN:HB3	37:1f:14:LEU:HG	1.98	0.46
55:1x:75:C:H2'	55:1x:76:8AN:C1'	2.45	0.46
1:2A:1821:A:H2'	1:2A:1822:G:C8	2.50	0.46
1:2A:2728:U:H2'	1:2A:2729:G:C8	2.50	0.46
5:2F:130:ALA:H	5:2F:142:TRP:CD1	2.33	0.46
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.49	0.46
21:2Z:163:LEU:HD23	21:2Z:163:LEU:HA	1.73	0.46
32:2a:501:C:OP1	43:2l:117:ARG:NH2	2.45	0.46
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	1.97	0.46
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.96	0.46
33:2b:77:ALA:HA	33:2b:80:ILE:HG22	1.96	0.46
34:2c:184:TYR:HA	34:2c:200:ALA:O	2.16	0.46
44:2m:38:GLY:O	44:2m:55:ARG:NH1	2.48	0.46
6:1G:132:ASN:HA	6:1G:157:ILE:O	2.15	0.46
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.97	0.46
15:1T:98:LYS:HB3	15:1T:100:TYR:CE2	2.50	0.46
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.50	0.46
32:1a:1367:C:H5'	41:1j:60:ARG:CZ	2.44	0.46
39:1h:36:LEU:C	39:1h:38:ILE:H	2.23	0.46
40:1i:17:VAL:HG23	40:1i:63:ILE:HG12	1.97	0.46
49:1r:66:LEU:O	49:1r:70:ILE:HG13	2.15	0.46
1:2A:121:G:H4'	1:2A:149:A:H5'	1.97	0.46
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.50	0.46
1:2A:1014:U:H2'	1:2A:1015:G:C8	2.50	0.46
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.16	0.46
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.79	0.46
6:2G:56:ALA:O	6:2G:60:LEU:HB2	2.16	0.46
26:24:57:GLU:CB	26:24:58:ARG:HD2	2.45	0.46
26:24:57:GLU:HA	26:24:58:ARG:HA	1.75	0.46
32:2a:1073:U:H2'	32:2a:1074:G:C8	2.50	0.46
33:2b:48:MET:HA	33:2b:51:LEU:HD12	1.96	0.46
39:2h:49:GLU:HG2	39:2h:62:TYR:HE2	1.80	0.46
40:2i:3:GLN:HE21	40:2i:20:ARG:NH2	2.14	0.46
44:2m:106:ASN:HB2	44:2m:107:ALA:H	1.57	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:2n:57:ARG:HG2	45:2n:58:LYS:N	2.31	0.46
7:1H:3:ARG:HE	7:1H:54:ARG:HH12	1.63	0.46
16:1U:117:GLN:H	16:1U:117:GLN:HG2	1.48	0.46
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.50	0.46
26:14:16:CYS:HB2	26:14:36:CYS:HB3	1.96	0.46
28:16:26:ASN:HD21	28:16:28:ARG:NH2	2.13	0.46
32:1a:1137:C:H5'	32:1a:1138:G:C4	2.51	0.46
44:1m:87:TYR:CZ	44:1m:91:ARG:HD2	2.50	0.46
47:1p:40:ASP:HB3	47:1p:48:TRP:HB3	1.98	0.46
1:2A:1359:A:C2	1:2A:1372:U:O4	2.68	0.46
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.97	0.46
1:2A:2167:U:H2'	1:2A:2168:G:H21	1.80	0.46
1:2A:2206:G:H5"	1:2A:2207:G:N7	2.31	0.46
1:2A:2788:C:N3	1:2A:2789:C:N4	2.64	0.46
6:2G:7:LEU:HD21	6:2G:107:LEU:HD12	1.97	0.46
8:2I:90:GLY:O	8:2I:121:LYS:NZ	2.44	0.46
13:2R:13:HIS:CE1	13:2R:16:HIS:HB2	2.51	0.46
26:24:26:SER:OG	26:24:27:THR:N	2.48	0.46
32:2a:713:G:H2'	32:2a:714:G:C8	2.51	0.46
32:2a:839:U:H3'	32:2a:840:C:H5'	1.98	0.46
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.51	0.46
32:2a:1277:C:O2'	32:2a:1279:A:H1'	2.15	0.46
32:2a:1331:G:O6	52:2u:7:ARG:NH2	2.47	0.46
35:2d:57:ARG:HH22	36:2e:107:ARG:HD3	1.81	0.46
44:2m:15:VAL:HG11	44:2m:48:LEU:HD11	1.97	0.46
53:2v:16:U:H2'	53:2v:17:G:O4'	2.14	0.46
1:1A:388:G:O2'	1:1A:389:G:N7	2.48	0.46
1:1A:686:G:N2	1:1A:788:A:H61	2.14	0.46
1:1A:1115:G:H2'	1:1A:1116:C:O4'	2.15	0.46
1:1A:1357:U:H2'	1:1A:1358:G:O4'	2.16	0.46
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.48	0.46
14:1S:41:ASP:O	14:1S:45:GLY:N	2.43	0.46
21:1Z:91:LEU:HD21	21:1Z:96:VAL:HG11	1.98	0.46
27:15:40:LYS:HD3	27:15:46:CYS:HA	1.97	0.46
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.14	0.46
35:1d:111:ALA:HB1	35:1d:116:GLN:HG2	1.96	0.46
41:1j:55:LYS:HE3	41:1j:56:HIS:CE1	2.50	0.46
42:1k:48:ILE:C	42:1k:50:TYR:H	2.23	0.46
1:2A:89:G:C6	1:2A:90:U:C4	3.04	0.46
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.30	0.46
1:2A:2127:G:O2'	1:2A:2173:A:N3	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2352:A:N6	1:2A:2365:G:O2'	2.49	0.46
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.16	0.46
6:2G:135:LEU:H	6:2G:135:LEU:HD12	1.80	0.46
21:2Z:7:ALA:O	21:2Z:62:PRO:HD3	2.15	0.46
32:2a:392:G:H2'	32:2a:393:A:C8	2.51	0.46
32:2a:976:G:OP1	45:2n:32:SER:N	2.45	0.46
32:2a:1228:C:P	44:2m:108:ARG:HH22	2.38	0.46
32:2a:1466:C:H2'	32:2a:1467:G:O4'	2.15	0.46
34:2c:52:LEU:HA	34:2c:70:VAL:HG22	1.98	0.46
38:2g:18:TYR:HB3	38:2g:59:LEU:HD22	1.97	0.46
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.16	0.46
40:2i:29:ASN:HD21	40:2i:65:VAL:N	2.12	0.46
44:2m:14:ARG:HB2	44:2m:17:VAL:HG23	1.97	0.46
48:2q:12:SER:HB3	48:2q:20:THR:HB	1.97	0.46
51:2t:82:SER:O	51:2t:86:ARG:HG3	2.15	0.46
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.51	0.46
22:10:43:THR:O	22:10:43:THR:HG23	2.16	0.46
23:11:44:PRO:HB2	23:11:46:LEU:HD13	1.98	0.46
32:1a:189(C):C:H2'	32:1a:189(D):C:O4'	2.14	0.46
32:1a:736:C:H2'	32:1a:737:A:H8	1.80	0.46
39:1h:121:ASP:HB2	39:1h:125:ARG:NH2	2.31	0.46
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.98	0.46
1:2A:647:G:H8	1:2A:647:G:O5'	1.99	0.46
1:2A:900:A:H2'	1:2A:901:A:C8	2.51	0.46
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.15	0.46
1:2A:1259:G:H2'	1:2A:1260:G:C8	2.50	0.46
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.97	0.46
32:2a:509:A:N3	32:2a:543:C:O2'	2.37	0.46
33:2b:76:GLN:HB2	33:2b:208:ILE:HG12	1.98	0.46
48:2q:64:PRO:HB3	48:2q:70:ARG:NH1	2.30	0.46
1:1A:1022:G:C5	1:1A:1140:C:C4	3.03	0.46
1:1A:1152:C:H4'	16:1U:77:SER:HA	1.98	0.46
1:1A:1784:A:H4'	1:1A:1785:A:O5'	2.15	0.46
1:1A:2439:A:H5'	1:1A:2439:A:H8	1.80	0.46
1:1A:2577:A:H5'	27:15:3:LYS:HD2	1.96	0.46
36:1e:41:VAL:O	36:1e:66:MET:HA	2.14	0.46
40:1i:23:ASN:ND2	40:1i:25:LYS:HG2	2.30	0.46
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.51	0.46
1:2A:2498:C:OP2	61:2A:3929:HOH:O	2.20	0.46
9:2N:62:VAL:HG22	9:2N:66:LYS:HD2	1.97	0.46
32:2a:141:A:H2'	32:2a:142:G:O4'	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:164:U:H2'	32:2a:165:C:C6	2.51	0.46
32:2a:229:U:O2'	47:2p:23:ASP:OD2	2.33	0.46
32:2a:508:C:OP1	35:2d:209:ARG:NH2	2.49	0.46
38:2g:38:LEU:O	38:2g:42:ILE:HG12	2.16	0.46
44:2m:10:PRO:HG3	44:2m:21:TYR:CD2	2.50	0.46
55:2x:8:4SU:O5'	55:2x:8:4SU:H6	2.15	0.46
1:1A:1683:C:H2'	1:1A:1684:C:C6	2.51	0.46
1:1A:1882:C:H2'	1:1A:1883:G:O4'	2.16	0.46
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.28	0.46
14:1S:5:THR:OG1	14:1S:8:GLU:HG3	2.15	0.46
19:1X:40:LYS:HG3	19:1X:51:VAL:HB	1.97	0.46
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.15	0.46
26:14:26:SER:OG	26:14:27:THR:N	2.49	0.46
28:16:14:THR:OG1	28:16:48:VAL:O	2.29	0.46
39:1h:81:HIS:ND1	39:1h:138:TRP:OXT	2.49	0.46
40:1i:9:ARG:HG2	40:1i:14:VAL:HG12	1.97	0.46
43:1l:109:GLY:HA3	43:1l:121:GLY:O	2.16	0.46
1:2A:579:G:H2'	1:2A:580:C:C6	2.51	0.46
1:2A:639:U:H2'	1:2A:640:C:C6	2.51	0.46
1:2A:1003:G:O2'	1:2A:1010:A:N1	2.44	0.46
1:2A:1710:C:H2'	1:2A:1711:C:H6	1.81	0.46
1:2A:1799:G:O2'	3:2D:181:GLU:OE2	2.26	0.46
1:2A:2006:C:H6	1:2A:2006:C:O5'	1.99	0.46
1:2A:2322:A:H2'	1:2A:2323:G:O4'	2.15	0.46
2:2B:90:A:N7	2:2B:91:C:H1'	2.30	0.46
34:2c:18:TRP:CD1	45:2n:54:PRO:HA	2.50	0.46
45:2n:10:ALA:HB2	45:2n:23:ARG:HE	1.80	0.46
54:2w:239:VAL:HG11	54:2w:262:ARG:HA	1.98	0.46
1:1A:222:A:H5"	1:1A:421:U:OP1	2.16	0.46
1:1A:615:G:OP2	5:1F:43:LYS:NZ	2.48	0.46
1:1A:784:A:H5'	1:1A:785:G:OP1	2.16	0.46
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.16	0.46
5:1F:95:ARG:HD3	5:1F:97:TYR:CZ	2.51	0.46
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.16	0.46
32:1a:302:G:O2'	32:1a:556:C:H5"	2.15	0.46
32:1a:501:C:H1'	32:1a:549:C:H1'	1.97	0.46
32:1a:833:U:H2'	32:1a:834:C:H6	1.81	0.46
32:1a:1402:4OC:OP2	61:1a:3802:HOH:O	2.21	0.46
33:1b:28:PHE:CD2	33:1b:190:THR:HA	2.51	0.46
36:1e:35:GLY:HA3	36:1e:112:LEU:HB3	1.98	0.46
38:1g:26:PHE:HD1	38:1g:101:LEU:HD22	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:8:A:H2'	1:2A:9:U:H6	1.81	0.46
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.80	0.46
11:2P:96:THR:HG22	11:2P:98:GLU:H	1.80	0.46
11:2P:124:LYS:HA	11:2P:144:GLU:HB3	1.98	0.46
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.98	0.46
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.51	0.46
45:2n:37:PHE:O	45:2n:39:LEU:HG	2.15	0.46
51:2t:14:LYS:HE2	51:2t:18:GLN:NE2	2.30	0.46
54:2w:198:THR:HB	54:2w:293:ILE:HB	1.97	0.46
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.50	0.46
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.46	0.46
1:1A:2144:U:H3'	1:1A:2146:C:C5	2.51	0.46
11:1P:113:LYS:HA	11:1P:129:ALA:O	2.16	0.46
32:1a:606:G:N2	32:1a:631:G:N7	2.63	0.46
36:1e:57:LYS:HG2	36:1e:61:TYR:CE2	2.50	0.46
38:1g:89:MET:HG3	38:1g:156:TRP:NE1	2.31	0.46
40:1i:5:TYR:CG	40:1i:6:GLY:N	2.84	0.46
49:1r:26:LEU:HD21	49:1r:39:VAL:HG13	1.97	0.46
1:2A:877:U:O2'	1:2A:900:A:N6	2.44	0.46
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.50	0.46
11:2P:28:GLY:O	11:2P:30:THR:N	2.47	0.46
19:2X:92:LEU:HD12	19:2X:92:LEU:HA	1.81	0.46
35:2d:57:ARG:NH2	36:2e:107:ARG:HD3	2.31	0.46
48:2q:48:GLU:HB3	48:2q:50:LYS:HG3	1.98	0.46
51:2t:10:LEU:HD12	51:2t:11:SER:H	1.81	0.46
1:1A:271(L):U:H4'	8:1I:50:ARG:CZ	2.45	0.46
1:1A:602:G:O2'	1:1A:655:A:N6	2.49	0.46
1:1A:796:C:H2'	1:1A:797:C:C6	2.50	0.46
1:1A:1800:C:OP2	3:1D:183:ARG:NH2	2.48	0.46
5:1F:135:LYS:HB2	5:1F:138:GLU:CD	2.41	0.46
13:1R:72:ASP:HB3	13:1R:75:LEU:HB3	1.98	0.46
16:1U:27:LEU:HB3	16:1U:31:SER:HB3	1.98	0.46
32:1a:116:A:H61	32:1a:313:A:H1'	1.80	0.46
35:1d:88:VAL:O	35:1d:92:VAL:HG23	2.16	0.46
45:1n:26:ARG:HD3	45:1n:43:CYS:HB3	1.98	0.46
54:1w:108:ILE:HD13	54:1w:161:GLU:HB3	1.98	0.46
1:2A:483:A:O2'	20:2Y:59:GLY:N	2.49	0.46
1:2A:538:G:H2'	1:2A:539:G:H8	1.80	0.46
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.51	0.46
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.79	0.46
3:2D:232:PRO:HB3	3:2D:244:ARG:CZ	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:337:C:H2'	32:2a:338:A:C8	2.51	0.46
32:2a:504:C:C2	32:2a:542:G:C2	3.04	0.46
32:2a:755:G:OP2	46:2o:65:ARG:HD2	2.15	0.46
32:2a:790:A:C6	32:2a:791:G:C6	3.04	0.46
32:2a:865:A:H2	32:2a:918:A:H4'	1.81	0.46
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.51	0.46
38:2g:51:GLN:HA	38:2g:55:GLY:HA2	1.98	0.46
44:2m:13:LYS:NZ	44:2m:21:TYR:OH	2.49	0.46
49:2r:35:ARG:O	49:2r:37:VAL:N	2.47	0.46
1:1A:735:A:N7	1:1A:761:A:H2	2.14	0.45
1:1A:888:C:O2	44:1m:83:ASP:HA	2.16	0.45
4:1E:28:ALA:HB3	4:1E:93:VAL:HG13	1.97	0.45
6:1G:148:MET:H	6:1G:148:MET:HG3	1.45	0.45
7:1H:37:VAL:HB	7:1H:68:THR:HG23	1.98	0.45
32:1a:232:G:H1'	32:1a:262:A:N1	2.31	0.45
32:1a:833:U:H2'	32:1a:834:C:C6	2.52	0.45
32:1a:1207:2MG:H2'	32:1a:1208:C:H6	1.81	0.45
38:1g:16:LEU:HD12	40:1i:42:ARG:HA	1.98	0.45
1:2A:519:U:H2'	1:2A:520:G:C8	2.51	0.45
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.51	0.45
25:23:4:LEU:N	25:23:37:LEU:O	2.43	0.45
25:23:11:SER:HA	25:23:31:LEU:HD11	1.98	0.45
32:2a:1255:G:O2'	32:2a:1259:C:O4'	2.31	0.45
34:2c:180:ALA:HA	34:2c:206:GLU:HB3	1.98	0.45
35:2d:20:TYR:CD1	35:2d:26:CYS:HB3	2.51	0.45
44:2m:59:TYR:CE1	44:2m:63:THR:HG21	2.52	0.45
1:1A:195:A:H5"	11:1P:46:LYS:NZ	2.31	0.45
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.52	0.45
1:1A:287:C:H2'	1:1A:288:C:H6	1.80	0.45
1:1A:621:A:OP2	11:1P:108:LYS:NZ	2.49	0.45
1:1A:2128:C:H4'	1:1A:2174:C:O2'	2.16	0.45
24:12:52:ASP:O	24:12:56:GLN:HG3	2.16	0.45
32:1a:688:G:H2'	32:1a:689:C:H6	1.80	0.45
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.51	0.45
32:1a:1268:A:N3	32:1a:1326:C:O2'	2.49	0.45
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.81	0.45
44:1m:82:MET:HE3	44:1m:82:MET:HB2	1.79	0.45
47:1p:40:ASP:OD2	47:1p:44:THR:OG1	2.30	0.45
54:1w:228:GLY:HA3	54:1w:232:VAL:HB	1.98	0.45
1:2A:602:G:O2'	1:2A:655:A:N6	2.49	0.45
1:2A:775:G:H4'	1:2A:776:G:H5'	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:796:C:H2'	1:2A:797:C:C6	2.51	0.45
1:2A:1683:C:H2'	1:2A:1684:C:C6	2.51	0.45
1:2A:2785:C:O2'	4:2E:66:HIS:ND1	2.46	0.45
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.16	0.45
14:2S:61:ASN:O	14:2S:64:GLU:HG2	2.15	0.45
26:24:1:MET:HE2	26:24:6:HIS:CD2	2.51	0.45
32:2a:8:A:N6	35:2d:209:ARG:HB2	2.31	0.45
32:2a:685:G:C2	32:2a:686:U:C4	3.04	0.45
32:2a:781:A:OP1	32:2a:1523:G:H5'	2.17	0.45
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.50	0.45
32:2a:1203:C:H2'	32:2a:1204:A:O4'	2.16	0.45
32:2a:1268:A:H2'	32:2a:1269:A:C8	2.51	0.45
50:2s:28:LYS:HD3	50:2s:47:HIS:HA	1.98	0.45
1:1A:505:A:OP2	61:1A:4140:HOH:O	2.20	0.45
1:1A:1426:G:O2'	1:1A:1572:A:N6	2.48	0.45
1:1A:2881:C:H2'	1:1A:2882:A:O4'	2.17	0.45
32:1a:1118:C:OP1	40:1i:104:ARG:NH1	2.43	0.45
33:1b:71:VAL:HG13	33:1b:164:VAL:HA	1.98	0.45
35:1d:8:VAL:HG22	35:1d:21:LEU:HD13	1.97	0.45
35:1d:63:LYS:HD2	35:1d:198:VAL:HG12	1.99	0.45
37:1f:19:LEU:HD21	37:1f:59:TYR:CE2	2.51	0.45
1:2A:870:A:OP1	12:2Q:6:ARG:HD3	2.16	0.45
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.32	0.45
1:2A:2117:A:H1'	1:2A:2118:U:H3'	1.98	0.45
2:2B:6:C:H42	2:2B:115:G:H1	1.62	0.45
6:2G:115:ARG:NH2	6:2G:137:GLU:OE1	2.50	0.45
14:2S:41:ASP:CG	14:2S:44:LYS:HG3	2.41	0.45
32:2a:1027:C:H3'	32:2a:1028:C:H6	1.81	0.45
32:2a:1038:C:H2'	32:2a:1039:C:C6	2.51	0.45
33:2b:115:LEU:O	33:2b:119:GLU:N	2.39	0.45
36:2e:110:LEU:HD13	36:2e:118:ILE:HD13	1.99	0.45
42:2k:99:GLN:HG2	42:2k:105:VAL:HG11	1.98	0.45
44:2m:81:LEU:HD22	44:2m:88:ARG:HB2	1.98	0.45
49:2r:48:GLY:O	49:2r:74:ARG:NH2	2.49	0.45
50:2s:40:ILE:HA	50:2s:44:MET:SD	2.57	0.45
1:1A:700:G:O2'	1:1A:1632:A:N3	2.49	0.45
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.26	0.45
1:1A:1936:A:OP1	1:1A:1937:A:H5'	2.17	0.45
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	1.97	0.45
7:1H:3:ARG:HG2	7:1H:6:ARG:HG3	1.98	0.45
21:1Z:138:GLU:H	21:1Z:156:LYS:NZ	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:11:3:LYS:HZ3	23:11:3:LYS:HG2	1.69	0.45
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.49	0.45
37:1f:23:LYS:HA	37:1f:26:ILE:HD12	1.97	0.45
54:1w:128:PHE:CZ	54:1w:132:LEU:HD11	2.52	0.45
1:2A:1357:U:H2'	1:2A:1358:G:O4'	2.16	0.45
1:2A:1826:G:H4'	3:2D:242:ARG:NH1	2.31	0.45
1:2A:2130:U:H5"	1:2A:2133:G:H5'	1.99	0.45
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.17	0.45
7:2H:159:GLU:HG2	7:2H:169:VAL:HG11	1.98	0.45
17:2V:56:SER:O	17:2V:100:ARG:N	2.49	0.45
32:2a:1279:A:H5"	32:2a:1280:A:OP1	2.15	0.45
32:2a:1304:G:C6	32:2a:1305:G:N1	2.84	0.45
34:2c:134:ILE:HG22	34:2c:168:ALA:HB3	1.97	0.45
35:2d:70:ILE:HD12	35:2d:70:ILE:HA	1.71	0.45
54:2w:105:ARG:H	54:2w:105:ARG:HG2	1.53	0.45
1:1A:477:A:C6	1:1A:478:A:C6	3.05	0.45
1:1A:1213:A:N3	1:1A:1238:G:O2'	2.42	0.45
1:1A:2291:U:OP1	1:1A:2380:C:O2'	2.26	0.45
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.52	0.45
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.17	0.45
32:1a:475:G:H2'	32:1a:476:G:H8	1.82	0.45
32:1a:948:C:H2'	32:1a:949:A:H8	1.81	0.45
32:1a:1129:C:N4	32:1a:1143:G:H1	2.14	0.45
32:1a:1147:C:O2'	40:1i:5:TYR:OH	2.30	0.45
34:1c:125:GLU:HG3	34:1c:189:ALA:HB1	1.98	0.45
36:1e:103:GLY:C	36:1e:106:PRO:HD2	2.40	0.45
55:1x:49:U:H2'	55:1x:50:C:C6	2.51	0.45
1:2A:244:A:C2	1:2A:255:A:C4	3.05	0.45
1:2A:551:G:O2'	1:2A:1220:A:N3	2.42	0.45
1:2A:652:C:C2'	1:2A:652(A):A:H5'	2.46	0.45
1:2A:2432:A:OP2	61:2A:3951:HOH:O	2.21	0.45
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.49	0.45
11:2P:96:THR:HG22	11:2P:98:GLU:N	2.31	0.45
25:23:8:LEU:O	25:23:32:GLN:N	2.40	0.45
32:2a:538:G:H2'	32:2a:539:A:H8	1.82	0.45
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.17	0.45
32:2a:757:U:H2'	32:2a:758:G:O4'	2.17	0.45
32:2a:1121:U:H2'	32:2a:1122:U:H6	1.81	0.45
36:2e:82:VAL:HG21	36:2e:138:ALA:HA	1.99	0.45
40:2i:88:TYR:HD2	40:2i:89:ASN:HD22	1.65	0.45
46:2o:7:GLU:O	46:2o:11:VAL:HG13	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:492:A:H2'	1:1A:493:G:O4'	2.17	0.45
1:1A:493:G:H2'	1:1A:494:G:O4'	2.17	0.45
1:1A:571:A:O2'	17:1V:78:LYS:HE2	2.17	0.45
1:1A:1339:G:H5"	19:1X:16:LYS:HD3	1.99	0.45
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.16	0.45
1:1A:2292:C:OP1	14:1S:17:ARG:NH2	2.37	0.45
11:1P:121:LYS:O	11:1P:123:LEU:N	2.45	0.45
18:1W:82:LEU:HB2	18:1W:98:LYS:HB2	1.98	0.45
26:14:9:LEU:HD23	26:14:9:LEU:HA	1.80	0.45
32:1a:92:C:H2'	32:1a:93:G:H8	1.80	0.45
32:1a:538:G:H5"	43:1l:114:LYS:HG2	1.98	0.45
32:1a:690:G:C6	32:1a:691:G:C6	3.04	0.45
32:1a:1006:C:H2'	32:1a:1007:C:C6	2.51	0.45
32:1a:1034:G:H3'	32:1a:1035:A:H8	1.80	0.45
32:1a:1060:C:O2'	41:1j:56:HIS:HD2	2.00	0.45
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.52	0.45
37:1f:21:LEU:O	37:1f:25:ILE:HG13	2.17	0.45
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.42	0.45
54:1w:105:ARG:HE	54:1w:203:PRO:HB2	1.82	0.45
1:2A:805:G:OP1	61:2A:3917:HOH:O	2.20	0.45
1:2A:2104:G:H1	1:2A:2185:C:H42	1.64	0.45
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.81	0.45
1:2A:2493:U:O2'	12:2Q:80:GLU:OE2	2.28	0.45
5:2F:122:LYS:HB3	5:2F:191:ARG:HG2	1.98	0.45
7:2H:55:PRO:HG2	7:2H:61:HIS:CE1	2.52	0.45
8:2I:89:TYR:O	8:2I:121:LYS:NZ	2.49	0.45
32:2a:736:C:H2'	32:2a:737:A:C8	2.51	0.45
32:2a:1119:C:OP1	40:2i:83:ARG:NH2	2.50	0.45
38:2g:120:ILE:HG22	38:2g:124:LEU:HD12	1.98	0.45
43:2l:6:THR:HG23	43:2l:9:GLN:OE1	2.17	0.45
1:1A:271(L):U:H4'	8:1I:50:ARG:NH2	2.32	0.45
1:1A:784:A:C5	3:1D:229:VAL:HG21	2.52	0.45
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.50	0.45
1:1A:1614:A:C2	18:1W:93:ALA:HB2	2.52	0.45
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.51	0.45
6:1G:66:GLN:OE1	6:1G:98:ARG:NE	2.46	0.45
11:1P:65:ARG:HD2	30:18:25:MET:SD	2.57	0.45
26:14:16:CYS:SG	26:14:17:GLY:N	2.90	0.45
34:1c:149:ALA:HA	34:1c:201:TYR:O	2.16	0.45
36:1e:148:VAL:O	36:1e:152:ARG:HG3	2.16	0.45
1:2A:616:G:H4'	5:2F:205:ARG:HD2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.49	0.45
1:2A:667:U:O2	30:28:2:PRO:HD2	2.17	0.45
1:2A:1187:G:H5"	17:2V:81:TYR:CE1	2.52	0.45
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.32	0.45
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.98	0.45
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.51	0.45
6:2G:108:ASN:HA	26:24:37:SER:HB2	1.99	0.45
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.51	0.45
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.99	0.45
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.16	0.45
28:26:11:LEU:HB2	28:26:21:TYR:HB2	1.99	0.45
32:2a:659:U:OP2	46:2o:8:LYS:NZ	2.42	0.45
32:2a:1259:C:C4	32:2a:1260:C:H1'	2.51	0.45
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.51	0.45
34:2c:7:PRO:HG2	34:2c:201:TYR:HE1	1.80	0.45
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.52	0.45
1:1A:234:C:H2'	1:1A:235:U:H6	1.82	0.45
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.17	0.45
1:1A:1510:G:H2'	1:1A:1511:C:C6	2.51	0.45
1:1A:2140:C:H2'	1:1A:2141:G:N7	2.32	0.45
1:1A:2144:U:H1'	1:1A:2148:G:N2	2.32	0.45
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.17	0.45
3:1D:260:ARG:HH22	3:1D:266:SER:HB2	1.81	0.45
12:1Q:82:ARG:NH2	61:1Q:301:HOH:O	2.33	0.45
35:1d:10:ARG:HB2	35:1d:40:PRO:HG3	1.98	0.45
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.17	0.45
1:2A:2136:C:N3	1:2A:2155:G:O6	2.49	0.45
2:2B:114:C:H4'	14:2S:46:VAL:HG12	1.98	0.45
5:2F:7:TYR:O	5:2F:21:ALA:HA	2.17	0.45
5:2F:110:LEU:HD11	5:2F:181:LEU:HD23	1.99	0.45
33:2b:70:PHE:HE2	33:2b:90:MET:HG3	1.82	0.45
34:2c:54:ARG:HB3	34:2c:69:HIS:HB2	1.99	0.45
34:2c:79:ARG:N	34:2c:82:GLU:HB3	2.22	0.45
35:2d:9:CYS:O	35:2d:13:ARG:HG3	2.16	0.45
38:2g:66:VAL:HG12	38:2g:70:LYS:HE2	1.98	0.45
40:2i:18:PHE:O	40:2i:61:ALA:HA	2.17	0.45
41:2j:27:ALA:O	41:2j:81:THR:HG21	2.16	0.45
1:1A:8:A:H2'	1:1A:9:U:C6	2.51	0.45
1:1A:1647:G:OP1	61:1A:4112:HOH:O	2.21	0.45
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.50	0.45
10:1O:63:VAL:HA	10:1O:106:LEU:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:266:G:H2'	32:1a:266:G:N3	2.32	0.45
32:1a:328:C:H4'	32:1a:329:A:H5'	1.99	0.45
32:1a:1127:G:H1'	32:1a:1280:A:C6	2.52	0.45
32:1a:1175:G:H2'	32:1a:1176:A:C8	2.52	0.45
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.23	0.45
32:1a:1404:5MC:O2	32:1a:1519:MA6:O2'	2.32	0.45
33:1b:55:PHE:CE1	33:1b:218:ALA:HA	2.40	0.45
34:1c:105:GLU:HG2	34:1c:106:VAL:H	1.81	0.45
50:1s:36:ARG:O	50:1s:70:LYS:HB3	2.17	0.45
1:2A:116:C:H2'	1:2A:117:G:O4'	2.17	0.45
2:2B:41:U:O4	6:2G:70:VAL:HG12	2.16	0.45
3:2D:165:ILE:HG23	3:2D:173:VAL:HG13	1.99	0.45
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.16	0.45
10:2O:70:LYS:HB3	10:2O:70:LYS:HE2	1.76	0.45
32:2a:232:G:H1'	32:2a:262:A:N1	2.32	0.45
32:2a:235:C:H2'	32:2a:236:G:H8	1.82	0.45
32:2a:434:U:H2'	32:2a:435:C:C6	2.52	0.45
32:2a:791:G:C6	32:2a:792:A:N7	2.84	0.45
32:2a:1186:G:H21	45:2n:61:TRP:C	2.25	0.45
32:2a:1269:A:H2	32:2a:1312:G:N3	2.15	0.45
37:2f:100:ASN:ND2	49:2r:23:LYS:HE3	2.32	0.45
47:2p:4:ILE:O	47:2p:66:PRO:HA	2.16	0.45
1:1A:236:C:H2'	1:1A:237:C:H6	1.80	0.45
1:1A:877:U:H2'	1:1A:878:A:H5"	1.99	0.45
1:1A:1833:U:O2'	1:1A:1969:A:N1	2.43	0.45
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.52	0.45
5:1F:161:GLU:HG2	5:1F:164:ARG:NH2	2.32	0.45
8:1I:114:LEU:HD13	8:1I:130:TYR:HD1	1.82	0.45
11:1P:96:THR:HG22	11:1P:98:GLU:H	1.82	0.45
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.99	0.45
37:1f:86:ARG:O	37:1f:87:ARG:HG2	2.16	0.45
46:1o:4:THR:OG1	46:1o:7:GLU:HG3	2.17	0.45
54:1w:212:LEU:HD22	54:1w:217:ILE:HD11	1.99	0.45
1:2A:892:G:H2'	1:2A:893:C:H4'	1.99	0.45
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.52	0.45
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.99	0.45
7:2H:46:GLU:HG3	7:2H:49:VAL:HG23	1.99	0.45
16:2U:102:GLU:HB3	16:2U:104:GLN:HE22	1.82	0.45
32:2a:745:C:H2'	32:2a:746:A:C8	2.52	0.45
32:2a:1493:A:C4	54:2w:115:THR:HA	2.52	0.45
33:2b:189:ASP:CG	33:2b:205:ASP:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:23:TYR:HB3	44:2m:67:GLU:HB3	1.98	0.45
46:2o:82:ILE:O	46:2o:86:GLY:N	2.50	0.45
1:1A:143(A):C:O2'	19:1X:2:LYS:NZ	2.37	0.44
1:1A:239:U:H2'	1:1A:240:G:O4'	2.17	0.44
1:1A:1268:A:C2	1:1A:2013:A:C4	3.05	0.44
1:1A:1902:C:H5'	3:1D:246:PRO:HD3	2.00	0.44
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.17	0.44
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	1.98	0.44
32:1a:624:C:H2'	32:1a:625:G:H8	1.82	0.44
32:1a:1006:C:N4	32:1a:1023:G:H1	2.15	0.44
32:1a:1389:C:H2'	32:1a:1390:U:O4'	2.16	0.44
38:1g:18:TYR:CD1	38:1g:59:LEU:HB2	2.52	0.44
45:1n:58:LYS:HE2	45:1n:58:LYS:HB3	1.80	0.44
1:2A:341:G:H2'	1:2A:342:G:O4'	2.17	0.44
1:2A:882:G:H1	1:2A:894:C:H42	1.63	0.44
1:2A:1152:C:H4'	16:2U:77:SER:HA	2.00	0.44
1:2A:1186:G:H2'	1:2A:1187:G:O4'	2.17	0.44
1:2A:2420:C:P	30:28:33:ASN:H	2.40	0.44
1:2A:2849:U:O4	15:2T:23:ARG:NH1	2.38	0.44
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.52	0.44
3:2D:164:GLN:OE1	3:2D:176:ARG:NH2	2.44	0.44
32:2a:137:C:H2'	32:2a:138:G:H8	1.81	0.44
32:2a:253:U:H2'	32:2a:254:G:H8	1.82	0.44
32:2a:1123:A:H4'	41:2j:36:GLY:HA3	1.99	0.44
32:2a:1133:G:C2	32:2a:1142:G:C2	3.05	0.44
32:2a:1327:C:H2'	32:2a:1328:C:H6	1.82	0.44
40:2i:111:ARG:HD2	45:2n:61:TRP:CD1	2.51	0.44
43:2l:24:VAL:HG12	43:2l:98:TYR:CE1	2.52	0.44
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.98	0.44
54:2w:103:ASP:O	54:2w:166:GLY:HA2	2.17	0.44
54:2w:260:LYS:HD3	54:2w:260:LYS:HA	1.79	0.44
1:1A:1026:U:OP1	61:1A:4142:HOH:O	2.21	0.44
1:1A:2587:A:N6	1:1A:2608:G:O2'	2.50	0.44
1:1A:2892:A:N6	1:1A:2893:G:N1	2.65	0.44
26:14:54:GLY:C	26:14:56:VAL:HA	2.43	0.44
32:1a:688:G:H5'	42:1k:46:GLY:C	2.43	0.44
32:1a:1006:C:H42	32:1a:1023:G:H1	1.65	0.44
32:1a:1157:A:H4'	32:1a:1158:C:O4'	2.16	0.44
32:1a:1317:C:N4	45:1n:19:ARG:HH21	2.15	0.44
38:1g:22:LEU:HG	38:1g:62:PHE:HE2	1.81	0.44
52:1u:18:TYR:CE1	52:1u:24:ARG:HB3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:411:G:OP2	1:2A:2406:U:O2'	2.33	0.44
1:2A:571:A:OP2	61:2A:3952:HOH:O	2.21	0.44
1:2A:702:G:C2	1:2A:731:C:C2	3.05	0.44
1:2A:2409:G:H2'	1:2A:2410:G:O4'	2.17	0.44
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.17	0.44
9:2N:85:ILE:HG21	9:2N:90:MET:HE2	1.99	0.44
26:24:41:PRO:HG3	26:24:49:PHE:CE2	2.52	0.44
32:2a:171:A:H2'	32:2a:172:A:C8	2.53	0.44
32:2a:458:C:H2'	32:2a:460:G:O4'	2.16	0.44
32:2a:838:G:H3'	32:2a:840:C:H41	1.82	0.44
32:2a:1071:C:H2'	32:2a:1072:G:H8	1.82	0.44
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.52	0.44
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.57	0.44
39:2h:31:PHE:O	39:2h:35:ILE:HG13	2.17	0.44
1:1A:2165:G:H22	1:1A:2171:A:H2'	1.82	0.44
1:1A:2356:C:H2'	1:1A:2357:U:O4'	2.17	0.44
6:1G:65:GLY:HA2	26:14:7:PRO:HG2	1.99	0.44
9:1N:97:ARG:HA	9:1N:100:GLU:HB2	2.00	0.44
16:1U:108:GLU:O	16:1U:112:ARG:HG2	2.18	0.44
32:1a:142:G:H2'	32:1a:143:A:H8	1.81	0.44
35:1d:8:VAL:O	35:1d:11:LEU:HB2	2.17	0.44
47:1p:4:ILE:O	47:1p:66:PRO:HA	2.17	0.44
1:2A:271(M):G:N2	8:2I:50:ARG:HD2	2.32	0.44
1:2A:373:U:H2'	1:2A:374:A:H8	1.82	0.44
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.18	0.44
1:2A:2273:A:O2'	1:2A:2274:A:H5'	2.17	0.44
14:2S:15:ARG:HD3	14:2S:25:ARG:HH21	1.81	0.44
14:2S:18:ILE:O	14:2S:21:THR:HG23	2.18	0.44
16:2U:117:GLN:H	16:2U:117:GLN:HG2	1.71	0.44
20:2Y:14:LEU:HD11	20:2Y:22:GLY:HA2	2.00	0.44
32:2a:189(L):G:H2'	32:2a:190:U:C6	2.52	0.44
32:2a:429:U:O3'	35:2d:22:LYS:NZ	2.50	0.44
32:2a:617:G:H4'	47:2p:44:THR:O	2.18	0.44
32:2a:973:G:O3'	45:2n:41:ARG:NH2	2.49	0.44
32:2a:1207:2MG:H2'	32:2a:1208:C:H6	1.81	0.44
33:2b:136:VAL:O	33:2b:139:LYS:HB2	2.18	0.44
34:2c:139:GLN:HG3	34:2c:143:GLU:OE1	2.18	0.44
35:2d:128:VAL:HG22	35:2d:146:ILE:HG13	1.97	0.44
38:2g:79:ARG:HE	38:2g:80:VAL:HA	1.83	0.44
46:2o:4:THR:OG1	46:2o:7:GLU:HG3	2.17	0.44
51:2t:77:ALA:O	51:2t:81:LYS:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:438:G:H2'	1:1A:440:G:C8	2.52	0.44
1:1A:818:G:H4'	1:1A:838:C:O3'	2.17	0.44
1:1A:1580:A:OP2	1:1A:1580:A:H8	2.00	0.44
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.33	0.44
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.53	0.44
1:1A:2405:G:O2'	1:1A:2406:U:OP1	2.25	0.44
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.52	0.44
11:1P:111:ARG:HB3	11:1P:128:HIS:CG	2.53	0.44
14:1S:61:ASN:HD21	14:1S:63:THR:HB	1.81	0.44
14:1S:83:LYS:HB3	14:1S:111:GLU:HG3	2.00	0.44
14:1S:110:LEU:HD12	14:1S:110:LEU:HA	1.83	0.44
26:14:58:ARG:HD3	50:1s:67:VAL:H	1.82	0.44
32:1a:131:C:H2'	32:1a:132:C:C6	2.53	0.44
32:1a:403:C:OP1	35:1d:137:SER:OG	2.33	0.44
33:1b:54:THR:HG23	33:1b:199:TYR:HB3	2.00	0.44
33:1b:92:TYR:HE1	33:1b:94:ASN:HB2	1.82	0.44
46:1o:25:THR:HG21	46:1o:69:TYR:HD2	1.82	0.44
1:2A:311:A:C6	1:2A:328:U:C4	3.06	0.44
1:2A:898:C:H2'	1:2A:899:A:O4'	2.17	0.44
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.47	0.44
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.17	0.44
1:2A:2441:C:OP2	1:2A:2586:C:O2'	2.31	0.44
1:2A:2661:G:H2'	1:2A:2662:A:C8	2.53	0.44
5:2F:40:GLN:HE22	5:2F:182:ASN:HB2	1.82	0.44
6:2G:46:ALA:HA	6:2G:49:ASP:HB2	2.00	0.44
32:2a:389:A:C6	32:2a:390:C:H1'	2.53	0.44
32:2a:985:C:H2'	32:2a:986:A:C8	2.53	0.44
32:2a:1111:A:N1	34:2c:177:THR:HA	2.33	0.44
32:2a:1121:U:O2'	32:2a:1122:U:H5'	2.17	0.44
32:2a:1169:A:H2'	32:2a:1170:A:C8	2.51	0.44
40:2i:53:VAL:O	40:2i:55:ALA:N	2.41	0.44
40:2i:118:LYS:H	40:2i:121:ARG:HB3	1.82	0.44
42:2k:98:LEU:O	42:2k:101:SER:OG	2.18	0.44
51:2t:26:ASN:HA	51:2t:71:THR:HG23	1.99	0.44
54:2w:134:PHE:O	54:2w:138:MET:HG2	2.17	0.44
54:2w:177:VAL:HG13	54:2w:196:THR:CG2	2.48	0.44
54:2w:336:LEU:HG	54:2w:340:LYS:HD2	2.00	0.44
1:1A:1045:A:C8	1:1A:1047:G:N2	2.86	0.44
1:1A:1068:G:C8	1:1A:1096:A:H1'	2.52	0.44
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.18	0.44
1:1A:2108:C:O2	1:1A:2182:G:N2	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:3:LEU:HD13	26:14:25:TYR:CZ	2.53	0.44
50:1s:40:ILE:HD11	50:1s:71:LEU:HD23	1.99	0.44
1:2A:2138:C:H42	1:2A:2153:G:H1	1.64	0.44
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.99	0.44
13:2R:26:LYS:HE2	13:2R:70:LEU:O	2.17	0.44
32:2a:664:G:P	49:2r:64:ARG:HH21	2.40	0.44
32:2a:735:C:H2'	32:2a:736:C:H6	1.82	0.44
33:2b:48:MET:HA	33:2b:51:LEU:HB2	2.00	0.44
40:2i:56:LEU:H	40:2i:56:LEU:HG	1.28	0.44
50:2s:10:PHE:CE2	50:2s:12:ASP:HA	2.53	0.44
52:2u:6:ARG:C	52:2u:8:THR:H	2.26	0.44
1:1A:784:A:C8	1:1A:792:G:C5	3.06	0.44
1:1A:826:U:H4'	11:1P:55:ARG:HB3	1.99	0.44
1:1A:862:G:H2'	1:1A:863:A:O4'	2.18	0.44
1:1A:1047:G:H2'	1:1A:1110:G:H1	1.82	0.44
1:1A:1614:A:C6	18:1W:87:PRO:HB3	2.53	0.44
32:1a:389:A:C5	32:1a:390:C:H1'	2.53	0.44
32:1a:666:G:H5'	32:1a:726:C:H1'	2.00	0.44
32:1a:1041:A:H2'	32:1a:1042:G:O4'	2.18	0.44
32:1a:1053:G:N7	32:1a:1200:C:H5"	2.33	0.44
32:1a:1397:C:H4'	32:1a:1398:A:O5'	2.17	0.44
34:1c:164:ARG:HD2	34:1c:166:GLU:OE1	2.17	0.44
36:1e:99:GLY:N	36:1e:117:ASP:OD1	2.38	0.44
46:1o:61:GLY:O	46:1o:65:ARG:HG3	2.17	0.44
1:2A:208:C:H2'	1:2A:209:C:C6	2.52	0.44
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.53	0.44
1:2A:2869:G:H2'	1:2A:2870:C:O4'	2.18	0.44
61:2A:4059:HOH:O	11:2P:37:GLY:HA3	2.18	0.44
25:23:28:LEU:HD23	25:23:28:LEU:HA	1.77	0.44
32:2a:137:C:H2'	32:2a:138:G:C8	2.53	0.44
36:2e:81:GLU:HG2	36:2e:90:VAL:HG13	1.98	0.44
41:2j:22:LYS:O	41:2j:26:ALA:N	2.51	0.44
42:2k:31:THR:HG22	42:2k:42:TRP:HB2	1.99	0.44
51:2t:50:GLU:HG3	51:2t:100:ILE:HD13	1.99	0.44
1:1A:185:U:H2'	1:1A:186:G:C8	2.53	0.44
4:1E:28:ALA:HB3	4:1E:93:VAL:CG1	2.47	0.44
12:1Q:138:ASP:OD2	21:1Z:81:ARG:NH1	2.49	0.44
16:1U:19:LYS:O	16:1U:22:LYS:HG3	2.18	0.44
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.75	0.44
32:1a:1126:U:O2'	32:1a:1127:G:H8	2.00	0.44
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:182:LYS:HB3	35:1d:182:LYS:HE2	1.77	0.44
1:2A:108:U:H2'	1:2A:109:G:H8	1.81	0.44
1:2A:514:A:N3	1:2A:581:C:O2'	2.44	0.44
1:2A:1448:G:H1'	1:2A:1528:A:N1	2.32	0.44
1:2A:1504:C:H2'	1:2A:1505:C:C6	2.53	0.44
1:2A:1587:A:H2'	1:2A:1588:C:C6	2.52	0.44
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.52	0.44
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.53	0.44
4:2E:31:CYS:HB3	4:2E:49:LEU:HB3	1.99	0.44
6:2G:109:VAL:HG21	6:2G:142:PRO:HB3	2.00	0.44
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.37	0.44
12:2Q:137:TYR:HB3	21:2Z:76:LEU:HD11	1.99	0.44
16:2U:104:GLN:HE21	16:2U:105:VAL:HG23	1.82	0.44
32:2a:1015:A:H2'	32:2a:1016:A:C8	2.53	0.44
32:2a:1060:C:C5'	41:2j:51:ARG:HG2	2.48	0.44
32:2a:1187:G:OP1	40:2i:113:LYS:HE3	2.17	0.44
32:2a:1342:C:H2'	32:2a:1343:G:C8	2.53	0.44
32:2a:1397:C:H4'	32:2a:1398:A:OP2	2.18	0.44
34:2c:71:ALA:O	34:2c:72:LYS:HD2	2.18	0.44
42:2k:80:VAL:HG21	42:2k:103:LEU:HD13	1.99	0.44
48:2q:67:LYS:O	48:2q:69:LYS:N	2.50	0.44
54:2w:302:ILE:HD12	54:2w:302:ILE:HA	1.80	0.44
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.51	0.44
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.53	0.44
1:1A:2058:A:N7	61:1A:4233:HOH:O	2.36	0.44
1:1A:2130:U:O2'	1:1A:2133:G:H4'	2.18	0.44
1:1A:2207:G:O2'	1:1A:2208:A:OP1	2.34	0.44
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.16	0.44
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.18	0.44
19:1X:43:VAL:HG21	19:1X:81:VAL:HG11	1.99	0.44
25:13:8:LEU:HB2	25:13:28:LEU:HD13	2.00	0.44
32:1a:76:C:N4	32:1a:77:G:O6	2.51	0.44
32:1a:334:C:H2'	32:1a:335:C:C6	2.52	0.44
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.53	0.44
32:1a:1327:C:H2'	32:1a:1328:C:C6	2.53	0.44
40:1i:37:PHE:HA	40:1i:40:LEU:HD12	2.00	0.44
49:1r:22:VAL:HG23	49:1r:56:THR:HA	1.99	0.44
1:2A:118:A:N3	1:2A:178:G:H1'	2.33	0.44
1:2A:530:G:C5	1:2A:2022:U:H5"	2.53	0.44
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.99	0.44
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:124:SER:HB2	6:2G:131:TYR:CE1	2.51	0.44
8:2I:114:LEU:HD11	8:2I:128:LEU:HB3	1.99	0.44
32:2a:1014:A:H5'	50:2s:14:HIS:CE1	2.53	0.44
32:2a:1143:G:H2'	32:2a:1144:G:O4'	2.18	0.44
33:2b:185:ILE:H	33:2b:185:ILE:HG13	1.64	0.44
34:2c:159:GLY:HA2	34:2c:193:TYR:CD1	2.53	0.44
51:2t:97:ALA:HB1	51:2t:98:PRO:HD2	2.00	0.44
1:1A:2155:G:H3'	1:1A:2156:G:H8	1.80	0.44
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.53	0.44
4:1E:120:TRP:CD1	4:1E:155:LYS:HB3	2.53	0.44
5:1F:116:ASP:OD2	11:1P:1:MET:HB3	2.17	0.44
5:1F:195:ASP:HB3	5:1F:198:ALA:H	1.82	0.44
6:1G:125:PHE:CZ	6:1G:173:LEU:HD12	2.53	0.44
7:1H:51:ARG:NH2	7:1H:53:GLU:OE1	2.51	0.44
10:1O:100:GLY:O	10:1O:119:PRO:HD2	2.18	0.44
11:1P:46:LYS:HE2	11:1P:46:LYS:HB3	1.81	0.44
26:14:57:GLU:HB3	26:14:58:ARG:HG2	1.99	0.44
32:1a:381:C:H2'	32:1a:382:A:O4'	2.17	0.44
32:1a:1179:A:H2'	32:1a:1180:A:O4'	2.18	0.44
33:1b:74:LYS:NZ	33:1b:206:ASP:OD1	2.51	0.44
34:1c:131:ARG:HA	34:1c:131:ARG:HD2	1.71	0.44
37:1f:100:ASN:HD21	49:1r:23:LYS:HE2	1.82	0.44
50:1s:31:ILE:O	50:1s:50:ALA:N	2.28	0.44
54:1w:182:ARG:O	54:1w:184:PRO:HD3	2.18	0.44
1:2A:10:G:H2'	1:2A:11:G:H8	1.81	0.44
1:2A:57:C:H2'	1:2A:58:G:O4'	2.18	0.44
1:2A:893:C:H2'	1:2A:894:C:C5	2.53	0.44
1:2A:2371:G:C2	1:2A:2372:G:C8	3.06	0.44
1:2A:2638:G:P	4:2E:82:ARG:HH22	2.39	0.44
6:2G:107:LEU:HA	6:2G:111:LEU:HD12	2.00	0.44
11:2P:1:MET:HG3	11:2P:5:ASP:HB2	2.00	0.44
32:2a:358:U:H2'	32:2a:359:U:C6	2.52	0.44
32:2a:538:G:H2'	32:2a:539:A:C8	2.52	0.44
32:2a:692:U:O2'	32:2a:694:A:N7	2.34	0.44
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	1.99	0.44
55:2x:75:C:H2'	55:2x:76:8AN:H1'	2.00	0.44
1:1A:27:G:C2	1:1A:512:G:N3	2.86	0.43
1:1A:826:U:OP1	61:1A:4105:HOH:O	2.21	0.43
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.51	0.43
2:1B:7:G:H5'	14:1S:29:PHE:CE2	2.53	0.43
4:1E:13:ARG:HD2	4:1E:20:ALA:HB1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:167:ALA:HB1	5:1F:173:VAL:HG11	1.99	0.43
26:14:69:LYS:HD3	50:1s:20:LEU:HD13	2.00	0.43
32:1a:523:A:H61	43:1l:92:0TD:CG	2.31	0.43
32:1a:595:G:H1'	32:1a:596:C:H5	1.83	0.43
32:1a:736:C:OP1	49:1r:72:ARG:NE	2.41	0.43
32:1a:1333:A:H3'	32:1a:1334:G:H8	1.83	0.43
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.99	0.43
44:1m:88:ARG:HG2	44:1m:98:VAL:HG22	1.99	0.43
51:1t:63:ILE:HG22	51:1t:77:ALA:HB1	2.00	0.43
55:1x:7:U:O2'	55:1x:49:U:OP2	2.36	0.43
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.53	0.43
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.52	0.43
1:2A:1462:C:H2'	1:2A:1463:C:O4'	2.18	0.43
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.53	0.43
1:2A:2118:U:O2'	1:2A:2149:G:H5'	2.18	0.43
1:2A:2377:A:O2'	14:2S:112:PHE:O	2.25	0.43
4:2E:14:ILE:HB	15:2T:14:TYR:CZ	2.53	0.43
5:2F:33:LEU:HD21	5:2F:112:MET:HB3	2.00	0.43
6:2G:16:ARG:HB2	6:2G:17:PRO:HD3	2.00	0.43
6:2G:163:ALA:HB1	6:2G:168:GLU:HB2	2.00	0.43
21:2Z:141:VAL:HB	21:2Z:144:LEU:HD12	2.00	0.43
22:20:49:LYS:HA	22:20:49:LYS:HD2	1.81	0.43
32:2a:130:A:O2'	32:2a:131:C:O5'	2.29	0.43
32:2a:1226:C:H3'	44:2m:96:LEU:HD21	2.00	0.43
32:2a:1367:C:H5'	41:2j:60:ARG:CZ	2.47	0.43
42:2k:79:SER:HB2	42:2k:106:LYS:HD3	2.00	0.43
45:2n:58:LYS:HE2	45:2n:58:LYS:HB3	1.83	0.43
52:2u:3:LYS:HB3	52:2u:14:TRP:CD1	2.52	0.43
1:1A:271(K):U:O2	8:1I:50:ARG:HG3	2.18	0.43
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.18	0.43
1:1A:1169:G:H2'	1:1A:1170:G:O4'	2.19	0.43
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.18	0.43
32:1a:502:G:C6	32:1a:503:C:C4	3.06	0.43
32:1a:618:C:N4	32:1a:621:A:N7	2.65	0.43
32:1a:620:C:N1	35:1d:135:LEU:HD13	2.32	0.43
32:1a:815:A:N7	32:1a:1509:C:O2'	2.47	0.43
32:1a:1288:A:H2'	32:1a:1289:A:C8	2.53	0.43
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	2.00	0.43
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.50	0.43
1:2A:86:C:H4'	1:2A:104:U:H1'	1.99	0.43
1:2A:570:G:H2'	1:2A:2030:A:C5	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1019:U:O2'	1:2A:1021:A:H2	2.02	0.43
1:2A:1428:C:N4	1:2A:1570:A:OP2	2.47	0.43
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.53	0.43
1:2A:2198:A:OP1	8:2I:33:ARG:NH2	2.51	0.43
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	2.01	0.43
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	2.00	0.43
7:2H:133:VAL:HG12	7:2H:141:VAL:HG13	1.99	0.43
15:2T:62:THR:HG23	15:2T:75:ILE:HG12	2.00	0.43
20:2Y:97:ARG:NH1	20:2Y:106:LEU:O	2.51	0.43
29:27:1:MET:HE3	29:27:3:ARG:NH2	2.33	0.43
32:2a:427:U:OP1	35:2d:13:ARG:NH1	2.49	0.43
32:2a:1117:G:H4'	40:2i:104:ARG:NH2	2.32	0.43
32:2a:1146:A:H2'	32:2a:1147:C:O4'	2.18	0.43
33:2b:141:GLU:O	33:2b:144:ARG:HB3	2.18	0.43
38:2g:69:VAL:HG21	38:2g:104:LEU:HD21	1.99	0.43
50:2s:23:ASN:HA	50:2s:27:GLU:CD	2.42	0.43
1:1A:1312:U:H4'	1:1A:1313:U:O5'	2.18	0.43
31:19:7:VAL:HG12	31:19:34:GLN:HB3	2.00	0.43
32:1a:78:G:C6	32:1a:91:C:N4	2.87	0.43
32:1a:157:G:H1	32:1a:164:U:H3	1.64	0.43
35:1d:19:LEU:HD23	35:1d:67:ILE:CG1	2.48	0.43
40:1i:100:GLY:O	40:1i:103:THR:HG22	2.19	0.43
44:1m:33:ALA:HB2	44:1m:64:TRP:HH2	1.83	0.43
44:1m:67:GLU:O	44:1m:71:ARG:HG3	2.18	0.43
49:1r:58:LEU:HD12	49:1r:63:GLN:NE2	2.33	0.43
54:1w:323:ASP:O	54:1w:327:VAL:HG23	2.18	0.43
1:2A:236:C:H2'	1:2A:237:C:C6	2.53	0.43
1:2A:995:C:O2	9:2N:3:THR:OG1	2.34	0.43
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	2.01	0.43
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.18	0.43
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.33	0.43
1:2A:1988:C:H2'	1:2A:1989:G:O4'	2.18	0.43
1:2A:2258:C:O2'	1:2A:2427:C:OP2	2.30	0.43
6:2G:96:ARG:N	6:2G:99:MET:HE2	2.33	0.43
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.18	0.43
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.18	0.43
17:2V:56:SER:HB3	17:2V:100:ARG:HB2	2.00	0.43
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.33	0.43
30:28:6:THR:HG23	30:28:62:LEU:HD23	2.00	0.43
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.53	0.43
32:2a:1252:A:H2'	32:2a:1253:G:O4'	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:29:ALA:HA	33:2b:32:ILE:HD12	2.00	0.43
33:2b:219:VAL:O	33:2b:223:ILE:HG22	2.18	0.43
35:2d:196:LEU:H	35:2d:196:LEU:HD12	1.83	0.43
36:2e:40:ARG:NH1	36:2e:68:GLU:HA	2.33	0.43
41:2j:32:ALA:HB3	41:2j:74:ILE:HD11	2.01	0.43
54:2w:177:VAL:HG13	54:2w:196:THR:HG23	1.99	0.43
55:2x:55:PSU:O2'	55:2x:57:G:N7	2.37	0.43
1:1A:144:C:H5'	19:1X:2:LYS:HD2	1.98	0.43
1:1A:234:C:H2'	1:1A:235:U:C6	2.54	0.43
1:1A:1399:C:OP1	19:1X:25:LYS:NZ	2.52	0.43
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.34	0.43
1:1A:2747:G:O6	1:1A:2755:C:H5"	2.17	0.43
1:1A:2853:C:H2'	1:1A:2854:G:C8	2.53	0.43
6:1G:9:ARG:NH1	6:1G:13:GLU:OE2	2.51	0.43
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	2.00	0.43
32:1a:474:G:H2'	32:1a:475:G:C8	2.53	0.43
32:1a:564:C:OP1	43:1l:15:ARG:NE	2.48	0.43
32:1a:1296:C:H4'	32:1a:1302:U:C5	2.53	0.43
34:1c:33:LEU:O	34:1c:37:GLN:N	2.51	0.43
42:1k:97:ALA:O	42:1k:101:SER:OG	2.35	0.43
43:1l:38:THR:OG1	43:1l:39:VAL:N	2.52	0.43
1:2A:242:G:C8	30:28:5:LYS:HG2	2.53	0.43
1:2A:601:C:O2'	1:2A:605:C:H5"	2.18	0.43
1:2A:646:A:H2'	1:2A:647:G:O4'	2.18	0.43
1:2A:876:C:H2'	1:2A:877:U:O4'	2.18	0.43
1:2A:924:C:H2'	1:2A:925:C:C6	2.53	0.43
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.29	0.43
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.54	0.43
1:2A:2396:G:H1'	23:21:30:VAL:HG12	2.01	0.43
3:2D:35:LYS:HB2	3:2D:36:PRO:HD2	2.01	0.43
3:2D:96:HIS:CD2	3:2D:102:LYS:HG2	2.54	0.43
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.33	0.43
25:23:7:LYS:NZ	25:23:34:GLU:HG3	2.32	0.43
32:2a:930:C:H2'	32:2a:931:C:O4'	2.19	0.43
32:2a:1005:A:P	32:2a:1006:C:H41	2.41	0.43
32:2a:1240:U:C2	38:2g:32:ARG:HD2	2.53	0.43
33:2b:133:LYS:HA	33:2b:136:VAL:HG22	2.00	0.43
44:2m:66:LEU:HD23	44:2m:66:LEU:HA	1.86	0.43
1:1A:576:U:H2'	1:1A:577:G:C8	2.53	0.43
1:1A:639:U:H2'	1:1A:640:C:C6	2.54	0.43
1:1A:922:U:H2'	1:1A:923:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1309:G:H4'	29:17:7:PRO:HB2	2.00	0.43
1:1A:1683:C:H2'	1:1A:1684:C:H6	1.82	0.43
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.53	0.43
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.18	0.43
7:1H:155:SER:HB3	7:1H:158:HIS:O	2.19	0.43
8:1I:40:THR:HG23	8:1I:43:ASN:H	1.83	0.43
24:12:53:LEU:HD12	24:12:53:LEU:HA	1.76	0.43
32:1a:418:C:H2'	32:1a:419:C:C6	2.53	0.43
32:1a:509:A:O2'	32:1a:510:A:OP1	2.33	0.43
32:1a:554:C:H2'	32:1a:555:C:C6	2.53	0.43
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.99	0.43
32:1a:1034:G:C2'	32:1a:1035:A:H5'	2.48	0.43
32:1a:1134:G:H3'	32:1a:1135:U:H6	1.84	0.43
32:1a:1144:G:N2	32:1a:1146:A:H62	2.16	0.43
32:1a:1343:G:H4'	40:1i:122:ALA:HB3	1.99	0.43
34:1c:129:ALA:HB3	34:1c:132:ARG:HD2	2.00	0.43
51:1t:16:HIS:O	51:1t:19:SER:OG	2.35	0.43
1:2A:171:G:H2'	1:2A:172:C:C6	2.53	0.43
1:2A:197:A:N6	1:2A:2430:A:H2'	2.33	0.43
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.51	0.43
1:2A:1472:A:H2'	1:2A:1473:G:O4'	2.18	0.43
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.18	0.43
1:2A:1856:G:H2'	1:2A:1857:G:O4'	2.18	0.43
1:2A:2129:C:H3'	1:2A:2130:U:C6	2.53	0.43
6:2G:12:TYR:HA	6:2G:16:ARG:HD3	1.99	0.43
17:2V:64:HIS:ND1	17:2V:92:THR:OG1	2.37	0.43
25:23:7:LYS:HZ3	25:23:34:GLU:HG3	1.84	0.43
32:2a:148:G:H2'	32:2a:149:A:C8	2.53	0.43
32:2a:636:U:H2'	32:2a:637:G:C8	2.53	0.43
32:2a:1176:A:C6	32:2a:1177:G:C6	3.07	0.43
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	2.00	0.43
33:2b:92:TYR:CD2	33:2b:151:GLY:HA3	2.53	0.43
34:2c:51:GLY:C	34:2c:70:VAL:HG13	2.43	0.43
37:2f:11:ASN:HB3	37:2f:14:LEU:HG	2.01	0.43
37:2f:96:PRO:HB3	49:2r:30:ASP:OD2	2.18	0.43
47:2p:3:LYS:O	47:2p:21:VAL:HA	2.19	0.43
51:2t:50:GLU:O	51:2t:100:ILE:HD11	2.18	0.43
1:1A:516:C:OP1	27:15:13:LYS:NZ	2.43	0.43
1:1A:2101:G:H3'	1:1A:2102:U:C6	2.53	0.43
1:1A:2576:G:O2'	1:1A:2579:C:OP2	2.26	0.43
21:1Z:67:LEU:HD23	21:1Z:67:LEU:HA	1.90	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:5:U:C4	35:1d:86:LYS:HE2	2.54	0.43
32:1a:292:G:N7	32:1a:293:G:H1'	2.34	0.43
32:1a:300:A:H2'	32:1a:301:G:O4'	2.19	0.43
32:1a:518:C:O2'	32:1a:530:G:N2	2.50	0.43
32:1a:730:G:C5	32:1a:731:G:H1'	2.54	0.43
32:1a:924:C:H2'	32:1a:925:G:C8	2.54	0.43
32:1a:1080:A:H5'	36:1e:14:ARG:NH2	2.32	0.43
32:1a:1317:C:H42	45:1n:19:ARG:HH21	1.65	0.43
34:1c:19:GLU:HG2	34:1c:54:ARG:NE	2.34	0.43
37:1f:82:ARG:HB2	37:1f:85:VAL:HG23	2.00	0.43
54:1w:250:VAL:HG21	54:1w:268:ILE:HG22	2.00	0.43
1:2A:315:G:H2'	1:2A:316:C:O4'	2.17	0.43
1:2A:660:G:H5'	5:2F:99:TYR:CE1	2.54	0.43
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.54	0.43
6:2G:51:ARG:O	6:2G:52:ILE:C	2.62	0.43
18:2W:71:VAL:HA	18:2W:107:LEU:HD23	2.01	0.43
20:2Y:20:TYR:CE2	20:2Y:43:ASN:HA	2.53	0.43
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.52	0.43
32:2a:598:U:H2'	32:2a:599:C:C6	2.54	0.43
32:2a:779:C:H2'	32:2a:780:A:O4'	2.19	0.43
32:2a:1012:U:H3	32:2a:1017:G:H1	1.66	0.43
32:2a:1070:U:H2'	32:2a:1071:C:H6	1.82	0.43
32:2a:1372:U:H2'	32:2a:1373:G:O4'	2.19	0.43
37:2f:6:VAL:HG22	37:2f:90:VAL:HG22	2.00	0.43
38:2g:50:ILE:HG21	38:2g:58:PRO:HA	1.99	0.43
46:2o:5:LYS:NZ	46:2o:5:LYS:H	2.16	0.43
54:2w:335:ILE:H	54:2w:335:ILE:HG13	1.62	0.43
1:1A:212:G:H2'	1:1A:213:A:O4'	2.18	0.43
1:1A:1045:A:H8	1:1A:1047:G:N2	2.17	0.43
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.53	0.43
1:1A:2347:C:OP1	28:16:38:LYS:NZ	2.45	0.43
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.19	0.43
6:1G:111:LEU:HA	6:1G:114:ILE:HG13	2.01	0.43
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.81	0.43
32:1a:297:G:N2	32:1a:300:A:OP2	2.48	0.43
32:1a:439:A:N1	32:1a:496:A:H1'	2.34	0.43
32:1a:458:C:H2'	32:1a:460:G:O4'	2.18	0.43
32:1a:662:G:H2'	32:1a:663:A:C8	2.54	0.43
32:1a:737:A:H2'	32:1a:738:C:H6	1.83	0.43
32:1a:1030:C:N4	32:1a:1030(A):G:N3	2.67	0.43
36:1e:93:PRO:HG2	39:1h:105:ARG:NH1	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:87:SER:HB3	39:1h:133:LEU:O	2.19	0.43
1:2A:784:A:H5'	1:2A:785:G:OP1	2.18	0.43
1:2A:1339:G:N2	1:2A:1603:A:H1'	2.33	0.43
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.53	0.43
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.19	0.43
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.53	0.43
7:2H:9:ILE:HB	7:2H:50:VAL:HB	2.00	0.43
8:2I:27:ARG:HD3	23:21:71:TYR:CE2	2.54	0.43
16:2U:69:CYS:HB3	16:2U:74:LEU:HD13	2.00	0.43
32:2a:457:C:H2'	32:2a:458:C:H6	1.84	0.43
32:2a:1265:G:C6	32:2a:1266:G:C6	3.07	0.43
36:2e:6:PHE:HD1	36:2e:6:PHE:HA	1.77	0.43
40:2i:26:VAL:HG12	40:2i:61:ALA:HB3	2.01	0.43
41:2j:61:GLU:OE1	45:2n:45:ARG:NE	2.49	0.43
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.18	0.43
54:2w:171:PHE:O	54:2w:201:VAL:HG21	2.18	0.43
1:1A:265:A:N1	1:1A:427:U:O2'	2.49	0.43
1:1A:720:C:H2'	1:1A:721:C:H6	1.83	0.43
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.19	0.43
1:1A:2447:G:OP2	61:1A:4145:HOH:O	2.22	0.43
2:1B:66:A:H61	2:1B:108:U:H2'	1.83	0.43
2:1B:73:A:C4	2:1B:105:A:C2	3.07	0.43
8:1I:44:LEU:HD23	8:1I:44:LEU:HA	1.83	0.43
32:1a:501:C:H2'	32:1a:502:G:H8	1.82	0.43
32:1a:924:C:H2'	32:1a:925:G:H8	1.83	0.43
32:1a:1268:A:O2'	52:1u:19:GLY:HA2	2.18	0.43
32:1a:1293:G:H2'	32:1a:1294:G:C8	2.53	0.43
35:1d:174:LEU:HD23	35:1d:185:PHE:HA	2.00	0.43
44:1m:78:ILE:HG12	44:1m:78:ILE:H	1.41	0.43
48:1q:53:LEU:HD22	48:1q:85:VAL:HG11	2.00	0.43
1:2A:414:C:H2'	1:2A:415:A:C8	2.54	0.43
1:2A:443:A:N7	5:2F:45:ARG:HG2	2.34	0.43
1:2A:2189:U:H2'	1:2A:2190:G:C8	2.54	0.43
2:2B:72:G:H1'	2:2B:105:A:H61	1.83	0.43
6:2G:112:PRO:HG3	26:24:43:TYR:CE2	2.54	0.43
28:26:6:ARG:HD3	28:26:24:GLU:OE2	2.18	0.43
32:2a:540:G:H2'	32:2a:541:G:O4'	2.19	0.43
32:2a:865:A:C2	32:2a:918:A:H4'	2.54	0.43
32:2a:1236:A:H2'	32:2a:1237:C:C6	2.54	0.43
32:2a:1360:A:H8	32:2a:1360:A:OP1	2.02	0.43
33:2b:19:HIS:CG	33:2b:20:GLU:N	2.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:207:ALA:O	33:2b:211:ILE:HG13	2.19	0.43
44:2m:86:CYS:SG	44:2m:87:TYR:N	2.92	0.43
54:2w:218:ARG:NH1	54:2w:220:ASP:OD2	2.52	0.43
1:1A:153:C:OP2	23:11:92:LYS:NZ	2.52	0.43
1:1A:251:A:C5	1:1A:252:G:H1'	2.54	0.43
1:1A:330:A:N7	1:1A:1210:A:O2'	2.42	0.43
1:1A:569:U:C4	1:1A:570:G:C6	3.07	0.43
1:1A:2115:G:H2'	1:1A:2117:A:H62	1.84	0.43
18:1W:5:ALA:C	18:1W:6:ILE:HG13	2.42	0.43
23:11:18:ILE:HG12	23:11:37:ILE:HG23	2.00	0.43
32:1a:1352:C:H2'	32:1a:1353:G:C8	2.53	0.43
32:1a:1516:G:H2'	32:1a:1518:MA6:OP2	2.19	0.43
40:1i:89:ASN:HA	40:1i:90:PRO:HD3	1.89	0.43
42:1k:98:LEU:HD23	42:1k:98:LEU:HA	1.75	0.43
50:1s:47:HIS:O	50:1s:62:ILE:HD12	2.19	0.43
1:2A:698:C:O2'	1:2A:734:A:N6	2.52	0.43
1:2A:1710:C:H2'	1:2A:1711:C:C6	2.54	0.43
1:2A:2097:C:H2'	1:2A:2098:U:C6	2.54	0.43
1:2A:2280:G:O2'	1:2A:2388:A:N1	2.43	0.43
1:2A:2378:A:C5	1:2A:2379:G:H1'	2.54	0.43
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.54	0.43
2:2B:48:A:H2'	2:2B:49:C:C6	2.54	0.43
3:2D:206:LEU:O	3:2D:211:ARG:HD3	2.18	0.43
8:2I:75:LEU:HD11	8:2I:105:HIS:CE1	2.53	0.43
10:2O:92:GLU:HG2	10:2O:113:LYS:HE3	2.01	0.43
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.67	0.43
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.51	0.43
20:2Y:35:TYR:CE2	20:2Y:69:ALA:HB3	2.54	0.43
32:2a:310:G:H5'	47:2p:31:LYS:HB2	2.01	0.43
32:2a:325:A:OP2	51:2t:70:SER:OG	2.24	0.43
32:2a:438:G:H4'	35:2d:123:HIS:CE1	2.53	0.43
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.34	0.43
32:2a:975:A:H5"	32:2a:1363(A):A:N6	2.33	0.43
33:2b:187:LEU:HA	33:2b:201:ILE:O	2.19	0.43
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.54	0.43
38:2g:137:LYS:HA	38:2g:140:ASP:HB2	2.01	0.43
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.52	0.43
44:2m:20:THR:C	44:2m:22:ILE:H	2.27	0.43
1:1A:26:G:C6	1:1A:27:G:N1	2.87	0.43
1:1A:572:A:H5"	1:1A:573:G:OP2	2.19	0.43
1:1A:720:C:H2'	1:1A:721:C:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:910:A:N1	1:1A:2277:G:H1'	2.34	0.43
2:1B:55:U:H2'	2:1B:56:G:O4'	2.19	0.43
32:1a:336:C:H2'	32:1a:337:C:C6	2.54	0.43
32:1a:620:C:C2	35:1d:135:LEU:HD13	2.54	0.43
32:1a:1016:A:O2'	32:1a:1217:C:O2'	2.22	0.43
32:1a:1496:C:H2'	32:1a:1497:G:O4'	2.18	0.43
33:1b:27:LYS:HD2	33:1b:193:ASP:OD1	2.18	0.43
34:1c:124:ILE:HD12	34:1c:196:LEU:HD22	2.00	0.43
45:1n:21:TYR:HE1	45:1n:23:ARG:CZ	2.32	0.43
47:1p:15:PRO:HD2	47:1p:42:ARG:HG2	2.00	0.43
49:1r:47:THR:O	49:1r:83:GLU:N	2.50	0.43
54:1w:223:ARG:NH1	54:1w:223:ARG:HB2	2.34	0.43
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.19	0.43
1:2A:2471:C:N4	1:2A:2476:A:O2'	2.52	0.43
3:2D:70:TRP:HB3	3:2D:190:TYR:CE2	2.54	0.43
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.54	0.43
9:2N:29:LYS:O	9:2N:33:LEU:HG	2.19	0.43
11:2P:46:LYS:HE2	11:2P:46:LYS:HB3	1.83	0.43
14:2S:38:GLN:HB2	14:2S:47:THR:HG23	2.00	0.43
32:2a:518:C:OP2	32:2a:530:G:O2'	2.31	0.43
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	2.01	0.43
35:2d:49:ARG:HE	35:2d:49:ARG:HB2	1.58	0.43
39:2h:85:ARG:NH1	39:2h:134:ILE:HG23	2.33	0.43
40:2i:88:TYR:HD2	40:2i:89:ASN:ND2	2.17	0.43
1:1A:581:C:H2'	1:1A:582:G:H8	1.84	0.42
1:1A:1235:G:OP1	61:1A:4140:HOH:O	2.22	0.42
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.84	0.42
1:1A:1478:G:O2'	1:1A:1558:A:N7	2.48	0.42
1:1A:2572:A:N7	4:1E:145:LYS:HB2	2.33	0.42
5:1F:184:TYR:CD2	5:1F:188:ARG:HD2	2.54	0.42
18:1W:4:LYS:HD3	18:1W:6:ILE:HD11	2.00	0.42
26:14:49:PHE:HD1	26:14:49:PHE:HA	1.69	0.42
32:1a:189(K):U:H2'	32:1a:189(L):G:H8	1.82	0.42
32:1a:202:U:O2'	32:1a:203:U:O5'	2.31	0.42
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.19	0.42
34:1c:16:ARG:HE	34:1c:16:ARG:HB3	1.49	0.42
34:1c:114:PRO:O	34:1c:118:GLN:NE2	2.51	0.42
34:1c:148:GLY:HA3	34:1c:172:ARG:H	1.84	0.42
34:1c:180:ALA:HB1	34:1c:203:PHE:CE1	2.54	0.42
35:1d:142:PRO:HB3	35:1d:186:LEU:O	2.19	0.42
50:1s:35:SER:HB3	50:1s:38:SER:OG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:55:LYS:HG2	50:1s:56:GLN:HG3	2.01	0.42
1:2A:466:A:N1	1:2A:795:C:O2'	2.52	0.42
1:2A:824:A:H1'	1:2A:2358:G:N7	2.34	0.42
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.52	0.42
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.51	0.42
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.54	0.42
1:2A:2113:U:H3'	1:2A:2115:G:H1	1.83	0.42
1:2A:2286:A:N1	28:26:24:GLU:O	2.52	0.42
1:2A:2682:U:H5'	4:2E:11:MET:O	2.19	0.42
1:2A:2740:A:C6	1:2A:2741:A:C6	3.07	0.42
2:2B:4:C:H42	2:2B:117:G:H1	1.67	0.42
4:2E:25:VAL:HG22	4:2E:183:LEU:HD11	2.00	0.42
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.54	0.42
5:2F:176:LEU:HD23	5:2F:176:LEU:HA	1.83	0.42
8:2I:87:LYS:HE2	8:2I:87:LYS:HB2	1.68	0.42
27:25:9:LYS:HD3	27:25:9:LYS:HA	1.85	0.42
32:2a:266:G:O3'	48:2q:67:LYS:HB2	2.18	0.42
32:2a:652:U:O4	32:2a:752:G:O2'	2.26	0.42
32:2a:1323:G:H2'	32:2a:1324:A:H8	1.83	0.42
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.19	0.42
34:2c:150:LYS:HD2	34:2c:201:TYR:HD2	1.85	0.42
40:2i:8:GLY:HA3	40:2i:15:ALA:HB3	2.01	0.42
41:2j:13:HIS:HB3	41:2j:68:HIS:CE1	2.54	0.42
47:2p:43:LYS:HG2	47:2p:48:TRP:CD2	2.54	0.42
50:2s:52:TYR:HA	50:2s:56:GLN:O	2.20	0.42
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.33	0.42
1:1A:1098:A:H5"	1:1A:1099:G:OP2	2.19	0.42
1:1A:1359:A:N6	1:1A:1372:U:H3	2.17	0.42
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.19	0.42
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.54	0.42
4:1E:168:MET:HE2	4:1E:168:MET:HB3	1.89	0.42
4:1E:175:VAL:O	4:1E:177:PRO:HD3	2.19	0.42
10:1O:64:ARG:HG2	10:1O:79:PHE:CD1	2.54	0.42
22:10:53:MET:HG3	22:10:59:LEU:HD23	2.01	0.42
32:1a:1288:A:N1	32:1a:1371:G:H1'	2.34	0.42
32:1a:1394:A:N1	32:1a:1500:A:O2'	2.45	0.42
39:1h:94:TYR:CE1	39:1h:132:GLU:HB2	2.54	0.42
54:1w:152:LEU:HD12	54:1w:152:LEU:HA	1.89	0.42
1:2A:1485:G:H2'	1:2A:1486:A:C8	2.54	0.42
1:2A:1754:C:H2'	1:2A:1755:A:O4'	2.19	0.42
1:2A:1857:G:O6	1:2A:1858:G:N1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:29:TYR:HD2	8:2I:30:LEU:HD23	1.83	0.42
32:2a:683:G:C6	32:2a:684:A:C6	3.07	0.42
43:2l:55:VAL:HG12	43:2l:69:TYR:HA	2.00	0.42
54:2w:102:MET:C	54:2w:104:GLU:H	2.26	0.42
1:1A:37:C:H2'	1:1A:38:A:C8	2.53	0.42
1:1A:272(H):C:H2'	1:1A:272(I):U:C6	2.54	0.42
1:1A:458:G:C8	29:17:37:LYS:HG2	2.55	0.42
1:1A:747:U:O2	1:1A:2014:A:H1'	2.18	0.42
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.54	0.42
3:1D:3:VAL:HG13	3:1D:17:THR:HB	2.00	0.42
4:1E:11:MET:HE2	4:1E:11:MET:HB3	1.96	0.42
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.36	0.42
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.84	0.42
29:17:24:THR:HG23	61:17:205:HOH:O	2.19	0.42
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.35	0.42
32:1a:363:A:C5	43:1l:31:PRO:HD2	2.55	0.42
35:1d:68:TYR:CE1	35:1d:97:LEU:HB3	2.54	0.42
35:1d:176:LEU:HD12	35:1d:177:ASP:H	1.85	0.42
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	2.00	0.42
40:1i:19:LEU:HD22	40:1i:59:PHE:HB3	2.01	0.42
1:2A:609:A:H2'	1:2A:610:G:O4'	2.19	0.42
1:2A:1263:U:C4	1:2A:1264:G:C6	3.07	0.42
2:2B:88:C:H2'	2:2B:89:G:O4'	2.19	0.42
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.53	0.42
32:2a:970:C:N4	40:2i:128:ARG:OXT	2.52	0.42
32:2a:1128:C:H4'	32:2a:1129:C:OP1	2.20	0.42
32:2a:1178:G:N2	32:2a:1181:G:OP2	2.47	0.42
32:2a:1278:U:C5'	32:2a:1279:A:H5'	2.48	0.42
32:2a:1469:G:H2'	32:2a:1470:G:H8	1.83	0.42
35:2d:191:ARG:HE	35:2d:200:GLU:CD	2.27	0.42
36:2e:92:LYS:HB3	36:2e:119:LEU:HB2	2.01	0.42
40:2i:23:ASN:CG	40:2i:25:LYS:HD3	2.45	0.42
40:2i:25:LYS:N	40:2i:25:LYS:HD2	2.35	0.42
1:1A:631:A:N3	1:1A:2415:G:O2'	2.46	0.42
1:1A:724:U:H2'	1:1A:725:G:O4'	2.19	0.42
1:1A:1783:A:H5'	1:1A:2608:G:H4'	2.02	0.42
4:1E:1:MET:HB3	4:1E:83:ASP:O	2.18	0.42
10:1O:16:ALA:HB2	10:1O:52:VAL:HG21	2.00	0.42
16:1U:39:LEU:HA	16:1U:39:LEU:HD23	1.77	0.42
32:1a:701:C:O2	32:1a:703:G:N1	2.52	0.42
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.19	0.42
33:1b:88:ALA:HB2	33:1b:219:VAL:HG23	2.01	0.42
34:1c:195:VAL:O	34:1c:196:LEU:HD12	2.20	0.42
35:1d:11:LEU:HD23	35:1d:66:ARG:HB3	2.00	0.42
46:1o:82:ILE:O	46:1o:86:GLY:N	2.53	0.42
51:1t:57:ARG:HH12	51:1t:100:ILE:CD1	2.33	0.42
54:1w:103:ASP:HB3	54:1w:169:GLY:HA2	2.01	0.42
1:2A:64:A:H2'	1:2A:65:C:O4'	2.20	0.42
1:2A:108:U:H2'	1:2A:109:G:C8	2.55	0.42
1:2A:657:U:H2'	1:2A:658:C:C6	2.53	0.42
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.55	0.42
7:2H:84:SER:HA	7:2H:133:VAL:O	2.18	0.42
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	2.01	0.42
10:2O:52:VAL:HG11	10:2O:58:VAL:HG11	2.01	0.42
32:2a:160:A:H2'	32:2a:161:A:O4'	2.19	0.42
32:2a:814:A:N7	32:2a:816:A:C4	2.87	0.42
32:2a:939:G:H2'	32:2a:940:C:C6	2.54	0.42
32:2a:1206:G:O4'	34:2c:194:GLY:N	2.52	0.42
44:2m:87:TYR:CE2	44:2m:91:ARG:HD2	2.55	0.42
1:1A:207:A:H2'	1:1A:208:C:O4'	2.17	0.42
1:1A:306:U:H2'	1:1A:307:G:O4'	2.20	0.42
1:1A:1754:C:N3	1:1A:2716:U:O2'	2.45	0.42
1:1A:1930:G:O2'	1:1A:1968:G:O6	2.25	0.42
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.20	0.42
1:1A:2137:C:H2'	1:1A:2138:C:C6	2.54	0.42
12:1Q:12:GLN:NE2	12:1Q:72:LYS:HG3	2.35	0.42
16:1U:16:LYS:HB3	16:1U:16:LYS:HE2	1.74	0.42
16:1U:102:GLU:HB3	16:1U:104:GLN:HE22	1.84	0.42
29:17:1:MET:HE3	29:17:3:ARG:NH2	2.34	0.42
32:1a:448:A:P	32:1a:485:G:H22	2.43	0.42
32:1a:1164:G:C6	32:1a:1173:G:C6	3.08	0.42
32:1a:1346:A:O3'	32:1a:1347:G:H4'	2.20	0.42
36:1e:68:GLU:HG3	36:1e:69:VAL:N	2.35	0.42
50:1s:32:LYS:HG2	50:1s:57:HIS:CE1	2.54	0.42
1:2A:614(C):A:C4	5:2F:180:GLY:HA2	2.54	0.42
1:2A:864:G:C6	1:2A:865:C:N4	2.87	0.42
1:2A:994:C:O2'	1:2A:996:A:OP1	2.33	0.42
3:2D:228:PRO:HD3	3:2D:235:GLY:HA3	2.02	0.42
5:2F:29:ASN:HD22	5:2F:32:LEU:HB2	1.85	0.42
5:2F:172:TRP:CD1	5:2F:172:TRP:H	2.37	0.42
23:21:67:ILE:N	23:21:68:PRO:HD2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:13:ARG:HA	26:24:22:ILE:O	2.19	0.42
30:28:32:LEU:O	30:28:36:LYS:HE3	2.19	0.42
32:2a:974:A:H8	32:2a:974:A:OP1	2.03	0.42
32:2a:1129:C:H1'	32:2a:1130:A:N7	2.34	0.42
32:2a:1133:G:H2'	32:2a:1134:G:C8	2.54	0.42
42:2k:38:ASN:HA	42:2k:39:PRO:HD3	1.89	0.42
1:1A:1002:G:H2'	1:1A:1003:G:O4'	2.20	0.42
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.83	0.42
1:1A:2319:G:N2	14:1S:3:ARG:HA	2.34	0.42
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.34	0.42
1:1A:2576:G:H1'	61:1A:4726:HOH:O	2.18	0.42
6:1G:70:VAL:HG11	6:1G:87:PRO:HB3	2.01	0.42
6:1G:83:ARG:H	6:1G:86:MET:CE	2.32	0.42
7:1H:35:VAL:O	7:1H:37:VAL:HG12	2.19	0.42
26:14:61:ARG:HG2	26:14:62:ARG:N	2.35	0.42
31:19:17:ILE:HD13	31:19:26:ILE:HD13	2.01	0.42
32:1a:406:G:O3'	35:1d:3:ARG:NH2	2.53	0.42
32:1a:598:U:H4'	39:1h:94:TYR:CD2	2.54	0.42
32:1a:979:C:O2	45:1n:19:ARG:NE	2.53	0.42
32:1a:1104:G:C2	32:1a:1105:A:C4	3.06	0.42
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.37	0.42
1:2A:662:G:H5"	11:2P:16:ARG:HG2	2.01	0.42
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.54	0.42
2:2B:50:G:OP1	14:2S:63:THR:OG1	2.27	0.42
4:2E:13:ARG:HG2	15:2T:58:ASN:HD21	1.84	0.42
5:2F:7:TYR:CD2	5:2F:24:LEU:HB2	2.55	0.42
8:2I:104:GLN:HB3	8:2I:105:HIS:H	1.62	0.42
10:2O:7:TYR:CZ	10:2O:44:LYS:HG3	2.55	0.42
12:2Q:42:ILE:O	12:2Q:95:ALA:N	2.48	0.42
21:2Z:61:LEU:HB2	21:2Z:65:GLN:HB2	2.02	0.42
32:2a:399:G:H2'	32:2a:400:C:C6	2.55	0.42
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.55	0.42
32:2a:1162:C:N4	32:2a:1174:G:H1	2.13	0.42
34:2c:156:ARG:HD3	34:2c:193:TYR:O	2.20	0.42
43:2l:119:LYS:C	43:2l:121:GLY:H	2.27	0.42
1:1A:125:G:C6	29:17:10:ARG:HG3	2.55	0.42
1:1A:381:G:O6	61:1A:4143:HOH:O	2.21	0.42
1:1A:466:A:N3	1:1A:683:C:H1'	2.35	0.42
1:1A:1062:G:N1	1:1A:1088:A:H2'	2.35	0.42
1:1A:2110:G:N1	1:1A:2120:G:H1'	2.34	0.42
32:1a:44:G:H2'	32:1a:45:U:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:687:A:N3	32:1a:688:G:H1'	2.35	0.42
32:1a:741:G:H2'	32:1a:742:G:O4'	2.19	0.42
32:1a:1134:G:H5'	32:1a:1135:U:OP2	2.19	0.42
33:1b:20:GLU:C	33:1b:39:ILE:HG23	2.45	0.42
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.19	0.42
36:1e:60:TYR:CD1	36:1e:64:ARG:HD2	2.54	0.42
46:1o:8:LYS:O	46:1o:12:ILE:HG13	2.19	0.42
1:2A:36:G:N3	1:2A:450:G:O2'	2.53	0.42
1:2A:687:C:H2'	1:2A:688:U:O4'	2.19	0.42
1:2A:884:C:N4	1:2A:893:C:C2	2.88	0.42
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.46	0.42
1:2A:2019:A:N7	27:25:9:LYS:HE3	2.35	0.42
1:2A:2842:G:H2'	1:2A:2843:G:O4'	2.20	0.42
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.20	0.42
14:2S:11:LYS:HD2	14:2S:15:ARG:NH1	2.34	0.42
23:21:8:SER:HB3	23:21:66:HIS:NE2	2.35	0.42
30:28:62:LEU:HB3	30:28:65:GLU:HG2	2.02	0.42
32:2a:255:G:H4'	48:2q:17:LYS:HD2	2.02	0.42
32:2a:325:A:H2'	32:2a:326:G:O4'	2.20	0.42
32:2a:674:G:H2'	32:2a:675:A:H8	1.85	0.42
32:2a:840:C:H4'	32:2a:841:U:OP1	2.19	0.42
32:2a:1001(A):G:H2'	32:2a:1002:G:O4'	2.20	0.42
32:2a:1206:G:H4'	34:2c:192:THR:C	2.44	0.42
36:2e:12:LEU:O	36:2e:30:ALA:HA	2.20	0.42
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.38	0.42
44:2m:78:ILE:HG22	44:2m:82:MET:HE2	2.01	0.42
50:2s:28:LYS:HB3	50:2s:28:LYS:HE3	1.92	0.42
54:2w:242:VAL:HG22	54:2w:249:MET:HB3	2.02	0.42
1:1A:372:G:H8	23:11:65:SER:O	2.03	0.42
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.55	0.42
1:1A:1680:U:O2'	1:1A:1763:G:N7	2.48	0.42
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.55	0.42
32:1a:321:A:N7	32:1a:328:C:O2'	2.49	0.42
32:1a:628:G:H2'	32:1a:629:G:C8	2.55	0.42
32:1a:1381:U:H1'	38:1g:79:ARG:CG	2.43	0.42
38:1g:69:VAL:HG22	38:1g:135:VAL:HG22	2.02	0.42
54:1w:349:ALA:HA	54:1w:350:ALA:HA	1.62	0.42
1:2A:141:A:H8	1:2A:1408:C:O2'	2.02	0.42
1:2A:208:C:H2'	1:2A:209:C:H6	1.85	0.42
1:2A:760:G:H2'	1:2A:761:A:O4'	2.19	0.42
1:2A:832:G:H5'	11:2P:45:LEU:HD22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:959:A:C6	1:2A:960:A:C6	3.08	0.42
1:2A:2138:C:N4	1:2A:2153:G:H1	2.18	0.42
5:2F:184:TYR:CZ	5:2F:188:ARG:HD2	2.55	0.42
7:2H:41:MET:HE2	7:2H:65:HIS:HA	2.01	0.42
7:2H:103:LEU:HB3	7:2H:115:VAL:HB	2.02	0.42
10:2O:29:ASN:OD1	10:2O:29:ASN:N	2.52	0.42
24:22:51:ARG:O	24:22:55:ARG:HG2	2.18	0.42
32:2a:41:G:H2'	32:2a:42:G:C8	2.55	0.42
32:2a:298:A:C6	32:2a:299:G:C2	3.07	0.42
32:2a:370:C:H2'	32:2a:371:G:C8	2.54	0.42
32:2a:983:A:N1	32:2a:1222:G:N2	2.67	0.42
32:2a:1190:G:O2'	34:2c:3:ASN:HB2	2.20	0.42
36:2e:51:VAL:O	36:2e:55:VAL:HG23	2.19	0.42
40:2i:27:THR:HG23	40:2i:62:TYR:HA	2.00	0.42
43:2l:110:VAL:CG2	43:2l:120:TYR:HB3	2.50	0.42
48:2q:66:SER:OG	48:2q:67:LYS:O	2.38	0.42
54:2w:312:VAL:HG21	54:2w:327:VAL:HG11	2.01	0.42
1:1A:956:G:H2'	1:1A:957:A:H2'	2.01	0.42
1:1A:1094:U:O3'	1:1A:1095:A:H8	2.02	0.42
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.19	0.42
1:1A:1826:G:H2'	1:1A:1827:C:O4'	2.19	0.42
6:1G:7:LEU:N	6:1G:104:GLU:OE1	2.53	0.42
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.85	0.42
12:1Q:37:LEU:HA	12:1Q:37:LEU:HD23	1.85	0.42
16:1U:17:ILE:HG23	16:1U:39:LEU:HD12	2.02	0.42
19:1X:84:ALA:HB3	19:1X:87:GLN:CD	2.45	0.42
23:11:70:VAL:O	23:11:74:VAL:HG13	2.20	0.42
32:1a:1277:C:O2'	32:1a:1279:A:H8	2.03	0.42
32:1a:1299:A:N3	32:1a:1299:A:H2'	2.33	0.42
38:1g:113:GLU:HG2	38:1g:118:VAL:HG22	2.01	0.42
52:1u:2:GLY:C	52:1u:4:GLY:H	2.28	0.42
1:2A:118:A:H1'	1:2A:178:G:O4'	2.20	0.42
1:2A:400:G:O6	61:2A:3946:HOH:O	2.19	0.42
1:2A:493:G:H2'	1:2A:494:G:O4'	2.20	0.42
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.55	0.42
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.45	0.42
6:2G:136:ARG:HA	6:2G:154:GLY:HA3	2.01	0.42
16:2U:102:GLU:OE2	17:2V:13:ARG:NH2	2.39	0.42
19:2X:44:GLU:O	19:2X:48:LYS:N	2.51	0.42
32:2a:404:U:H2'	32:2a:405:U:C6	2.55	0.42
32:2a:751:U:H4'	46:2o:24:SER:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.42	0.42
34:2c:53:ALA:HB2	34:2c:115:LEU:HG	2.01	0.42
41:2j:17:ASP:CG	41:2j:70:ARG:HH21	2.28	0.42
54:2w:217:ILE:HA	54:2w:242:VAL:O	2.20	0.42
1:1A:226:G:N2	1:1A:228:A:H62	2.18	0.42
1:1A:565:C:H2'	1:1A:566:U:O4'	2.20	0.42
1:1A:626:U:O4	11:1P:107:LYS:HE3	2.20	0.42
1:1A:1005:C:H2'	1:1A:1006:C:C6	2.55	0.42
1:1A:1142(A):A:C4	1:1A:1144:G:N7	2.87	0.42
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.20	0.42
1:1A:1359:A:H2'	1:1A:1360:A:H5'	2.02	0.42
1:1A:1364:G:N7	23:11:3:LYS:HE2	2.34	0.42
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.20	0.42
1:1A:2507:C:H4'	54:1w:233:ASN:O	2.20	0.42
7:1H:94:TYR:HA	7:1H:106:THR:O	2.19	0.42
8:1I:101:LEU:HD22	8:1I:140:LEU:HD11	2.01	0.42
10:1O:59:LYS:NZ	10:1O:89:ASN:HD21	2.18	0.42
23:11:49:VAL:HG21	23:11:67:ILE:HG23	2.02	0.42
32:1a:20:U:H2'	32:1a:21:G:O4'	2.20	0.42
32:1a:327:A:H1'	32:1a:329:A:O4'	2.20	0.42
32:1a:620:C:H2'	32:1a:621:A:O4'	2.19	0.42
32:1a:767:A:H2'	32:1a:768:A:O4'	2.20	0.42
32:1a:826:C:H2'	32:1a:827:U:H6	1.83	0.42
32:1a:1088:G:H21	32:1a:1168:A:H61	1.67	0.42
32:1a:1152:A:H5'	41:1j:13:HIS:ND1	2.35	0.42
32:1a:1157:A:H61	32:1a:1178:G:N2	2.18	0.42
32:1a:1391:U:H2'	32:1a:1392:G:H8	1.82	0.42
35:1d:61:LYS:HD2	35:1d:207:TYR:OH	2.20	0.42
40:1i:4:TYR:CE1	40:1i:88:TYR:HA	2.54	0.42
1:2A:195:A:H5"	11:2P:46:LYS:NZ	2.35	0.42
1:2A:234:C:H2'	1:2A:235:U:C6	2.54	0.42
1:2A:1184:G:OP1	25:23:30:ARG:NH1	2.51	0.42
1:2A:1277:G:O2'	13:2R:24:GLN:HG2	2.19	0.42
1:2A:1818:U:O2'	3:2D:154:LYS:O	2.31	0.42
1:2A:2554:U:H2'	1:2A:2555:U:C6	2.54	0.42
2:2B:40:U:O2'	2:2B:42:C:H5'	2.20	0.42
4:2E:175:VAL:O	4:2E:177:PRO:HD3	2.20	0.42
6:2G:72:ARG:NH1	6:2G:87:PRO:HG3	2.35	0.42
15:2T:119:LYS:O	15:2T:123:GLN:HG3	2.20	0.42
32:2a:266:G:N3	32:2a:266:G:H5"	2.35	0.42
32:2a:722:A:H2'	32:2a:724:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.82	0.42
32:2a:1316:G:H4'	45:2n:18:VAL:HG13	2.01	0.42
38:2g:150:ALA:HA	42:2k:59:TYR:HB3	2.02	0.42
45:2n:27:CYS:SG	45:2n:29:ARG:HB2	2.60	0.42
48:2q:29:HIS:CE1	48:2q:32:TYR:HD2	2.38	0.42
49:2r:60:ALA:O	49:2r:64:ARG:HG3	2.19	0.42
1:1A:86:C:H4'	1:1A:104:U:H1'	2.01	0.41
1:1A:945:A:C4	1:1A:2448:A:C2	3.08	0.41
1:1A:1059:G:H2'	1:1A:1060:U:C6	2.54	0.41
1:1A:1915:5MU:OP1	54:1w:112:ARG:NH2	2.53	0.41
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.55	0.41
16:1U:43:GLY:HA3	17:1V:73:SER:OG	2.19	0.41
19:1X:44:GLU:HG3	19:1X:51:VAL:HG23	2.01	0.41
20:1Y:55:TYR:CE1	20:1Y:61:ILE:HG21	2.55	0.41
32:1a:302:G:N3	32:1a:556:C:H4'	2.35	0.41
32:1a:625:G:H4'	47:1p:16:HIS:CG	2.55	0.41
32:1a:946:A:C6	32:1a:947:G:C6	3.08	0.41
32:1a:1058:G:C6	32:1a:1059:C:C4	3.08	0.41
32:1a:1123:A:O2'	41:1j:37:PRO:O	2.35	0.41
34:1c:85:ARG:HG3	34:1c:86:VAL:N	2.35	0.41
47:1p:19:ILE:HD13	47:1p:51:VAL:HG22	2.02	0.41
47:1p:39:TYR:CD2	47:1p:73:LEU:HD11	2.55	0.41
51:1t:91:LEU:HD23	51:1t:91:LEU:HA	1.81	0.41
1:2A:764:A:O4'	3:2D:213:ARG:HG3	2.20	0.41
1:2A:1160:G:C6	1:2A:1161:C:C4	3.08	0.41
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.55	0.41
1:2A:2029:G:H2'	1:2A:2031:A:OP1	2.20	0.41
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.54	0.41
1:2A:2553:G:H1'	1:2A:2582:G:N3	2.34	0.41
1:2A:2721:A:H5"	61:2A:4297:HOH:O	2.19	0.41
5:2F:133:ASN:N	5:2F:138:GLU:OE1	2.53	0.41
12:2Q:1:MET:HE3	12:2Q:1:MET:HB2	1.81	0.41
17:2V:55:ALA:HA	17:2V:101:GLY:HA2	2.02	0.41
29:27:1:MET:HE3	29:27:3:ARG:CZ	2.49	0.41
32:2a:59:A:H5"	32:2a:387:U:H5"	2.02	0.41
32:2a:164:U:H2'	32:2a:165:C:H6	1.85	0.41
32:2a:397:A:H3'	32:2a:397:A:N3	2.35	0.41
32:2a:743:U:H2'	32:2a:744:C:C6	2.54	0.41
32:2a:1338:G:C6	32:2a:1339:A:C6	3.08	0.41
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.52	0.41
34:2c:178:LEU:HD23	34:2c:178:LEU:HA	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:45:ASP:O	38:2g:49:ILE:HG13	2.20	0.41
44:2m:95:GLY:O	44:2m:110:ARG:HG3	2.19	0.41
1:1A:118:A:O5'	1:1A:119:A:H5"	2.19	0.41
1:1A:140:G:N3	1:1A:142:A:N6	2.61	0.41
1:1A:287:C:H2'	1:1A:288:C:C6	2.55	0.41
1:1A:479:A:N3	1:1A:481:G:H5"	2.35	0.41
1:1A:1422:G:H1'	1:1A:1496:A:N1	2.35	0.41
1:1A:2064:C:H2'	1:1A:2065:C:C6	2.55	0.41
1:1A:2134:A:H2'	1:1A:2135:A:H8	1.81	0.41
1:1A:2162:G:H4'	1:1A:2172:U:H5'	2.02	0.41
21:1Z:124:ILE:HD12	21:1Z:124:ILE:HA	1.89	0.41
32:1a:70:G:H1	32:1a:99:U:H3	1.68	0.41
32:1a:114:U:O2'	32:1a:115:G:H5'	2.20	0.41
32:1a:441:A:N6	32:1a:493:G:O2'	2.53	0.41
32:1a:453:A:H4'	47:1p:72:ARG:HB2	2.01	0.41
32:1a:719:C:O2'	49:1r:49:LYS:HB3	2.19	0.41
32:1a:1190:G:H5'	34:1c:176:HIS:CE1	2.55	0.41
32:1a:1253:G:C2	32:1a:1254:C:C2	3.08	0.41
32:1a:1304:G:C5	32:1a:1305:G:C6	3.09	0.41
32:1a:1445:C:C4	32:1a:1446:U:C4	3.08	0.41
33:1b:195:ASP:N	33:1b:195:ASP:OD1	2.51	0.41
40:1i:87:GLN:HG3	40:1i:88:TYR:N	2.35	0.41
1:2A:531:C:H4'	1:2A:532:A:H5"	2.02	0.41
1:2A:1138:G:N3	9:2N:106:MET:HE2	2.35	0.41
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.35	0.41
1:2A:2143:C:H42	1:2A:2148:G:H1	1.68	0.41
1:2A:2370:G:C6	1:2A:2371:G:C6	3.08	0.41
1:2A:2875:C:H2'	1:2A:2876:G:O4'	2.20	0.41
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.55	0.41
6:2G:107:LEU:HD23	6:2G:111:LEU:HD12	2.02	0.41
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.20	0.41
13:2R:98:LEU:HB2	13:2R:113:LEU:HD11	2.02	0.41
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.33	0.41
32:2a:22:G:H4'	32:2a:885:G:C8	2.55	0.41
32:2a:522:C:H41	43:2l:53:ARG:NH1	2.18	0.41
32:2a:949:A:H1'	32:2a:1364:U:H3	1.85	0.41
32:2a:954:G:H2'	32:2a:955:U:C6	2.55	0.41
32:2a:1080:A:OP1	36:2e:47:LYS:HD3	2.20	0.41
32:2a:1366:C:O3'	41:2j:60:ARG:NH2	2.52	0.41
36:2e:71:LEU:O	36:2e:72:GLN:NE2	2.53	0.41
37:2f:35:ALA:CA	37:2f:67:MET:HB3	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2o:29:VAL:HG13	46:2o:63:ARG:HG3	2.01	0.41
50:2s:31:ILE:HG22	50:2s:32:LYS:O	2.21	0.41
50:2s:31:ILE:O	50:2s:50:ALA:N	2.51	0.41
51:2t:13:LEU:O	51:2t:17:ARG:HG3	2.20	0.41
51:2t:53:LEU:HD23	51:2t:53:LEU:HA	1.86	0.41
51:2t:64:ASP:OD2	51:2t:81:LYS:NZ	2.32	0.41
1:1A:9:U:N3	1:1A:2629:A:H2	2.12	0.41
1:1A:548:A:H4'	1:1A:549:G:OP2	2.18	0.41
1:1A:817:C:H4'	1:1A:932:G:C5	2.56	0.41
1:1A:996:A:OP2	16:1U:93:LYS:NZ	2.41	0.41
1:1A:1756:G:H4'	1:1A:1758:G:O4'	2.19	0.41
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.60	0.41
5:1F:46:ARG:HB3	5:1F:48:THR:HG23	2.01	0.41
7:1H:152:ARG:HA	7:1H:152:ARG:HD3	1.80	0.41
13:1R:26:LYS:HE2	13:1R:70:LEU:O	2.19	0.41
32:1a:323:U:H5'	51:1t:23:ARG:HB2	2.03	0.41
32:1a:688:G:H2'	32:1a:689:C:C6	2.55	0.41
34:1c:42:LEU:O	34:1c:46:GLU:N	2.53	0.41
38:1g:26:PHE:O	38:1g:30:ILE:HG13	2.19	0.41
43:1l:8:ASN:OD1	48:1q:34:LYS:HE2	2.19	0.41
50:1s:40:ILE:HA	50:1s:44:MET:SD	2.60	0.41
1:2A:250:G:H2'	1:2A:251:A:C8	2.56	0.41
1:2A:724:U:H2'	1:2A:725:G:O4'	2.20	0.41
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.56	0.41
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.55	0.41
1:2A:2124:G:H1	1:2A:2174:C:H42	1.67	0.41
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.54	0.41
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.20	0.41
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.85	0.41
8:2I:40:THR:OG1	8:2I:43:ASN:ND2	2.54	0.41
8:2I:69:LYS:NZ	8:2I:137:PRO:O	2.47	0.41
19:2X:60:ARG:HH22	29:27:47:ARG:NH1	2.18	0.41
21:2Z:144:LEU:HD23	21:2Z:144:LEU:HA	1.81	0.41
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.55	0.41
35:2d:150:GLU:C	35:2d:152:SER:H	2.29	0.41
35:2d:173:TRP:CE2	35:2d:189:PRO:HG3	2.56	0.41
36:2e:31:LEU:HD12	36:2e:45:PHE:HB2	2.02	0.41
40:2i:17:VAL:HG21	40:2i:81:ILE:N	2.35	0.41
40:2i:86:VAL:HG11	40:2i:93:ARG:NE	2.33	0.41
40:2i:112:LYS:HA	40:2i:119:ALA:HA	2.02	0.41
40:2i:116:LYS:HD2	40:2i:122:ALA:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:2l:33:ARG:O	43:2l:85:ILE:HG12	2.20	0.41
43:2l:52:LEU:HG	54:2w:299:SER:HB2	2.03	0.41
1:1A:271(P):C:O3'	8:1I:42:SER:HB2	2.20	0.41
1:1A:478:A:C6	1:1A:480:A:C6	3.09	0.41
1:1A:824:A:H1'	1:1A:2358:G:N7	2.35	0.41
1:1A:1088:A:H5'	1:1A:1089:G:H8	1.85	0.41
1:1A:1805:U:O2	3:1D:50:THR:HB	2.21	0.41
1:1A:1903:G:OP1	3:1D:241:PRO:HB2	2.20	0.41
1:1A:2090:G:H21	23:11:45:ASN:CG	2.23	0.41
5:1F:36:VAL:HG22	5:1F:101:LEU:HD21	2.03	0.41
10:1O:104:ARG:NH2	15:1T:43:GLN:OE1	2.51	0.41
15:1T:127:ALA:C	15:1T:129:ARG:N	2.74	0.41
18:1W:20:VAL:HG11	18:1W:44:ALA:HA	2.01	0.41
19:1X:61:GLY:HA3	19:1X:73:ARG:O	2.21	0.41
32:1a:1001(A):G:H2'	32:1a:1002:G:O4'	2.21	0.41
32:1a:1084:G:H5'	32:1a:1102:A:OP2	2.20	0.41
32:1a:1370:G:C2	32:1a:1371:G:C8	3.09	0.41
34:1c:23:TYR:HA	41:1j:11:PHE:CE2	2.55	0.41
34:1c:155:GLY:HA3	34:1c:196:LEU:HG	2.02	0.41
37:1f:3:ARG:HA	37:1f:65:VAL:O	2.20	0.41
44:1m:16:ASP:HA	44:1m:30:ALA:HB1	2.02	0.41
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.21	0.41
47:1p:1:MET:HE2	47:1p:1:MET:N	2.35	0.41
52:1u:12:LYS:HB3	52:1u:17:THR:O	2.21	0.41
54:1w:285:LEU:HG	54:1w:289:ARG:NH1	2.35	0.41
1:2A:27:G:O2'	1:2A:28:A:OP2	2.35	0.41
1:2A:200:U:O2	1:2A:386:G:N2	2.54	0.41
1:2A:483:A:H3'	1:2A:484:C:H6	1.85	0.41
1:2A:2336:A:H61	22:20:43:THR:CG2	2.34	0.41
1:2A:2841:C:H2'	1:2A:2842:G:H8	1.85	0.41
4:2E:167:VAL:HG12	4:2E:170:LEU:HD11	2.02	0.41
5:2F:14:PRO:HD2	5:2F:127:GLU:OE1	2.20	0.41
9:2N:56:ASN:N	9:2N:125:GLY:O	2.48	0.41
10:2O:54:GLU:OE1	61:2O:301:HOH:O	2.21	0.41
21:2Z:92:SER:O	21:2Z:94:GLU:N	2.53	0.41
21:2Z:157:LEU:HB3	21:2Z:161:VAL:HG22	2.01	0.41
28:26:11:LEU:N	28:26:21:TYR:O	2.51	0.41
32:2a:411:A:O2'	32:2a:413:G:H5'	2.20	0.41
33:2b:53:ARG:HG3	33:2b:56:ARG:HH22	1.85	0.41
34:2c:12:LEU:HD23	34:2c:12:LEU:HA	1.85	0.41
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:145:LYS:O	36:2e:149:GLU:HB2	2.20	0.41
40:2i:3:GLN:HG2	40:2i:20:ARG:NH2	2.32	0.41
51:2t:87:LYS:O	51:2t:91:LEU:HG	2.20	0.41
54:2w:132:LEU:HD23	54:2w:132:LEU:HA	1.90	0.41
1:1A:1500:G:O2'	3:1D:100:GLY:O	2.34	0.41
1:1A:2316:C:H2'	1:1A:2317:C:H6	1.85	0.41
7:1H:117:PRO:HA	7:1H:118:PRO:HD2	1.96	0.41
21:1Z:1:MET:HE1	21:1Z:133:ILE:HG22	2.02	0.41
30:18:34:TRP:CG	30:18:35:GLN:N	2.88	0.41
32:1a:554:C:H2'	32:1a:555:C:H6	1.85	0.41
32:1a:1324:A:C6	32:1a:1325:C:C4	3.08	0.41
32:1a:1332:A:H2'	32:1a:1333:A:C8	2.56	0.41
34:1c:22:TRP:CH2	34:1c:32:LEU:HB2	2.55	0.41
42:1k:91:ARG:HH21	49:1r:87:ARG:NH2	2.18	0.41
44:1m:86:CYS:O	44:1m:90:LEU:HB2	2.20	0.41
1:2A:265:A:H1'	1:2A:266:G:O4'	2.20	0.41
1:2A:1464:C:H2'	1:2A:1465:G:H8	1.85	0.41
1:2A:2014:A:H2'	1:2A:2015:A:C8	2.55	0.41
1:2A:2121:G:H1	1:2A:2177:C:N4	2.17	0.41
3:2D:5:LYS:HE3	3:2D:5:LYS:HB3	1.92	0.41
8:2I:6:LEU:HD11	8:2I:37:VAL:HG23	2.02	0.41
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	2.02	0.41
12:2Q:58:PHE:HB3	12:2Q:61:GLY:O	2.21	0.41
12:2Q:116:GLU:OE2	12:2Q:119:ARG:NH2	2.36	0.41
19:2X:11:PRO:HG2	19:2X:13:LEU:HD21	2.02	0.41
19:2X:72:LYS:NZ	19:2X:75:ASP:OD1	2.48	0.41
32:2a:828:A:H2'	32:2a:829:G:O4'	2.21	0.41
32:2a:857:C:H2'	32:2a:858:G:O4'	2.20	0.41
32:2a:922:G:H2'	32:2a:923:A:C8	2.56	0.41
32:2a:923:A:OP1	36:2e:21:ALA:HB2	2.20	0.41
33:2b:71:VAL:HG23	33:2b:164:VAL:HA	2.02	0.41
34:2c:164:ARG:NH1	34:2c:166:GLU:OE1	2.54	0.41
38:2g:65:ALA:HB3	38:2g:124:LEU:HD23	2.02	0.41
42:2k:15:ALA:HA	42:2k:76:GLY:O	2.21	0.41
1:1A:286:C:H2'	1:1A:287:C:C6	2.56	0.41
1:1A:299:A:N1	1:1A:322:A:O2'	2.47	0.41
1:1A:1087:G:P	1:1A:1087:G:H8	2.44	0.41
1:1A:1093:G:H3'	1:1A:1094:U:H5"	2.02	0.41
1:1A:2106:G:H2'	1:1A:2107:C:C6	2.56	0.41
13:1R:98:LEU:HD12	27:15:57:VAL:HG11	2.03	0.41
32:1a:16:A:N1	32:1a:919:A:H2	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:93:G:H2'	32:1a:96:U:C6	2.56	0.41
32:1a:165:C:H2'	32:1a:166:G:H8	1.85	0.41
32:1a:841:U:C2	32:1a:848:C:H1'	2.56	0.41
32:1a:1493:A:H4'	53:1v:19:U:O2	2.20	0.41
35:1d:36:ARG:HB3	35:1d:38:TYR:CZ	2.55	0.41
41:1j:43:ARG:HB3	41:1j:67:THR:OG1	2.20	0.41
45:1n:3:ARG:HD2	45:1n:3:ARG:HA	1.82	0.41
1:2A:299:A:N1	1:2A:322:A:O2'	2.42	0.41
1:2A:582:G:H2'	1:2A:583:G:C8	2.55	0.41
1:2A:848:G:O6	1:2A:928:G:H2'	2.20	0.41
1:2A:910:A:N1	1:2A:2277:G:H1'	2.35	0.41
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.55	0.41
1:2A:1766:U:H2'	1:2A:1767:C:C6	2.55	0.41
3:2D:38:LYS:HE2	3:2D:39:LYS:N	2.36	0.41
3:2D:146:GLU:HG2	3:2D:152:GLY:C	2.45	0.41
6:2G:146:TYR:O	6:2G:149:VAL:HG22	2.20	0.41
7:2H:152:ARG:HA	7:2H:152:ARG:HD3	1.86	0.41
14:2S:25:ARG:HD2	14:2S:42:ASP:OD2	2.21	0.41
16:2U:76:TYR:CE2	16:2U:80:ILE:HG13	2.56	0.41
23:21:73:LEU:HD22	23:21:97:LEU:HB2	2.03	0.41
24:22:35:LEU:HD21	24:22:49:LYS:HE3	2.03	0.41
32:2a:37:U:O2'	32:2a:500:G:H4'	2.20	0.41
32:2a:93:G:H2'	32:2a:96:U:O4'	2.20	0.41
32:2a:272:C:H2'	32:2a:273:A:C8	2.55	0.41
32:2a:407:G:H5"	35:2d:115:ARG:HB2	2.01	0.41
32:2a:564:C:O2'	39:2h:91:ARG:NH1	2.46	0.41
32:2a:586:C:O2'	32:2a:878:G:H4'	2.20	0.41
32:2a:1041:A:H2'	32:2a:1042:G:O4'	2.20	0.41
32:2a:1060:C:H2'	32:2a:1061:G:H8	1.86	0.41
32:2a:1095:U:H2'	32:2a:1096:C:C6	2.55	0.41
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.85	0.41
1:1A:588:U:O4	1:1A:670:A:H1'	2.21	0.41
1:1A:1568:G:H4'	3:1D:59:LYS:HB3	2.03	0.41
1:1A:1637:A:H2'	1:1A:1638:C:O4'	2.20	0.41
1:1A:1688:U:H1'	1:1A:1701:A:C6	2.55	0.41
1:1A:1814:G:C4'	3:1D:51:VAL:HG21	2.51	0.41
1:1A:2370:G:C6	1:1A:2371:G:C6	3.09	0.41
4:1E:181:LEU:HD23	4:1E:181:LEU:HA	1.89	0.41
5:1F:60:SER:OG	5:1F:61:GLY:N	2.54	0.41
7:1H:60:ARG:HE	7:1H:60:ARG:HB3	1.66	0.41
22:10:49:LYS:HD2	22:10:49:LYS:HA	1.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:751:U:H4'	46:1o:24:SER:HA	2.03	0.41
33:1b:186:ALA:HB3	33:1b:197:VAL:HG11	2.03	0.41
34:1c:36:ASP:HA	34:1c:39:ILE:HD12	2.03	0.41
34:1c:178:LEU:C	34:1c:180:ALA:H	2.29	0.41
35:1d:13:ARG:HB3	35:1d:38:TYR:O	2.20	0.41
35:1d:121:VAL:O	35:1d:134:ASP:HA	2.19	0.41
35:1d:134:ASP:OD1	35:1d:134:ASP:N	2.52	0.41
44:1m:15:VAL:HG12	44:1m:19:LEU:HD11	2.02	0.41
1:2A:177:G:OP2	1:2A:177:G:N2	2.43	0.41
1:2A:2070:G:C2	1:2A:2442:C:C2	3.08	0.41
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.56	0.41
1:2A:2390:U:P	30:28:35:GLN:HE22	2.44	0.41
1:2A:2784:C:H1'	4:2E:37:ARG:NH1	2.36	0.41
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.02	0.41
8:2I:134:PRO:C	8:2I:136:VAL:H	2.28	0.41
14:2S:15:ARG:HE	14:2S:88:ASP:CG	2.27	0.41
17:2V:50:PRO:HG2	17:2V:51:VAL:HG23	2.03	0.41
28:26:38:LYS:HB2	28:26:49:HIS:CE1	2.56	0.41
32:2a:278:G:OP2	48:2q:41:LYS:NZ	2.54	0.41
32:2a:1272:G:N2	32:2a:1273:G:C8	2.80	0.41
35:2d:112:VAL:HG22	35:2d:116:GLN:NE2	2.36	0.41
40:2i:102:LEU:H	40:2i:102:LEU:HD23	1.85	0.41
1:1A:271(R):G:O6	61:1A:4144:HOH:O	2.21	0.41
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.56	0.41
1:1A:1044:G:H1'	1:1A:1048:A:H1'	2.03	0.41
1:1A:1091:G:C2	1:1A:1101:U:H1'	2.55	0.41
1:1A:2404:C:O3'	11:1P:77:ARG:NH2	2.54	0.41
1:1A:2471:C:N4	1:1A:2476:A:O2'	2.50	0.41
1:1A:2721:A:H2'	1:1A:2722:G:O4'	2.21	0.41
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.56	0.41
8:1I:4:ILE:HD11	8:1I:44:LEU:HD23	2.02	0.41
8:1I:72:LEU:HD23	8:1I:75:LEU:HD21	2.03	0.41
13:1R:13:HIS:CE1	13:1R:16:HIS:HB2	2.56	0.41
19:1X:34:ALA:O	19:1X:77:LYS:NZ	2.53	0.41
29:17:3:ARG:HA	29:17:3:ARG:HD3	1.88	0.41
32:1a:292:G:C5	32:1a:293:G:H1'	2.56	0.41
32:1a:373:A:H2'	32:1a:374:A:H8	1.86	0.41
32:1a:539:A:H2'	32:1a:540:G:C8	2.55	0.41
32:1a:1260:C:H4'	32:1a:1284:C:H5'	2.02	0.41
32:1a:1291:G:H5"	38:1g:41:ARG:NH2	2.36	0.41
32:1a:1316:G:N2	32:1a:1318:A:H3'	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1399:C:C2	32:1a:1401:G:C5	3.09	0.41
32:1a:1521:G:H2'	32:1a:1522:U:C6	2.56	0.41
35:1d:160:GLN:HG3	35:1d:160:GLN:H	1.67	0.41
44:1m:106:ASN:OD1	44:1m:106:ASN:N	2.53	0.41
55:1x:20:H2U:O2'	55:1x:21:H2U:O5'	2.38	0.41
1:2A:27:G:C2	1:2A:512:G:N3	2.89	0.41
1:2A:38:A:H2'	1:2A:39:C:C6	2.56	0.41
1:2A:221:A:O4'	1:2A:233:A:H1'	2.20	0.41
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.55	0.41
1:2A:1268:A:C2	1:2A:2013:A:C4	3.09	0.41
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.56	0.41
1:2A:2101:G:N1	1:2A:2187:G:O6	2.53	0.41
1:2A:2241:A:H2'	1:2A:2242:G:C8	2.56	0.41
1:2A:2853:C:H2'	1:2A:2854:G:H8	1.86	0.41
7:2H:58:GLU:H	7:2H:58:GLU:HG2	1.62	0.41
32:2a:552:U:O2	43:2l:31:PRO:HB3	2.21	0.41
32:2a:622:A:C8	32:2a:623:C:C6	3.09	0.41
32:2a:841:U:H6	32:2a:841:U:P	2.43	0.41
32:2a:1030(D):A:H3'	32:2a:1031:G:H8	1.86	0.41
33:2b:7:VAL:HG12	33:2b:8:LYS:H	1.85	0.41
55:2x:48:G:C4	55:2x:59:C:H1'	2.56	0.41
1:1A:68:G:H2'	1:1A:69:C:O4'	2.21	0.41
1:1A:483:A:O4'	20:1Y:48:ALA:HB1	2.21	0.41
1:1A:530:G:N1	1:1A:2023:G:OP1	2.33	0.41
1:1A:545:G:OP1	1:1A:545:G:H4'	2.21	0.41
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.54	0.41
1:1A:1252:G:N3	16:1U:33:ARG:HG2	2.36	0.41
1:1A:1300:U:H4'	1:1A:1301:A:H5'	2.03	0.41
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.21	0.41
1:1A:2128:C:O2'	1:1A:2174:C:H4'	2.21	0.41
1:1A:2145:C:O2'	1:1A:2147:G:O6	2.39	0.41
1:1A:2555:U:O2	54:1w:223:ARG:NH1	2.54	0.41
1:1A:2836:U:H2'	1:1A:2837:G:C8	2.56	0.41
2:1B:87:G:N2	2:1B:89:G:H3'	2.36	0.41
3:1D:20:ASP:OD1	3:1D:20:ASP:N	2.50	0.41
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.85	0.41
3:1D:246:PRO:O	3:1D:254:THR:HG22	2.20	0.41
5:1F:68:LYS:HE3	5:1F:68:LYS:HB3	1.83	0.41
10:1O:1:MET:HE3	10:1O:32:TYR:CZ	2.54	0.41
10:1O:64:ARG:O	10:1O:82:ASN:HA	2.21	0.41
16:1U:59:ARG:O	16:1U:63:VAL:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:10:10:THR:HG22	22:10:12:ASN:H	1.86	0.41
24:12:61:LEU:HD23	24:12:61:LEU:HA	1.87	0.41
25:13:39:ASP:OD2	25:13:44:ARG:NH2	2.54	0.41
32:1a:164:U:H2'	32:1a:165:C:C6	2.56	0.41
32:1a:336:C:H2'	32:1a:337:C:H6	1.86	0.41
32:1a:1001:A:N6	32:1a:1001(A):G:O6	2.54	0.41
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.21	0.41
32:1a:1342:C:H4'	40:1i:125:TYR:HB3	2.03	0.41
32:1a:1374:A:C4	32:1a:1375:A:C8	3.09	0.41
33:1b:22:LYS:HG2	33:1b:40:HIS:CE1	2.56	0.41
34:1c:22:TRP:CZ3	34:1c:32:LEU:HB2	2.56	0.41
36:1e:15:ARG:HD2	36:1e:26:PHE:CD1	2.56	0.41
40:1i:27:THR:O	40:1i:63:ILE:HD12	2.21	0.41
42:1k:52:GLY:H	42:1k:55:LYS:HE2	1.86	0.41
43:1l:53:ARG:HB2	43:1l:93:LEU:HD11	2.03	0.41
47:1p:19:ILE:HD12	47:1p:37:GLY:HA3	2.03	0.41
51:1t:45:GLN:HB2	51:1t:91:LEU:HD13	2.03	0.41
54:1w:319:PHE:CE2	54:1w:335:ILE:HG12	2.56	0.41
55:1x:52:G:C6	55:1x:63:G:C6	3.09	0.41
1:2A:271(H):G:H5'	23:21:81:LYS:HD3	2.03	0.41
1:2A:323:G:HO2'	1:2A:1205:U:H3	1.61	0.41
1:2A:580:C:H2'	1:2A:581:C:H6	1.83	0.41
1:2A:886:C:H1'	1:2A:890:A:N6	2.36	0.41
1:2A:1006:C:C2	1:2A:1138:G:N2	2.89	0.41
1:2A:1657:C:H2'	1:2A:1658:C:H6	1.86	0.41
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.56	0.41
1:2A:2114:A:H2	1:2A:2171:A:H61	1.69	0.41
1:2A:2280:G:O6	22:20:14:ARG:HD3	2.21	0.41
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.55	0.41
1:2A:2785:C:H2'	1:2A:2786:U:O4'	2.20	0.41
2:2B:95:C:H2'	2:2B:96:U:C6	2.56	0.41
3:2D:123:ALA:O	3:2D:131:LEU:HD21	2.21	0.41
25:23:43:ILE:O	25:23:47:VAL:HG23	2.21	0.41
26:24:53:GLU:H	26:24:53:GLU:HG3	1.51	0.41
28:26:38:LYS:HB3	28:26:38:LYS:HE3	1.86	0.41
32:2a:60:A:N1	32:2a:107:G:O2'	2.48	0.41
32:2a:391:G:OP1	47:2p:28:ARG:NH2	2.46	0.41
32:2a:455:C:H2'	32:2a:456:C:C6	2.56	0.41
32:2a:691:G:H2'	32:2a:692:U:C6	2.56	0.41
32:2a:1014:A:C2	32:2a:1219:U:H1'	2.56	0.41
32:2a:1318:A:O2'	50:2s:37:ARG:HD2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1517:G:H2'	32:2a:1518:MA6:H8	2.02	0.41
33:2b:187:LEU:HD11	33:2b:203:GLY:HA3	2.02	0.41
34:2c:20:SER:HB2	45:2n:54:PRO:HG3	2.03	0.41
34:2c:181:ASN:N	34:2c:205:GLY:O	2.51	0.41
38:2g:15:ASP:OD1	38:2g:19:GLY:N	2.53	0.41
43:2l:88:GLY:O	43:2l:99:HIS:HD2	2.03	0.41
54:2w:347:GLN:O	54:2w:351:LEU:HB2	2.21	0.41
1:1A:1069:A:H2	1:1A:1095:A:HO2'	1.65	0.41
1:1A:1072:C:H1'	1:1A:1092:C:H41	1.86	0.41
1:1A:1709:U:H2'	1:1A:1710:C:C6	2.56	0.41
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.21	0.41
2:1B:48:A:H2'	2:1B:49:C:C6	2.57	0.41
2:1B:96:U:H2'	2:1B:97:G:C8	2.56	0.41
7:1H:84:SER:HA	7:1H:133:VAL:O	2.21	0.41
10:1O:64:ARG:HG2	10:1O:79:PHE:CD2	2.57	0.41
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.64	0.41
32:1a:266:G:H5"	32:1a:268:C:H41	1.86	0.41
32:1a:473:G:H2'	32:1a:474:G:C8	2.56	0.41
32:1a:721:G:H4'	32:1a:722:A:O4'	2.21	0.41
32:1a:909:A:H2'	32:1a:910:C:O4'	2.21	0.41
32:1a:1076:C:C2	32:1a:1082:G:C2	3.10	0.41
44:1m:45:VAL:HG13	44:1m:48:LEU:HD11	2.03	0.41
44:1m:65:LYS:HG2	44:1m:69:GLU:HB3	2.03	0.41
45:1n:4:LYS:HA	45:1n:7:ILE:HG22	2.03	0.41
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.84	0.41
1:2A:1392:A:C6	1:2A:1393:A:C6	3.09	0.41
1:2A:1504:C:H2'	1:2A:1505:C:H6	1.85	0.41
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.31	0.41
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.20	0.41
1:2A:2867:G:O2'	1:2A:2868:A:OP2	2.38	0.41
8:2I:79:ILE:HB	8:2I:144:VAL:HG13	2.02	0.41
15:2T:127:ALA:C	15:2T:129:ARG:N	2.76	0.41
16:2U:27:LEU:HB3	16:2U:31:SER:HB3	2.03	0.41
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.56	0.41
26:24:58:ARG:HD3	44:2m:80:ARG:NH1	2.36	0.41
32:2a:189(L):G:H2'	32:2a:190:U:H6	1.86	0.41
32:2a:649:G:H2'	32:2a:650:G:O4'	2.21	0.41
32:2a:1151:A:O4'	41:2j:39:PRO:HB2	2.19	0.41
32:2a:1289:A:N1	32:2a:1371:G:O2'	2.48	0.41
34:2c:8:ILE:CD1	34:2c:184:TYR:HB3	2.51	0.41
34:2c:114:PRO:O	34:2c:118:GLN:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:13:ARG:O	35:2d:39:PRO:HA	2.21	0.41
37:2f:95:GLU:HA	37:2f:96:PRO:HD3	1.94	0.41
40:2i:16:ARG:O	40:2i:63:ILE:HA	2.21	0.41
42:2k:20:TYR:CZ	42:2k:83:ILE:HD13	2.55	0.41
1:1A:817:C:O2'	1:1A:839:U:H5"	2.21	0.40
1:1A:2305:A:H2'	1:1A:2306:C:O4'	2.21	0.40
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.56	0.40
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.51	0.40
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.29	0.40
21:1Z:163:LEU:HD12	21:1Z:163:LEU:HA	1.90	0.40
32:1a:900:A:H2'	32:1a:901:A:C8	2.56	0.40
32:1a:922:G:C6	32:1a:923:A:C6	3.09	0.40
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.48	0.40
32:1a:1296:C:H5"	44:1m:44:ARG:HH22	1.85	0.40
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.55	0.40
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.56	0.40
37:1f:33:TYR:OH	37:1f:78:GLU:HG3	2.21	0.40
43:1l:71:PRO:HG2	43:1l:102:ARG:HG2	2.03	0.40
1:2A:720:C:H2'	1:2A:721:C:C6	2.57	0.40
1:2A:1248:G:C2	16:2U:3:ARG:HD2	2.56	0.40
1:2A:2129:C:N4	1:2A:2159:G:N1	2.37	0.40
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.21	0.40
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.86	0.40
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	2.02	0.40
4:2E:134:ILE:HA	4:2E:137:HIS:CD2	2.56	0.40
6:2G:145:THR:HB	6:2G:148:MET:HG2	2.02	0.40
32:2a:564:C:H5'	43:2l:10:LEU:HD13	2.02	0.40
32:2a:993:G:H4'	32:2a:994:A:OP2	2.21	0.40
32:2a:1113:C:H42	32:2a:1187:G:H1	1.69	0.40
32:2a:1130:A:H4'	40:2i:3:GLN:NE2	2.36	0.40
32:2a:1168:A:C6	32:2a:1169:A:C6	3.09	0.40
32:2a:1228:C:H4'	44:2m:116:THR:HA	2.03	0.40
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.56	0.40
33:2b:163:PHE:HA	33:2b:185:ILE:O	2.20	0.40
33:2b:213:LEU:O	33:2b:217:ARG:HG2	2.22	0.40
42:2k:20:TYR:O	42:2k:30:VAL:HA	2.21	0.40
42:2k:21:ILE:HD12	42:2k:95:ILE:HG12	2.04	0.40
42:2k:110:ASP:OD1	42:2k:112:THR:OG1	2.35	0.40
1:1A:1676:A:H2'	1:1A:1677:A:O4'	2.21	0.40
1:1A:2255:G:O2'	55:1x:2:G:O2'	2.31	0.40
1:1A:2691:C:O3'	1:1A:2871:C:H4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2788:C:H2'	1:1A:2789:C:O4'	2.21	0.40
7:1H:121:ILE:HD13	7:1H:121:ILE:HA	1.83	0.40
10:1O:107:ARG:CZ	15:1T:36:GLU:HG3	2.51	0.40
26:14:14:ILE:HA	26:14:31:ILE:O	2.21	0.40
32:1a:1346:A:H5"	40:1i:120:ARG:NH1	2.37	0.40
32:1a:1424:C:H2'	32:1a:1425:U:O4'	2.20	0.40
33:1b:52:GLU:HG2	33:1b:56:ARG:HH12	1.87	0.40
34:1c:119:ARG:O	34:1c:123:GLN:HG3	2.20	0.40
35:1d:81:GLU:OE1	35:1d:139:ARG:NH2	2.30	0.40
36:1e:107:ARG:HG3	36:1e:108:ALA:N	2.36	0.40
37:1f:61:LEU:HB3	37:1f:63:TYR:CE2	2.56	0.40
48:1q:5:VAL:HA	48:1q:59:ILE:O	2.22	0.40
1:2A:8:A:H2'	1:2A:9:U:C6	2.57	0.40
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.43	0.40
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.21	0.40
1:2A:340:A:H2'	1:2A:341:G:O4'	2.21	0.40
1:2A:635:C:O2'	1:2A:639:U:OP1	2.35	0.40
1:2A:947:G:H2'	1:2A:948:G:C8	2.56	0.40
1:2A:1847:A:H3'	1:2A:1848:A:H5'	2.02	0.40
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.22	0.40
2:2B:17:C:H2'	2:2B:18:G:O4'	2.21	0.40
5:2F:37:VAL:O	5:2F:41:LEU:HG	2.21	0.40
5:2F:148:LEU:HD11	5:2F:193:VAL:HG21	2.03	0.40
12:2Q:58:PHE:O	12:2Q:59:ARG:HB2	2.22	0.40
21:2Z:150:LEU:HD23	21:2Z:150:LEU:HA	1.87	0.40
24:22:53:LEU:O	24:22:57:ILE:HG13	2.20	0.40
32:2a:518:C:OP1	54:2w:179:ARG:NH1	2.51	0.40
32:2a:580:U:H2'	32:2a:581:G:O4'	2.21	0.40
32:2a:779:C:O2'	42:2k:120:ARG:HD3	2.21	0.40
32:2a:1342:C:H2'	32:2a:1343:G:H8	1.85	0.40
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.36	0.40
33:2b:71:VAL:HG21	33:2b:164:VAL:HG22	2.03	0.40
39:2h:29:SER:HB3	39:2h:32:LYS:HG3	2.03	0.40
40:2i:78:LYS:HE2	40:2i:78:LYS:HB3	1.79	0.40
42:2k:69:ALA:O	42:2k:73:MET:HG3	2.21	0.40
44:2m:105:THR:O	44:2m:106:ASN:C	2.64	0.40
51:2t:43:LEU:HD23	51:2t:43:LEU:HA	1.95	0.40
1:1A:428:A:H8	1:1A:428:A:OP2	2.05	0.40
1:1A:609:A:H2'	1:1A:610:G:O4'	2.22	0.40
1:1A:784:A:O4'	3:1D:227:ASN:ND2	2.55	0.40
1:1A:1342:A:O2'	1:1A:1344:G:OP2	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1963:U:H4'	1:1A:1964:G:OP1	2.22	0.40
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.50	0.40
12:1Q:45:GLN:OE1	12:1Q:45:GLN:N	2.42	0.40
17:1V:10:LYS:NZ	17:1V:23:GLU:OE2	2.37	0.40
21:1Z:1:MET:SD	21:1Z:1:MET:N	2.90	0.40
32:1a:222:U:H2'	32:1a:223:U:C6	2.56	0.40
32:1a:374:A:C6	32:1a:375:U:C4	3.09	0.40
32:1a:456:C:C2	32:1a:476:G:C2	3.10	0.40
32:1a:1010:G:N2	32:1a:1020:U:H1'	2.36	0.40
32:1a:1030(D):A:H3'	32:1a:1031:G:O4'	2.21	0.40
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	2.04	0.40
40:1i:49:PRO:HB3	40:1i:82:ALA:HB2	2.03	0.40
43:1l:36:VAL:HG22	43:1l:82:VAL:HG22	2.03	0.40
1:2A:272:G:H4'	1:2A:272(A):U:H5"	2.04	0.40
1:2A:843:G:C2	1:2A:936:C:C2	3.10	0.40
1:2A:1212:G:H1'	1:2A:1236:G:N2	2.36	0.40
1:2A:1876:A:H2'	1:2A:1877:A:C8	2.56	0.40
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.56	0.40
1:2A:2162:G:O2'	1:2A:2172:U:H5'	2.22	0.40
1:2A:2321:G:H5"	1:2A:2322:A:OP2	2.22	0.40
1:2A:2521:C:O2'	1:2A:2564:A:N3	2.47	0.40
1:2A:2539:C:H4'	31:29:3:VAL:HG21	2.03	0.40
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.56	0.40
2:2B:59:A:H2'	2:2B:60:C:O4'	2.21	0.40
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.69	0.40
7:2H:121:ILE:HG12	7:2H:140:LYS:HD3	2.03	0.40
16:2U:34:LYS:NZ	16:2U:37:GLU:OE1	2.41	0.40
19:2X:27:THR:HG23	19:2X:80:ILE:HG12	2.03	0.40
32:2a:255:G:H2'	32:2a:256:U:C6	2.56	0.40
32:2a:684:A:H1'	42:2k:38:ASN:HB3	2.03	0.40
32:2a:1015:A:H4'	45:2n:15:LYS:NZ	2.36	0.40
32:2a:1226:C:OP1	44:2m:91:ARG:NH2	2.50	0.40
38:2g:111:ARG:HD2	38:2g:123:GLU:HB2	2.02	0.40
41:2j:74:ILE:HA	41:2j:74:ILE:HD12	1.70	0.40
44:2m:25:ILE:HD11	44:2m:60:VAL:HG13	2.04	0.40
51:2t:59:ALA:O	51:2t:63:ILE:HG13	2.21	0.40
1:1A:38:A:H2'	1:1A:39:C:C6	2.57	0.40
1:1A:57:C:H2'	1:1A:58:G:O4'	2.22	0.40
1:1A:1243:G:H2'	1:1A:1244:G:O4'	2.21	0.40
1:1A:1803:A:H4'	3:1D:259:THR:HG23	2.04	0.40
1:1A:2102:U:H2'	1:1A:2103:C:C5	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2352:A:N6	1:1A:2365:G:O2'	2.55	0.40
1:1A:2389:G:H5"	1:1A:2390:U:O4'	2.21	0.40
5:1F:196:LEU:HD23	5:1F:196:LEU:HA	1.84	0.40
6:1G:95:ARG:HA	6:1G:99:MET:HB2	2.04	0.40
6:1G:145:THR:HG22	6:1G:146:TYR:H	1.87	0.40
12:1Q:118:LEU:HB2	12:1Q:131:ILE:HD13	2.04	0.40
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	2.03	0.40
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.36	0.40
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.56	0.40
32:1a:1413:A:H2	32:1a:1487:G:H22	1.69	0.40
33:1b:223:ILE:HG13	33:1b:224:GLN:N	2.36	0.40
39:1h:4:ASP:OD2	39:1h:85:ARG:NE	2.41	0.40
43:1l:110:VAL:HG23	43:1l:120:TYR:HB3	2.01	0.40
54:1w:111:ILE:HB	54:1w:158:VAL:HG23	2.03	0.40
54:1w:229:GLY:HA3	55:1x:76:8AN:H5'A	2.03	0.40
1:2A:207:A:H2'	1:2A:208:C:O4'	2.22	0.40
1:2A:500:G:N1	1:2A:503:A:OP2	2.54	0.40
1:2A:1401:G:H2'	1:2A:1402:C:O4'	2.22	0.40
1:2A:2319:G:H22	14:2S:3:ARG:HH21	1.70	0.40
1:2A:2335:A:C8	1:2A:2337:G:C5	3.09	0.40
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.35	0.40
3:2D:171:ASP:O	3:2D:187:GLY:N	2.49	0.40
32:2a:424:G:H2'	32:2a:425:G:C8	2.54	0.40
32:2a:436:C:H2'	32:2a:437:U:H6	1.86	0.40
32:2a:457:C:H2'	32:2a:458:C:C6	2.56	0.40
32:2a:990:C:H2'	32:2a:991:U:O4'	2.21	0.40
32:2a:1124:G:H5"	41:2j:35:SER:OG	2.22	0.40
5:1F:178:PRO:HB2	5:1F:201:VAL:CG2	2.51	0.40
15:1T:84:GLN:HG2	15:1T:85:LYS:HG2	2.03	0.40
32:1a:148:G:H2'	32:1a:149:A:C8	2.56	0.40
32:1a:348:G:O2'	32:1a:349:A:H5'	2.22	0.40
32:1a:976:G:C8	32:1a:1358:U:C2	3.10	0.40
32:1a:1228:C:H2'	32:1a:1229:A:H8	1.87	0.40
32:1a:1243:C:C2	32:1a:1295:G:C2	3.10	0.40
32:1a:1412:C:H2'	32:1a:1413:A:H8	1.86	0.40
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	2.03	0.40
45:1n:9:LYS:HE3	45:1n:9:LYS:HB2	1.90	0.40
1:2A:30:G:C5	1:2A:31:C:C4	3.09	0.40
1:2A:194:G:H2'	1:2A:195:A:O4'	2.21	0.40
1:2A:262:A:H2'	1:2A:263:C:O4'	2.21	0.40
1:2A:299:A:H5"	20:2Y:86:ARG:HH21	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:401:A:H2'	1:2A:402:A:O4'	2.22	0.40
1:2A:658:C:H2'	1:2A:659:C:C6	2.56	0.40
1:2A:675:A:C6	1:2A:676:A:C6	3.09	0.40
1:2A:1453:U:OP1	13:2R:77:ARG:HD3	2.22	0.40
1:2A:1485:G:H2'	1:2A:1486:A:H8	1.86	0.40
1:2A:1530:C:H42	1:2A:1539:G:H1	1.70	0.40
1:2A:2287:A:C8	1:2A:2289:G:C8	3.09	0.40
2:2B:24:G:O4'	2:2B:26:A:N6	2.48	0.40
2:2B:58:A:H2'	2:2B:59:A:O4'	2.21	0.40
5:2F:170:LEU:HD13	5:2F:172:TRP:CZ2	2.56	0.40
6:2G:20:ILE:H	6:2G:20:ILE:HG13	1.69	0.40
6:2G:66:GLN:HG3	26:24:6:HIS:CE1	2.56	0.40
7:2H:127:GLU:C	7:2H:129:THR:H	2.29	0.40
32:2a:16:A:O2'	36:2e:16:THR:HB	2.21	0.40
32:2a:107:G:H2'	32:2a:108:G:O4'	2.22	0.40
32:2a:714:G:H2'	32:2a:715:A:C8	2.56	0.40
32:2a:1206:G:C6	32:2a:1207:2MG:C5	3.10	0.40
32:2a:1308:U:H5"	44:2m:98:VAL:HG22	2.03	0.40
36:2e:95:ALA:O	36:2e:97:GLY:N	2.55	0.40
39:2h:34:GLU:HB3	39:2h:118:VAL:CG1	2.51	0.40
54:2w:184:PRO:C	54:2w:186:THR:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	25	56
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	25	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	25 56
5	2F	201/210 (96%)	186 (92%)	14 (7%)	1 (0%)	25 56
6	1G	179/182 (98%)	154 (86%)	22 (12%)	3 (2%)	7 26
6	2G	179/182 (98%)	160 (89%)	14 (8%)	5 (3%)	4 14
7	1H	172/180 (96%)	163 (95%)	7 (4%)	2 (1%)	11 34
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	22 51
8	1I	144/148 (97%)	126 (88%)	18 (12%)	0	100 100
8	2I	144/148 (97%)	118 (82%)	21 (15%)	5 (4%)	3 10
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100 100
9	2N	138/140 (99%)	135 (98%)	3 (2%)	0	100 100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100 100
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16 44
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100 100
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	19 48
12	1Q	139/141 (99%)	131 (94%)	6 (4%)	2 (1%)	9 30
12	2Q	139/141 (99%)	127 (91%)	10 (7%)	2 (1%)	9 30
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
13	2R	116/118 (98%)	108 (93%)	8 (7%)	0	100 100
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100 100
14	2S	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	14 42
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16 44
15	2T	129/146 (88%)	120 (93%)	9 (7%)	0	100 100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
16	2U	114/118 (97%)	114 (100%)	0	0	100 100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6 21
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	13 39
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
19	1X	93/96 (97%)	91 (98%)	2 (2%)	0	100 100
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	13 39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	2Y	105/110 (96%)	91 (87%)	13 (12%)	1 (1%)	13 39
21	1Z	148/206 (72%)	130 (88%)	13 (9%)	5 (3%)	3 11
21	2Z	156/206 (76%)	138 (88%)	15 (10%)	3 (2%)	6 23
22	10	74/85 (87%)	73 (99%)	1 (1%)	0	100 100
22	20	74/85 (87%)	70 (95%)	4 (5%)	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12 37
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100 100
24	12	68/72 (94%)	68 (100%)	0	0	100 100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
26	14	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2 7
26	24	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1 2
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
31	29	35/37 (95%)	35 (100%)	0	0	100 100
33	1b	229/256 (90%)	190 (83%)	32 (14%)	7 (3%)	3 12
33	2b	229/256 (90%)	193 (84%)	32 (14%)	4 (2%)	7 26
34	1c	204/239 (85%)	174 (85%)	26 (13%)	4 (2%)	6 21
34	2c	204/239 (85%)	176 (86%)	28 (14%)	0	100 100
35	1d	206/209 (99%)	186 (90%)	19 (9%)	1 (0%)	25 56
35	2d	206/209 (99%)	191 (93%)	15 (7%)	0	100 100
36	1e	146/162 (90%)	130 (89%)	14 (10%)	2 (1%)	9 30
36	2e	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	5 20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
38	1g	153/156 (98%)	131 (86%)	20 (13%)	2 (1%)	10	32
38	2g	153/156 (98%)	138 (90%)	12 (8%)	3 (2%)	6	21
39	1h	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	19	48
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	16	44
40	2i	125/128 (98%)	108 (86%)	16 (13%)	1 (1%)	16	44
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	5	20
41	2j	94/105 (90%)	81 (86%)	12 (13%)	1 (1%)	12	37
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	14	42
42	2k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	7	24
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
43	2l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
44	1m	116/126 (92%)	106 (91%)	9 (8%)	1 (1%)	14	42
44	2m	114/126 (90%)	98 (86%)	14 (12%)	2 (2%)	7	24
45	1n	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	1p	80/88 (91%)	67 (84%)	13 (16%)	0	100	100
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	13	39
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	64 (79%)	17 (21%)	0	100	100
50	2s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	11	34
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5	20
51	2t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	5	20
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
54	1w	247/354 (70%)	227 (92%)	17 (7%)	3 (1%)	11 34
54	2w	251/354 (71%)	232 (92%)	17 (7%)	2 (1%)	16 44
56	1z	3/7 (43%)	2 (67%)	1 (33%)	0	100 100
56	2z	2/7 (29%)	2 (100%)	0	0	100 100
All	All	11848/12850 (92%)	10869 (92%)	880 (7%)	99 (1%)	16 44

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	96	ARG
6	1G	126	ASP
12	1Q	16	ARG
21	1Z	53	ILE
26	14	55	ARG
33	1b	17	PHE
33	1b	125	PRO
33	1b	126	GLU
34	1c	66	VAL
44	1m	67	GLU
54	1w	206	GLU
5	2F	130	ALA
7	2H	126	PRO
33	2b	17	PHE
36	2e	65	ASN
38	2g	80	VAL
44	2m	106	ASN
50	2s	13	ASP
54	2w	300	GLU
7	1H	126	PRO
15	1T	37	GLY
20	1Y	54	LYS
23	11	3	LYS
26	14	49	PHE
34	1c	129	ALA
36	1e	21	ALA
39	1h	37	ARG
51	1t	47	GLY
54	1w	207	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	42	GLY
6	2G	49	ASP
6	2G	52	ILE
10	2O	5	GLN
12	2Q	16	ARG
17	2V	79	VAL
21	2Z	52	SER
33	2b	22	LYS
33	2b	125	PRO
41	2j	31	GLY
42	2k	49	GLY
51	2t	95	ALA
7	1H	159	GLU
17	1V	79	VAL
33	1b	20	GLU
33	1b	116	GLU
33	1b	124	SER
38	1g	131	LYS
54	1w	208	GLU
6	2G	43	LEU
8	2I	104	GLN
26	24	47	GLN
33	2b	78	GLN
38	2g	4	ARG
51	2t	102	GLY
54	2w	208	GLU
4	1E	52	LEU
6	1G	47	LYS
17	1V	100	ARG
34	1c	65	ALA
4	2E	52	LEU
6	2G	47	LYS
8	2I	42	SER
8	2I	80	PRO
8	2I	117	GLU
12	2Q	60	ARG
20	2Y	54	LYS
26	24	62	ARG
21	1Z	157	LEU
26	14	59	PHE
38	1g	4	ARG
41	1j	78	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	1k	49	GLY
14	2S	51	ALA
21	2Z	31	ARG
21	2Z	93	ASP
26	24	29	PRO
26	24	56	VAL
38	2g	54	THR
21	1Z	156	LYS
40	1i	126	SER
40	2i	54	ASP
42	2k	87	THR
44	2m	12	ASN
21	1Z	137	ILE
33	1b	231	GLU
11	2P	122	PRO
26	24	50	VAL
21	1Z	120	ILE
51	1t	98	PRO
36	1e	69	VAL
34	1c	81	GLY
35	1d	136	PRO
41	1j	77	PRO
8	2I	106	GLY
36	2e	69	VAL
36	2e	96	PRO
12	1Q	15	GLY
48	2q	33	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	215/218 (99%)	204 (95%)	11 (5%)	20 51
3	2D	215/218 (99%)	203 (94%)	12 (6%)	17 47
4	1E	164/166 (99%)	156 (95%)	8 (5%)	21 52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	2E	164/166 (99%)	157 (96%)	7 (4%)	25 57
5	1F	160/166 (96%)	148 (92%)	12 (8%)	11 33
5	2F	159/166 (96%)	143 (90%)	16 (10%)	6 20
6	1G	143/156 (92%)	123 (86%)	20 (14%)	3 9
6	2G	143/156 (92%)	126 (88%)	17 (12%)	4 14
7	1H	144/148 (97%)	131 (91%)	13 (9%)	8 25
7	2H	144/148 (97%)	131 (91%)	13 (9%)	8 25
8	1I	113/124 (91%)	105 (93%)	8 (7%)	12 35
8	2I	105/124 (85%)	85 (81%)	20 (19%)	1 4
9	1N	118/119 (99%)	108 (92%)	10 (8%)	8 27
9	2N	118/119 (99%)	107 (91%)	11 (9%)	7 23
10	1O	100/100 (100%)	98 (98%)	2 (2%)	50 81
10	2O	100/100 (100%)	96 (96%)	4 (4%)	27 60
11	1P	115/116 (99%)	100 (87%)	15 (13%)	3 11
11	2P	115/116 (99%)	103 (90%)	12 (10%)	5 18
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	23 55
12	2Q	111/111 (100%)	103 (93%)	8 (7%)	12 34
13	1R	101/101 (100%)	100 (99%)	1 (1%)	73 91
13	2R	101/101 (100%)	99 (98%)	2 (2%)	50 81
14	1S	86/88 (98%)	80 (93%)	6 (7%)	12 36
14	2S	85/88 (97%)	77 (91%)	8 (9%)	7 23
15	1T	115/127 (91%)	104 (90%)	11 (10%)	7 22
15	2T	113/127 (89%)	109 (96%)	4 (4%)	31 65
16	1U	93/94 (99%)	88 (95%)	5 (5%)	18 48
16	2U	93/94 (99%)	86 (92%)	7 (8%)	11 33
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42 75
17	2V	80/82 (98%)	76 (95%)	4 (5%)	20 51
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33 67
18	2W	90/92 (98%)	85 (94%)	5 (6%)	17 47
19	1X	77/78 (99%)	74 (96%)	3 (4%)	27 61
19	2X	77/78 (99%)	73 (95%)	4 (5%)	19 50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	16 44
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	9 29
21	1Z	135/179 (75%)	117 (87%)	18 (13%)	3 10
21	2Z	137/179 (76%)	116 (85%)	21 (15%)	2 7
22	10	61/67 (91%)	60 (98%)	1 (2%)	58 85
22	20	61/67 (91%)	59 (97%)	2 (3%)	33 67
23	11	80/83 (96%)	74 (92%)	6 (8%)	11 33
23	21	80/83 (96%)	77 (96%)	3 (4%)	28 62
24	12	65/67 (97%)	60 (92%)	5 (8%)	10 31
24	22	65/67 (97%)	62 (95%)	3 (5%)	23 55
25	13	51/52 (98%)	45 (88%)	6 (12%)	4 14
25	23	50/52 (96%)	45 (90%)	5 (10%)	6 20
26	14	59/63 (94%)	52 (88%)	7 (12%)	4 14
26	24	53/63 (84%)	45 (85%)	8 (15%)	2 8
27	15	50/52 (96%)	46 (92%)	4 (8%)	10 30
27	25	50/52 (96%)	46 (92%)	4 (8%)	10 30
28	16	51/52 (98%)	44 (86%)	7 (14%)	3 10
28	26	50/52 (96%)	48 (96%)	2 (4%)	27 60
29	17	41/42 (98%)	39 (95%)	2 (5%)	21 52
29	27	41/42 (98%)	37 (90%)	4 (10%)	6 21
30	18	54/55 (98%)	52 (96%)	2 (4%)	29 63
30	28	54/55 (98%)	52 (96%)	2 (4%)	29 63
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	31 (91%)	3 (9%)	8 26
33	1b	192/220 (87%)	166 (86%)	26 (14%)	3 10
33	2b	187/220 (85%)	161 (86%)	26 (14%)	3 9
34	1c	142/188 (76%)	124 (87%)	18 (13%)	3 12
34	2c	140/188 (74%)	129 (92%)	11 (8%)	10 30
35	1d	169/181 (93%)	160 (95%)	9 (5%)	19 49
35	2d	173/181 (96%)	153 (88%)	20 (12%)	4 15
36	1e	113/123 (92%)	100 (88%)	13 (12%)	4 15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	2e	114/123 (93%)	103 (90%)	11 (10%)	7 22
37	1f	84/90 (93%)	78 (93%)	6 (7%)	12 35
37	2f	85/90 (94%)	79 (93%)	6 (7%)	12 35
38	1g	119/127 (94%)	109 (92%)	10 (8%)	9 28
38	2g	120/127 (94%)	109 (91%)	11 (9%)	7 24
39	1h	114/119 (96%)	102 (90%)	12 (10%)	5 18
39	2h	114/119 (96%)	103 (90%)	11 (10%)	7 22
40	1i	90/99 (91%)	78 (87%)	12 (13%)	3 10
40	2i	89/99 (90%)	77 (86%)	12 (14%)	3 10
41	1j	66/92 (72%)	56 (85%)	10 (15%)	2 7
41	2j	69/92 (75%)	65 (94%)	4 (6%)	17 45
42	1k	82/99 (83%)	70 (85%)	12 (15%)	2 8
42	2k	83/99 (84%)	74 (89%)	9 (11%)	5 17
43	1l	96/108 (89%)	87 (91%)	9 (9%)	7 23
43	2l	96/108 (89%)	88 (92%)	8 (8%)	9 28
44	1m	89/101 (88%)	70 (79%)	19 (21%)	1 3
44	2m	88/101 (87%)	81 (92%)	7 (8%)	10 30
45	1n	49/50 (98%)	40 (82%)	9 (18%)	1 4
45	2n	49/50 (98%)	45 (92%)	4 (8%)	9 29
46	1o	78/80 (98%)	71 (91%)	7 (9%)	8 25
46	2o	78/80 (98%)	69 (88%)	9 (12%)	4 15
47	1p	69/74 (93%)	56 (81%)	13 (19%)	1 4
47	2p	68/74 (92%)	57 (84%)	11 (16%)	2 6
48	1q	94/97 (97%)	82 (87%)	12 (13%)	3 12
48	2q	94/97 (97%)	86 (92%)	8 (8%)	8 27
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32 66
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32 66
50	1s	69/80 (86%)	60 (87%)	9 (13%)	3 11
50	2s	67/80 (84%)	59 (88%)	8 (12%)	4 14
51	1t	70/82 (85%)	68 (97%)	2 (3%)	37 71
51	2t	70/82 (85%)	67 (96%)	3 (4%)	25 57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	1u	18/22 (82%)	17 (94%)	1 (6%)	17 47
52	2u	18/22 (82%)	17 (94%)	1 (6%)	17 47
54	1w	204/299 (68%)	183 (90%)	21 (10%)	6 19
54	2w	204/299 (68%)	171 (84%)	33 (16%)	2 6
56	1z	2/3 (67%)	2 (100%)	0	100 100
56	2z	2/3 (67%)	2 (100%)	0	100 100
All	All	9699/10668 (91%)	8836 (91%)	863 (9%)	8 25

All (863) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	34	VAL
3	1D	38	LYS
3	1D	39	LYS
3	1D	71	ASP
3	1D	127	VAL
3	1D	155	LEU
3	1D	183	ARG
3	1D	200	ASP
3	1D	229	VAL
3	1D	273	ARG
4	1E	1	MET
4	1E	41	LYS
4	1E	75	VAL
4	1E	87	GLU
4	1E	93	VAL
4	1E	94	GLU
4	1E	116	VAL
4	1E	195	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	78	ILE
5	1F	140	LEU
5	1F	165	ARG
5	1F	191	ARG
5	1F	192	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	201	VAL
5	1F	204	ASN
6	1G	3	LEU
6	1G	28	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	49	ASP
6	1G	58	GLN
6	1G	66	GLN
6	1G	82	LEU
6	1G	95	ARG
6	1G	115	ARG
6	1G	116	ASP
6	1G	126	ASP
6	1G	133	LEU
6	1G	140	ILE
6	1G	145	THR
6	1G	148	MET
6	1G	150	ASP
6	1G	159	VAL
6	1G	162	THR
6	1G	174	GLU
7	1H	13	LYS
7	1H	24	VAL
7	1H	37	VAL
7	1H	46	GLU
7	1H	49	VAL
7	1H	81	GLU
7	1H	84	SER
7	1H	85	LYS
7	1H	92	ILE
7	1H	114	VAL
7	1H	122	THR
7	1H	130	ARG
7	1H	138	LYS
8	1I	1	MET
8	1I	12	LEU
8	1I	78	THR
8	1I	108	THR
8	1I	109	ILE
8	1I	116	LEU
8	1I	127	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1I	140	LEU
9	1N	5	VAL
9	1N	10	GLU
9	1N	28	THR
9	1N	34	LEU
9	1N	46	VAL
9	1N	62	VAL
9	1N	65	LYS
9	1N	96	GLU
9	1N	137	LYS
9	1N	140	VAL
10	1O	25	LEU
10	1O	108	GLU
11	1P	29	LYS
11	1P	55	ARG
11	1P	56	SER
11	1P	65	ARG
11	1P	74	GLU
11	1P	75	ILE
11	1P	95	VAL
11	1P	98	GLU
11	1P	99	LEU
11	1P	101	VAL
11	1P	126	VAL
11	1P	135	LEU
11	1P	147	LEU
11	1P	148	LEU
11	1P	149	GLU
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	38	GLU
12	1Q	75	THR
13	1R	114	VAL
14	1S	3	ARG
14	1S	46	VAL
14	1S	49	VAL
14	1S	68	GLN
14	1S	73	LEU
14	1S	110	LEU
15	1T	1	MET
15	1T	6	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	1T	13	ARG
15	1T	28	VAL
15	1T	34	VAL
15	1T	41	ARG
15	1T	65	LYS
15	1T	67	SER
15	1T	84	GLN
15	1T	96	ARG
15	1T	128	GLU
16	1U	31	SER
16	1U	74	LEU
16	1U	95	LEU
16	1U	108	GLU
16	1U	117	GLN
17	1V	79	VAL
17	1V	98	GLU
18	1W	11	ARG
18	1W	17	VAL
18	1W	60	ASN
19	1X	57	LEU
19	1X	66	LEU
19	1X	88	LYS
20	1Y	23	ARG
20	1Y	34	LYS
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	106	LEU
21	1Z	1	MET
21	1Z	4	ARG
21	1Z	24	LEU
21	1Z	31	ARG
21	1Z	33	LEU
21	1Z	41	LEU
21	1Z	42	VAL
21	1Z	53	ILE
21	1Z	72	ARG
21	1Z	84	GLU
21	1Z	94	GLU
21	1Z	121	HIS
21	1Z	126	VAL
21	1Z	150	LEU
21	1Z	153	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	161	VAL
22	10	49	LYS
23	11	3	LYS
23	11	37	ILE
23	11	40	ARG
23	11	46	LEU
23	11	74	VAL
23	11	95	LEU
24	12	2	LYS
24	12	3	LEU
24	12	9	GLN
24	12	19	VAL
24	12	41	ILE
25	13	6	VAL
25	13	23	LEU
25	13	31	LEU
25	13	54	VAL
25	13	56	VAL
25	13	60	GLU
26	14	27	THR
26	14	49	PHE
26	14	50	VAL
26	14	53	GLU
26	14	56	VAL
26	14	59	PHE
26	14	61	ARG
27	15	6	VAL
27	15	16	ARG
27	15	20	ARG
27	15	57	VAL
28	16	7	ILE
28	16	9	LEU
28	16	14	THR
28	16	47	THR
28	16	48	VAL
28	16	52	VAL
28	16	54	ILE
29	17	24	THR
29	17	43	THR
30	18	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	18	23	VAL
33	1b	7	VAL
33	1b	11	LEU
33	1b	15	VAL
33	1b	17	PHE
33	1b	21	ARG
33	1b	35	GLU
33	1b	44	LEU
33	1b	48	MET
33	1b	49	GLU
33	1b	53	ARG
33	1b	71	VAL
33	1b	75	LYS
33	1b	107	THR
33	1b	108	ILE
33	1b	111	ARG
33	1b	112	VAL
33	1b	128	GLU
33	1b	145	LEU
33	1b	150	SER
33	1b	165	VAL
33	1b	189	ASP
33	1b	191	ASP
33	1b	195	ASP
33	1b	208	ILE
33	1b	221	LEU
33	1b	233	SER
34	1c	3	ASN
34	1c	16	ARG
34	1c	28	GLN
34	1c	49	SER
34	1c	64	VAL
34	1c	91	LEU
34	1c	101	LEU
34	1c	106	VAL
34	1c	120	VAL
34	1c	130	VAL
34	1c	132	ARG
34	1c	138	VAL
34	1c	143	GLU
34	1c	144	SER
34	1c	165	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	172	ARG
34	1c	192	THR
34	1c	196	LEU
35	1d	17	VAL
35	1d	28	SER
35	1d	34	GLU
35	1d	83	SER
35	1d	85	LYS
35	1d	92	VAL
35	1d	101	LEU
35	1d	120	LEU
35	1d	129	ASN
36	1e	12	LEU
36	1e	31	LEU
36	1e	34	VAL
36	1e	41	VAL
36	1e	68	GLU
36	1e	75	THR
36	1e	78	HIS
36	1e	79	GLU
36	1e	100	VAL
36	1e	105	VAL
36	1e	120	THR
36	1e	151	LEU
36	1e	152	ARG
37	1f	15	ASP
37	1f	19	LEU
37	1f	45	LEU
37	1f	55	ASP
37	1f	72	VAL
37	1f	91	VAL
38	1g	12	LEU
38	1g	13	GLN
38	1g	21	VAL
38	1g	27	ILE
38	1g	38	LEU
38	1g	53	LYS
38	1g	61	VAL
38	1g	66	VAL
38	1g	80	VAL
38	1g	140	ASP
39	1h	2	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	1h	19	VAL
39	1h	25	ASP
39	1h	26	VAL
39	1h	51	VAL
39	1h	63	LEU
39	1h	98	LYS
39	1h	115	SER
39	1h	121	ASP
39	1h	127	LEU
39	1h	133	LEU
39	1h	137	VAL
40	1i	9	ARG
40	1i	23	ASN
40	1i	41	VAL
40	1i	54	ASP
40	1i	60	ASP
40	1i	64	THR
40	1i	65	VAL
40	1i	87	GLN
40	1i	92	TYR
40	1i	96	LEU
40	1i	108	VAL
40	1i	128	ARG
41	1j	8	LEU
41	1j	34	VAL
41	1j	35	SER
41	1j	38	ILE
41	1j	42	THR
41	1j	62	HIS
41	1j	66	ARG
41	1j	81	THR
41	1j	85	LEU
41	1j	98	ILE
42	1k	28	THR
42	1k	31	THR
42	1k	33	THR
42	1k	48	ILE
42	1k	63	LEU
42	1k	84	VAL
42	1k	87	THR
42	1k	96	ARG
42	1k	98	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	1k	101	SER
42	1k	105	VAL
42	1k	117	ASN
43	1l	18	VAL
43	1l	22	SER
43	1l	60	LEU
43	1l	61	THR
43	1l	62	SER
43	1l	66	VAL
43	1l	67	THR
43	1l	81	SER
43	1l	104	VAL
44	1m	9	ILE
44	1m	12	ASN
44	1m	15	VAL
44	1m	34	LEU
44	1m	43	THR
44	1m	47	ASP
44	1m	48	LEU
44	1m	49	THR
44	1m	54	VAL
44	1m	67	GLU
44	1m	69	GLU
44	1m	73	GLU
44	1m	78	ILE
44	1m	82	MET
44	1m	90	LEU
44	1m	103	THR
44	1m	106	ASN
44	1m	109	THR
44	1m	116	THR
45	1n	7	ILE
45	1n	11	LYS
45	1n	15	LYS
45	1n	18	VAL
45	1n	22	THR
45	1n	32	SER
45	1n	33	VAL
45	1n	46	GLU
45	1n	60	SER
46	1o	3	ILE
46	1o	10	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	1o	11	VAL
46	1o	13	GLN
46	1o	25	THR
46	1o	39	LEU
46	1o	56	LEU
47	1p	1	MET
47	1p	8	ARG
47	1p	16	HIS
47	1p	20	VAL
47	1p	21	VAL
47	1p	45	THR
47	1p	49	LEU
47	1p	50	LYS
47	1p	54	GLU
47	1p	62	VAL
47	1p	67	THR
47	1p	74	LEU
47	1p	76	GLN
48	1q	7	THR
48	1q	15	MET
48	1q	43	LEU
48	1q	50	LYS
48	1q	52	LYS
48	1q	60	ILE
48	1q	63	ARG
48	1q	66	SER
48	1q	73	VAL
48	1q	86	GLU
48	1q	97	SER
48	1q	99	SER
49	1r	22	VAL
49	1r	86	VAL
50	1s	4	SER
50	1s	19	VAL
50	1s	28	LYS
50	1s	32	LYS
50	1s	37	ARG
50	1s	41	VAL
50	1s	63	THR
50	1s	66	MET
50	1s	77	THR
51	1t	24	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1t	85	MET
52	1u	9	ARG
54	1w	102	MET
54	1w	108	ILE
54	1w	119	GLU
54	1w	125	ARG
54	1w	136	GLU
54	1w	143	GLU
54	1w	145	LEU
54	1w	152	LEU
54	1w	157	LYS
54	1w	158	VAL
54	1w	180	VAL
54	1w	185	VAL
54	1w	188	THR
54	1w	196	THR
54	1w	206	GLU
54	1w	223	ARG
54	1w	288	THR
54	1w	299	SER
54	1w	302	ILE
54	1w	320	THR
54	1w	333	THR
3	2D	22	SER
3	2D	27	THR
3	2D	32	SER
3	2D	38	LYS
3	2D	136	ILE
3	2D	162	SER
3	2D	173	VAL
3	2D	183	ARG
3	2D	200	ASP
3	2D	229	VAL
3	2D	259	THR
3	2D	260	ARG
4	2E	27	LEU
4	2E	75	VAL
4	2E	77	ILE
4	2E	93	VAL
4	2E	116	VAL
4	2E	134	ILE
4	2E	188	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	2F	15	SER
5	2F	20	LEU
5	2F	70	THR
5	2F	74	ARG
5	2F	132	VAL
5	2F	133	ASN
5	2F	137	LYS
5	2F	140	LEU
5	2F	144	LYS
5	2F	153	SER
5	2F	158	THR
5	2F	165	ARG
5	2F	181	LEU
5	2F	183	VAL
5	2F	190	GLU
5	2F	197	ASP
6	2G	3	LEU
6	2G	5	VAL
6	2G	7	LEU
6	2G	15	VAL
6	2G	31	VAL
6	2G	34	LEU
6	2G	43	LEU
6	2G	70	VAL
6	2G	88	ILE
6	2G	91	ARG
6	2G	109	VAL
6	2G	135	LEU
6	2G	140	ILE
6	2G	152	LEU
6	2G	159	VAL
6	2G	165	THR
6	2G	172	LEU
7	2H	23	ARG
7	2H	24	VAL
7	2H	37	VAL
7	2H	58	GLU
7	2H	63	SER
7	2H	70	THR
7	2H	84	SER
7	2H	92	ILE
7	2H	107	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	2H	113	VAL
7	2H	119	GLU
7	2H	130	ARG
7	2H	134	SER
8	2I	7	GLU
8	2I	19	VAL
8	2I	31	LEU
8	2I	38	LEU
8	2I	43	ASN
8	2I	47	LEU
8	2I	58	LEU
8	2I	61	ARG
8	2I	68	LEU
8	2I	75	LEU
8	2I	77	LEU
8	2I	87	LYS
8	2I	101	LEU
8	2I	105	HIS
8	2I	108	THR
8	2I	114	LEU
8	2I	117	GLU
8	2I	127	VAL
8	2I	129	THR
8	2I	144	VAL
9	2N	5	VAL
9	2N	10	GLU
9	2N	28	THR
9	2N	32	THR
9	2N	34	LEU
9	2N	38	HIS
9	2N	43	THR
9	2N	48	MET
9	2N	58	ASP
9	2N	61	ARG
9	2N	62	VAL
10	2O	1	MET
10	2O	52	VAL
10	2O	69	ILE
10	2O	108	GLU
11	2P	29	LYS
11	2P	42	SER
11	2P	55	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	2P	71	VAL
11	2P	75	ILE
11	2P	96	THR
11	2P	98	GLU
11	2P	99	LEU
11	2P	125	VAL
11	2P	132	LYS
11	2P	135	LEU
11	2P	149	GLU
12	2Q	6	ARG
12	2Q	7	MET
12	2Q	18	LYS
12	2Q	38	GLU
12	2Q	75	THR
12	2Q	85	LYS
12	2Q	98	LYS
12	2Q	127	ILE
13	2R	102	GLU
13	2R	114	VAL
14	2S	3	ARG
14	2S	21	THR
14	2S	36	TYR
14	2S	69	VAL
14	2S	78	LEU
14	2S	80	LEU
14	2S	85	VAL
14	2S	110	LEU
15	2T	6	LEU
15	2T	28	VAL
15	2T	89	VAL
15	2T	118	ARG
16	2U	36	ARG
16	2U	55	ARG
16	2U	74	LEU
16	2U	77	SER
16	2U	100	VAL
16	2U	108	GLU
16	2U	117	GLN
17	2V	46	VAL
17	2V	53	GLU
17	2V	73	SER
17	2V	79	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	2W	4	LYS
18	2W	6	ILE
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
19	2X	14	SER
19	2X	35	THR
19	2X	82	GLN
19	2X	92	LEU
20	2Y	11	ASP
20	2Y	23	ARG
20	2Y	34	LYS
20	2Y	72	VAL
20	2Y	75	ILE
20	2Y	99	CYS
20	2Y	106	LEU
21	2Z	5	LEU
21	2Z	33	LEU
21	2Z	39	VAL
21	2Z	46	LYS
21	2Z	47	VAL
21	2Z	50	GLN
21	2Z	57	ILE
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	74	VAL
21	2Z	76	LEU
21	2Z	91	LEU
21	2Z	121	HIS
21	2Z	124	ILE
21	2Z	126	VAL
21	2Z	141	VAL
21	2Z	145	GLU
21	2Z	149	SER
21	2Z	154	ASP
21	2Z	161	VAL
22	20	10	THR
22	20	14	ARG
23	21	74	VAL
23	21	83	GLU
23	21	95	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	22	3	LEU
24	22	26	ARG
24	22	59	ARG
25	23	31	LEU
25	23	53	LEU
25	23	54	VAL
25	23	56	VAL
25	23	59	VAL
26	24	3	GLU
26	24	22	ILE
26	24	27	THR
26	24	50	VAL
26	24	52	THR
26	24	53	GLU
26	24	56	VAL
26	24	67	TYR
27	25	6	VAL
27	25	16	ARG
27	25	55	ARG
27	25	58	LEU
28	26	28	ARG
28	26	48	VAL
29	27	1	MET
29	27	23	ARG
29	27	24	THR
29	27	43	THR
30	28	14	VAL
30	28	23	VAL
31	29	4	ARG
31	29	26	ILE
31	29	33	LYS
33	2b	7	VAL
33	2b	23	ARG
33	2b	30	ARG
33	2b	37	ASN
33	2b	44	LEU
33	2b	67	THR
33	2b	71	VAL
33	2b	79	ASP
33	2b	87	ARG
33	2b	112	VAL
33	2b	118	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	122	PHE
33	2b	127	ILE
33	2b	130	ARG
33	2b	136	VAL
33	2b	140	HIS
33	2b	154	LEU
33	2b	158	LEU
33	2b	164	VAL
33	2b	172	ILE
33	2b	185	ILE
33	2b	189	ASP
33	2b	191	ASP
33	2b	196	LEU
33	2b	223	ILE
33	2b	224	GLN
34	2c	14	ILE
34	2c	15	THR
34	2c	36	ASP
34	2c	49	SER
34	2c	166	GLU
34	2c	182	ILE
34	2c	188	LEU
34	2c	191	THR
34	2c	195	VAL
34	2c	202	ILE
34	2c	207	VAL
35	2d	8	VAL
35	2d	11	LEU
35	2d	28	SER
35	2d	34	GLU
35	2d	45	GLN
35	2d	67	ILE
35	2d	70	ILE
35	2d	83	SER
35	2d	85	LYS
35	2d	105	VAL
35	2d	115	ARG
35	2d	126	ILE
35	2d	135	LEU
35	2d	141	ARG
35	2d	155	LEU
35	2d	158	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	162	LEU
35	2d	170	VAL
35	2d	196	LEU
35	2d	201	GLN
36	2e	5	ASP
36	2e	6	PHE
36	2e	24	ARG
36	2e	25	ARG
36	2e	34	VAL
36	2e	50	GLU
36	2e	51	VAL
36	2e	67	VAL
36	2e	75	THR
36	2e	79	GLU
36	2e	120	THR
37	2f	1	MET
37	2f	8	ILE
37	2f	21	LEU
37	2f	66	GLU
37	2f	69	GLU
37	2f	75	LEU
38	2g	9	VAL
38	2g	13	GLN
38	2g	16	LEU
38	2g	79	ARG
38	2g	80	VAL
38	2g	90	GLU
38	2g	120	ILE
38	2g	129	GLU
38	2g	135	VAL
38	2g	155	ARG
38	2g	156	TRP
39	2h	8	ASP
39	2h	25	ASP
39	2h	26	VAL
39	2h	51	VAL
39	2h	63	LEU
39	2h	98	LYS
39	2h	105	ARG
39	2h	118	VAL
39	2h	127	LEU
39	2h	133	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	2h	137	VAL
40	2i	7	THR
40	2i	17	VAL
40	2i	27	THR
40	2i	28	VAL
40	2i	54	ASP
40	2i	56	LEU
40	2i	64	THR
40	2i	86	VAL
40	2i	89	ASN
40	2i	108	VAL
40	2i	124	GLN
40	2i	128	ARG
41	2j	8	LEU
41	2j	47	PHE
41	2j	89	ASP
41	2j	92	THR
42	2k	30	VAL
42	2k	33	THR
42	2k	38	ASN
42	2k	41	THR
42	2k	80	VAL
42	2k	84	VAL
42	2k	105	VAL
42	2k	109	VAL
42	2k	117	ASN
43	2l	6	THR
43	2l	18	VAL
43	2l	24	VAL
43	2l	33	ARG
43	2l	34	ARG
43	2l	67	THR
43	2l	91	LYS
43	2l	104	VAL
44	2m	4	ILE
44	2m	15	VAL
44	2m	32	GLU
44	2m	67	GLU
44	2m	77	ASN
44	2m	106	ASN
44	2m	117	VAL
45	2n	7	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	2n	18	VAL
45	2n	22	THR
45	2n	33	VAL
46	2o	5	LYS
46	2o	11	VAL
46	2o	24	SER
46	2o	25	THR
46	2o	38	ARG
46	2o	39	LEU
46	2o	72	ARG
46	2o	76	GLU
46	2o	87	ILE
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG
47	2p	20	VAL
47	2p	21	VAL
47	2p	28	ARG
47	2p	31	LYS
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	76	GLN
48	2q	13	ASP
48	2q	60	ILE
48	2q	63	ARG
48	2q	65	ILE
48	2q	66	SER
48	2q	73	VAL
48	2q	76	LEU
48	2q	86	GLU
49	2r	37	VAL
49	2r	45	SER
50	2s	7	LYS
50	2s	16	LEU
50	2s	28	LYS
50	2s	33	THR
50	2s	49	ILE
50	2s	79	THR
50	2s	81	ARG
50	2s	83	HIS
51	2t	30	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	2t	71	THR
51	2t	88	VAL
52	2u	8	THR
54	2w	103	ASP
54	2w	105	ARG
54	2w	106	ASP
54	2w	109	VAL
54	2w	119	GLU
54	2w	125	ARG
54	2w	129	ASN
54	2w	143	GLU
54	2w	145	LEU
54	2w	158	VAL
54	2w	163	ARG
54	2w	175	SER
54	2w	177	VAL
54	2w	180	VAL
54	2w	182	ARG
54	2w	183	VAL
54	2w	185	VAL
54	2w	188	THR
54	2w	189	GLN
54	2w	209	ASP
54	2w	222	MET
54	2w	225	SER
54	2w	248	ILE
54	2w	262	ARG
54	2w	267	MET
54	2w	283	GLU
54	2w	302	ILE
54	2w	320	THR
54	2w	322	HIS
54	2w	327	VAL
54	2w	333	THR
54	2w	335	ILE
54	2w	336	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (142) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	164	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
8	1I	43	ASN
8	1I	139	GLN
9	1N	8	GLN
10	1O	89	ASN
11	1P	84	ASN
12	1Q	12	GLN
12	1Q	57	HIS
12	1Q	89	ASN
13	1R	71	GLN
14	1S	61	ASN
14	1S	95	HIS
15	1T	58	ASN
15	1T	84	GLN
16	1U	81	HIS
16	1U	94	ASN
18	1W	60	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	32	HIS
21	1Z	73	GLN
21	1Z	121	HIS
21	1Z	151	HIS
22	10	35	ASN
24	12	43	GLN
24	12	70	GLN
25	13	32	GLN
26	14	46	GLN
30	18	35	GLN
33	1b	16	HIS
33	1b	19	HIS
33	1b	37	ASN
33	1b	40	HIS
33	1b	135	GLN
34	1c	6	HIS
34	1c	118	GLN
34	1c	136	GLN
34	1c	170	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	77	ASN
35	1d	123	HIS
35	1d	125	HIS
35	1d	160	GLN
35	1d	161	ASN
36	1e	78	HIS
37	1f	13	ASN
37	1f	84	ASN
37	1f	100	ASN
38	1g	51	GLN
38	1g	86	GLN
38	1g	109	ASN
40	1i	29	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	87	GLN
40	1i	89	ASN
40	1i	117	HIS
40	1i	124	GLN
41	1j	21	GLN
41	1j	56	HIS
41	1j	69	ASN
42	1k	93	GLN
43	1l	80	HIS
46	1o	50	HIS
46	1o	62	GLN
47	1p	76	GLN
49	1r	63	GLN
50	1s	83	HIS
51	1t	90	GLN
54	1w	178	HIS
54	1w	189	GLN
54	1w	258	GLN
54	1w	315	HIS
54	1w	322	HIS
4	2E	48	GLN
5	2F	29	ASN
5	2F	69	HIS
6	2G	26	GLN
6	2G	79	ASN
8	2I	43	ASN
10	2O	89	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	2Q	12	GLN
12	2Q	89	ASN
13	2R	13	HIS
13	2R	24	GLN
13	2R	61	HIS
13	2R	71	GLN
15	2T	58	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	43	ASN
21	2Z	50	GLN
21	2Z	55	HIS
21	2Z	73	GLN
22	20	29	GLN
24	22	9	GLN
24	22	70	GLN
26	24	40	HIS
28	26	20	ASN
30	28	35	GLN
31	29	20	HIS
33	2b	45	GLN
33	2b	95	GLN
33	2b	224	GLN
34	2c	37	GLN
34	2c	181	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
37	2f	7	ASN
37	2f	100	ASN
38	2g	37	ASN
38	2g	97	GLN
38	2g	109	ASN
40	2i	3	GLN
40	2i	29	ASN
40	2i	89	ASN
40	2i	124	GLN
41	2j	56	HIS
41	2j	68	HIS
42	2k	99	GLN
42	2k	116	HIS
42	2k	117	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	2l	80	HIS
43	2l	99	HIS
44	2m	12	ASN
47	2p	13	HIS
47	2p	16	HIS
49	2r	63	GLN
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	18	GLN
51	2t	45	GLN
54	2w	129	ASN
54	2w	193	HIS
54	2w	315	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	449 (15%)	30 (1%)
1	2A	2791/2915 (95%)	458 (16%)	19 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	18 (15%)	0
32	1a	1497/1521 (98%)	295 (19%)	0
32	2a	1501/1521 (98%)	279 (18%)	0
53	1v	8/24 (33%)	1 (12%)	0
53	2v	8/24 (33%)	1 (12%)	0
55	1x	72/74 (97%)	12 (16%)	0
55	2x	72/74 (97%)	5 (6%)	0
All	All	9050/9310 (97%)	1527 (16%)	49 (0%)

All (1527) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	55	G
1	1A	60	G
1	1A	71	A
1	1A	74	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	139	G
1	1A	196	A
1	1A	197	A
1	1A	200	U
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	224	G
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	265	A
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	345	A
1	1A	352	G
1	1A	362	U
1	1A	363	G
1	1A	363(B)	G
1	1A	370	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	412	A
1	1A	428	A
1	1A	436	C
1	1A	442	G
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	513	A
1	1A	529	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	586	A
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(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	726	G
1	1A	730	C
1	1A	764	A
1	1A	765	G
1	1A	775	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	802	A
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	878	A
1	1A	880	G
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	899	A
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	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1004	C
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1033	U
1	1A	1039	G
1	1A	1040	C
1	1A	1041	C
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1060	U
1	1A	1063	G
1	1A	1064	C
1	1A	1066	U
1	1A	1067	A
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1083	U
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1093	G
1	1A	1094	U
1	1A	1095	A
1	1A	1096	A
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1220	A
1	1A	1241	A
1	1A	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1308	A
1	1A	1321	A
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C
1	1A	1421	G
1	1A	1428	C
1	1A	1437	C
1	1A	1439	A
1	1A	1445	A
1	1A	1450	G
1	1A	1453	U
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C
1	1A	1478	G
1	1A	1482	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1493	C
1	1A	1494	A
1	1A	1497	U
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1607	C
1	1A	1608	A
1	1A	1609	A
1	1A	1634	A
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1758	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1786	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1816	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1848	A
1	1A	1853	A
1	1A	1861	G
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
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	2062	A
1	1A	2069	G
1	1A	2093	G
1	1A	2099	U
1	1A	2101	G
1	1A	2102	U
1	1A	2104	G
1	1A	2105	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2108	C
1	1A	2112	G
1	1A	2113	U
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2120	G
1	1A	2123	G
1	1A	2124	G
1	1A	2126	A
1	1A	2127	G
1	1A	2128	C
1	1A	2130	U
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2138	C
1	1A	2139	C
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2151	G
1	1A	2154	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2162	G
1	1A	2163	C
1	1A	2164	C
1	1A	2166	G
1	1A	2168	G
1	1A	2170	A
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2175	C
1	1A	2176	A
1	1A	2178	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2182	G
1	1A	2184	G
1	1A	2185	C
1	1A	2186	G
1	1A	2187	G
1	1A	2190	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2278	A
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2335	A
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2383	G
1	1A	2385	C
1	1A	2391	G
1	1A	2406	U
1	1A	2407	G
1	1A	2410	G
1	1A	2422	A
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2434	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2582	G
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2682	U
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2718	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2780	G
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2849	U
1	1A	2872	G
1	1A	2873	A
1	1A	2880	C
1	1A	2894	G
1	1A	2895	U
2	1B	13	A
2	1B	24	G
2	1B	25	A
2	1B	45	A
2	1B	56	G
2	1B	57	A
2	1B	73	A
2	1B	106	G
2	1B	110	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	76	C
32	1a	78	G
32	1a	91	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	97	G
32	1a	101	A
32	1a	102	G
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	122	G
32	1a	131	C
32	1a	137	C
32	1a	143	A
32	1a	144	G
32	1a	146	G
32	1a	163	C
32	1a	165	C
32	1a	174	C
32	1a	182	U
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	223	U
32	1a	227	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	281	G
32	1a	289	G
32	1a	316	G
32	1a	317	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	349	A
32	1a	350	G
32	1a	352	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	444	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	474	G
32	1a	485	G
32	1a	492	G
32	1a	496	A
32	1a	498	U
32	1a	499	A
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	517	G
32	1a	518	C
32	1a	521	G
32	1a	528	C
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	564	C
32	1a	572	A
32	1a	573	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	618	C
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	657	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	694	A
32	1a	695	A
32	1a	703	G
32	1a	707	C
32	1a	721	G
32	1a	723	U
32	1a	733	A
32	1a	749	C
32	1a	753	A
32	1a	755	G
32	1a	777	A
32	1a	786	G
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	802	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	828	A
32	1a	834	C
32	1a	838	G
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	857	C
32	1a	859	A
32	1a	876	G
32	1a	884	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	936	C
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	983	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1004	A
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1011	G
32	1a	1013	G
32	1a	1016	A
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1035	A
32	1a	1036	G
32	1a	1038	C
32	1a	1039	C
32	1a	1040	U
32	1a	1043	C
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1054	C
32	1a	1057	G
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1092	A
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1113	C
32	1a	1122	U
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1129	C
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1159	U
32	1a	1162	C
32	1a	1166	G
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1222	G
32	1a	1226	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1244	C
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1297	C
32	1a	1298	C
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1303	C
32	1a	1312	G
32	1a	1317	C
32	1a	1320	C
32	1a	1322	C
32	1a	1323	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1327	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	1398	A
32	1a	1402	4OC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1447	A
32	1a	1452	C
32	1a	1460	A
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1494	G
32	1a	1497	G
32	1a	1499	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
53	1v	22	U
55	1x	6	G
55	1x	9	A
55	1x	18	G
55	1x	20	H2U
55	1x	21	H2U
55	1x	22	A
55	1x	37	MIA
55	1x	46	A
55	1x	48	G
55	1x	49	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	1x	51	C
55	1x	54	5MU
1	2A	8	A
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	61	G
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	76	C
1	2A	84	A
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	237	C
1	2A	248	G
1	2A	249	C
1	2A	271(B)	C
1	2A	271(K)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	324	A
1	2A	327	G
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	386	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	434	U
1	2A	435	C
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	496	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	573	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	575	A
1	2A	586	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(A)	A
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	762	U
1	2A	775	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	832	G
1	2A	847	U
1	2A	859	G
1	2A	874	G
1	2A	878	A
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	897	C
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	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1033	U
1	2A	1039	G
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1114	G
1	2A	1115	G
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1155	A
1	2A	1171	G
1	2A	1202	C
1	2A	1205	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1244	G
1	2A	1247	A
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1342	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1400	G
1	2A	1416	G
1	2A	1417	C
1	2A	1419	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1543	C
1	2A	1554	A
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	1587	A
1	2A	1608	A
1	2A	1609	A
1	2A	1639	U
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1675	C
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1745	C
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1860	G
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1884	A
1	2A	1896	G
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	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2051	A
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2080	G
1	2A	2103	C
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2113	U
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2138	C
1	2A	2139	C
1	2A	2142	C
1	2A	2146	C
1	2A	2149	G
1	2A	2150	U
1	2A	2153	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2160	G
1	2A	2161	C
1	2A	2162	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2173	A
1	2A	2175	C
1	2A	2178	C
1	2A	2183	C
1	2A	2184	G
1	2A	2185	C
1	2A	2186	G
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2193	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2325	G
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2372	G
1	2A	2376	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2396	G
1	2A	2406	U
1	2A	2407	G
1	2A	2410	G
1	2A	2422	A
1	2A	2423	U
1	2A	2424	C
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2459	A
1	2A	2469	A
1	2A	2476	A
1	2A	2478	A
1	2A	2480	C
1	2A	2490	G
1	2A	2492	U
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2585	U
1	2A	2602	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2752	C
1	2A	2757	A
1	2A	2759	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
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	2873	A
1	2A	2876	G
1	2A	2880	C
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	4	C
2	2B	9	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	25	A
2	2B	35	U
2	2B	41	U
2	2B	42	C
2	2B	50	G
2	2B	53	A
2	2B	56	G
2	2B	73	A
2	2B	85	G
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	120	A
32	2a	9	G
32	2a	22	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
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	146	G
32	2a	156	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	195	A
32	2a	197	A
32	2a	200	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	274	A
32	2a	289	G
32	2a	294	U
32	2a	321	A
32	2a	328	C
32	2a	329	A
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	367	U
32	2a	369	C
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	395	C
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	422	C
32	2a	429	U
32	2a	430	A
32	2a	438	G
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	482	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	485	G
32	2a	492	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	521	G
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	592	G
32	2a	596	C
32	2a	607	A
32	2a	630	G
32	2a	641	U
32	2a	650	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	666	G
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	693	G
32	2a	702	A
32	2a	703	G
32	2a	717	C
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	733	A
32	2a	755	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	874	G
32	2a	884	U
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	1001	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1013	G
32	2a	1022	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(D)	A
32	2a	1032	G
32	2a	1038	C
32	2a	1040	U
32	2a	1041	A
32	2a	1042	G
32	2a	1044	A
32	2a	1045	C
32	2a	1046	A
32	2a	1056	U
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1084	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1104	G
32	2a	1113	C
32	2a	1117	G
32	2a	1121	U
32	2a	1122	U
32	2a	1125	U
32	2a	1126	U
32	2a	1128	C
32	2a	1129	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1141	C
32	2a	1142	G
32	2a	1146	A
32	2a	1151	A
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1159	U
32	2a	1181	G
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1212	U
32	2a	1214	C
32	2a	1220	G
32	2a	1227	A
32	2a	1228	C
32	2a	1233	G
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1245	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1278	U
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1289	A
32	2a	1299	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1300	G
32	2a	1301	U
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1319	A
32	2a	1320	C
32	2a	1322	C
32	2a	1323	G
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1383	C
32	2a	1397	C
32	2a	1398	A
32	2a	1402	4OC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1475	G
32	2a	1487	G
32	2a	1497	G
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1532	U
53	2v	22	U
55	2x	16	C
55	2x	18	G
55	2x	19	G
55	2x	21	H2U
55	2x	37	MIA

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	199	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	764	A
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
1	1A	1174	A
1	1A	1176	G
1	1A	1420	U
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1653	G
1	1A	1992	G
1	1A	2126	A
1	1A	2133	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	266	G
1	2A	277	C
1	2A	528	A
1	2A	669	G
1	2A	752	A
1	2A	827	U
1	2A	893	C
1	2A	896	A
1	2A	1210	A
1	2A	1379	A
1	2A	1530	C
1	2A	1653	G
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2406	U
1	2A	2689	U
1	2A	2756	U

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

66 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	$\#\|Z\| > 2$
55	5MU	1x	54	55	19,22,23	1.37	3 (15%)	27,32,35	1.81	5 (18%)
55	8AN	2x	76	57,56,55	17,24,25	1.12	2 (11%)	13,35,38	2.86	2 (15%)
43	0TD	1l	92	43	8,9,10	4.74	2 (25%)	6,11,13	5.96	3 (50%)
32	UR3	2a	1498	32	19,22,23	1.02	0	26,32,35	1.68	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.99	5 (23%)
32	PSU	1a	516	57,32	18,21,22	1.40	2 (11%)	21,30,33	2.00	4 (19%)
32	MA6	1a	1518	32	19,26,27	1.02	2 (10%)	18,38,41	1.99	3 (16%)
32	5MC	2a	1400	32	19,22,23	1.48	3 (15%)	26,32,35	1.25	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	M2G	2a	966	32	20,27,28	1.30	3 (15%)	19,40,43	1.07	2 (10%)
32	MA6	1a	1519	32	19,26,27	1.05	2 (10%)	18,38,41	2.02	3 (16%)
32	5MC	2a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.18	2 (7%)
1	OMU	1A	2552	57,1	19,22,23	1.25	3 (15%)	25,31,34	1.67	5 (20%)
32	5MC	2a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.10	3 (11%)
55	PSU	1x	55	55	18,21,22	1.30	2 (11%)	21,30,33	2.03	4 (19%)
1	OMU	2A	2552	57,1	19,22,23	1.21	3 (15%)	25,31,34	1.70	5 (20%)
1	PSU	1A	1911	1	18,21,22	1.41	3 (16%)	21,30,33	2.11	5 (23%)
1	5MU	1A	1939	57,1	19,22,23	1.41	5 (26%)	27,32,35	2.06	5 (18%)
1	PSU	2A	1911	1	18,21,22	1.38	3 (16%)	21,30,33	2.02	4 (19%)
1	5MU	2A	1939	57,1	19,22,23	1.40	5 (26%)	27,32,35	2.22	6 (22%)
55	PSU	2x	39	55	18,21,22	1.43	3 (16%)	21,30,33	1.71	4 (19%)
55	H2U	1x	20	55	18,21,22	0.93	2 (11%)	19,30,33	1.01	1 (5%)
1	5MU	1A	1915	1	19,22,23	1.39	5 (26%)	27,32,35	2.29	6 (22%)
32	5MC	2a	1407	32	19,22,23	1.50	3 (15%)	26,32,35	1.24	3 (11%)
1	2MA	1A	2503	57,1	18,25,26	0.72	0	20,37,40	1.91	3 (15%)
1	5MU	2A	1915	57,1	19,22,23	1.46	6 (31%)	27,32,35	2.18	6 (22%)
55	4SU	1x	8	55	18,21,22	1.85	4 (22%)	25,30,33	1.78	4 (16%)
32	5MC	1a	967	32	19,22,23	1.57	3 (15%)	26,32,35	1.16	2 (7%)
55	8AN	1x	76	57,56,55	17,24,25	1.11	2 (11%)	13,35,38	2.84	2 (15%)
55	MIA	1x	37	55	17,24,32	1.00	1 (5%)	16,35,47	1.34	2 (12%)
1	2MA	2A	2503	57,1	18,25,26	0.70	0	20,37,40	1.93	4 (20%)
55	MIA	2x	37	55	17,24,32	0.99	1 (5%)	16,35,47	1.49	3 (18%)
55	PSU	1x	32	57,55	18,21,22	1.30	2 (11%)	21,30,33	1.94	4 (19%)
55	H2U	2x	20	55	18,21,22	0.96	2 (11%)	19,30,33	0.95	1 (5%)
1	OMG	1A	2251	57,55,1	19,26,27	0.94	1 (5%)	21,38,41	1.21	3 (14%)
32	2MG	2a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.18	1 (6%)
32	MA6	2a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	1.82	3 (16%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	0.88	0
55	PSU	1x	39	55	18,21,22	1.37	2 (11%)	21,30,33	1.89	4 (19%)
32	4OC	1a	1402	57,32	20,23,24	0.75	0	25,32,35	0.98	2 (8%)
55	PSU	2x	32	55	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
1	OMC	2A	1920	1	19,22,23	0.81	0	25,31,34	0.82	0
32	5MC	1a	1407	32	19,22,23	1.53	3 (15%)	26,32,35	0.97	2 (7%)
32	UR3	1a	1498	32	19,22,23	1.13	2 (10%)	26,32,35	1.74	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	1A	2605	57,1	18,21,22	1.32	2 (11%)	21,30,33	2.02	5 (23%)
1	5MC	2A	1942	1	19,22,23	1.52	3 (15%)	26,32,35	1.19	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.36	2 (11%)	21,30,33	2.27	4 (19%)
32	2MG	1a	1207	57,32	18,26,27	0.90	1 (5%)	16,38,41	1.34	3 (18%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	1.98	4 (19%)
32	PSU	2a	516	57,32	18,21,22	1.40	2 (11%)	21,30,33	1.95	5 (23%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.19	2 (7%)
1	OMG	2A	2251	55,1	19,26,27	0.97	1 (5%)	21,38,41	1.01	2 (9%)
43	0TD	2l	92	43	8,9,10	4.52	1 (12%)	6,11,13	8.81	3 (50%)
32	5MC	1a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.21	3 (11%)
1	5MC	2A	1962	57,1	19,22,23	1.52	3 (15%)	26,32,35	1.16	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
55	5MU	2x	54	55	19,22,23	1.40	4 (21%)	27,32,35	2.05	6 (22%)
32	G7M	2a	527	57,32	20,26,27	1.20	2 (10%)	16,39,42	0.64	0
32	4OC	2a	1402	57,32	20,23,24	0.79	0	25,32,35	0.94	1 (4%)
32	MA6	2a	1519	32	19,26,27	1.02	2 (10%)	18,38,41	1.92	3 (16%)
1	5MC	1A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.27	3 (11%)
55	H2U	1x	21	55	18,21,22	0.94	2 (11%)	19,30,33	0.93	1 (5%)
32	G7M	1a	527	32	20,26,27	1.16	2 (10%)	16,39,42	0.51	0
55	4SU	2x	8	55	18,21,22	1.80	4 (22%)	25,30,33	2.12	5 (20%)
55	H2U	2x	21	55	18,21,22	0.99	2 (11%)	19,30,33	0.88	1 (5%)
32	M2G	1a	966	32	20,27,28	1.38	2 (10%)	19,40,43	1.11	2 (10%)
1	5MC	1A	1962	57,1	19,22,23	1.60	3 (15%)	26,32,35	1.06	2 (7%)

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
55	5MU	1x	54	55	-	2/7/25/26	0/2/2/2
55	8AN	2x	76	57,56,55	-	1/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	1/7/12/14	-
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	57,32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
55	H2U	1x	20	55	-	2/7/38/39	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	1/3/25/26	0/3/3/3
1	5MU	2A	1915	57,1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	57,56,55	-	1/3/25/26	0/3/3/3
55	MIA	1x	37	55	-	2/3/25/34	0/3/3/3
1	2MA	2A	2503	57,1	-	1/3/25/26	0/3/3/3
55	MIA	2x	37	55	-	2/3/25/34	0/3/3/3
55	PSU	1x	32	57,55	-	0/7/25/26	0/2/2/2
55	H2U	2x	20	55	-	0/7/38/39	0/2/2/2
1	OMG	1A	2251	57,55,1	-	0/5/27/28	0/3/3/3
32	2MG	2a	1207	32	-	2/5/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
55	PSU	1x	39	55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	57,32	-	3/9/29/30	0/2/2/2
55	PSU	2x	32	55	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	57,32	-	0/5/27/28	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	2a	516	57,32	-	1/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	57,32	-	1/3/25/26	0/3/3/3
32	4OC	2a	1402	57,32	-	3/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	5MC	1A	1942	1	-	1/7/25/26	0/2/2/2
55	H2U	1x	21	55	-	4/7/38/39	0/2/2/2
32	G7M	1a	527	32	-	2/3/25/26	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	H2U	2x	21	55	-	2/7/38/39	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.57	1.69	1.82
43	2l	92	0TD	CB-SB	-12.33	1.69	1.82
32	2a	967	5MC	C5-C4	6.37	1.48	1.44
32	1a	1404	5MC	C5-C4	6.36	1.48	1.44
32	2a	1404	5MC	C5-C4	5.86	1.48	1.44
1	1A	1962	5MC	C5-C4	5.83	1.48	1.44
32	1a	1400	5MC	C5-C4	5.79	1.48	1.44
32	1a	967	5MC	C5-C4	5.79	1.48	1.44
1	1A	1942	5MC	C5-C4	5.67	1.48	1.44
32	1a	1407	5MC	C5-C4	5.36	1.48	1.44
1	2A	1962	5MC	C5-C4	5.25	1.48	1.44
32	2a	1400	5MC	C5-C4	5.21	1.48	1.44
32	2a	1407	5MC	C5-C4	5.13	1.48	1.44
1	2A	1942	5MC	C5-C4	5.07	1.48	1.44
55	2x	8	4SU	C4-S4	-4.88	1.60	1.68
55	1x	8	4SU	C4-S4	-4.68	1.60	1.68
32	1a	966	M2G	C2-N3	4.10	1.36	1.30
55	1x	8	4SU	C4-N3	-3.98	1.33	1.37
55	2x	39	PSU	C6-C5	3.81	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	516	PSU	C6-C5	3.78	1.39	1.35
32	2a	966	M2G	C2-N3	3.75	1.35	1.30
55	2x	55	PSU	C6-C5	3.63	1.39	1.35
32	2a	516	PSU	C6-C5	3.61	1.39	1.35
1	1A	1911	PSU	C6-C5	3.55	1.39	1.35
1	2A	1911	PSU	C6-C5	3.55	1.39	1.35
32	1a	527	G7M	C5-C4	3.54	1.46	1.39
55	1x	39	PSU	C6-C5	3.50	1.39	1.35
55	2x	32	PSU	C6-C5	3.48	1.39	1.35
43	1l	92	0TD	CB-CA	-3.43	1.53	1.54
32	2a	527	G7M	C5-C4	3.41	1.45	1.39
55	1x	55	PSU	C6-C5	3.25	1.38	1.35
1	2A	1917	PSU	C6-C5	3.17	1.38	1.35
55	1x	32	PSU	C6-C5	3.14	1.38	1.35
55	2x	8	4SU	C4-N3	-3.12	1.34	1.37
1	1A	1917	PSU	C6-C5	3.12	1.38	1.35
1	2A	1942	5MC	C6-C5	3.05	1.39	1.34
1	1A	1942	5MC	C6-C5	3.02	1.39	1.34
32	2a	1404	5MC	C6-C5	2.97	1.39	1.34
32	1a	966	M2G	C2-N2	2.95	1.40	1.35
32	1a	1498	UR3	C2-N1	2.87	1.42	1.38
1	2A	1939	5MU	C6-C5	2.86	1.39	1.34
55	2x	54	5MU	C6-C5	2.85	1.39	1.34
1	1A	2552	OMU	C4-N3	-2.83	1.33	1.38
32	2a	1407	5MC	C6-C5	2.83	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.82	1.33	1.38
1	1A	1917	PSU	C4-N3	-2.82	1.33	1.38
55	1x	54	5MU	C6-C5	2.81	1.39	1.34
55	2x	39	PSU	C4-N3	-2.81	1.33	1.38
1	1A	1915	5MU	C6-C5	2.81	1.39	1.34
55	1x	39	PSU	C4-N3	-2.81	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.81	1.33	1.38
1	1A	2605	PSU	C4-N3	-2.80	1.33	1.38
32	2a	966	M2G	C2-N2	2.79	1.40	1.35
1	2A	1915	5MU	C6-C5	2.78	1.39	1.34
55	2x	8	4SU	C5-C4	-2.77	1.39	1.42
55	2x	21	H2U	C2-N3	-2.76	1.33	1.38
1	2A	2251	OMG	C6-N1	-2.76	1.33	1.37
1	1A	2251	OMG	C6-N1	-2.75	1.33	1.37
1	1A	1939	5MU	C4-N3	-2.75	1.33	1.38
55	1x	37	MIA	C2-N3	2.73	1.36	1.32
1	2A	2605	PSU	C6-C5	2.71	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	21	H2U	C4-N3	-2.71	1.33	1.37
55	2x	76	8AN	C6-C5	-2.70	1.33	1.43
1	1A	1962	5MC	C6-C5	2.68	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.68	1.33	1.38
1	2A	2552	OMU	C4-N3	-2.65	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.65	1.33	1.38
1	1A	1915	5MU	C4-N3	-2.65	1.33	1.38
32	1a	1400	5MC	C6-C5	2.65	1.38	1.34
32	1a	516	PSU	C4-N3	-2.65	1.33	1.38
1	1A	1939	5MU	C6-N1	-2.64	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.64	1.33	1.38
55	1x	54	5MU	C4-N3	-2.64	1.33	1.38
55	2x	54	5MU	C4-N3	-2.63	1.33	1.38
55	2x	20	H2U	C2-N3	-2.62	1.33	1.38
32	1a	1407	5MC	C6-C5	2.61	1.38	1.34
55	1x	8	4SU	C5-C4	-2.60	1.39	1.42
55	2x	37	MIA	C2-N3	2.60	1.36	1.32
32	1a	1404	5MC	C6-C5	2.59	1.38	1.34
55	1x	8	4SU	C2-N3	-2.58	1.33	1.38
1	2A	1917	PSU	C4-N3	-2.57	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.57	1.33	1.38
55	1x	21	H2U	C2-N3	-2.56	1.33	1.38
1	1A	2552	OMU	C2-N3	-2.56	1.33	1.38
55	1x	76	8AN	C6-C5	-2.56	1.33	1.43
55	1x	20	H2U	C2-N3	-2.55	1.33	1.38
32	2a	967	5MC	C6-C5	2.55	1.38	1.34
32	2a	516	PSU	C4-N3	-2.54	1.34	1.38
1	1A	2605	PSU	C6-C5	2.51	1.38	1.35
1	2A	1962	5MC	C6-C5	2.50	1.38	1.34
32	2a	1404	5MC	C6-N1	-2.50	1.33	1.38
1	1A	1939	5MU	C6-C5	2.49	1.38	1.34
55	1x	20	H2U	C4-N3	-2.47	1.33	1.37
1	2A	1915	5MU	C2-N1	2.46	1.42	1.38
32	1a	967	5MC	C6-C5	2.46	1.38	1.34
32	1a	1404	5MC	C6-N1	-2.45	1.33	1.38
32	1a	1207	2MG	C6-N1	-2.45	1.34	1.37
32	2a	527	G7M	C6-N1	-2.44	1.34	1.37
55	2x	32	PSU	C4-N3	-2.44	1.34	1.38
32	2a	1518	MA6	C6-C5	-2.44	1.41	1.44
1	2A	1939	5MU	C6-N1	-2.43	1.33	1.38
55	2x	54	5MU	C2-N1	2.41	1.42	1.38
32	1a	1518	MA6	C6-C5	-2.41	1.41	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	55	PSU	C4-N3	-2.40	1.34	1.38
1	1A	1915	5MU	C2-N1	2.40	1.42	1.38
32	2a	1400	5MC	C6-C5	2.40	1.38	1.34
32	1a	1519	MA6	C6-C5	-2.38	1.41	1.44
55	1x	76	8AN	C5-N7	-2.37	1.31	1.39
1	2A	1915	5MU	C4-C5	2.36	1.48	1.44
32	1a	1400	5MC	C6-N1	-2.35	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.35	1.34	1.37
32	2a	1519	MA6	C6-C5	-2.32	1.41	1.44
55	1x	32	PSU	C4-N3	-2.32	1.34	1.38
32	2a	967	5MC	C6-N1	-2.31	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.30	1.34	1.38
55	2x	54	5MU	C4-C5	2.30	1.48	1.44
1	2A	1915	5MU	C6-N1	-2.29	1.34	1.38
55	1x	55	PSU	C4-N3	-2.29	1.34	1.38
55	1x	21	H2U	C4-N3	-2.28	1.33	1.37
55	1x	54	5MU	C2-N1	2.25	1.42	1.38
1	1A	2552	OMU	C5-C4	-2.25	1.38	1.43
55	2x	76	8AN	C5-N7	-2.23	1.31	1.39
1	2A	2552	OMU	C2-N3	-2.23	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.22	1.34	1.38
55	2x	8	4SU	C2-N1	2.22	1.41	1.38
32	1a	1407	5MC	C6-N1	-2.21	1.34	1.38
1	2A	2552	OMU	C5-C4	-2.20	1.38	1.43
1	2A	1915	5MU	C2-N3	-2.19	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.18	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.18	1.34	1.38
32	1a	527	G7M	C6-N1	-2.18	1.34	1.37
1	1A	1911	PSU	C2-N3	-2.17	1.33	1.37
1	2A	1942	5MC	C6-N1	-2.16	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.15	1.34	1.38
1	2A	1939	5MU	C2-N1	2.14	1.41	1.38
55	2x	20	H2U	C4-N3	-2.12	1.34	1.37
1	1A	1939	5MU	C2-N1	2.12	1.41	1.38
1	1A	1962	5MC	C6-N1	-2.12	1.34	1.38
32	2a	966	M2G	C6-N1	-2.11	1.34	1.37
32	2a	1518	MA6	C6-N1	2.11	1.35	1.32
1	1A	1915	5MU	C6-N1	-2.11	1.34	1.38
32	1a	1519	MA6	C6-N1	2.10	1.35	1.32
55	2x	39	PSU	C2-N3	-2.09	1.34	1.37
32	1a	1498	UR3	C6-C5	2.09	1.39	1.35
32	1a	967	5MC	C6-N1	-2.07	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1519	MA6	C6-N1	2.04	1.35	1.32
32	1a	1518	MA6	C6-N1	2.03	1.35	1.32
1	2A	1911	PSU	C2-N3	-2.01	1.34	1.37
1	1A	1915	5MU	C2-N3	-2.00	1.34	1.38

All (204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-21.15	64.35	102.36
43	1l	92	0TD	CSB-SB-CB	-14.05	77.11	102.36
55	1x	76	8AN	C4'-O4'-C1'	-7.66	102.91	109.92
55	2x	76	8AN	C4'-O4'-C1'	-7.59	102.97	109.92
1	2A	2605	PSU	N1-C2-N3	7.00	122.55	115.17
1	1A	1911	PSU	N1-C2-N3	6.71	122.24	115.17
32	2a	1498	UR3	C4-N3-C2	-6.69	119.19	124.58
1	2A	2503	2MA	C2-N3-C4	6.69	120.86	115.46
1	1A	2503	2MA	C2-N3-C4	6.58	120.77	115.46
55	2x	76	8AN	N3-C2-N1	-6.57	119.75	128.67
32	1a	1498	UR3	C4-N3-C2	-6.57	119.30	124.58
1	1A	1917	PSU	N1-C2-N3	6.43	121.95	115.17
55	1x	76	8AN	N3-C2-N1	-6.32	120.10	128.67
55	2x	55	PSU	N1-C2-N3	6.26	121.77	115.17
1	2A	1911	PSU	N1-C2-N3	6.18	121.68	115.17
55	1x	55	PSU	N1-C2-N3	6.15	121.66	115.17
55	2x	32	PSU	N1-C2-N3	6.14	121.65	115.17
32	1a	516	PSU	N1-C2-N3	6.10	121.60	115.17
32	2a	516	PSU	N1-C2-N3	6.06	121.56	115.17
55	2x	8	4SU	C4-N3-C2	-6.05	121.52	127.31
1	2A	1917	PSU	N1-C2-N3	6.01	121.51	115.17
55	1x	39	PSU	N1-C2-N3	5.84	121.33	115.17
32	1a	1518	MA6	N3-C2-N1	-5.72	120.90	128.67
1	1A	1915	5MU	C4-N3-C2	-5.62	119.98	127.34
55	1x	32	PSU	N1-C2-N3	5.61	121.08	115.17
1	2A	1915	5MU	N3-C2-N1	5.59	122.17	114.89
1	1A	1915	5MU	N3-C2-N1	5.56	122.12	114.89
1	1A	2605	PSU	N1-C2-N3	5.48	120.94	115.17
1	2A	1939	5MU	C4-N3-C2	-5.46	120.19	127.34
55	2x	54	5MU	N3-C2-N1	5.43	121.95	114.89
55	2x	8	4SU	C5-C4-N3	5.39	119.76	114.75
32	1a	1519	MA6	N3-C2-N1	-5.38	121.37	128.67
1	2A	1915	5MU	C4-N3-C2	-5.38	120.29	127.34
32	2a	1519	MA6	N3-C2-N1	-5.34	121.42	128.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	39	PSU	N1-C2-N3	5.20	120.66	115.17
55	1x	8	4SU	C4-N3-C2	-5.14	122.39	127.31
32	1a	1519	MA6	C2-N1-C6	5.11	121.85	116.84
32	2a	1518	MA6	N3-C2-N1	-5.09	121.76	128.67
1	2A	1939	5MU	N3-C2-N1	5.06	121.48	114.89
1	2A	1939	5MU	C5-C4-N3	4.93	119.61	115.32
1	1A	1915	5MU	O4-C4-C5	-4.93	119.28	124.92
32	1a	1518	MA6	C2-N1-C6	4.92	121.66	116.84
55	1x	8	4SU	C5-C4-N3	4.91	119.32	114.75
1	1A	1939	5MU	C4-N3-C2	-4.90	120.91	127.34
1	2A	2605	PSU	C4-N3-C2	-4.82	119.74	126.37
55	2x	54	5MU	C4-N3-C2	-4.81	121.03	127.34
1	2A	1939	5MU	O4-C4-C5	-4.80	119.43	124.92
1	1A	1915	5MU	C5-C4-N3	4.76	119.47	115.32
1	1A	1939	5MU	O4-C4-C5	-4.72	119.52	124.92
1	2A	2552	OMU	C4-N3-C2	-4.59	120.91	126.61
32	2a	1518	MA6	C2-N1-C6	4.58	121.33	116.84
1	1A	2605	PSU	C4-N3-C2	-4.54	120.11	126.37
55	1x	54	5MU	O4-C4-C5	-4.43	119.85	124.92
1	1A	1939	5MU	N3-C2-N1	4.42	120.65	114.89
32	2a	1519	MA6	C2-N1-C6	4.41	121.16	116.84
1	1A	1911	PSU	C4-N3-C2	-4.36	120.36	126.37
1	2A	1915	5MU	C5-C4-N3	4.32	119.08	115.32
1	1A	2552	OMU	C4-N3-C2	-4.29	121.28	126.61
1	2A	1911	PSU	C4-N3-C2	-4.26	120.51	126.37
1	1A	1939	5MU	C5-C6-N1	-4.20	118.75	123.31
1	1A	1939	5MU	C5-C4-N3	4.16	118.94	115.32
1	1A	1917	PSU	C4-N3-C2	-4.16	120.64	126.37
55	1x	55	PSU	C4-N3-C2	-4.15	120.65	126.37
32	1a	516	PSU	C4-N3-C2	-4.04	120.80	126.37
55	2x	32	PSU	C4-N3-C2	-4.04	120.80	126.37
1	2A	2552	OMU	N3-C2-N1	4.04	120.15	114.89
55	2x	55	PSU	C4-N3-C2	-4.04	120.80	126.37
55	1x	32	PSU	C4-N3-C2	-4.03	120.81	126.37
55	1x	54	5MU	N3-C2-N1	4.01	120.11	114.89
1	1A	2552	OMU	N3-C2-N1	4.00	120.10	114.89
55	1x	54	5MU	C4-N3-C2	-4.00	122.10	127.34
1	2A	1917	PSU	C4-N3-C2	-3.99	120.88	126.37
55	2x	8	4SU	N3-C2-N1	3.96	120.04	114.89
55	2x	8	4SU	C5-C4-S4	-3.95	119.79	124.31
55	1x	54	5MU	C5-C4-N3	3.95	118.75	115.32
55	1x	37	MIA	N3-C2-N1	-3.89	123.40	128.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	39	PSU	C4-N3-C2	-3.88	121.03	126.37
1	2A	1939	5MU	C5-C6-N1	-3.88	119.10	123.31
32	2a	516	PSU	C4-N3-C2	-3.87	121.03	126.37
1	2A	2605	PSU	O2-C2-N1	-3.86	118.81	122.79
1	2A	1915	5MU	O4-C4-C5	-3.79	120.58	124.92
55	2x	32	PSU	O2-C2-N1	-3.73	118.94	122.79
1	2A	1917	PSU	O2-C2-N1	-3.71	118.96	122.79
1	1A	1942	5MC	C5-C6-N1	-3.71	119.29	123.31
55	2x	54	5MU	O4-C4-C5	-3.69	120.70	124.92
55	1x	55	PSU	O2-C2-N1	-3.68	119.00	122.79
1	2A	2552	OMU	C5-C4-N3	3.67	119.95	114.80
32	2a	1404	5MC	C5-C6-N1	-3.64	119.36	123.31
55	2x	54	5MU	C5-C4-N3	3.63	118.48	115.32
55	1x	32	PSU	O2-C2-N1	-3.63	119.05	122.79
55	2x	37	MIA	N3-C2-N1	-3.62	123.75	128.67
1	1A	1915	5MU	C5-C6-N1	-3.59	119.41	123.31
1	2A	1962	5MC	C5-C6-N1	-3.58	119.43	123.31
32	1a	1404	5MC	C5-C6-N1	-3.57	119.44	123.31
32	1a	967	5MC	C5-C6-N1	-3.55	119.45	123.31
1	1A	1917	PSU	O2-C2-N1	-3.55	119.13	122.79
1	1A	2552	OMU	C5-C4-N3	3.54	119.77	114.80
1	2A	1915	5MU	C5-C6-N1	-3.54	119.47	123.31
32	2a	967	5MC	C5-C6-N1	-3.53	119.48	123.31
55	1x	8	4SU	N3-C2-N1	3.47	119.41	114.89
32	2a	1519	MA6	C4-C5-N7	-3.39	105.75	109.34
1	1A	2605	PSU	O2-C2-N1	-3.29	119.39	122.79
32	2a	1498	UR3	C5-C4-N3	3.28	119.36	115.04
1	1A	1962	5MC	C5-C6-N1	-3.27	119.76	123.31
32	1a	1519	MA6	C4-C5-N7	-3.27	105.89	109.34
43	2l	92	0TD	OD2-CG-CB	3.23	120.13	113.15
55	2x	37	MIA	C4-C5-N7	-3.18	105.98	109.34
1	1A	1942	5MC	C5-C4-N3	-3.13	118.55	121.75
1	2A	1942	5MC	C5-C6-N1	-3.10	119.94	123.31
32	1a	1498	UR3	C5-C4-N3	3.09	119.11	115.04
1	2A	1942	5MC	C5-C4-N3	-3.09	118.59	121.75
1	1A	1962	5MC	C5-C4-N3	-3.06	118.62	121.75
32	2a	1400	5MC	C5-C6-N1	-3.04	120.01	123.31
55	2x	39	PSU	C4-N3-C2	-3.03	122.19	126.37
32	1a	1400	5MC	C5-C6-N1	-3.02	120.04	123.31
32	1a	516	PSU	O2-C2-N1	-3.01	119.69	122.79
32	2a	516	PSU	O2-C2-N1	-3.00	119.69	122.79
43	1l	92	0TD	OD2-CG-CB	3.00	119.62	113.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1911	PSU	O2-C2-N1	-3.00	119.70	122.79
32	2a	1407	5MC	C5-C4-N3	-2.93	118.76	121.75
32	2a	1207	2MG	C8-N7-C5	2.91	107.51	102.55
55	1x	54	5MU	C5-C6-N1	-2.91	120.16	123.31
32	2a	1407	5MC	O2-C2-N3	-2.89	117.77	122.33
55	2x	55	PSU	O2-C2-N1	-2.88	119.81	122.79
32	1a	1400	5MC	C5-C4-N3	-2.87	118.81	121.75
1	2A	1911	PSU	O2-C2-N1	-2.87	119.83	122.79
32	1a	966	M2G	C8-N7-C5	2.85	107.40	102.55
32	1a	1404	5MC	C5-C4-N3	-2.84	118.85	121.75
55	1x	39	PSU	O2-C2-N1	-2.83	119.87	122.79
32	1a	1207	2MG	C8-N7-C5	2.82	107.35	102.55
1	1A	1915	5MU	O2-C2-N1	-2.82	119.12	122.80
32	2a	1404	5MC	C5-C4-N3	-2.82	118.87	121.75
55	2x	54	5MU	C5-C6-N1	-2.81	120.26	123.31
32	2a	966	M2G	C8-N7-C5	2.81	107.33	102.55
1	2A	2251	OMG	C8-N7-C5	2.78	107.29	102.55
1	1A	2503	2MA	C2-N1-C6	2.74	122.32	118.10
32	2a	1518	MA6	C4-C5-N7	-2.74	106.44	109.34
55	2x	54	5MU	O2-C2-N1	-2.72	119.25	122.80
32	2a	1407	5MC	C5-C6-N1	-2.72	120.36	123.31
1	2A	2552	OMU	O4-C4-C5	-2.71	120.48	125.16
1	1A	2251	OMG	O6-C6-C5	-2.71	118.96	124.32
32	1a	1407	5MC	C5-C6-N1	-2.70	120.38	123.31
32	1a	1518	MA6	C4-C5-N7	-2.69	106.50	109.34
1	2A	2503	2MA	C4-C5-N7	-2.68	106.50	109.34
1	1A	2251	OMG	C8-N7-C5	2.65	107.06	102.55
1	1A	2552	OMU	O4-C4-C5	-2.64	120.61	125.16
1	2A	2605	PSU	C5-C6-N1	-2.61	118.51	122.14
32	2a	1400	5MC	C1'-N1-C6	-2.61	116.85	121.15
55	2x	20	H2U	C5-C6-N1	-2.60	103.66	111.52
32	1a	1407	5MC	C5-C4-N3	-2.58	119.11	121.75
1	2A	1939	5MU	O2-C2-N1	-2.58	119.44	122.80
1	2A	1962	5MC	C5-C4-N3	-2.57	119.12	121.75
55	1x	37	MIA	C4-C5-N7	-2.55	106.64	109.34
1	1A	2552	OMU	O2-C2-N1	-2.53	119.50	122.80
32	2a	1400	5MC	C5-C4-N3	-2.51	119.18	121.75
1	2A	2552	OMU	O2-C2-N1	-2.50	119.54	122.80
1	2A	2503	2MA	C5-C6-N1	-2.49	117.89	120.84
55	2x	39	PSU	C6-C5-C4	-2.46	116.51	118.17
1	2A	2503	2MA	C2-N1-C6	2.43	121.83	118.10
55	1x	8	4SU	C5-C4-S4	-2.43	121.53	124.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2503	2MA	C4-C5-N7	-2.42	106.78	109.34
32	1a	1498	UR3	C6-N1-C2	-2.39	119.85	121.80
32	1a	1207	2MG	N1-C2-N2	2.39	119.00	116.56
1	1A	2251	OMG	C5-C6-N1	2.35	118.55	114.07
32	1a	516	PSU	C6-C5-C4	-2.34	116.59	118.17
32	2a	967	5MC	C5-C4-N3	-2.34	119.36	121.75
1	1A	2605	PSU	C5-C6-N1	-2.33	118.90	122.14
32	2a	516	PSU	O4'-C1'-C2'	2.32	108.36	105.15
32	1a	967	5MC	C5-C4-N3	-2.28	119.42	121.75
1	1A	1911	PSU	C5-C6-N1	-2.26	119.00	122.14
32	1a	966	M2G	C5-C6-N1	2.24	118.34	114.07
32	1a	1404	5MC	CM5-C5-C6	-2.24	119.82	122.85
32	1a	1498	UR3	C3U-N3-C4	2.23	120.96	117.87
1	1A	1942	5MC	N1-C2-N3	2.22	122.66	118.80
32	2a	1402	4OC	CM4-N4-C4	-2.20	118.15	122.45
1	1A	2605	PSU	O4-C4-C5	-2.20	118.53	124.01
32	1a	1207	2MG	N2-C2-N3	-2.20	117.70	120.51
55	1x	55	PSU	C5-C6-N1	-2.18	119.11	122.14
32	1a	1402	4OC	C6-C5-C4	2.18	119.62	117.00
1	2A	2251	OMG	C5-C6-N1	2.17	118.21	114.07
1	2A	1915	5MU	O2-C2-N1	-2.17	119.97	122.80
1	1A	1917	PSU	C5-C6-N1	-2.17	119.14	122.14
55	1x	39	PSU	C5-C6-N1	-2.16	119.14	122.14
1	1A	1911	PSU	O2-C2-N3	-2.14	118.06	121.86
55	2x	55	PSU	C5-C6-N1	-2.14	119.17	122.14
55	2x	32	PSU	C6-C5-C4	-2.13	116.73	118.17
43	2l	92	0TD	OD1-CG-CB	-2.12	118.00	122.44
55	2x	39	PSU	O2-C2-N1	-2.12	120.61	122.79
55	1x	32	PSU	C6-C5-C4	-2.10	116.75	118.17
32	1a	1498	UR3	C1'-N1-C2	2.10	120.47	117.04
32	2a	966	M2G	C5-C6-N1	2.09	118.05	114.07
32	1a	1402	4OC	O2-C2-N3	-2.08	119.05	122.33
55	1x	20	H2U	N3-C2-N1	2.08	118.74	116.65
55	2x	21	H2U	O2-C2-N1	2.07	125.59	123.10
55	2x	8	4SU	C1'-N1-C2	2.07	121.31	117.59
32	2a	1400	5MC	O2-C2-N3	-2.06	119.08	122.33
1	2A	1917	PSU	C5-C6-N1	-2.05	119.30	122.14
55	1x	21	H2U	O4-C4-N3	2.05	123.46	120.30
55	2x	37	MIA	C1'-N9-C4	-2.05	123.05	126.64
1	2A	1911	PSU	C6-C5-C4	-2.05	116.79	118.17
32	2a	516	PSU	C5-C6-N1	-2.02	119.34	122.14
43	1l	92	0TD	OD1-CG-CB	-2.02	118.22	122.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	967	5MC	CM5-C5-C6	-2.01	120.13	122.85
1	2A	1917	PSU	O4'-C1'-C2'	2.01	107.93	105.15

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1402	4OC	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB
55	1x	21	H2U	C4'-C5'-O5'-P
55	1x	37	MIA	O4'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
32	2a	1519	MA6	O4'-C4'-C5'-O5'
55	1x	20	H2U	O4'-C4'-C5'-O5'
55	1x	20	H2U	C3'-C4'-C5'-O5'
55	1x	21	H2U	C3'-C4'-C5'-O5'
55	1x	37	MIA	C3'-C4'-C5'-O5'
55	2x	37	MIA	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
55	1x	21	H2U	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
55	2x	37	MIA	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	1x	76	8AN	C4'-C5'-O5'-P
55	1x	54	5MU	O4'-C4'-C5'-O5'
55	1x	54	5MU	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
32	2a	967	5MC	O4'-C4'-C5'-O5'
1	1A	1915	5MU	O4'-C4'-C5'-O5'
32	2a	516	PSU	O4'-C1'-C5-C4
55	2x	21	H2U	C2'-C1'-N1-C6
55	2x	21	H2U	C2'-C1'-N1-C2
1	2A	2503	2MA	C4'-C5'-O5'-P
32	2a	527	G7M	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	2503	2MA	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C2'-O2'-CM2
55	1x	21	H2U	O4'-C1'-N1-C6
32	1a	527	G7M	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
32	2a	1402	4OC	C2'-C1'-N1-C2
1	1A	1942	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

28 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	76	8AN	1	0
43	1l	92	0TD	1	0
32	1a	516	PSU	1	0
32	1a	1518	MA6	2	0
32	1a	1519	MA6	2	0
32	2a	1404	5MC	1	0
1	1A	2552	OMU	1	0
1	1A	1939	5MU	1	0
1	2A	1939	5MU	1	0
55	1x	20	H2U	1	0
1	1A	1915	5MU	2	0
1	1A	2503	2MA	1	0
55	1x	8	4SU	1	0
55	1x	76	8AN	4	0
32	2a	1207	2MG	2	0
32	2a	1518	MA6	4	0
1	1A	1920	OMC	1	0
32	1a	1402	4OC	2	0
32	1a	1207	2MG	2	0
55	2x	55	PSU	1	0
1	2A	2251	OMG	1	0
32	1a	1404	5MC	1	0
32	2a	1402	4OC	2	0
32	2a	1519	MA6	3	0
1	1A	1942	5MC	1	0
55	1x	21	H2U	1	0
55	2x	8	4SU	1	0
32	1a	966	M2G	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2664 ligands modelled in this entry, 2662 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	SF4	2d	303	35	0,12,12	-	-	-		
60	SF4	1d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	303	35	-	-	0/6/5/5
60	SF4	1d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1d	302	SF4	1	0

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, 95^{th} 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%)	-0.32	180 (6%) 27 21	9, 24, 87, 101	0
1	2A	2789/2915 (95%)	0.09	145 (5%) 34 26	22, 43, 83, 100	0
2	1B	120/121 (99%)	-0.24	0 100 100	20, 40, 53, 78	0
2	2B	120/121 (99%)	0.64	0 100 100	45, 64, 73, 84	0
3	1D	275/276 (99%)	-0.56	1 (0%) 89 85	12, 24, 38, 68	0
3	2D	275/276 (99%)	-0.21	3 (1%) 77 71	20, 36, 48, 68	0
4	1E	204/206 (99%)	-0.56	0 100 100	10, 25, 46, 60	0
4	2E	204/206 (99%)	-0.06	1 (0%) 87 83	23, 41, 57, 68	0
5	1F	203/210 (96%)	-0.44	0 100 100	10, 27, 57, 78	0
5	2F	203/210 (96%)	0.22	2 (0%) 79 73	22, 51, 66, 78	0
6	1G	181/182 (99%)	0.51	8 (4%) 39 32	34, 51, 66, 77	0
6	2G	181/182 (99%)	1.14	23 (12%) 9 8	58, 66, 76, 84	0
7	1H	174/180 (96%)	0.01	3 (1%) 69 61	26, 39, 53, 60	0
7	2H	174/180 (96%)	1.01	17 (9%) 14 11	53, 69, 79, 85	0
8	1I	146/148 (98%)	0.52	2 (1%) 73 66	31, 58, 68, 72	0
8	2I	146/148 (98%)	0.60	4 (2%) 56 47	42, 61, 68, 75	0
9	1N	140/140 (100%)	-0.57	1 (0%) 84 79	15, 24, 45, 61	0
9	2N	140/140 (100%)	0.23	1 (0%) 84 79	30, 49, 63, 70	0
10	1O	122/122 (100%)	-0.55	0 100 100	16, 26, 43, 47	0
10	2O	122/122 (100%)	-0.15	0 100 100	30, 39, 54, 60	0
11	1P	149/150 (99%)	-0.34	0 100 100	10, 32, 53, 66	0
11	2P	149/150 (99%)	0.33	1 (0%) 84 79	29, 53, 68, 75	0
12	1Q	141/141 (100%)	-0.40	2 (1%) 73 66	16, 27, 42, 53	0
12	2Q	141/141 (100%)	0.29	3 (2%) 63 55	32, 49, 60, 66	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%)	-0.66	0 100 100	15, 22, 35, 47	0
13	2R	118/118 (100%)	-0.17	0 100 100	29, 38, 50, 59	0
14	1S	110/112 (98%)	-0.15	1 (0%) 81 75	29, 40, 52, 58	0
14	2S	110/112 (98%)	0.95	11 (10%) 14 11	48, 59, 67, 71	0
15	1T	131/146 (89%)	-0.34	2 (1%) 71 64	20, 30, 58, 65	0
15	2T	131/146 (89%)	0.07	1 (0%) 82 77	34, 43, 66, 71	0
16	1U	116/118 (98%)	-0.69	1 (0%) 81 75	11, 17, 29, 47	0
16	2U	116/118 (98%)	0.04	0 100 100	29, 46, 58, 66	0
17	1V	101/101 (100%)	-0.60	0 100 100	11, 24, 42, 59	0
17	2V	101/101 (100%)	0.25	0 100 100	30, 54, 66, 73	0
18	1W	112/113 (99%)	-0.66	1 (0%) 81 75	11, 18, 36, 68	0
18	2W	112/113 (99%)	-0.20	0 100 100	27, 37, 52, 75	0
19	1X	95/96 (98%)	-0.42	0 100 100	15, 27, 51, 64	0
19	2X	95/96 (98%)	0.28	3 (3%) 50 42	37, 47, 62, 75	0
20	1Y	107/110 (97%)	-0.12	3 (2%) 55 46	22, 35, 53, 73	0
20	2Y	107/110 (97%)	0.64	5 (4%) 37 30	45, 58, 70, 77	0
21	1Z	154/206 (74%)	0.16	3 (1%) 66 58	26, 44, 62, 66	0
21	2Z	160/206 (77%)	0.81	7 (4%) 39 32	49, 63, 73, 76	0
22	10	76/85 (89%)	-0.50	1 (1%) 74 67	18, 25, 44, 58	0
22	20	76/85 (89%)	0.49	5 (6%) 26 19	38, 49, 62, 72	0
23	11	97/98 (98%)	-0.25	1 (1%) 79 73	16, 31, 57, 63	0
23	21	97/98 (98%)	0.09	1 (1%) 79 73	28, 44, 64, 68	0
24	12	70/72 (97%)	-0.24	0 100 100	24, 36, 48, 64	0
24	22	70/72 (97%)	0.40	1 (1%) 73 66	46, 56, 67, 71	0
25	13	59/60 (98%)	-0.54	0 100 100	15, 21, 42, 59	0
25	23	59/60 (98%)	0.10	0 100 100	39, 46, 63, 66	0
26	14	69/71 (97%)	1.10	12 (17%) 5 4	44, 68, 82, 86	0
26	24	69/71 (97%)	1.55	15 (21%) 3 3	60, 74, 81, 88	0
27	15	59/60 (98%)	-0.75	0 100 100	9, 19, 37, 44	0
27	25	59/60 (98%)	-0.15	1 (1%) 69 61	22, 39, 53, 64	0
28	16	53/54 (98%)	-0.48	0 100 100	23, 29, 38, 46	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%)	-0.02	0 100 100	37, 46, 55, 60	0
29	17	48/49 (97%)	-0.34	2 (4%) 41 33	12, 18, 43, 52	0
29	27	48/49 (97%)	-0.03	1 (2%) 63 55	23, 31, 51, 63	0
30	18	64/65 (98%)	-0.71	0 100 100	15, 21, 28, 39	0
30	28	64/65 (98%)	0.11	0 100 100	33, 42, 49, 55	0
31	19	37/37 (100%)	-0.44	0 100 100	17, 27, 45, 45	0
31	29	37/37 (100%)	0.55	0 100 100	44, 51, 59, 61	0
32	1a	1488/1521 (97%)	0.72	127 (8%) 18 14	21, 61, 84, 99	0
32	2a	1491/1521 (98%)	0.71	129 (8%) 17 13	31, 61, 85, 98	0
33	1b	231/256 (90%)	1.16	35 (15%) 6 5	50, 67, 76, 83	0
33	2b	231/256 (90%)	1.29	48 (20%) 3 3	56, 71, 79, 86	0
34	1c	206/239 (86%)	1.25	28 (13%) 8 7	56, 69, 77, 80	0
34	2c	206/239 (86%)	1.23	31 (15%) 6 6	59, 70, 77, 84	0
35	1d	208/209 (99%)	0.94	18 (8%) 17 13	47, 61, 71, 78	0
35	2d	208/209 (99%)	0.63	8 (3%) 44 36	47, 57, 66, 71	0
36	1e	148/162 (91%)	0.36	1 (0%) 84 79	33, 54, 65, 75	0
36	2e	148/162 (91%)	0.59	7 (4%) 37 30	44, 57, 66, 76	0
37	1f	100/101 (99%)	0.48	2 (2%) 64 56	42, 56, 64, 68	0
37	2f	100/101 (99%)	0.63	4 (4%) 43 35	53, 61, 68, 71	0
38	1g	155/156 (99%)	0.89	14 (9%) 17 12	53, 64, 76, 80	0
38	2g	155/156 (99%)	1.10	18 (11%) 11 9	58, 68, 77, 82	0
39	1h	137/138 (99%)	0.48	4 (2%) 54 45	44, 55, 62, 68	0
39	2h	137/138 (99%)	0.43	0 100 100	47, 58, 65, 73	0
40	1i	127/128 (99%)	1.56	29 (22%) 2 3	51, 69, 74, 80	0
40	2i	127/128 (99%)	1.71	43 (33%) 1 1	61, 73, 77, 82	0
41	1j	97/105 (92%)	1.59	27 (27%) 2 2	56, 72, 80, 83	0
41	2j	96/105 (91%)	1.99	41 (42%) 1 1	61, 74, 81, 84	0
42	1k	114/129 (88%)	0.35	4 (3%) 47 39	28, 54, 66, 73	0
42	2k	114/129 (88%)	0.53	7 (6%) 28 21	45, 59, 70, 80	0
43	1l	121/132 (91%)	0.45	6 (4%) 35 28	35, 48, 60, 67	0
43	2l	121/132 (91%)	0.16	1 (0%) 82 77	40, 47, 57, 68	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	118/126 (93%)	1.41	25 (21%) 3 3	56, 68, 74, 78	0
44	2m	116/126 (92%)	1.58	30 (25%) 2 2	60, 71, 76, 77	0
45	1n	60/61 (98%)	1.60	14 (23%) 2 3	57, 69, 74, 76	0
45	2n	60/61 (98%)	1.75	20 (33%) 1 1	63, 72, 77, 78	0
46	1o	88/89 (98%)	0.36	2 (2%) 61 52	35, 53, 64, 68	0
46	2o	88/89 (98%)	0.69	7 (7%) 20 15	45, 58, 67, 73	0
47	1p	82/88 (93%)	1.28	17 (20%) 3 3	52, 61, 71, 79	0
47	2p	82/88 (93%)	0.68	5 (6%) 28 21	46, 56, 63, 70	0
48	1q	99/105 (94%)	0.52	2 (2%) 64 56	43, 53, 65, 68	0
48	2q	99/105 (94%)	0.26	2 (2%) 64 56	43, 54, 63, 69	0
49	1r	68/88 (77%)	0.27	0 100 100	41, 52, 67, 71	0
49	2r	68/88 (77%)	0.73	3 (4%) 39 32	52, 60, 69, 76	0
50	1s	83/93 (89%)	1.83	31 (37%) 1 1	63, 72, 79, 81	0
50	2s	83/93 (89%)	1.85	33 (39%) 1 1	67, 76, 82, 84	0
51	1t	96/106 (90%)	0.64	6 (6%) 27 21	47, 58, 67, 78	0
51	2t	96/106 (90%)	0.67	4 (4%) 41 33	44, 55, 67, 70	0
52	1u	23/27 (85%)	1.96	8 (34%) 1 1	56, 68, 71, 75	0
52	2u	23/27 (85%)	1.42	6 (26%) 2 2	64, 69, 74, 78	0
53	1v	9/24 (37%)	0.61	2 (22%) 3 3	39, 41, 73, 83	0
53	2v	9/24 (37%)	1.19	3 (33%) 1 1	49, 53, 80, 87	0
54	1w	249/354 (70%)	0.18	6 (2%) 59 51	15, 48, 66, 80	0
54	2w	253/354 (71%)	0.40	6 (2%) 59 51	32, 55, 72, 82	0
55	1x	65/74 (87%)	0.11	0 100 100	16, 50, 66, 71	0
55	2x	65/74 (87%)	0.40	0 100 100	32, 60, 73, 79	0
56	1z	5/7 (71%)	0.82	1 (20%) 3 3	16, 20, 34, 50	0
56	2z	4/7 (57%)	0.57	1 (25%) 2 2	33, 35, 36, 40	0
All	All	21074/22160 (95%)	0.30	1341 (6%) 27 20	9, 50, 77, 101	0

All (1341) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	2112	G	9.0
1	2A	2147	G	8.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2146	C	8.7
1	2A	2145	C	8.7
1	1A	2117	A	8.3
1	2A	2159	G	8.3
1	2A	2138	C	8.1
1	1A	2114	A	8.1
1	1A	2113	U	8.0
1	1A	1068	G	7.9
1	2A	2111	C	7.8
1	2A	2160	G	7.8
1	1A	2179	C	7.6
1	1A	2178	C	7.4
1	2A	2158	A	7.2
1	1A	2135	A	7.1
1	1A	2141	G	7.1
1	2A	2134	A	7.0
1	2A	2117	A	6.7
1	1A	2110	G	6.6
1	1A	1072	C	6.6
1	1A	2120	G	6.6
45	1n	2	ALA	6.5
1	2A	2110	G	6.5
1	1A	1088	A	6.5
1	2A	2148	G	6.5
1	2A	2144	U	6.3
1	1A	1058	G	6.2
1	1A	1093	G	6.2
1	1A	2116	G	6.2
1	2A	2105	C	6.1
1	1A	1071	G	6.1
1	1A	2159	G	6.1
26	24	49	PHE	6.1
1	2A	2136	C	6.0
44	1m	2	ALA	6.0
1	2A	2135	A	6.0
1	2A	2137	C	6.0
1	1A	1069	A	5.9
1	1A	2115	G	5.9
1	2A	2115	G	5.9
1	1A	1100	C	5.9
22	20	9	SER	5.9
1	2A	2120	G	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2104	G	5.8
1	2A	2182	G	5.7
1	1A	2129	C	5.7
1	1A	1087	G	5.6
38	2g	81	GLY	5.6
7	1H	2	SER	5.6
1	2A	2143	C	5.6
1	1A	1099	G	5.5
1	2A	2112	G	5.5
1	1A	2109	U	5.5
1	2A	2149	G	5.5
32	1a	1003	G	5.5
50	1s	13	ASP	5.5
40	1i	15	ALA	5.5
1	1A	2174	C	5.4
45	2n	2	ALA	5.4
1	1A	1062	G	5.3
1	1A	1063	G	5.3
1	1A	2160	G	5.3
1	1A	2111	C	5.3
1	1A	2136	C	5.3
1	1A	2121	G	5.3
1	1A	1059	G	5.2
1	2A	2165	G	5.2
23	21	2	SER	5.2
1	1A	2122	U	5.2
32	2a	1286	A	5.2
44	2m	118	ALA	5.2
1	2A	2793	G	5.2
1	2A	2108	C	5.2
1	2A	2128	C	5.2
1	2A	2100	G	5.2
1	1A	2180	U	5.1
1	1A	2158	A	5.1
1	1A	2168	G	5.1
32	1a	1286	A	5.1
1	2A	2109	U	5.1
1	1A	1057	A	5.1
50	2s	2	PRO	5.1
1	2A	2139	C	5.0
1	2A	2123	G	5.0
1	1A	2145	C	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2129	C	5.0
1	2A	2181	G	5.0
26	14	56	VAL	5.0
41	2j	34	VAL	5.0
1	1A	1086	A	5.0
50	1s	8	GLY	4.9
1	1A	2123	G	4.9
1	1A	1081	U	4.9
52	1u	23	PRO	4.9
1	1A	2167	U	4.9
1	2A	2114	A	4.9
1	2A	2169	A	4.8
1	1A	2165	G	4.8
1	1A	2156	G	4.8
1	2A	2133	G	4.8
32	1a	1021	G	4.8
1	1A	1064	C	4.8
1	1A	2105	C	4.8
1	2A	2157	G	4.8
1	1A	1098	A	4.7
1	2A	2126	A	4.7
38	2g	80	VAL	4.7
1	1A	1060	U	4.7
1	2A	2130	U	4.7
1	1A	1176	G	4.7
1	1A	2181	G	4.7
1	2A	2101	G	4.7
21	2Z	174	VAL	4.7
1	2A	2154	G	4.6
1	1A	1067	A	4.6
1	1A	2134	A	4.6
1	1A	2147	G	4.6
1	2A	2155	G	4.6
1	2A	2118	U	4.6
1	1A	1073	A	4.6
1	1A	2106	G	4.6
1	1A	1094	U	4.5
1	1A	2137	C	4.5
32	2a	1033	G	4.5
38	2g	156	TRP	4.5
1	1A	2169	A	4.5
1	2A	2177	C	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2133	G	4.5
1	1A	2119	A	4.5
1	1A	2173	A	4.5
40	2i	102	LEU	4.5
1	1A	1091	G	4.5
1	1A	2148	G	4.5
1	2A	2125	G	4.5
1	1A	2108	C	4.5
1	2A	2178	C	4.5
45	1n	7	ILE	4.4
1	2A	2174	C	4.4
34	1c	189	ALA	4.4
41	1j	34	VAL	4.4
1	1A	1082	U	4.4
1	2A	2113	U	4.4
1	2A	2122	U	4.4
50	1s	84	GLY	4.4
1	2A	2184	G	4.4
32	1a	1036	G	4.4
32	2a	1032	G	4.4
1	2A	2163	C	4.4
1	1A	2118	U	4.4
1	1A	2130	U	4.4
1	1A	1101	U	4.3
1	1A	2138	C	4.3
1	2A	2183	C	4.3
1	1A	2124	G	4.3
1	2A	2162	G	4.3
1	2A	2168	G	4.3
1	1A	2175	C	4.3
50	1s	71	LEU	4.3
32	1a	1024	G	4.3
7	2H	2	SER	4.3
41	1j	4	ILE	4.3
1	1A	2805	G	4.2
44	1m	6	GLY	4.2
41	2j	68	HIS	4.2
41	1j	76	ASN	4.2
1	2A	2127	G	4.2
42	2k	13	GLN	4.2
1	1A	2170	A	4.2
32	1a	1001	A	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1092	C	4.2
40	1i	2	GLU	4.2
53	2v	14	A	4.2
32	1a	1002	G	4.1
1	2A	2185	C	4.1
1	2A	2804	C	4.1
32	2a	1027	C	4.1
32	2a	1030(B)	C	4.1
1	1A	1074	G	4.1
1	1A	2125	G	4.1
1	2A	2121	G	4.1
1	2A	2140	C	4.1
1	2A	2179	C	4.1
40	2i	11	LYS	4.1
1	2A	2166	G	4.1
32	1a	1034	G	4.1
32	2a	1003	G	4.1
41	2j	37	PRO	4.1
44	1m	97	PRO	4.1
43	1l	64	TYR	4.1
1	1A	2107	C	4.1
32	1a	1531	A	4.0
1	2A	2156	G	4.0
1	1A	1080	C	4.0
32	1a	1029	C	4.0
51	1t	103	GLY	4.0
1	1A	1089	G	4.0
1	1A	2127	G	4.0
1	2A	2116	G	4.0
1	1A	2102	U	4.0
1	1A	2142	C	4.0
1	2A	2151	G	4.0
32	1a	1026	G	4.0
38	1g	84	ASN	4.0
52	1u	9	ARG	3.9
32	2a	1026	G	3.9
38	1g	34	GLY	3.9
45	2n	4	LYS	3.9
40	1i	64	THR	3.9
49	2r	68	LYS	3.9
38	1g	80	VAL	3.9
1	2A	2150	U	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	16	LEU	3.9
41	2j	75	ILE	3.9
26	14	54	GLY	3.9
51	2t	103	GLY	3.9
1	1A	2166	G	3.9
1	1A	2182	G	3.9
1	1A	1079	C	3.8
1	1A	2146	C	3.8
26	24	51	ASP	3.8
41	2j	20	ALA	3.8
12	2Q	59	ARG	3.8
34	1c	109	PRO	3.8
50	2s	35	SER	3.8
51	1t	9	ASN	3.8
1	2A	2131	G	3.8
1	2A	2142	C	3.8
32	1a	1030(B)	C	3.8
1	2A	2119	A	3.8
54	2w	351	LEU	3.8
33	1b	129	GLU	3.8
33	2b	200	ILE	3.8
1	2A	2152	G	3.8
32	2a	1035	A	3.8
40	1i	67	GLY	3.8
1	1A	2103	C	3.8
1	1A	2143	C	3.8
1	1A	2164	C	3.8
44	2m	70	LEU	3.8
1	2A	2893	G	3.8
54	1w	350	ALA	3.7
44	2m	100	GLY	3.7
32	1a	1025	U	3.7
32	2a	1532	U	3.7
50	1s	20	LEU	3.7
1	1A	1070	A	3.7
32	1a	1028	C	3.7
32	1a	1035	A	3.7
44	2m	102	ARG	3.7
56	1z	3	ALA	3.7
1	2A	11	G	3.7
1	2A	2802	G	3.7
33	2b	10	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1257	U	3.7
34	1c	184	TYR	3.7
44	1m	102	ARG	3.7
41	2j	74	ILE	3.7
32	2a	1001	A	3.7
1	1A	2183	C	3.7
1	2A	2175	C	3.7
32	1a	1027	C	3.7
1	2A	2141	G	3.7
32	1a	1032	G	3.7
33	1b	237	ALA	3.7
32	1a	1447	A	3.7
1	1A	2157	G	3.7
1	1A	2162	G	3.7
1	1A	2187	G	3.7
1	2A	2124	G	3.7
26	24	59	PHE	3.6
50	2s	68	GLY	3.6
1	1A	1077	A	3.6
50	2s	13	ASP	3.6
1	1A	1090	U	3.6
1	1A	2144	U	3.6
1	1A	2131	G	3.6
32	2a	1030(C)	G	3.6
47	1p	42	ARG	3.6
40	1i	105	ASP	3.6
1	1A	1078	U	3.6
39	1h	87	SER	3.6
1	1A	2104	G	3.6
32	2a	1031	G	3.6
34	2c	207	VAL	3.6
6	2G	146	TYR	3.6
26	14	59	PHE	3.6
1	1A	2161	C	3.6
32	1a	999	C	3.6
26	14	52	THR	3.6
22	10	9	SER	3.6
1	1A	2793	G	3.6
38	2g	83	ALA	3.6
32	1a	1000	U	3.5
29	17	46	VAL	3.5
1	2A	2894	G	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1002	G	3.5
53	2v	15	A	3.5
1	2A	2107	C	3.5
32	1a	1354	C	3.5
32	1a	1033	G	3.5
45	1n	5	ALA	3.5
1	1A	2139	C	3.5
1	2A	2103	C	3.5
38	1g	85	TYR	3.5
50	2s	9	VAL	3.5
1	2A	2170	A	3.5
1	2A	2176	A	3.5
38	1g	156	TRP	3.5
1	1A	2149	G	3.5
1	1A	2152	G	3.5
32	1a	1030(A)	G	3.5
1	2A	2164	C	3.5
38	2g	79	ARG	3.4
1	1A	2792	G	3.4
21	1Z	2	GLU	3.4
1	1A	2177	C	3.4
1	2A	2188	C	3.4
32	1a	1037	C	3.4
48	1q	100	LYS	3.4
40	2i	103	THR	3.4
33	2b	44	LEU	3.4
23	11	2	SER	3.4
1	1A	2154	G	3.4
1	2A	2106	G	3.4
32	2a	1030(A)	G	3.4
41	2j	47	PHE	3.4
34	1c	193	TYR	3.4
51	1t	10	LEU	3.4
1	1A	1076	C	3.4
1	2A	2186	G	3.4
32	2a	1223	C	3.4
32	2a	1253	G	3.4
1	2A	2167	U	3.4
26	24	50	VAL	3.4
16	1U	117	GLN	3.3
52	1u	24	ARG	3.3
1	1A	1509	C	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1038	C	3.3
40	2i	97	LYS	3.3
1	2A	1533	G	3.3
1	1A	2790	A	3.3
33	2b	237	ALA	3.3
54	1w	189	GLN	3.3
33	2b	7	VAL	3.3
40	2i	108	VAL	3.3
12	2Q	61	GLY	3.3
41	1j	36	GLY	3.3
1	1A	2897	U	3.3
1	1A	10	G	3.3
32	2a	1034	G	3.3
32	2a	1036	G	3.3
20	1Y	78	ALA	3.3
12	2Q	60	ARG	3.3
22	20	10	THR	3.3
50	1s	9	VAL	3.3
34	2c	13	GLY	3.3
1	1A	2140	C	3.3
22	20	11	ARG	3.3
33	2b	34	ALA	3.3
44	1m	118	ALA	3.3
50	2s	24	ALA	3.3
1	1A	11	G	3.3
32	2a	1024	G	3.3
32	2a	1144	G	3.3
1	1A	2892	A	3.3
6	2G	139	LEU	3.3
33	2b	11	LEU	3.3
1	1A	1065	U	3.2
40	1i	13	ALA	3.2
1	1A	886	C	3.2
1	1A	2896	C	3.2
21	2Z	146	ILE	3.2
40	1i	14	VAL	3.2
1	1A	1173	G	3.2
1	1A	2151	G	3.2
35	1d	58	LEU	3.2
1	1A	1046	A	3.2
32	2a	1004	A	3.2
6	2G	142	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	1u	15	ARG	3.2
15	1T	131	ALA	3.2
45	2n	21	TYR	3.2
50	2s	4	SER	3.2
47	2p	16	HIS	3.2
1	1A	1102	C	3.2
1	1A	2163	C	3.2
32	1a	1043	C	3.2
32	2a	1030	C	3.2
32	2a	1119	C	3.2
1	1A	548	A	3.2
1	1A	1045	A	3.2
1	1A	2155	G	3.2
33	2b	93	VAL	3.2
41	1j	40	LEU	3.2
41	2j	67	THR	3.2
1	1A	2128	C	3.2
1	2A	1536	C	3.2
40	2i	42	ARG	3.2
41	1j	5	ARG	3.2
40	2i	43	ALA	3.2
45	2n	7	ILE	3.2
1	1A	1056	G	3.2
1	1A	2894	G	3.2
32	1a	1009	G	3.2
32	1a	1224	G	3.2
32	2a	1000	U	3.2
14	2S	32	LEU	3.2
41	2j	65	LEU	3.2
41	2j	42	THR	3.2
37	2f	54	LYS	3.2
40	2i	12	GLU	3.2
1	2A	2161	C	3.2
32	1a	1363	C	3.2
32	2a	1029	C	3.2
41	2j	91	PRO	3.2
41	1j	32	ALA	3.1
44	2m	30	ALA	3.1
33	1b	15	VAL	3.1
1	1A	1174	A	3.1
32	2a	1447	A	3.1
34	1c	115	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	1s	5	LEU	3.1
1	2A	2180	U	3.1
32	1a	1020	U	3.1
32	1a	1532	U	3.1
1	1A	2802	G	3.1
12	1Q	60	ARG	3.1
1	2A	2803	C	3.1
32	1a	1039	C	3.1
41	2j	44	VAL	3.1
47	2p	82	GLN	3.1
6	2G	147	ASP	3.1
34	1c	52	LEU	3.1
40	1i	17	VAL	3.1
40	2i	5	TYR	3.1
33	2b	72	GLY	3.1
44	1m	103	THR	3.1
50	2s	84	GLY	3.1
1	2A	2172	U	3.1
50	2s	3	ARG	3.1
33	2b	39	ILE	3.1
1	1A	2893	G	3.1
1	2A	2319	G	3.1
32	2a	1224	G	3.1
33	2b	236	TYR	3.1
41	1j	33	GLN	3.1
33	1b	17	PHE	3.1
40	1i	9	ARG	3.1
1	2A	2102	U	3.1
54	2w	208	GLU	3.1
1	1A	2801(A)	A	3.1
32	1a	1004	A	3.1
50	2s	40	ILE	3.1
41	2j	40	LEU	3.0
38	1g	9	VAL	3.0
42	2k	14	VAL	3.0
3	1D	276	LYS	3.0
26	24	64	GLY	3.0
45	1n	3	ARG	3.0
32	2a	1124	G	3.0
32	2a	1221	G	3.0
50	1s	2	PRO	3.0
1	1A	2150	U	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	91	C	3.0
33	2b	218	ALA	3.0
34	2c	129	ALA	3.0
44	2m	73	GLU	3.0
54	2w	205	ALA	3.0
50	2s	15	LEU	3.0
14	2S	3	ARG	3.0
34	1c	2	GLY	3.0
38	2g	154	TYR	3.0
43	2l	64	TYR	3.0
33	1b	107	THR	3.0
41	2j	100	THR	3.0
1	1A	2132	U	3.0
1	1A	2185	C	3.0
32	1a	1019	C	3.0
33	2b	164	VAL	3.0
35	1d	102	ASP	3.0
44	2m	7	VAL	3.0
35	1d	65	ARG	3.0
40	2i	10	ARG	3.0
54	1w	102	MET	3.0
40	1i	7	THR	3.0
40	2i	7	THR	3.0
44	2m	49	THR	3.0
44	2m	63	THR	3.0
1	1A	2207	G	3.0
32	1a	1023	G	3.0
32	1a	1030	C	3.0
32	1a	1031	G	3.0
32	2a	1043	C	3.0
34	2c	79	ARG	3.0
1	1A	890	A	3.0
50	2s	16	LEU	3.0
20	2Y	54	LYS	3.0
26	24	56	VAL	3.0
36	2e	74	GLY	2.9
41	1j	93	GLY	2.9
1	1A	2794	C	2.9
1	1A	2153	G	2.9
1	2A	1042	G	2.9
6	2G	52	ILE	2.9
40	1i	19	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	22	THR	2.9
34	1c	71	ALA	2.9
22	20	68	GLU	2.9
38	1g	118	VAL	2.9
34	2c	21	ARG	2.9
1	1A	1083	U	2.9
1	1A	1097	U	2.9
40	1i	6	GLY	2.9
32	1a	1260	C	2.9
50	1s	33	THR	2.9
1	1A	887	A	2.9
1	1A	1177	A	2.9
33	1b	20	GLU	2.9
40	2i	96	LEU	2.9
26	24	67	TYR	2.9
33	1b	236	TYR	2.9
44	2m	23	TYR	2.9
6	2G	15	VAL	2.9
14	2S	49	VAL	2.9
26	24	30	GLU	2.9
33	1b	230	VAL	2.9
40	2i	14	VAL	2.9
40	2i	109	VAL	2.9
1	2A	2896	C	2.9
32	2a	1006	C	2.9
32	2a	1028	C	2.9
32	2a	1284	C	2.9
41	1j	78	ASN	2.9
1	1A	1095	A	2.9
1	2A	2792	G	2.9
32	1a	631	G	2.9
32	2a	1001(A)	G	2.9
47	1p	80	PHE	2.9
3	2D	38	LYS	2.9
50	1s	62	ILE	2.9
14	2S	36	TYR	2.9
26	14	63	TYR	2.9
54	2w	185	VAL	2.9
32	2a	91	C	2.8
32	2a	999	C	2.8
34	2c	7	PRO	2.8
1	2A	1171	G	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2805	G	2.8
1	2A	2897	U	2.8
32	1a	78	G	2.8
32	1a	1001(A)	G	2.8
41	2j	27	ALA	2.8
42	2k	75	TYR	2.8
14	2S	93	LYS	2.8
29	27	48	LYS	2.8
1	1A	888	C	2.8
1	1A	2126	A	2.8
32	1a	1041	A	2.8
32	2a	1018	C	2.8
1	2A	271(K)	U	2.8
36	1e	17	ALA	2.8
45	2n	30	ALA	2.8
49	2r	20	ALA	2.8
20	2Y	1	MET	2.8
45	2n	31	ARG	2.8
1	2A	10	G	2.8
1	2A	1112	G	2.8
32	1a	630	G	2.8
32	1a	1258	G	2.8
32	2a	1222	G	2.8
33	1b	19	HIS	2.8
22	20	84	LEU	2.8
33	1b	10	LEU	2.8
35	1d	87	GLY	2.8
36	2e	109	ILE	2.8
34	2c	71	ALA	2.8
35	2d	149	ALA	2.8
45	1n	10	ALA	2.8
54	1w	349	ALA	2.8
7	2H	59	ARG	2.8
40	1i	10	ARG	2.8
41	2j	5	ARG	2.8
32	1a	1040	U	2.8
38	1g	154	TYR	2.8
7	2H	71	LEU	2.8
6	2G	20	ILE	2.8
41	2j	76	ASN	2.8
41	2j	93	GLY	2.8
7	2H	60	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	2P	15	ARG	2.8
46	2o	88	ARG	2.8
32	2a	1531	A	2.8
1	2A	888	C	2.8
32	1a	1362	C	2.8
32	2a	1116	C	2.8
40	2i	125	TYR	2.8
45	1n	17	LYS	2.8
1	2A	2153	G	2.7
33	2b	165	VAL	2.7
50	1s	38	SER	2.7
33	2b	22	LYS	2.7
6	2G	35	GLU	2.7
33	2b	17	PHE	2.7
1	1A	1103	A	2.7
26	24	52	THR	2.7
1	1A	34	C	2.7
1	2A	277	C	2.7
1	2A	2789	C	2.7
32	2a	1147	C	2.7
40	1i	117	HIS	2.7
6	2G	2	PRO	2.7
35	2d	183	GLY	2.7
41	1j	77	PRO	2.7
33	2b	186	ALA	2.7
38	1g	83	ALA	2.7
50	2s	67	VAL	2.7
33	2b	133	LYS	2.7
40	2i	126	SER	2.7
1	2A	2807	G	2.7
32	1a	1042	G	2.7
8	2I	86	THR	2.7
35	1d	158	ILE	2.7
38	2g	85	TYR	2.7
40	1i	62	TYR	2.7
32	2a	1030(D)	A	2.7
1	2A	2794	C	2.7
32	2a	1137	C	2.7
7	2H	19	VAL	2.7
56	2z	4	ALA	2.7
34	2c	204	LEU	2.7
39	1h	54	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	34	TYR	2.7
50	1s	77	THR	2.7
32	1a	1253	G	2.7
32	2a	79	G	2.7
1	2A	652(B)	A	2.7
20	1Y	23	ARG	2.7
50	1s	29	ARG	2.7
43	1l	18	VAL	2.7
1	1A	889	C	2.7
1	1A	2803	C	2.7
32	1a	1008	C	2.7
32	2a	1039	C	2.7
26	14	57	GLU	2.7
26	24	63	TYR	2.7
44	1m	49	THR	2.7
26	14	17	GLY	2.7
41	2j	77	PRO	2.7
35	1d	86	LYS	2.6
32	2a	1190	G	2.6
33	1b	97	TRP	2.6
40	1i	76	ALA	2.6
44	2m	5	ALA	2.6
1	1A	1460	A	2.6
41	2j	21	GLN	2.6
34	2c	178	LEU	2.6
33	2b	70	PHE	2.6
32	2a	1037	C	2.6
50	1s	14	HIS	2.6
50	2s	38	SER	2.6
33	1b	232	PRO	2.6
44	2m	6	GLY	2.6
51	1t	14	LYS	2.6
1	1A	1066	U	2.6
1	2A	2808	U	2.6
39	1h	93	VAL	2.6
33	1b	225	ALA	2.6
40	1i	56	LEU	2.6
53	1v	14	A	2.6
32	1a	79	G	2.6
32	1a	1047	G	2.6
32	2a	1009	G	2.6
32	2a	1010	G	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1310	G	2.6
32	1a	1018	C	2.6
38	2g	82	GLY	2.6
40	1i	39	GLY	2.6
7	1H	3	ARG	2.6
14	1S	3	ARG	2.6
40	2i	64	THR	2.6
34	2c	62	ASP	2.6
32	1a	1257	U	2.6
40	2i	94	ALA	2.6
32	2a	1146	A	2.6
32	2a	1285	A	2.6
8	1I	113	ARG	2.6
44	1m	68	GLY	2.6
44	2m	65	LYS	2.6
45	2n	3	ARG	2.6
1	2A	2318	G	2.6
26	24	32	TYR	2.6
32	1a	1215	G	2.6
32	1a	1353	G	2.6
32	2a	1311	G	2.6
50	2s	20	LEU	2.6
26	24	31	ILE	2.6
49	2r	43	PHE	2.6
42	2k	117	ASN	2.6
44	2m	106	ASN	2.6
33	2b	234	PRO	2.6
35	1d	23	GLY	2.6
7	2H	45	VAL	2.6
33	2b	71	VAL	2.6
42	1k	14	VAL	2.6
50	1s	11	VAL	2.6
40	1i	43	ALA	2.5
44	1m	56	LEU	2.6
1	2A	2751	G	2.5
32	1a	73	G	2.5
32	2a	1023	G	2.5
32	2a	1182	G	2.5
32	2a	1363	C	2.5
32	2a	1388	C	2.5
20	2Y	57	GLN	2.5
34	1c	107	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	56	GLN	2.5
32	1a	991	U	2.5
34	1c	110	ASN	2.5
43	1l	91	LYS	2.5
45	2n	17	LYS	2.5
33	1b	36	ARG	2.5
33	2b	228	GLY	2.5
40	2i	67	GLY	2.5
37	2f	6	VAL	2.5
44	2m	117	VAL	2.5
50	1s	39	THR	2.5
32	2a	959	A	2.5
40	2i	56	LEU	2.5
52	2u	21	TYR	2.5
48	1q	99	SER	2.5
38	2g	27	ILE	2.5
32	1a	1366	C	2.5
32	2a	1259	C	2.5
1	1A	1175	U	2.5
1	1A	2184	G	2.5
1	2A	1537	G	2.5
32	1a	1131	G	2.5
32	1a	1355	G	2.5
32	2a	1131	G	2.5
32	2a	1273	G	2.5
45	2n	9	LYS	2.5
41	2j	53	PRO	2.5
6	1G	48	GLU	2.5
14	2S	61	ASN	2.5
8	2I	81	VAL	2.5
40	2i	17	VAL	2.5
40	2i	79	LEU	2.5
44	2m	34	LEU	2.5
47	1p	44	THR	2.5
6	2G	73	ALA	2.5
6	2G	157	ILE	2.5
34	1c	77	ILE	2.5
7	1H	6	ARG	2.5
51	1t	8	ARG	2.5
32	2a	1219	U	2.5
1	2A	652(T)	C	2.5
32	1a	1317	C	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1019	C	2.5
32	2a	1260	C	2.5
50	2s	47	HIS	2.5
34	2c	158	GLY	2.5
40	2i	2	GLU	2.5
1	1A	2190	G	2.5
32	1a	1202	G	2.5
32	2a	631	G	2.5
32	2a	951	G	2.5
20	1Y	1	MET	2.5
40	2i	106	ALA	2.5
44	2m	51	ALA	2.5
52	1u	18	TYR	2.5
40	1i	126	SER	2.5
44	1m	27	LYS	2.5
35	1d	160	GLN	2.5
1	1A	2176	A	2.5
32	1a	1285	A	2.5
33	2b	130	ARG	2.5
40	2i	66	ARG	2.5
40	2i	104	ARG	2.5
47	2p	48	TRP	2.5
52	2u	23	PRO	2.5
1	2A	2132	U	2.5
12	1Q	61	GLY	2.5
33	1b	227	GLY	2.5
50	2s	17	GLU	2.5
33	1b	229	VAL	2.5
1	1A	2804	C	2.5
32	2a	1214	C	2.5
15	1T	130	ALA	2.5
41	2j	48	THR	2.5
1	2A	2190	G	2.4
32	1a	438	G	2.4
32	1a	993	G	2.4
32	2a	1017	G	2.4
32	2a	1048	G	2.4
32	2a	1272	G	2.4
42	2k	126	ARG	2.4
50	2s	34	TRP	2.4
50	2s	76	PRO	2.4
1	2A	2171	A	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	26	GLY	2.4
42	1k	98	LEU	2.4
45	1n	47	LEU	2.4
50	2s	64	GLU	2.4
32	1a	1012	U	2.4
44	2m	54	VAL	2.4
38	2g	2	ALA	2.4
50	1s	40	ILE	2.4
50	1s	50	ALA	2.4
51	2t	97	ALA	2.4
8	2I	141	LYS	2.4
21	2Z	136	PHE	2.4
29	17	48	LYS	2.4
34	1c	128	PHE	2.4
41	2j	57	LYS	2.4
50	1s	79	THR	2.4
1	2A	645	C	2.4
1	2A	889	C	2.4
1	2A	1178	C	2.4
32	2a	1109	C	2.4
34	1c	48	TYR	2.4
6	2G	115	ARG	2.4
41	1j	46	ARG	2.4
32	2a	1220	G	2.4
8	1I	106	GLY	2.4
40	2i	19	LEU	2.4
50	2s	22	LEU	2.4
21	2Z	1	MET	2.4
34	1c	207	VAL	2.4
1	2A	1847	A	2.4
1	2A	2173	A	2.4
32	2a	1248	A	2.4
32	1a	202	U	2.4
33	2b	172	ILE	2.4
46	2o	87	ILE	2.4
53	2v	22	U	2.4
50	1s	24	ALA	2.4
41	2j	54	PHE	2.4
45	2n	36	PHE	2.4
41	1j	67	THR	2.4
43	1l	61	THR	2.4
47	1p	38	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	190	ARG	2.4
32	1a	1038	C	2.4
32	1a	1115	C	2.4
32	2a	995	C	2.4
24	22	46	GLN	2.4
50	1s	35	SER	2.4
6	2G	152	LEU	2.4
33	1b	44	LEU	2.4
41	2j	56	HIS	2.4
45	2n	38	GLY	2.4
40	1i	35	GLU	2.4
1	1A	2186	G	2.4
1	2A	883	G	2.4
32	1a	1108	G	2.4
32	1a	1120	G	2.4
32	2a	630	G	2.4
33	2b	201	ILE	2.4
34	2c	202	ILE	2.4
36	2e	21	ALA	2.4
54	2w	350	ALA	2.4
33	2b	163	PHE	2.4
41	2j	63	PHE	2.4
44	1m	37	THR	2.4
40	2i	92	TYR	2.4
45	1n	29	ARG	2.4
50	2s	80	TYR	2.4
52	1u	10	ARG	2.4
1	1A	2188	C	2.4
32	1a	1140	C	2.4
32	1a	1335	C	2.4
40	2i	105	ASP	2.4
44	1m	64	TRP	2.4
50	2s	46	GLY	2.4
54	2w	190	GLY	2.4
9	1N	9	VAL	2.4
33	1b	231	GLU	2.4
26	24	15	ILE	2.4
45	2n	42	ILE	2.4
45	2n	37	PHE	2.4
50	1s	10	PHE	2.4
32	1a	216	G	2.4
32	1a	978	A	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	998	G	2.4
32	1a	1049	U	2.4
32	1a	1503	A	2.4
50	2s	61	TYR	2.3
14	2S	54	LEU	2.3
33	1b	131	PRO	2.3
47	1p	76	GLN	2.3
47	1p	82	GLN	2.3
54	1w	348	LEU	2.3
40	2i	69	GLY	2.3
40	2i	72	GLY	2.3
33	2b	20	GLU	2.3
32	1a	92	C	2.3
32	1a	979	C	2.3
34	1c	163	ALA	2.3
34	1c	88	ARG	2.3
35	1d	153	ARG	2.3
38	1g	78	ARG	2.3
44	1m	3	ARG	2.3
50	2s	29	ARG	2.3
41	1j	100	THR	2.3
45	2n	13	THR	2.3
52	2u	17	THR	2.3
32	1a	960	U	2.3
32	2a	1150	U	2.3
34	2c	111	LEU	2.3
1	2A	229	A	2.3
32	1a	1005	A	2.3
32	1a	1016	A	2.3
32	1a	1151	A	2.3
32	2a	532	A	2.3
32	2a	974	A	2.3
40	2i	49	PRO	2.3
40	2i	85	LEU	2.3
32	2a	1225	A	2.3
32	2a	1251	A	2.3
1	2A	100	G	2.3
18	1W	112	GLY	2.3
20	2Y	93	GLY	2.3
45	1n	4	LYS	2.3
47	1p	13	HIS	2.3
7	2H	35	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	195	VAL	2.3
41	1j	44	VAL	2.3
33	1b	42	ILE	2.3
41	1j	38	ILE	2.3
44	2m	78	ILE	2.3
26	24	26	SER	2.3
47	1p	47	ASP	2.3
6	2G	50	ALA	2.3
33	1b	105	PHE	2.3
40	2i	82	ALA	2.3
38	2g	78	ARG	2.3
41	1j	66	ARG	2.3
43	1l	89	ARG	2.3
1	1A	1075	C	2.3
1	1A	2791	C	2.3
32	1a	1367	C	2.3
32	2a	980	C	2.3
32	2a	1149	C	2.3
32	2a	1321	C	2.3
41	1j	87	THR	2.3
46	1o	25	THR	2.3
33	1b	11	LEU	2.3
34	2c	32	LEU	2.3
50	1s	16	LEU	2.3
1	2A	9	U	2.3
32	1a	204	U	2.3
32	1a	950	U	2.3
32	1a	992	U	2.3
44	1m	87	TYR	2.3
50	2s	6	LYS	2.3
33	2b	136	VAL	2.3
35	1d	6	GLY	2.3
44	2m	24	GLY	2.3
40	2i	63	ILE	2.3
44	1m	9	ILE	2.3
45	1n	42	ILE	2.3
47	1p	48	TRP	2.3
1	1A	275	G	2.3
32	1a	1011	G	2.3
32	1a	1030(C)	G	2.3
32	1a	1304	G	2.3
32	1a	1361	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	945	G	2.3
32	2a	1171	G	2.3
33	2b	161	ALA	2.3
41	2j	30	SER	2.3
46	2o	25	THR	2.3
47	1p	22	THR	2.3
52	1u	17	THR	2.3
32	1a	1007	C	2.3
32	2a	1262	C	2.3
35	1d	154	ASN	2.3
44	2m	31	LYS	2.3
50	1s	18	LYS	2.3
32	1a	90	U	2.3
42	1k	75	TYR	2.3
33	2b	230	VAL	2.3
45	2n	33	VAL	2.3
47	2p	2	VAL	2.3
50	2s	45	VAL	2.3
52	1u	2	GLY	2.3
7	2H	58	GLU	2.3
32	2a	975	A	2.3
36	2e	45	PHE	2.3
44	1m	28	ALA	2.3
44	2m	69	GLU	2.3
41	2j	73	ASP	2.3
1	2A	171	G	2.3
1	2A	1114	G	2.3
1	2A	2207	G	2.3
7	2H	64	LEU	2.3
19	2X	95	LEU	2.3
32	1a	1138	G	2.3
32	2a	1011	G	2.3
32	2a	1117	G	2.3
32	2a	1202	G	2.3
47	1p	73	LEU	2.3
7	2H	21	PRO	2.3
50	2s	63	THR	2.3
35	2d	154	ASN	2.2
1	1A	885	C	2.2
1	2A	2474	C	2.2
32	1a	1452	C	2.2
32	2a	1112	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1326	C	2.2
33	1b	18	GLY	2.2
34	1c	185	GLY	2.2
34	2c	205	GLY	2.2
35	2d	112	VAL	2.2
41	1j	31	GLY	2.2
50	1s	61	TYR	2.2
50	2s	52	TYR	2.2
53	1v	22	U	2.2
40	2i	18	PHE	2.2
33	2b	173	ALA	2.2
35	2d	132	ARG	2.2
38	2g	5	ARG	2.2
52	2u	24	ARG	2.2
1	1A	229	A	2.2
32	2a	1123	A	2.2
6	1G	49	ASP	2.2
44	1m	16	ASP	2.2
32	1a	1010	G	2.2
32	2a	1274	G	2.2
33	1b	127	ILE	2.2
33	2b	38	GLY	2.2
33	2b	162	ILE	2.2
35	1d	171	GLY	2.2
32	1a	1121	U	2.2
32	2a	1125	U	2.2
1	2A	279	C	2.2
1	2A	1041	C	2.2
33	1b	53	ARG	2.2
33	1b	152	PHE	2.2
35	1d	131	ARG	2.2
45	2n	35	ARG	2.2
52	2u	15	ARG	2.2
33	1b	128	GLU	2.2
33	1b	188	ALA	2.2
34	2c	189	ALA	2.2
38	1g	2	ALA	2.2
40	1i	106	ALA	2.2
40	1i	47	LEU	2.2
41	1j	65	LEU	2.2
50	2s	71	LEU	2.2
47	1p	43	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	528	A	2.2
1	2A	2749	A	2.2
32	1a	532	A	2.2
32	2a	1287	A	2.2
34	1c	73	PRO	2.2
33	2b	15	VAL	2.2
34	2c	69	HIS	2.2
41	2j	13	HIS	2.2
41	2j	52	GLY	2.2
46	2o	20	GLY	2.2
46	2o	86	GLY	2.2
44	2m	21	TYR	2.2
45	1n	21	TYR	2.2
6	1G	51	ARG	2.2
50	2s	10	PHE	2.2
1	1A	271(K)	U	2.2
6	1G	50	ALA	2.2
32	1a	77	G	2.2
32	1a	102	G	2.2
32	2a	976	G	2.2
32	2a	1020	U	2.2
32	2a	1089	G	2.2
33	2b	123	ALA	2.2
6	2G	100	TRP	2.2
35	2d	157	LEU	2.2
37	1f	48	LEU	2.2
37	2f	21	LEU	2.2
40	1i	102	LEU	2.2
47	1p	6	LEU	2.2
1	2A	1040	C	2.2
3	2D	276	LYS	2.2
6	2G	36	LYS	2.2
32	2a	1007	C	2.2
41	2j	99	LYS	2.2
40	2i	91	ASP	2.2
40	2i	123	PRO	2.2
14	2S	31	SER	2.2
1	1A	278	A	2.2
7	2H	37	VAL	2.2
32	2a	965	A	2.2
32	2a	1005	A	2.2
32	2a	1183	A	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1252	A	2.2
33	1b	223	ILE	2.2
33	2b	41	ILE	2.2
44	1m	54	VAL	2.2
50	1s	68	GLY	2.2
33	2b	40	HIS	2.2
38	2g	13	GLN	2.2
33	2b	94	ASN	2.2
34	2c	23	TYR	2.2
34	2c	128	PHE	2.2
41	1j	54	PHE	2.2
41	2j	66	ARG	2.2
42	1k	117	ASN	2.2
44	1m	55	ARG	2.2
51	2t	25	ARG	2.2
34	2c	65	ALA	2.2
6	2G	53	LEU	2.2
1	2A	2895	U	2.2
32	1a	1212	U	2.2
44	1m	65	LYS	2.2
46	2o	31	LEU	2.2
1	1A	274	G	2.2
32	1a	64	G	2.2
32	2a	1258	G	2.2
1	2A	886	C	2.2
1	2A	1043	C	2.2
32	1a	615	C	2.2
32	1a	1114	C	2.2
32	1a	1119	C	2.2
32	1a	1149	C	2.2
32	1a	1284	C	2.2
32	2a	1128	C	2.2
33	2b	189	ASP	2.2
35	2d	5	ILE	2.2
44	2m	25	ILE	2.2
5	2F	6	VAL	2.2
34	1c	76	VAL	2.2
40	1i	65	VAL	2.2
40	2i	86	VAL	2.2
5	2F	208	GLY	2.1
38	1g	82	GLY	2.1
42	2k	31	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	1n	55	GLY	2.1
46	1o	89	GLY	2.1
7	2H	61	HIS	2.1
1	1A	2171	A	2.1
1	2A	896	A	2.1
32	1a	1318	A	2.1
33	2b	36	ARG	2.1
33	2b	152	PHE	2.1
40	2i	107	ARG	2.1
41	2j	70	ARG	2.1
54	1w	309	GLN	2.1
47	1p	58	TYR	2.1
33	2b	29	ALA	2.1
34	2c	196	LEU	2.1
41	2j	7	LYS	2.1
44	2m	27	LYS	2.1
6	2G	18	GLU	2.1
33	1b	134	GLU	2.1
33	2b	129	GLU	2.1
35	1d	163	GLU	2.1
1	1A	12	U	2.1
32	2a	1126	U	2.1
32	2a	1148	U	2.1
41	2j	39	PRO	2.1
41	2j	41	PRO	2.1
47	1p	68	ASP	2.1
44	1m	119	GLY	2.1
51	1t	11	SER	2.1
26	14	61	ARG	2.1
32	1a	93	G	2.1
32	1a	1006	C	2.1
32	1a	1107	C	2.1
32	1a	1132	C	2.1
32	1a	1220	G	2.1
32	2a	436	C	2.1
32	2a	1022	G	2.1
32	2a	1249	C	2.1
32	2a	1283	G	2.1
32	2a	1355	G	2.1
35	1d	132	ARG	2.1
37	2f	47	ARG	2.1
38	2g	155	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	79	THR	2.1
7	2H	123	PHE	2.1
40	1i	18	PHE	2.1
40	2i	33	PHE	2.1
3	2D	2	ALA	2.1
21	2Z	125	LEU	2.1
26	14	69	LYS	2.1
6	1G	151	ALA	2.1
41	1j	88	LEU	2.1
50	1s	15	LEU	2.1
51	2t	74	LYS	2.1
32	2a	1256	A	2.1
33	1b	62	ALA	2.1
38	1g	7	ALA	2.1
34	1c	44	GLU	2.1
1	1A	1026	U	2.1
1	2A	614(A)	U	2.1
26	14	41	PRO	2.1
7	2H	43	VAL	2.1
35	1d	170	VAL	2.1
7	2H	100	GLY	2.1
19	2X	68	ARG	2.1
26	24	54	GLY	2.1
34	2c	155	GLY	2.1
40	2i	8	GLY	2.1
40	2i	115	GLY	2.1
45	2n	29	ARG	2.1
14	2S	34	HIS	2.1
26	14	66	SER	2.1
43	1l	17	LYS	2.1
33	2b	138	LEU	2.1
41	2j	85	LEU	2.1
14	2S	55	ALA	2.1
32	1a	990	C	2.1
32	1a	1137	C	2.1
32	1a	1243	C	2.1
32	2a	1066	C	2.1
44	1m	5	ALA	2.1
50	2s	75	ALA	2.1
6	1G	146	TYR	2.1
19	2X	69	TYR	2.1
47	1p	39	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1048	G	2.1
32	2a	80	G	2.1
32	2a	993	G	2.1
26	14	53	GLU	2.1
50	1s	53	ASN	2.1
1	1A	1096	A	2.1
1	2A	890	A	2.1
32	2a	1016	A	2.1
32	2a	1236	A	2.1
6	1G	144	ILE	2.1
6	2G	77	ILE	2.1
9	2N	140	VAL	2.1
34	1c	106	VAL	2.1
41	1j	49	VAL	2.1
44	1m	98	VAL	2.1
20	2Y	5	MET	2.1
34	2c	172	ARG	2.1
34	2c	185	GLY	2.1
35	1d	16	GLY	2.1
41	2j	60	ARG	2.1
33	2b	140	HIS	2.1
41	1j	14	LYS	2.1
7	2H	134	SER	2.1
34	1c	34	LEU	2.1
36	2e	120	THR	2.1
42	2k	41	THR	2.1
41	2j	35	SER	2.1
34	2c	160	ALA	2.1
38	2g	25	ALA	2.1
41	2j	18	ALA	2.1
44	1m	21	TYR	2.1
47	1p	17	TYR	2.1
1	1A	1532	C	2.1
32	1a	76	C	2.1
32	1a	1054	C	2.1
32	1a	1214	C	2.1
32	2a	1145	C	2.1
41	1j	37	PRO	2.1
21	1Z	146	ILE	2.1
36	2e	13	ILE	2.1
1	1A	652(A)	A	2.1
1	1A	883	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	197	A	2.1
32	2a	949	A	2.1
32	2a	1130	A	2.1
32	2a	1365	G	2.1
6	2G	149	VAL	2.1
34	2c	106	VAL	2.1
44	2m	15	VAL	2.1
33	2b	83	MET	2.1
1	1A	9	U	2.1
1	1A	2808	U	2.1
32	2a	960	U	2.1
32	2a	1235	U	2.1
44	2m	104	ARG	2.1
41	1j	22	LYS	2.1
34	2c	203	PHE	2.1
6	2G	175	LEU	2.0
45	1n	39	LEU	2.0
6	1G	145	THR	2.0
6	2G	138	GLN	2.0
34	1c	192	THR	2.0
37	1f	57	GLN	2.0
41	2j	81	THR	2.0
44	1m	43	THR	2.0
45	1n	22	THR	2.0
33	1b	109	SER	2.0
40	1i	119	ALA	2.0
45	2n	5	ALA	2.0
4	2E	151	TYR	2.0
6	2G	137	GLU	2.0
27	25	59	GLU	2.0
44	2m	32	GLU	2.0
34	2c	84	ILE	2.0
32	1a	1246	C	2.0
32	1a	1352	C	2.0
32	2a	1129	C	2.0
48	2q	9	VAL	2.0
52	2u	14	TRP	2.0
1	1A	529	A	2.0
1	2A	887	A	2.0
7	2H	120	GLY	2.0
32	2a	983	A	2.0
21	1Z	136	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	122	PHE	2.0
39	1h	90	GLY	2.0
21	2Z	121	HIS	2.0
34	1c	43	LEU	2.0
34	1c	175	LEU	2.0
34	2c	34	LEU	2.0
35	2d	186	LEU	2.0
50	1s	74	PHE	2.0
32	1a	1222	G	2.0
32	1a	1365	G	2.0
34	1c	177	THR	2.0
15	2T	130	ALA	2.0
34	1c	121	ALA	2.0
36	2e	20	GLN	2.0
40	1i	45	ALA	2.0
50	1s	12	ASP	2.0
35	1d	208	SER	2.0
48	2q	99	SER	2.0
21	2Z	2	GLU	2.0
33	1b	31	TYR	2.0
34	2c	182	ILE	2.0
40	1i	21	PRO	2.0
41	1j	39	PRO	2.0
33	2b	48	MET	2.0
14	2S	30	ARG	2.0
44	2m	29	ARG	2.0
47	2p	20	VAL	2.0
50	1s	41	VAL	2.0
8	2I	38	LEU	2.0
33	1b	196	LEU	2.0
33	2b	121	LEU	2.0
38	2g	26	PHE	2.0
38	2g	34	GLY	2.0
46	2o	61	GLY	2.0
1	2A	34	C	2.0
1	2A	1179	C	2.0
32	1a	840	C	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, 95^{th} 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
55	H2U	1x	21	20/21	0.74	0.16	66,85,89,106	0
55	H2U	2x	21	20/21	0.74	0.17	76,84,91,98	0
55	H2U	2x	20	20/21	0.75	0.14	68,78,83,86	0
32	2MG	1a	1207	24/25	0.82	0.16	65,74,83,85	0
55	PSU	2x	55	20/21	0.82	0.12	62,69,77,82	0
32	2MG	2a	1207	24/25	0.84	0.15	61,71,77,79	0
55	PSU	2x	32	20/21	0.87	0.12	54,62,67,68	0
55	5MU	2x	54	21/22	0.88	0.11	62,68,75,80	0
43	0TD	1l	92	10/11	0.88	0.13	44,49,53,68	0
55	MIA	2x	37	22/30	0.89	0.11	53,62,64,66	0
32	PSU	1a	516	20/21	0.90	0.11	54,61,65,66	0
55	5MU	1x	54	21/22	0.90	0.13	51,61,69,73	0
55	H2U	1x	20	20/21	0.90	0.10	52,67,79,79	0
55	PSU	1x	55	20/21	0.90	0.11	52,59,69,71	0
32	G7M	2a	527	24/25	0.90	0.12	47,56,60,65	0
1	5MU	2A	1915	21/22	0.91	0.11	41,49,55,60	0
32	M2G	2a	966	25/26	0.91	0.13	46,56,67,71	0
32	PSU	2a	516	20/21	0.91	0.12	47,60,66,67	0
55	PSU	2x	39	20/21	0.91	0.10	43,60,64,66	0
43	0TD	2l	92	10/11	0.92	0.10	43,48,51,59	0
55	PSU	1x	32	20/21	0.92	0.11	50,54,63,66	0
32	M2G	1a	966	25/26	0.92	0.11	40,49,55,57	0
32	5MC	2a	967	21/22	0.93	0.12	52,56,65,68	0
55	MIA	1x	37	22/30	0.94	0.09	41,51,55,60	0
32	5MC	2a	1400	21/22	0.94	0.12	45,55,60,62	0
55	PSU	1x	39	20/21	0.94	0.10	35,44,51,55	0
32	5MC	1a	967	21/22	0.94	0.10	42,48,59,64	0
32	4OC	2a	1402	22/23	0.95	0.10	39,44,48,49	0
32	UR3	2a	1498	21/22	0.95	0.09	38,43,47,53	0
32	MA6	2a	1518	24/25	0.95	0.10	34,45,51,52	0
32	MA6	2a	1519	24/25	0.95	0.11	39,43,50,51	0
1	5MU	1A	1915	21/22	0.95	0.08	36,44,48,53	0
55	4SU	2x	8	20/21	0.95	0.09	45,63,67,68	0
1	PSU	2A	1911	20/21	0.95	0.09	40,47,49,51	0
1	PSU	1A	1911	20/21	0.95	0.08	25,38,41,42	0
1	PSU	2A	1917	20/21	0.95	0.09	39,47,54,57	0
32	G7M	1a	527	24/25	0.95	0.09	35,47,52,54	0
32	5MC	2a	1404	21/22	0.96	0.09	30,36,39,43	0
32	5MC	2a	1407	21/22	0.96	0.09	29,37,42,48	0
1	5MC	2A	1942	21/22	0.96	0.08	29,37,41,44	0
32	5MC	1a	1407	21/22	0.96	0.11	20,30,37,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MA6	1a	1519	24/25	0.96	0.09	23,29,36,40	0
1	PSU	1A	1917	20/21	0.96	0.09	31,40,44,45	0
55	4SU	1x	8	20/21	0.96	0.08	29,40,45,45	0
32	5MC	1a	1400	21/22	0.96	0.10	39,46,49,50	0
32	4OC	1a	1402	22/23	0.96	0.08	32,37,40,43	0
32	5MC	1a	1404	21/22	0.96	0.08	27,31,34,38	0
1	OMC	2A	1920	21/22	0.96	0.08	41,45,50,51	0
1	OMC	1A	1920	21/22	0.97	0.08	28,34,41,42	0
1	5MC	1A	1942	21/22	0.97	0.07	14,24,29,31	0
1	5MC	1A	1962	21/22	0.97	0.09	16,24,26,32	0
1	OMG	2A	2251	24/25	0.97	0.07	22,28,34,35	0
1	2MA	2A	2503	23/24	0.97	0.07	20,23,27,30	0
1	PSU	2A	2605	20/21	0.97	0.07	20,25,29,31	0
32	UR3	1a	1498	21/22	0.97	0.07	26,32,34,37	0
55	8AN	2x	76	22/23	0.97	0.08	27,32,34,43	0
1	5MU	1A	1939	21/22	0.98	0.06	11,16,20,22	0
1	5MC	2A	1962	21/22	0.98	0.07	26,30,36,40	0
1	OMG	1A	2251	24/25	0.98	0.07	9,12,14,19	0
1	2MA	1A	2503	23/24	0.98	0.06	8,11,13,14	0
1	OMU	2A	2552	21/22	0.98	0.08	19,25,29,31	0
1	OMU	1A	2552	21/22	0.98	0.06	11,16,19,20	0
1	PSU	1A	2605	20/21	0.98	0.07	13,15,19,22	0
32	MA6	1a	1518	24/25	0.98	0.07	21,29,31,34	0
55	8AN	1x	76	22/23	0.98	0.06	10,14,18,21	0
1	5MU	2A	1939	21/22	0.98	0.07	22,25,28,33	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1X	105	1/1	0.52	0.26	58,58,58,58	0
57	MG	2A	3835	1/1	0.56	0.16	58,58,58,58	0
57	MG	2a	1731	1/1	0.61	0.20	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3593	1/1	0.62	0.26	65,65,65,65	0
57	MG	1A	3524	1/1	0.63	0.24	57,57,57,57	0
57	MG	2A	3049	1/1	0.63	0.30	55,55,55,55	0
57	MG	2A	3490	1/1	0.63	0.26	54,54,54,54	0
57	MG	1A	3848	1/1	0.63	0.24	42,42,42,42	0
57	MG	1A	4032	1/1	0.63	0.43	75,75,75,75	0
57	MG	1B	233	1/1	0.63	0.22	74,74,74,74	0
57	MG	2A	3094	1/1	0.64	0.37	71,71,71,71	0
57	MG	1A	3917	1/1	0.65	0.15	20,20,20,20	0
57	MG	2B	207	1/1	0.66	0.21	64,64,64,64	0
57	MG	2A	3808	1/1	0.66	0.20	62,62,62,62	0
57	MG	1a	3675	1/1	0.67	0.34	65,65,65,65	0
57	MG	2A	3335	1/1	0.67	0.24	47,47,47,47	0
57	MG	2A	3118	1/1	0.68	0.19	65,65,65,65	0
57	MG	1A	3949	1/1	0.68	0.19	59,59,59,59	0
57	MG	1a	3681	1/1	0.69	0.31	57,57,57,57	0
57	MG	2A	3694	1/1	0.69	0.18	53,53,53,53	0
57	MG	2A	3263	1/1	0.69	0.14	51,51,51,51	0
57	MG	2a	1740	1/1	0.69	0.29	68,68,68,68	0
57	MG	2A	3083	1/1	0.70	0.18	77,77,77,77	0
57	MG	1B	236	1/1	0.70	0.27	58,58,58,58	0
57	MG	1A	4077	1/1	0.70	0.20	39,39,39,39	0
57	MG	2A	3626	1/1	0.70	0.22	66,66,66,66	0
57	MG	1a	3563	1/1	0.70	0.28	65,65,65,65	0
57	MG	2a	1747	1/1	0.70	0.27	69,69,69,69	0
57	MG	2A	3816	1/1	0.71	0.14	50,50,50,50	0
57	MG	2A	3622	1/1	0.71	0.15	55,55,55,55	0
57	MG	1a	3613	1/1	0.71	0.23	46,46,46,46	0
57	MG	1A	3496	1/1	0.71	0.11	55,55,55,55	0
57	MG	2A	3700	1/1	0.71	0.18	40,40,40,40	0
57	MG	2A	3295	1/1	0.71	0.22	55,55,55,55	0
57	MG	1A	3773	1/1	0.72	0.17	53,53,53,53	0
57	MG	1A	3970	1/1	0.72	0.22	67,67,67,67	0
57	MG	1B	219	1/1	0.72	0.15	46,46,46,46	0
57	MG	1A	3383	1/1	0.73	0.12	54,54,54,54	0
57	MG	1A	3808	1/1	0.73	0.13	38,38,38,38	0
57	MG	2f	201	1/1	0.73	0.22	48,48,48,48	0
57	MG	1a	3655	1/1	0.74	0.25	62,62,62,62	0
57	MG	1A	4031	1/1	0.74	0.15	66,66,66,66	0
57	MG	1A	3969	1/1	0.74	0.28	51,51,51,51	0
57	MG	2A	3803	1/1	0.74	0.13	57,57,57,57	0
57	MG	2A	3162	1/1	0.74	0.24	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3804	1/1	0.74	0.12	44,44,44,44	0
57	MG	2i	201	1/1	0.74	0.14	58,58,58,58	0
57	MG	2A	3334	1/1	0.75	0.19	48,48,48,48	0
57	MG	2A	3033	1/1	0.75	0.16	44,44,44,44	0
57	MG	1B	222	1/1	0.75	0.14	42,42,42,42	0
57	MG	2A	3519	1/1	0.75	0.16	46,46,46,46	0
57	MG	2A	3163	1/1	0.75	0.13	51,51,51,51	0
57	MG	2R	201	1/1	0.75	0.16	38,38,38,38	0
57	MG	2A	3246	1/1	0.75	0.26	49,49,49,49	0
57	MG	1A	3685	1/1	0.75	0.14	57,57,57,57	0
57	MG	1A	3866	1/1	0.75	0.22	52,52,52,52	0
57	MG	2a	1757	1/1	0.75	0.20	58,58,58,58	0
57	MG	2A	3326	1/1	0.75	0.28	62,62,62,62	0
57	MG	2A	3746	1/1	0.75	0.28	80,80,80,80	0
57	MG	2A	3396	1/1	0.76	0.18	57,57,57,57	0
57	MG	1A	4064	1/1	0.76	0.16	38,38,38,38	0
57	MG	2a	1732	1/1	0.76	0.28	75,75,75,75	0
57	MG	1a	3624	1/1	0.76	0.38	62,62,62,62	0
57	MG	1A	3344	1/1	0.76	0.19	63,63,63,63	0
57	MG	1A	3854	1/1	0.76	0.13	9,9,9,9	0
57	MG	1A	3464	1/1	0.76	0.21	56,56,56,56	0
57	MG	1a	3595	1/1	0.76	0.26	48,48,48,48	0
57	MG	1A	3514	1/1	0.77	0.28	50,50,50,50	0
57	MG	1A	3810	1/1	0.77	0.22	46,46,46,46	0
57	MG	2A	3499	1/1	0.77	0.19	48,48,48,48	0
57	MG	1I	201	1/1	0.77	0.15	56,56,56,56	0
57	MG	1U	212	1/1	0.77	0.55	53,53,53,53	0
57	MG	1x	108	1/1	0.77	0.15	66,66,66,66	0
57	MG	1A	3770	1/1	0.77	0.16	8,8,8,8	0
57	MG	2A	3310	1/1	0.77	0.16	56,56,56,56	0
57	MG	1A	4081	1/1	0.77	0.21	39,39,39,39	0
57	MG	1A	3430	1/1	0.77	0.20	52,52,52,52	0
57	MG	1A	3611	1/1	0.77	0.12	13,13,13,13	0
57	MG	2A	3804	1/1	0.77	0.15	64,64,64,64	0
57	MG	1a	3712	1/1	0.78	0.18	66,66,66,66	0
57	MG	1x	106	1/1	0.78	0.11	60,60,60,60	0
57	MG	2B	202	1/1	0.78	0.22	61,61,61,61	0
57	MG	2B	203	1/1	0.78	0.19	60,60,60,60	0
57	MG	1A	3999	1/1	0.78	0.11	43,43,43,43	0
57	MG	2B	210	1/1	0.78	0.23	63,63,63,63	0
57	MG	1A	3520	1/1	0.78	0.16	44,44,44,44	0
57	MG	2a	1655	1/1	0.78	0.15	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3633	1/1	0.78	0.21	63,63,63,63	0
57	MG	1A	3244	1/1	0.78	0.13	45,45,45,45	0
57	MG	2A	3352	1/1	0.78	0.14	52,52,52,52	0
57	MG	2A	3247	1/1	0.78	0.22	49,49,49,49	0
57	MG	1A	3742	1/1	0.78	0.17	17,17,17,17	0
57	MG	2a	1759	1/1	0.78	0.15	66,66,66,66	0
57	MG	2A	3275	1/1	0.78	0.16	50,50,50,50	0
57	MG	2g	201	1/1	0.78	0.15	60,60,60,60	0
57	MG	2A	3515	1/1	0.78	0.18	43,43,43,43	0
57	MG	1B	232	1/1	0.79	0.20	58,58,58,58	0
57	MG	1A	3282	1/1	0.79	0.12	40,40,40,40	0
57	MG	1a	3676	1/1	0.79	0.21	74,74,74,74	0
57	MG	1a	3679	1/1	0.79	0.21	66,66,66,66	0
57	MG	1B	235	1/1	0.79	0.12	40,40,40,40	0
57	MG	1A	3409	1/1	0.79	0.26	59,59,59,59	0
57	MG	1A	3892	1/1	0.79	0.18	66,66,66,66	0
57	MG	2A	3348	1/1	0.79	0.11	60,60,60,60	0
57	MG	1A	4034	1/1	0.79	0.16	44,44,44,44	0
57	MG	2A	3030	1/1	0.79	0.12	56,56,56,56	0
57	MG	1A	3507	1/1	0.79	0.15	60,60,60,60	0
57	MG	2a	1610	1/1	0.79	0.17	48,48,48,48	0
57	MG	1a	3506	1/1	0.79	0.17	65,65,65,65	0
57	MG	1a	3533	1/1	0.79	0.12	59,59,59,59	0
57	MG	1a	3541	1/1	0.79	0.26	56,56,56,56	0
57	MG	1A	3630	1/1	0.79	0.14	34,34,34,34	0
57	MG	2A	3144	1/1	0.79	0.13	56,56,56,56	0
57	MG	1A	3510	1/1	0.79	0.33	50,50,50,50	0
57	MG	1A	3381	1/1	0.79	0.16	49,49,49,49	0
57	MG	2A	3646	1/1	0.79	0.09	44,44,44,44	0
57	MG	1A	3972	1/1	0.79	0.16	57,57,57,57	0
57	MG	1a	3646	1/1	0.79	0.12	59,59,59,59	0
57	MG	1A	3977	1/1	0.80	0.16	23,23,23,23	0
57	MG	1a	3564	1/1	0.80	0.16	57,57,57,57	0
57	MG	2A	3361	1/1	0.80	0.24	57,57,57,57	0
57	MG	1A	3791	1/1	0.80	0.18	42,42,42,42	0
57	MG	1a	3602	1/1	0.80	0.14	53,53,53,53	0
57	MG	1a	3719	1/1	0.80	0.20	58,58,58,58	0
57	MG	1A	4004	1/1	0.80	0.16	54,54,54,54	0
57	MG	1a	3503	1/1	0.80	0.26	74,74,74,74	0
57	MG	2A	3548	1/1	0.80	0.13	53,53,53,53	0
57	MG	1a	3630	1/1	0.80	0.12	51,51,51,51	0
57	MG	2A	3602	1/1	0.80	0.11	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	26	101	1/1	0.80	0.14	44,44,44,44	0
57	MG	2A	3276	1/1	0.80	0.17	57,57,57,57	0
57	MG	1A	3919	1/1	0.80	0.15	52,52,52,52	0
57	MG	2a	1667	1/1	0.80	0.32	47,47,47,47	0
57	MG	2a	1690	1/1	0.80	0.15	53,53,53,53	0
57	MG	2a	1714	1/1	0.80	0.16	47,47,47,47	0
57	MG	1A	3900	1/1	0.80	0.15	18,18,18,18	0
57	MG	2A	3643	1/1	0.80	0.28	68,68,68,68	0
57	MG	1a	3659	1/1	0.80	0.16	56,56,56,56	0
57	MG	2A	3663	1/1	0.80	0.13	39,39,39,39	0
57	MG	2A	3669	1/1	0.80	0.13	59,59,59,59	0
57	MG	1E	311	1/1	0.80	0.14	50,50,50,50	0
57	MG	2A	3117	1/1	0.80	0.20	56,56,56,56	0
57	MG	2A	3703	1/1	0.80	0.21	59,59,59,59	0
57	MG	2A	3728	1/1	0.80	0.11	53,53,53,53	0
57	MG	2j	202	1/1	0.80	0.15	53,53,53,53	0
57	MG	2A	3500	1/1	0.81	0.12	26,26,26,26	0
57	MG	2A	3810	1/1	0.81	0.14	36,36,36,36	0
57	MG	1a	3664	1/1	0.81	0.37	61,61,61,61	0
57	MG	1a	3673	1/1	0.81	0.18	48,48,48,48	0
57	MG	1B	214	1/1	0.81	0.17	36,36,36,36	0
57	MG	2A	3557	1/1	0.81	0.23	57,57,57,57	0
57	MG	1A	3246	1/1	0.81	0.47	36,36,36,36	0
57	MG	2A	3594	1/1	0.81	0.14	33,33,33,33	0
57	MG	1A	3442	1/1	0.81	0.10	55,55,55,55	0
57	MG	1A	4009	1/1	0.81	0.16	39,39,39,39	0
57	MG	1a	3702	1/1	0.81	0.17	62,62,62,62	0
57	MG	2A	3629	1/1	0.81	0.14	38,38,38,38	0
57	MG	1A	4027	1/1	0.81	0.09	41,41,41,41	0
57	MG	2a	1668	1/1	0.81	0.39	56,56,56,56	0
57	MG	2A	3641	1/1	0.81	0.20	61,61,61,61	0
57	MG	1A	3817	1/1	0.81	0.19	40,40,40,40	0
57	MG	1A	3446	1/1	0.81	0.17	46,46,46,46	0
57	MG	1B	237	1/1	0.81	0.15	52,52,52,52	0
57	MG	1A	3613	1/1	0.81	0.18	45,45,45,45	0
57	MG	1A	3201	1/1	0.81	0.08	37,37,37,37	0
57	MG	2a	1750	1/1	0.81	0.25	63,63,63,63	0
57	MG	1A	3871	1/1	0.81	0.10	53,53,53,53	0
57	MG	2A	3075	1/1	0.81	0.29	46,46,46,46	0
57	MG	2a	1769	1/1	0.81	0.14	52,52,52,52	0
57	MG	1A	3662	1/1	0.81	0.12	10,10,10,10	0
57	MG	1a	3647	1/1	0.81	0.13	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1Y	202	1/1	0.81	0.08	46,46,46,46	0
57	MG	18	104	1/1	0.81	0.19	38,38,38,38	0
57	MG	2A	3715	1/1	0.82	0.13	39,39,39,39	0
57	MG	2A	3340	1/1	0.82	0.21	37,37,37,37	0
57	MG	1a	3615	1/1	0.82	0.27	59,59,59,59	0
57	MG	15	3209	1/1	0.82	0.16	45,45,45,45	0
57	MG	2A	3031	1/1	0.82	0.12	43,43,43,43	0
57	MG	2A	3385	1/1	0.82	0.30	50,50,50,50	0
57	MG	1a	3628	1/1	0.82	0.22	46,46,46,46	0
57	MG	1A	3807	1/1	0.82	0.10	22,22,22,22	0
57	MG	1a	3631	1/1	0.82	0.24	61,61,61,61	0
57	MG	1A	3450	1/1	0.82	0.18	52,52,52,52	0
57	MG	2A	3502	1/1	0.82	0.22	53,53,53,53	0
57	MG	1A	3756	1/1	0.82	0.12	70,70,70,70	0
57	MG	2A	3098	1/1	0.82	0.30	61,61,61,61	0
57	MG	1a	3518	1/1	0.82	0.12	59,59,59,59	0
57	MG	1A	3097	1/1	0.82	0.13	40,40,40,40	0
57	MG	1a	3540	1/1	0.82	0.12	50,50,50,50	0
57	MG	2a	1631	1/1	0.82	0.18	58,58,58,58	0
57	MG	2a	1635	1/1	0.82	0.24	56,56,56,56	0
57	MG	2a	1636	1/1	0.82	0.21	52,52,52,52	0
57	MG	1A	3656	1/1	0.82	0.09	30,30,30,30	0
57	MG	1A	3785	1/1	0.82	0.18	45,45,45,45	0
57	MG	2A	3621	1/1	0.82	0.16	49,49,49,49	0
57	MG	2A	3188	1/1	0.82	0.17	59,59,59,59	0
57	MG	1A	3588	1/1	0.82	0.08	6,6,6,6	0
57	MG	1a	3574	1/1	0.82	0.13	48,48,48,48	0
57	MG	1a	3579	1/1	0.82	0.25	68,68,68,68	0
57	MG	2A	3640	1/1	0.82	0.19	50,50,50,50	0
57	MG	2A	3269	1/1	0.82	0.17	54,54,54,54	0
57	MG	1a	3682	1/1	0.82	0.12	54,54,54,54	0
57	MG	2a	1751	1/1	0.82	0.22	60,60,60,60	0
57	MG	1a	3699	1/1	0.82	0.12	46,46,46,46	0
57	MG	2A	3660	1/1	0.82	0.12	60,60,60,60	0
57	MG	2a	1760	1/1	0.82	0.16	48,48,48,48	0
57	MG	1A	3793	1/1	0.82	0.12	24,24,24,24	0
57	MG	2a	1774	1/1	0.82	0.29	57,57,57,57	0
57	MG	1A	3794	1/1	0.82	0.21	32,32,32,32	0
57	MG	1a	3607	1/1	0.82	0.30	75,75,75,75	0
57	MG	1l	201	1/1	0.82	0.14	55,55,55,55	0
57	MG	1A	3087	1/1	0.82	0.15	37,37,37,37	0
57	MG	2A	3758	1/1	0.83	0.19	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3783	1/1	0.83	0.17	29,29,29,29	0
57	MG	2A	3364	1/1	0.83	0.21	44,44,44,44	0
57	MG	1B	223	1/1	0.83	0.09	40,40,40,40	0
57	MG	2A	3093	1/1	0.83	0.27	55,55,55,55	0
57	MG	2A	3403	1/1	0.83	0.22	55,55,55,55	0
57	MG	1B	231	1/1	0.83	0.13	51,51,51,51	0
57	MG	1A	3719	1/1	0.83	0.16	52,52,52,52	0
57	MG	2A	3114	1/1	0.83	0.12	39,39,39,39	0
57	MG	1A	3350	1/1	0.83	0.14	47,47,47,47	0
57	MG	1A	3367	1/1	0.83	0.17	42,42,42,42	0
57	MG	1A	3283	1/1	0.83	0.16	35,35,35,35	0
57	MG	2D	304	1/1	0.83	0.23	40,40,40,40	0
57	MG	1a	3570	1/1	0.83	0.11	53,53,53,53	0
57	MG	2A	3549	1/1	0.83	0.15	60,60,60,60	0
57	MG	1A	3936	1/1	0.83	0.09	41,41,41,41	0
57	MG	2a	1625	1/1	0.83	0.26	51,51,51,51	0
57	MG	2a	1630	1/1	0.83	0.26	69,69,69,69	0
57	MG	2A	3585	1/1	0.83	0.23	56,56,56,56	0
57	MG	2a	1634	1/1	0.83	0.15	51,51,51,51	0
57	MG	1A	3449	1/1	0.83	0.10	50,50,50,50	0
57	MG	1a	3689	1/1	0.83	0.24	55,55,55,55	0
57	MG	1a	3696	1/1	0.83	0.26	60,60,60,60	0
57	MG	2a	1661	1/1	0.83	0.26	51,51,51,51	0
57	MG	1F	310	1/1	0.83	0.10	44,44,44,44	0
57	MG	2A	3266	1/1	0.83	0.14	48,48,48,48	0
57	MG	2a	1677	1/1	0.83	0.25	61,61,61,61	0
57	MG	2a	1688	1/1	0.83	0.31	54,54,54,54	0
57	MG	1A	3832	1/1	0.83	0.14	43,43,43,43	0
57	MG	2a	1710	1/1	0.83	0.27	64,64,64,64	0
57	MG	2A	3273	1/1	0.83	0.28	60,60,60,60	0
57	MG	1S	203	1/1	0.83	0.11	56,56,56,56	0
57	MG	1A	4075	1/1	0.83	0.15	49,49,49,49	0
57	MG	1A	4076	1/1	0.83	0.17	55,55,55,55	0
57	MG	2A	3301	1/1	0.83	0.12	46,46,46,46	0
57	MG	1A	3315	1/1	0.83	0.14	35,35,35,35	0
57	MG	1a	3625	1/1	0.83	0.18	57,57,57,57	0
57	MG	2A	3331	1/1	0.83	0.14	58,58,58,58	0
57	MG	1x	111	1/1	0.83	0.18	52,52,52,52	0
57	MG	13	102	1/1	0.83	0.17	40,40,40,40	0
57	MG	1A	3119	1/1	0.83	0.27	45,45,45,45	0
57	MG	1A	3568	1/1	0.83	0.27	55,55,55,55	0
57	MG	1A	3690	1/1	0.83	0.11	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3357	1/1	0.83	0.16	54,54,54,54	0
57	MG	1A	4002	1/1	0.83	0.14	69,69,69,69	0
57	MG	2A	3748	1/1	0.83	0.09	41,41,41,41	0
57	MG	2A	3628	1/1	0.84	0.11	30,30,30,30	0
57	MG	1A	3503	1/1	0.84	0.14	34,34,34,34	0
57	MG	2A	3387	1/1	0.84	0.24	38,38,38,38	0
57	MG	1B	227	1/1	0.84	0.20	65,65,65,65	0
57	MG	1a	3668	1/1	0.84	0.23	64,64,64,64	0
57	MG	2A	3421	1/1	0.84	0.29	61,61,61,61	0
57	MG	2A	3440	1/1	0.84	0.11	54,54,54,54	0
57	MG	2A	3458	1/1	0.84	0.13	52,52,52,52	0
57	MG	2A	3476	1/1	0.84	0.20	46,46,46,46	0
57	MG	1v	101	1/1	0.84	0.27	77,77,77,77	0
57	MG	2A	3681	1/1	0.84	0.23	47,47,47,47	0
57	MG	1A	3907	1/1	0.84	0.17	59,59,59,59	0
57	MG	2A	3122	1/1	0.84	0.13	42,42,42,42	0
57	MG	1A	3393	1/1	0.84	0.18	47,47,47,47	0
57	MG	1a	3559	1/1	0.84	0.19	70,70,70,70	0
57	MG	2a	1683	1/1	0.84	0.22	55,55,55,55	0
57	MG	1A	3593	1/1	0.84	0.12	26,26,26,26	0
57	MG	2A	3729	1/1	0.84	0.18	53,53,53,53	0
57	MG	2A	3177	1/1	0.84	0.17	60,60,60,60	0
57	MG	1A	3788	1/1	0.84	0.11	46,46,46,46	0
57	MG	2A	3757	1/1	0.84	0.17	51,51,51,51	0
57	MG	2A	3343	1/1	0.84	0.33	64,64,64,64	0
57	MG	2A	3581	1/1	0.84	0.22	41,41,41,41	0
57	MG	2a	1743	1/1	0.84	0.20	52,52,52,52	0
57	MG	2A	3584	1/1	0.84	0.12	46,46,46,46	0
57	MG	2A	3347	1/1	0.84	0.14	51,51,51,51	0
57	MG	1A	3941	1/1	0.84	0.12	21,21,21,21	0
57	MG	2a	1753	1/1	0.84	0.23	51,51,51,51	0
57	MG	1A	3439	1/1	0.84	0.20	58,58,58,58	0
57	MG	2A	3355	1/1	0.84	0.15	53,53,53,53	0
57	MG	2A	3830	1/1	0.84	0.21	50,50,50,50	0
57	MG	2A	3606	1/1	0.84	0.16	19,19,19,19	0
57	MG	2a	1772	1/1	0.84	0.17	59,59,59,59	0
57	MG	2A	3610	1/1	0.84	0.17	64,64,64,64	0
57	MG	1a	3577	1/1	0.84	0.29	51,51,51,51	0
57	MG	1A	3889	1/1	0.84	0.18	39,39,39,39	0
57	MG	1A	3669	1/1	0.84	0.14	18,18,18,18	0
57	MG	2j	201	1/1	0.84	0.10	55,55,55,55	0
57	MG	2B	215	1/1	0.84	0.17	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3590	1/1	0.85	0.14	41,41,41,41	0
57	MG	1A	3780	1/1	0.85	0.17	42,42,42,42	0
57	MG	1F	311	1/1	0.85	0.10	44,44,44,44	0
57	MG	1A	3698	1/1	0.85	0.14	55,55,55,55	0
57	MG	2B	211	1/1	0.85	0.11	49,49,49,49	0
57	MG	1A	3605	1/1	0.85	0.11	47,47,47,47	0
57	MG	1A	3061	1/1	0.85	0.28	49,49,49,49	0
57	MG	2D	305	1/1	0.85	0.12	45,45,45,45	0
57	MG	2G	201	1/1	0.85	0.22	53,53,53,53	0
57	MG	2A	3349	1/1	0.85	0.18	47,47,47,47	0
57	MG	1A	3479	1/1	0.85	0.16	45,45,45,45	0
57	MG	1A	3918	1/1	0.85	0.12	56,56,56,56	0
57	MG	1a	3692	1/1	0.85	0.18	50,50,50,50	0
57	MG	10	101	1/1	0.85	0.13	41,41,41,41	0
57	MG	1A	3345	1/1	0.85	0.26	45,45,45,45	0
57	MG	2A	3174	1/1	0.85	0.18	47,47,47,47	0
57	MG	1B	224	1/1	0.85	0.17	54,54,54,54	0
57	MG	1A	3797	1/1	0.85	0.09	28,28,28,28	0
57	MG	1a	3716	1/1	0.85	0.17	51,51,51,51	0
57	MG	2A	3405	1/1	0.85	0.23	49,49,49,49	0
57	MG	2A	3416	1/1	0.85	0.11	50,50,50,50	0
57	MG	2A	3668	1/1	0.85	0.18	57,57,57,57	0
57	MG	1A	3798	1/1	0.85	0.10	42,42,42,42	0
57	MG	2A	3436	1/1	0.85	0.13	47,47,47,47	0
57	MG	2A	3693	1/1	0.85	0.23	52,52,52,52	0
57	MG	2A	3254	1/1	0.85	0.10	55,55,55,55	0
57	MG	2a	1692	1/1	0.85	0.23	67,67,67,67	0
57	MG	2a	1695	1/1	0.85	0.30	54,54,54,54	0
57	MG	1b	302	1/1	0.85	0.15	75,75,75,75	0
57	MG	2A	3464	1/1	0.85	0.24	66,66,66,66	0
57	MG	2a	1719	1/1	0.85	0.12	41,41,41,41	0
57	MG	2a	1724	1/1	0.85	0.12	50,50,50,50	0
57	MG	2A	3704	1/1	0.85	0.22	59,59,59,59	0
57	MG	2A	3709	1/1	0.85	0.17	32,32,32,32	0
57	MG	2A	3467	1/1	0.85	0.26	49,49,49,49	0
57	MG	1A	3942	1/1	0.85	0.10	26,26,26,26	0
57	MG	2A	3484	1/1	0.85	0.19	36,36,36,36	0
57	MG	2A	3734	1/1	0.85	0.14	67,67,67,67	0
57	MG	1A	3947	1/1	0.85	0.14	62,62,62,62	0
57	MG	2A	3272	1/1	0.85	0.20	56,56,56,56	0
57	MG	1a	3520	1/1	0.85	0.12	56,56,56,56	0
57	MG	1a	3638	1/1	0.85	0.16	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	3523	1/1	0.85	0.11	51,51,51,51	0
57	MG	2a	1762	1/1	0.85	0.26	58,58,58,58	0
57	MG	1A	3654	1/1	0.85	0.10	55,55,55,55	0
57	MG	1A	4055	1/1	0.85	0.11	30,30,30,30	0
57	MG	2A	3806	1/1	0.85	0.11	50,50,50,50	0
57	MG	2a	1777	1/1	0.85	0.29	53,53,53,53	0
57	MG	1A	3951	1/1	0.85	0.12	56,56,56,56	0
57	MG	2A	3321	1/1	0.85	0.23	48,48,48,48	0
57	MG	1A	3958	1/1	0.85	0.11	63,63,63,63	0
57	MG	1F	304	1/1	0.85	0.11	19,19,19,19	0
57	MG	1a	3672	1/1	0.85	0.11	51,51,51,51	0
57	MG	2A	3209	1/1	0.86	0.13	46,46,46,46	0
57	MG	1a	3606	1/1	0.86	0.25	49,49,49,49	0
57	MG	1A	3538	1/1	0.86	0.12	38,38,38,38	0
57	MG	1A	3314	1/1	0.86	0.17	29,29,29,29	0
57	MG	2A	3824	1/1	0.86	0.12	20,20,20,20	0
57	MG	1F	305	1/1	0.86	0.11	44,44,44,44	0
57	MG	1a	3507	1/1	0.86	0.12	52,52,52,52	0
57	MG	1a	3511	1/1	0.86	0.16	54,54,54,54	0
57	MG	1a	3515	1/1	0.86	0.13	58,58,58,58	0
57	MG	1v	102	1/1	0.86	0.12	41,41,41,41	0
57	MG	1x	101	1/1	0.86	0.22	52,52,52,52	0
57	MG	1x	105	1/1	0.86	0.18	45,45,45,45	0
57	MG	2A	3282	1/1	0.86	0.18	48,48,48,48	0
57	MG	1A	3586	1/1	0.86	0.11	22,22,22,22	0
57	MG	2A	3298	1/1	0.86	0.19	54,54,54,54	0
57	MG	2E	301	1/1	0.86	0.19	58,58,58,58	0
57	MG	2E	304	1/1	0.86	0.12	55,55,55,55	0
57	MG	1A	3635	1/1	0.86	0.13	34,34,34,34	0
57	MG	2Q	203	1/1	0.86	0.12	50,50,50,50	0
57	MG	2Q	204	1/1	0.86	0.19	43,43,43,43	0
57	MG	1A	4036	1/1	0.86	0.12	30,30,30,30	0
57	MG	2U	201	1/1	0.86	0.23	49,49,49,49	0
57	MG	2W	201	1/1	0.86	0.39	45,45,45,45	0
57	MG	2A	3314	1/1	0.86	0.16	52,52,52,52	0
57	MG	2a	1602	1/1	0.86	0.11	63,63,63,63	0
57	MG	2a	1607	1/1	0.86	0.25	45,45,45,45	0
57	MG	2A	3316	1/1	0.86	0.08	52,52,52,52	0
57	MG	2a	1617	1/1	0.86	0.13	45,45,45,45	0
57	MG	1A	4038	1/1	0.86	0.15	23,23,23,23	0
57	MG	2A	3324	1/1	0.86	0.09	52,52,52,52	0
57	MG	2A	3325	1/1	0.86	0.11	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3624	1/1	0.86	0.13	46,46,46,46	0
57	MG	1T	202	1/1	0.86	0.14	47,47,47,47	0
57	MG	1U	202	1/1	0.86	0.29	36,36,36,36	0
57	MG	2A	3039	1/1	0.86	0.19	51,51,51,51	0
57	MG	1a	3657	1/1	0.86	0.16	55,55,55,55	0
57	MG	2A	3056	1/1	0.86	0.13	49,49,49,49	0
57	MG	1a	3550	1/1	0.86	0.19	44,44,44,44	0
57	MG	1a	3551	1/1	0.86	0.24	64,64,64,64	0
57	MG	2a	1681	1/1	0.86	0.20	45,45,45,45	0
57	MG	2A	3090	1/1	0.86	0.21	58,58,58,58	0
57	MG	2A	3653	1/1	0.86	0.29	46,46,46,46	0
57	MG	2a	1689	1/1	0.86	0.32	54,54,54,54	0
57	MG	1a	3557	1/1	0.86	0.19	59,59,59,59	0
57	MG	1U	204	1/1	0.86	0.13	41,41,41,41	0
57	MG	1A	3382	1/1	0.86	0.26	61,61,61,61	0
57	MG	2A	3109	1/1	0.86	0.33	51,51,51,51	0
57	MG	2a	1711	1/1	0.86	0.12	54,54,54,54	0
57	MG	2A	3110	1/1	0.86	0.15	46,46,46,46	0
57	MG	2A	3692	1/1	0.86	0.18	48,48,48,48	0
57	MG	1A	3592	1/1	0.86	0.09	34,34,34,34	0
57	MG	2a	1730	1/1	0.86	0.12	46,46,46,46	0
57	MG	1A	3759	1/1	0.86	0.11	38,38,38,38	0
57	MG	1A	3763	1/1	0.86	0.16	52,52,52,52	0
57	MG	2a	1736	1/1	0.86	0.12	35,35,35,35	0
57	MG	2A	3392	1/1	0.86	0.20	45,45,45,45	0
57	MG	10	107	1/1	0.86	0.17	49,49,49,49	0
57	MG	2A	3142	1/1	0.86	0.25	48,48,48,48	0
57	MG	11	102	1/1	0.86	0.10	26,26,26,26	0
57	MG	2A	3723	1/1	0.86	0.14	40,40,40,40	0
57	MG	2A	3412	1/1	0.86	0.22	42,42,42,42	0
57	MG	2A	3160	1/1	0.86	0.08	60,60,60,60	0
57	MG	2A	3733	1/1	0.86	0.13	37,37,37,37	0
57	MG	1a	3590	1/1	0.86	0.18	52,52,52,52	0
57	MG	2a	1761	1/1	0.86	0.17	61,61,61,61	0
57	MG	2A	3740	1/1	0.86	0.13	50,50,50,50	0
57	MG	1a	3591	1/1	0.86	0.23	61,61,61,61	0
57	MG	2A	3168	1/1	0.86	0.18	55,55,55,55	0
57	MG	2A	3453	1/1	0.86	0.16	53,53,53,53	0
57	MG	1a	3693	1/1	0.86	0.21	46,46,46,46	0
57	MG	2A	3766	1/1	0.86	0.15	55,55,55,55	0
57	MG	2A	3776	1/1	0.86	0.14	50,50,50,50	0
57	MG	1A	3088	1/1	0.86	0.24	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3207	1/1	0.86	0.14	65,65,65,65	0
57	MG	2A	3199	1/1	0.86	0.16	41,41,41,41	0
57	MG	2x	108	1/1	0.86	0.27	50,50,50,50	0
57	MG	1a	3555	1/1	0.87	0.22	55,55,55,55	0
57	MG	1A	3356	1/1	0.87	0.13	41,41,41,41	0
57	MG	1A	3864	1/1	0.87	0.09	18,18,18,18	0
57	MG	1a	3695	1/1	0.87	0.25	48,48,48,48	0
57	MG	2A	3201	1/1	0.87	0.18	54,54,54,54	0
57	MG	2A	3488	1/1	0.87	0.23	44,44,44,44	0
57	MG	1A	4010	1/1	0.87	0.10	30,30,30,30	0
57	MG	2A	3820	1/1	0.87	0.11	48,48,48,48	0
57	MG	2A	3235	1/1	0.87	0.19	50,50,50,50	0
57	MG	2A	3238	1/1	0.87	0.35	57,57,57,57	0
57	MG	2A	3831	1/1	0.87	0.07	38,38,38,38	0
57	MG	1A	3251	1/1	0.87	0.09	49,49,49,49	0
57	MG	2A	3508	1/1	0.87	0.15	34,34,34,34	0
57	MG	1a	3701	1/1	0.87	0.22	60,60,60,60	0
57	MG	1A	3470	1/1	0.87	0.42	37,37,37,37	0
57	MG	2A	3525	1/1	0.87	0.16	25,25,25,25	0
57	MG	2A	3528	1/1	0.87	0.19	37,37,37,37	0
57	MG	2A	3546	1/1	0.87	0.17	38,38,38,38	0
57	MG	1a	3705	1/1	0.87	0.09	53,53,53,53	0
57	MG	1a	3707	1/1	0.87	0.14	57,57,57,57	0
57	MG	2A	3268	1/1	0.87	0.17	48,48,48,48	0
57	MG	2A	3571	1/1	0.87	0.14	48,48,48,48	0
57	MG	2F	304	1/1	0.87	0.13	41,41,41,41	0
57	MG	2A	3573	1/1	0.87	0.31	48,48,48,48	0
57	MG	2A	3574	1/1	0.87	0.12	57,57,57,57	0
57	MG	1P	203	1/1	0.87	0.23	36,36,36,36	0
57	MG	1A	3765	1/1	0.87	0.18	48,48,48,48	0
57	MG	1A	3600	1/1	0.87	0.10	19,19,19,19	0
57	MG	1T	203	1/1	0.87	0.16	43,43,43,43	0
57	MG	2A	3591	1/1	0.87	0.24	47,47,47,47	0
57	MG	1A	3473	1/1	0.87	0.12	50,50,50,50	0
57	MG	2a	1603	1/1	0.87	0.16	55,55,55,55	0
57	MG	1A	4037	1/1	0.87	0.18	52,52,52,52	0
57	MG	1a	3598	1/1	0.87	0.21	44,44,44,44	0
57	MG	1A	3610	1/1	0.87	0.18	34,34,34,34	0
57	MG	1V	203	1/1	0.87	0.32	25,25,25,25	0
57	MG	1A	4040	1/1	0.87	0.11	51,51,51,51	0
57	MG	1A	4052	1/1	0.87	0.11	32,32,32,32	0
57	MG	1A	3167	1/1	0.87	0.27	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3004	1/1	0.87	0.30	56,56,56,56	0
57	MG	2A	3019	1/1	0.87	0.20	50,50,50,50	0
57	MG	1A	3787	1/1	0.87	0.13	25,25,25,25	0
57	MG	2A	3630	1/1	0.87	0.12	50,50,50,50	0
57	MG	2a	1662	1/1	0.87	0.16	35,35,35,35	0
57	MG	2a	1663	1/1	0.87	0.18	61,61,61,61	0
57	MG	2A	3632	1/1	0.87	0.14	60,60,60,60	0
57	MG	1A	3178	1/1	0.87	0.14	28,28,28,28	0
57	MG	2A	3635	1/1	0.87	0.14	49,49,49,49	0
57	MG	1a	3627	1/1	0.87	0.14	47,47,47,47	0
57	MG	12	101	1/1	0.87	0.10	43,43,43,43	0
57	MG	1A	3923	1/1	0.87	0.10	66,66,66,66	0
57	MG	2A	3644	1/1	0.87	0.27	57,57,57,57	0
57	MG	1A	3928	1/1	0.87	0.20	53,53,53,53	0
57	MG	1a	3636	1/1	0.87	0.20	56,56,56,56	0
57	MG	2A	3346	1/1	0.87	0.24	44,44,44,44	0
57	MG	2a	1700	1/1	0.87	0.14	56,56,56,56	0
57	MG	2A	3076	1/1	0.87	0.16	33,33,33,33	0
57	MG	17	103	1/1	0.87	0.11	33,33,33,33	0
57	MG	1A	3931	1/1	0.87	0.15	48,48,48,48	0
57	MG	2A	3676	1/1	0.87	0.23	44,44,44,44	0
57	MG	2A	3677	1/1	0.87	0.17	46,46,46,46	0
57	MG	2A	3091	1/1	0.87	0.15	33,33,33,33	0
57	MG	1A	3614	1/1	0.87	0.13	47,47,47,47	0
57	MG	1A	3499	1/1	0.87	0.16	42,42,42,42	0
57	MG	1A	3500	1/1	0.87	0.10	38,38,38,38	0
57	MG	2A	3362	1/1	0.87	0.11	50,50,50,50	0
57	MG	1A	3284	1/1	0.87	0.20	48,48,48,48	0
57	MG	1A	3187	1/1	0.87	0.20	40,40,40,40	0
57	MG	1A	3137	1/1	0.87	0.09	35,35,35,35	0
57	MG	2A	3711	1/1	0.87	0.14	43,43,43,43	0
57	MG	2A	3714	1/1	0.87	0.24	37,37,37,37	0
57	MG	1A	3317	1/1	0.87	0.14	39,39,39,39	0
57	MG	1A	3146	1/1	0.87	0.28	46,46,46,46	0
57	MG	1A	3153	1/1	0.87	0.07	26,26,26,26	0
57	MG	2A	3123	1/1	0.87	0.20	62,62,62,62	0
57	MG	2A	3408	1/1	0.87	0.24	55,55,55,55	0
57	MG	1A	3445	1/1	0.87	0.18	52,52,52,52	0
57	MG	2a	1770	1/1	0.87	0.12	52,52,52,52	0
57	MG	1a	3677	1/1	0.87	0.17	49,49,49,49	0
57	MG	2A	3418	1/1	0.87	0.10	45,45,45,45	0
57	MG	1A	3822	1/1	0.87	0.25	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3754	1/1	0.87	0.17	47,47,47,47	0
57	MG	1A	3155	1/1	0.87	0.10	18,18,18,18	0
57	MG	1A	3352	1/1	0.87	0.16	44,44,44,44	0
57	MG	2A	3445	1/1	0.87	0.28	57,57,57,57	0
57	MG	1a	3684	1/1	0.87	0.13	59,59,59,59	0
57	MG	2A	3778	1/1	0.87	0.11	35,35,35,35	0
57	MG	1A	3890	1/1	0.88	0.23	48,48,48,48	0
57	MG	2A	3304	1/1	0.88	0.14	46,46,46,46	0
57	MG	2A	3084	1/1	0.88	0.20	52,52,52,52	0
57	MG	2A	3833	1/1	0.88	0.11	58,58,58,58	0
57	MG	2A	3086	1/1	0.88	0.11	46,46,46,46	0
57	MG	2A	3089	1/1	0.88	0.18	47,47,47,47	0
57	MG	2A	3319	1/1	0.88	0.13	47,47,47,47	0
57	MG	2B	206	1/1	0.88	0.20	47,47,47,47	0
57	MG	1A	3891	1/1	0.88	0.11	25,25,25,25	0
57	MG	1A	3743	1/1	0.88	0.11	8,8,8,8	0
57	MG	10	109	1/1	0.88	0.14	46,46,46,46	0
57	MG	1a	3685	1/1	0.88	0.16	59,59,59,59	0
57	MG	1A	3899	1/1	0.88	0.17	53,53,53,53	0
57	MG	2A	3108	1/1	0.88	0.35	51,51,51,51	0
57	MG	1a	3596	1/1	0.88	0.37	47,47,47,47	0
57	MG	2A	3615	1/1	0.88	0.11	35,35,35,35	0
57	MG	2E	305	1/1	0.88	0.12	62,62,62,62	0
57	MG	2E	308	1/1	0.88	0.09	18,18,18,18	0
57	MG	2A	3619	1/1	0.88	0.10	54,54,54,54	0
57	MG	1A	3651	1/1	0.88	0.18	46,46,46,46	0
57	MG	2O	201	1/1	0.88	0.16	53,53,53,53	0
57	MG	1A	3800	1/1	0.88	0.16	35,35,35,35	0
57	MG	2A	3623	1/1	0.88	0.18	50,50,50,50	0
57	MG	1A	3596	1/1	0.88	0.13	39,39,39,39	0
57	MG	1A	4020	1/1	0.88	0.29	47,47,47,47	0
57	MG	2A	3627	1/1	0.88	0.16	56,56,56,56	0
57	MG	1a	3609	1/1	0.88	0.23	49,49,49,49	0
57	MG	28	101	1/1	0.88	0.15	49,49,49,49	0
57	MG	1A	3080	1/1	0.88	0.27	26,26,26,26	0
57	MG	2A	3351	1/1	0.88	0.15	49,49,49,49	0
57	MG	2A	3131	1/1	0.88	0.19	55,55,55,55	0
57	MG	2A	3136	1/1	0.88	0.19	49,49,49,49	0
57	MG	2a	1614	1/1	0.88	0.25	43,43,43,43	0
57	MG	1A	3414	1/1	0.88	0.10	33,33,33,33	0
57	MG	1a	3618	1/1	0.88	0.19	63,63,63,63	0
57	MG	1a	3710	1/1	0.88	0.11	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3668	1/1	0.88	0.14	22,22,22,22	0
57	MG	2A	3370	1/1	0.88	0.19	27,27,27,27	0
57	MG	1a	3715	1/1	0.88	0.12	44,44,44,44	0
57	MG	1D	311	1/1	0.88	0.09	27,27,27,27	0
57	MG	2A	3388	1/1	0.88	0.21	35,35,35,35	0
57	MG	2A	3390	1/1	0.88	0.12	40,40,40,40	0
57	MG	2A	3169	1/1	0.88	0.15	51,51,51,51	0
57	MG	2A	3171	1/1	0.88	0.12	42,42,42,42	0
57	MG	1E	306	1/1	0.88	0.21	32,32,32,32	0
57	MG	1A	3269	1/1	0.88	0.11	31,31,31,31	0
57	MG	2a	1669	1/1	0.88	0.19	54,54,54,54	0
57	MG	2a	1671	1/1	0.88	0.22	58,58,58,58	0
57	MG	2A	3180	1/1	0.88	0.13	44,44,44,44	0
57	MG	2A	3690	1/1	0.88	0.17	42,42,42,42	0
57	MG	1f	201	1/1	0.88	0.22	40,40,40,40	0
57	MG	1A	3819	1/1	0.88	0.08	44,44,44,44	0
57	MG	1A	3779	1/1	0.88	0.34	17,17,17,17	0
57	MG	1a	3632	1/1	0.88	0.31	54,54,54,54	0
57	MG	2a	1691	1/1	0.88	0.19	54,54,54,54	0
57	MG	2A	3210	1/1	0.88	0.20	58,58,58,58	0
57	MG	2A	3212	1/1	0.88	0.24	56,56,56,56	0
57	MG	2A	3705	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	3451	1/1	0.88	0.17	42,42,42,42	0
57	MG	2A	3236	1/1	0.88	0.11	49,49,49,49	0
57	MG	1A	3325	1/1	0.88	0.13	44,44,44,44	0
57	MG	2A	3459	1/1	0.88	0.08	34,34,34,34	0
57	MG	2a	1723	1/1	0.88	0.12	48,48,48,48	0
57	MG	2A	3239	1/1	0.88	0.13	50,50,50,50	0
57	MG	1G	203	1/1	0.88	0.06	54,54,54,54	0
57	MG	1A	3944	1/1	0.88	0.21	52,52,52,52	0
57	MG	1a	3649	1/1	0.88	0.20	66,66,66,66	0
57	MG	2A	3255	1/1	0.88	0.10	55,55,55,55	0
57	MG	1A	3384	1/1	0.88	0.12	41,41,41,41	0
57	MG	2A	3265	1/1	0.88	0.23	50,50,50,50	0
57	MG	2A	3747	1/1	0.88	0.12	59,59,59,59	0
57	MG	1A	3377	1/1	0.88	0.25	40,40,40,40	0
57	MG	2A	3752	1/1	0.88	0.21	57,57,57,57	0
57	MG	1A	3733	1/1	0.88	0.12	12,12,12,12	0
57	MG	1A	3954	1/1	0.88	0.15	59,59,59,59	0
57	MG	2A	3509	1/1	0.88	0.14	48,48,48,48	0
57	MG	1A	3739	1/1	0.88	0.10	26,26,26,26	0
57	MG	1A	3874	1/1	0.88	0.17	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4084	1/1	0.88	0.14	53,53,53,53	0
57	MG	2A	3052	1/1	0.88	0.11	48,48,48,48	0
57	MG	2A	3789	1/1	0.88	0.14	49,49,49,49	0
57	MG	2A	3802	1/1	0.88	0.14	69,69,69,69	0
57	MG	2a	1773	1/1	0.88	0.24	56,56,56,56	0
57	MG	2A	3530	1/1	0.88	0.14	42,42,42,42	0
57	MG	2A	3533	1/1	0.88	0.15	29,29,29,29	0
57	MG	2a	1778	1/1	0.88	0.18	55,55,55,55	0
57	MG	2A	3535	1/1	0.88	0.13	23,23,23,23	0
57	MG	1a	3569	1/1	0.88	0.22	42,42,42,42	0
57	MG	2A	3292	1/1	0.88	0.18	51,51,51,51	0
57	MG	2A	3813	1/1	0.88	0.16	57,57,57,57	0
57	MG	1B	208	1/1	0.88	0.17	44,44,44,44	0
57	MG	2l	202	1/1	0.88	0.07	47,47,47,47	0
57	MG	2r	101	1/1	0.88	0.28	62,62,62,62	0
57	MG	2v	101	1/1	0.88	0.35	46,46,46,46	0
57	MG	2x	104	1/1	0.88	0.26	59,59,59,59	0
57	MG	1A	3477	1/1	0.88	0.19	46,46,46,46	0
58	K	1A	3537	1/1	0.88	0.18	65,65,65,65	0
57	MG	1a	3717	1/1	0.89	0.13	52,52,52,52	0
57	MG	1A	3821	1/1	0.89	0.16	58,58,58,58	0
57	MG	1a	3720	1/1	0.89	0.19	58,58,58,58	0
57	MG	1A	3229	1/1	0.89	0.23	49,49,49,49	0
57	MG	2A	3369	1/1	0.89	0.26	31,31,31,31	0
57	MG	2F	301	1/1	0.89	0.12	30,30,30,30	0
57	MG	2F	302	1/1	0.89	0.11	41,41,41,41	0
57	MG	2A	3631	1/1	0.89	0.19	51,51,51,51	0
57	MG	1B	201	1/1	0.89	0.10	42,42,42,42	0
57	MG	2A	3178	1/1	0.89	0.13	45,45,45,45	0
57	MG	1f	202	1/1	0.89	0.28	54,54,54,54	0
57	MG	2A	3638	1/1	0.89	0.26	33,33,33,33	0
57	MG	1B	207	1/1	0.89	0.24	40,40,40,40	0
57	MG	1A	3518	1/1	0.89	0.17	52,52,52,52	0
57	MG	1B	209	1/1	0.89	0.21	50,50,50,50	0
57	MG	2Z	301	1/1	0.89	0.12	50,50,50,50	0
57	MG	2A	3205	1/1	0.89	0.09	44,44,44,44	0
57	MG	1A	3142	1/1	0.89	0.11	28,28,28,28	0
57	MG	2A	3651	1/1	0.89	0.20	45,45,45,45	0
57	MG	1A	3194	1/1	0.89	0.10	43,43,43,43	0
57	MG	2A	3654	1/1	0.89	0.10	69,69,69,69	0
57	MG	1A	3858	1/1	0.89	0.11	37,37,37,37	0
57	MG	2a	1611	1/1	0.89	0.10	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3410	1/1	0.89	0.12	37,37,37,37	0
57	MG	2A	3228	1/1	0.89	0.13	46,46,46,46	0
57	MG	1A	3386	1/1	0.89	0.20	42,42,42,42	0
57	MG	1A	3769	1/1	0.89	0.13	14,14,14,14	0
57	MG	2A	3002	1/1	0.89	0.29	35,35,35,35	0
57	MG	1A	3973	1/1	0.89	0.15	48,48,48,48	0
57	MG	2A	3682	1/1	0.89	0.10	50,50,50,50	0
57	MG	2A	3685	1/1	0.89	0.19	61,61,61,61	0
57	MG	2a	1649	1/1	0.89	0.17	50,50,50,50	0
57	MG	2A	3687	1/1	0.89	0.13	49,49,49,49	0
57	MG	2a	1656	1/1	0.89	0.21	72,72,72,72	0
57	MG	1A	3565	1/1	0.89	0.08	45,45,45,45	0
57	MG	1A	3979	1/1	0.89	0.22	30,30,30,30	0
57	MG	2A	3249	1/1	0.89	0.13	42,42,42,42	0
57	MG	1A	3636	1/1	0.89	0.10	32,32,32,32	0
57	MG	1A	3480	1/1	0.89	0.10	33,33,33,33	0
57	MG	1a	3528	1/1	0.89	0.19	46,46,46,46	0
57	MG	2a	1670	1/1	0.89	0.23	50,50,50,50	0
57	MG	1A	3570	1/1	0.89	0.28	55,55,55,55	0
57	MG	1A	4007	1/1	0.89	0.10	19,19,19,19	0
57	MG	1A	3573	1/1	0.89	0.20	44,44,44,44	0
57	MG	1a	3542	1/1	0.89	0.15	52,52,52,52	0
57	MG	1A	3575	1/1	0.89	0.09	24,24,24,24	0
57	MG	1A	4019	1/1	0.89	0.08	21,21,21,21	0
57	MG	2A	3718	1/1	0.89	0.17	57,57,57,57	0
57	MG	1A	3492	1/1	0.89	0.18	50,50,50,50	0
57	MG	1A	4021	1/1	0.89	0.08	25,25,25,25	0
57	MG	2A	3277	1/1	0.89	0.21	39,39,39,39	0
57	MG	2A	3730	1/1	0.89	0.11	46,46,46,46	0
57	MG	2a	1706	1/1	0.89	0.22	59,59,59,59	0
57	MG	1A	3247	1/1	0.89	0.08	51,51,51,51	0
57	MG	2A	3290	1/1	0.89	0.15	52,52,52,52	0
57	MG	1A	3672	1/1	0.89	0.12	37,37,37,37	0
57	MG	2a	1716	1/1	0.89	0.27	48,48,48,48	0
57	MG	1A	3916	1/1	0.89	0.22	18,18,18,18	0
57	MG	1a	3567	1/1	0.89	0.09	56,56,56,56	0
57	MG	2A	3299	1/1	0.89	0.17	49,49,49,49	0
57	MG	2a	1728	1/1	0.89	0.29	61,61,61,61	0
57	MG	1A	3590	1/1	0.89	0.10	24,24,24,24	0
57	MG	1A	3591	1/1	0.89	0.10	34,34,34,34	0
57	MG	2A	3541	1/1	0.89	0.14	51,51,51,51	0
57	MG	2A	3102	1/1	0.89	0.20	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3086	1/1	0.89	0.10	35,35,35,35	0
57	MG	1A	3705	1/1	0.89	0.12	47,47,47,47	0
57	MG	2A	3551	1/1	0.89	0.12	45,45,45,45	0
57	MG	2A	3554	1/1	0.89	0.14	42,42,42,42	0
57	MG	1A	3706	1/1	0.89	0.10	39,39,39,39	0
57	MG	2a	1752	1/1	0.89	0.18	54,54,54,54	0
57	MG	2A	3566	1/1	0.89	0.17	49,49,49,49	0
57	MG	2a	1754	1/1	0.89	0.17	40,40,40,40	0
57	MG	1a	3580	1/1	0.89	0.11	38,38,38,38	0
57	MG	1a	3584	1/1	0.89	0.21	59,59,59,59	0
57	MG	1A	3206	1/1	0.89	0.17	48,48,48,48	0
57	MG	1A	3933	1/1	0.89	0.08	20,20,20,20	0
57	MG	1a	3592	1/1	0.89	0.11	55,55,55,55	0
57	MG	2a	1768	1/1	0.89	0.27	65,65,65,65	0
57	MG	2A	3332	1/1	0.89	0.13	66,66,66,66	0
57	MG	2A	3127	1/1	0.89	0.17	46,46,46,46	0
57	MG	2A	3817	1/1	0.89	0.14	33,33,33,33	0
57	MG	1a	3593	1/1	0.89	0.19	51,51,51,51	0
57	MG	2A	3339	1/1	0.89	0.29	47,47,47,47	0
57	MG	2a	1775	1/1	0.89	0.08	57,57,57,57	0
57	MG	2A	3829	1/1	0.89	0.12	56,56,56,56	0
57	MG	1A	3723	1/1	0.89	0.11	39,39,39,39	0
57	MG	2A	3137	1/1	0.89	0.23	43,43,43,43	0
57	MG	2A	3345	1/1	0.89	0.10	40,40,40,40	0
57	MG	2A	3607	1/1	0.89	0.10	46,46,46,46	0
57	MG	2A	3141	1/1	0.89	0.15	36,36,36,36	0
57	MG	2A	3611	1/1	0.89	0.14	37,37,37,37	0
57	MG	1A	4067	1/1	0.89	0.15	42,42,42,42	0
57	MG	2A	3143	1/1	0.89	0.18	56,56,56,56	0
57	MG	1A	3458	1/1	0.89	0.12	43,43,43,43	0
57	MG	2x	103	1/1	0.89	0.15	31,31,31,31	0
57	MG	1A	3460	1/1	0.89	0.15	34,34,34,34	0
57	MG	1a	3604	1/1	0.89	0.29	58,58,58,58	0
57	MG	1A	3060	1/1	0.89	0.15	35,35,35,35	0
57	MG	2A	3146	1/1	0.90	0.18	50,50,50,50	0
57	MG	2A	3153	1/1	0.90	0.09	42,42,42,42	0
57	MG	2A	3158	1/1	0.90	0.15	55,55,55,55	0
57	MG	2A	3159	1/1	0.90	0.10	53,53,53,53	0
57	MG	2E	302	1/1	0.90	0.16	52,52,52,52	0
57	MG	1A	3368	1/1	0.90	0.10	33,33,33,33	0
57	MG	1a	3594	1/1	0.90	0.25	35,35,35,35	0
57	MG	1A	3343	1/1	0.90	0.16	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1Z	302	1/1	0.90	0.10	49,49,49,49	0
57	MG	1A	3432	1/1	0.90	0.21	44,44,44,44	0
57	MG	10	106	1/1	0.90	0.09	44,44,44,44	0
57	MG	2F	305	1/1	0.90	0.13	45,45,45,45	0
57	MG	1a	3721	1/1	0.90	0.10	55,55,55,55	0
57	MG	1A	3952	1/1	0.90	0.07	43,43,43,43	0
57	MG	2A	3383	1/1	0.90	0.23	50,50,50,50	0
57	MG	1A	3784	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	3434	1/1	0.90	0.11	45,45,45,45	0
57	MG	1A	3961	1/1	0.90	0.10	15,15,15,15	0
57	MG	2V	202	1/1	0.90	0.08	38,38,38,38	0
57	MG	2A	3642	1/1	0.90	0.14	45,45,45,45	0
57	MG	2Y	201	1/1	0.90	0.08	52,52,52,52	0
57	MG	1A	3868	1/1	0.90	0.14	38,38,38,38	0
57	MG	25	103	1/1	0.90	0.11	35,35,35,35	0
57	MG	1A	3686	1/1	0.90	0.17	37,37,37,37	0
57	MG	16	102	1/1	0.90	0.10	52,52,52,52	0
57	MG	2A	3649	1/1	0.90	0.13	55,55,55,55	0
57	MG	1B	210	1/1	0.90	0.09	44,44,44,44	0
57	MG	1A	3519	1/1	0.90	0.17	43,43,43,43	0
57	MG	1x	107	1/1	0.90	0.17	56,56,56,56	0
57	MG	2A	3655	1/1	0.90	0.10	22,22,22,22	0
57	MG	2A	3656	1/1	0.90	0.10	47,47,47,47	0
57	MG	2A	3217	1/1	0.90	0.16	49,49,49,49	0
57	MG	2A	3223	1/1	0.90	0.30	50,50,50,50	0
57	MG	2a	1628	1/1	0.90	0.13	36,36,36,36	0
57	MG	19	101	1/1	0.90	0.12	36,36,36,36	0
57	MG	1A	3879	1/1	0.90	0.10	43,43,43,43	0
57	MG	2A	3419	1/1	0.90	0.09	56,56,56,56	0
57	MG	1A	3886	1/1	0.90	0.10	10,10,10,10	0
57	MG	2A	3679	1/1	0.90	0.13	52,52,52,52	0
57	MG	2a	1641	1/1	0.90	0.24	34,34,34,34	0
57	MG	2A	3430	1/1	0.90	0.15	45,45,45,45	0
57	MG	2a	1651	1/1	0.90	0.25	51,51,51,51	0
57	MG	2A	3433	1/1	0.90	0.23	52,52,52,52	0
57	MG	1A	3307	1/1	0.90	0.09	31,31,31,31	0
57	MG	2A	3005	1/1	0.90	0.24	54,54,54,54	0
57	MG	2A	3441	1/1	0.90	0.09	43,43,43,43	0
57	MG	2A	3444	1/1	0.90	0.14	43,43,43,43	0
57	MG	2a	1665	1/1	0.90	0.20	46,46,46,46	0
57	MG	2A	3012	1/1	0.90	0.13	31,31,31,31	0
57	MG	1A	3981	1/1	0.90	0.10	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3987	1/1	0.90	0.11	26,26,26,26	0
57	MG	2A	3253	1/1	0.90	0.11	51,51,51,51	0
57	MG	1A	3249	1/1	0.90	0.15	44,44,44,44	0
57	MG	1A	3607	1/1	0.90	0.08	15,15,15,15	0
57	MG	2a	1678	1/1	0.90	0.24	46,46,46,46	0
57	MG	2A	3469	1/1	0.90	0.09	50,50,50,50	0
57	MG	2A	3475	1/1	0.90	0.16	44,44,44,44	0
57	MG	1A	3795	1/1	0.90	0.14	28,28,28,28	0
57	MG	2A	3264	1/1	0.90	0.13	50,50,50,50	0
57	MG	2A	3046	1/1	0.90	0.21	47,47,47,47	0
57	MG	2A	3719	1/1	0.90	0.13	58,58,58,58	0
57	MG	1A	3527	1/1	0.90	0.38	42,42,42,42	0
57	MG	2a	1694	1/1	0.90	0.27	52,52,52,52	0
57	MG	2A	3493	1/1	0.90	0.12	27,27,27,27	0
57	MG	1a	3653	1/1	0.90	0.19	56,56,56,56	0
57	MG	1a	3654	1/1	0.90	0.11	61,61,61,61	0
57	MG	1a	3531	1/1	0.90	0.17	63,63,63,63	0
57	MG	2A	3507	1/1	0.90	0.11	36,36,36,36	0
57	MG	2a	1712	1/1	0.90	0.20	43,43,43,43	0
57	MG	2A	3739	1/1	0.90	0.17	71,71,71,71	0
57	MG	1A	3039	1/1	0.90	0.10	20,20,20,20	0
57	MG	2a	1717	1/1	0.90	0.11	39,39,39,39	0
57	MG	2A	3742	1/1	0.90	0.07	53,53,53,53	0
57	MG	2A	3743	1/1	0.90	0.07	30,30,30,30	0
57	MG	1a	3538	1/1	0.90	0.23	55,55,55,55	0
57	MG	1A	3562	1/1	0.90	0.07	32,32,32,32	0
57	MG	1B	238	1/1	0.90	0.14	46,46,46,46	0
57	MG	2A	3278	1/1	0.90	0.16	57,57,57,57	0
57	MG	2A	3280	1/1	0.90	0.08	41,41,41,41	0
57	MG	2A	3529	1/1	0.90	0.13	47,47,47,47	0
57	MG	1A	4018	1/1	0.90	0.12	35,35,35,35	0
57	MG	2A	3761	1/1	0.90	0.27	72,72,72,72	0
57	MG	1A	3915	1/1	0.90	0.13	44,44,44,44	0
57	MG	1A	3217	1/1	0.90	0.17	33,33,33,33	0
57	MG	2A	3294	1/1	0.90	0.19	46,46,46,46	0
57	MG	1A	3447	1/1	0.90	0.25	32,32,32,32	0
57	MG	2A	3296	1/1	0.90	0.29	39,39,39,39	0
57	MG	1A	4022	1/1	0.90	0.12	34,34,34,34	0
57	MG	2a	1755	1/1	0.90	0.23	54,54,54,54	0
57	MG	1A	3631	1/1	0.90	0.08	17,17,17,17	0
57	MG	1a	3680	1/1	0.90	0.22	48,48,48,48	0
57	MG	2A	3805	1/1	0.90	0.19	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	3560	1/1	0.90	0.19	62,62,62,62	0
57	MG	1A	3355	1/1	0.90	0.08	31,31,31,31	0
57	MG	2a	1763	1/1	0.90	0.21	60,60,60,60	0
57	MG	2a	1764	1/1	0.90	0.16	53,53,53,53	0
57	MG	2a	1767	1/1	0.90	0.14	61,61,61,61	0
57	MG	2A	3311	1/1	0.90	0.13	57,57,57,57	0
57	MG	1F	312	1/1	0.90	0.22	41,41,41,41	0
57	MG	1A	3498	1/1	0.90	0.26	65,65,65,65	0
57	MG	1A	3291	1/1	0.90	0.15	47,47,47,47	0
57	MG	2A	3819	1/1	0.90	0.18	49,49,49,49	0
57	MG	1a	3691	1/1	0.90	0.10	55,55,55,55	0
57	MG	2A	3821	1/1	0.90	0.14	62,62,62,62	0
57	MG	1N	201	1/1	0.90	0.21	47,47,47,47	0
57	MG	2A	3827	1/1	0.90	0.20	56,56,56,56	0
57	MG	2A	3828	1/1	0.90	0.20	38,38,38,38	0
57	MG	2f	202	1/1	0.90	0.10	52,52,52,52	0
57	MG	1A	3580	1/1	0.90	0.09	42,42,42,42	0
57	MG	1A	3335	1/1	0.90	0.18	43,43,43,43	0
57	MG	1a	3578	1/1	0.90	0.15	69,69,69,69	0
57	MG	1A	3934	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3825	1/1	0.90	0.09	51,51,51,51	0
57	MG	2A	3139	1/1	0.90	0.14	28,28,28,28	0
57	MG	2A	3140	1/1	0.90	0.12	54,54,54,54	0
57	MG	2x	101	1/1	0.90	0.25	51,51,51,51	0
57	MG	1A	3829	1/1	0.90	0.16	31,31,31,31	0
57	MG	1A	3456	1/1	0.90	0.09	41,41,41,41	0
57	MG	1A	3844	1/1	0.90	0.17	26,26,26,26	0
57	MG	1A	3946	1/1	0.90	0.14	46,46,46,46	0
57	MG	1A	4043	1/1	0.91	0.10	50,50,50,50	0
57	MG	1A	3295	1/1	0.91	0.24	43,43,43,43	0
57	MG	1V	208	1/1	0.91	0.07	48,48,48,48	0
57	MG	2A	3243	1/1	0.91	0.20	42,42,42,42	0
57	MG	2A	3245	1/1	0.91	0.14	58,58,58,58	0
57	MG	2A	3503	1/1	0.91	0.12	33,33,33,33	0
57	MG	1a	3599	1/1	0.91	0.22	33,33,33,33	0
57	MG	1a	3601	1/1	0.91	0.27	47,47,47,47	0
57	MG	2A	3823	1/1	0.91	0.13	33,33,33,33	0
57	MG	1A	4053	1/1	0.91	0.08	28,28,28,28	0
57	MG	2A	3511	1/1	0.91	0.10	20,20,20,20	0
57	MG	2A	3514	1/1	0.91	0.09	24,24,24,24	0
57	MG	1A	3692	1/1	0.91	0.16	36,36,36,36	0
57	MG	1a	3605	1/1	0.91	0.15	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3361	1/1	0.91	0.28	36,36,36,36	0
57	MG	2A	3256	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3834	1/1	0.91	0.09	38,38,38,38	0
57	MG	2A	3259	1/1	0.91	0.09	46,46,46,46	0
57	MG	1A	3306	1/1	0.91	0.12	40,40,40,40	0
57	MG	1a	3608	1/1	0.91	0.15	41,41,41,41	0
57	MG	1A	4069	1/1	0.91	0.10	33,33,33,33	0
57	MG	2A	3536	1/1	0.91	0.15	38,38,38,38	0
57	MG	2B	208	1/1	0.91	0.20	47,47,47,47	0
57	MG	2A	3014	1/1	0.91	0.13	41,41,41,41	0
57	MG	2A	3015	1/1	0.91	0.16	53,53,53,53	0
57	MG	2B	212	1/1	0.91	0.16	58,58,58,58	0
57	MG	1A	3818	1/1	0.91	0.14	41,41,41,41	0
57	MG	2B	216	1/1	0.91	0.16	57,57,57,57	0
57	MG	2A	3022	1/1	0.91	0.26	54,54,54,54	0
57	MG	2A	3024	1/1	0.91	0.28	42,42,42,42	0
57	MG	1A	3110	1/1	0.91	0.14	31,31,31,31	0
57	MG	2A	3555	1/1	0.91	0.14	29,29,29,29	0
57	MG	2E	303	1/1	0.91	0.23	47,47,47,47	0
57	MG	1A	3371	1/1	0.91	0.08	35,35,35,35	0
57	MG	2A	3565	1/1	0.91	0.09	39,39,39,39	0
57	MG	1a	3623	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3568	1/1	0.91	0.11	28,28,28,28	0
57	MG	2A	3570	1/1	0.91	0.22	46,46,46,46	0
57	MG	1A	3721	1/1	0.91	0.15	29,29,29,29	0
57	MG	2A	3279	1/1	0.91	0.10	39,39,39,39	0
57	MG	1A	3028	1/1	0.91	0.15	17,17,17,17	0
57	MG	2A	3577	1/1	0.91	0.15	47,47,47,47	0
57	MG	2A	3281	1/1	0.91	0.12	34,34,34,34	0
57	MG	1A	3728	1/1	0.91	0.11	36,36,36,36	0
57	MG	2A	3288	1/1	0.91	0.08	45,45,45,45	0
57	MG	2T	201	1/1	0.91	0.08	39,39,39,39	0
57	MG	2A	3587	1/1	0.91	0.21	43,43,43,43	0
57	MG	2U	204	1/1	0.91	0.12	53,53,53,53	0
57	MG	1B	203	1/1	0.91	0.23	39,39,39,39	0
57	MG	1A	3511	1/1	0.91	0.14	30,30,30,30	0
57	MG	2A	3057	1/1	0.91	0.13	45,45,45,45	0
57	MG	2A	3069	1/1	0.91	0.15	29,29,29,29	0
57	MG	1A	3836	1/1	0.91	0.09	44,44,44,44	0
57	MG	1A	3837	1/1	0.91	0.12	49,49,49,49	0
57	MG	1A	3955	1/1	0.91	0.18	41,41,41,41	0
57	MG	2A	3608	1/1	0.91	0.16	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3609	1/1	0.91	0.16	38,38,38,38	0
57	MG	1A	3838	1/1	0.91	0.10	13,13,13,13	0
57	MG	2A	3303	1/1	0.91	0.09	51,51,51,51	0
57	MG	1a	3640	1/1	0.91	0.08	40,40,40,40	0
57	MG	1a	3642	1/1	0.91	0.09	41,41,41,41	0
57	MG	1A	3960	1/1	0.91	0.15	14,14,14,14	0
57	MG	2a	1618	1/1	0.91	0.10	46,46,46,46	0
57	MG	2a	1623	1/1	0.91	0.24	41,41,41,41	0
57	MG	1A	3204	1/1	0.91	0.12	44,44,44,44	0
57	MG	1A	3845	1/1	0.91	0.17	23,23,23,23	0
57	MG	1a	3517	1/1	0.91	0.23	44,44,44,44	0
57	MG	2A	3095	1/1	0.91	0.22	53,53,53,53	0
57	MG	2a	1633	1/1	0.91	0.20	49,49,49,49	0
57	MG	2A	3322	1/1	0.91	0.18	43,43,43,43	0
57	MG	1A	3454	1/1	0.91	0.14	38,38,38,38	0
57	MG	2A	3099	1/1	0.91	0.08	43,43,43,43	0
57	MG	1A	3165	1/1	0.91	0.07	18,18,18,18	0
57	MG	2a	1645	1/1	0.91	0.13	51,51,51,51	0
57	MG	2a	1648	1/1	0.91	0.15	43,43,43,43	0
57	MG	2A	3107	1/1	0.91	0.29	45,45,45,45	0
57	MG	1a	3521	1/1	0.91	0.18	46,46,46,46	0
57	MG	1B	230	1/1	0.91	0.07	49,49,49,49	0
57	MG	1a	3660	1/1	0.91	0.20	40,40,40,40	0
57	MG	2a	1659	1/1	0.91	0.37	54,54,54,54	0
57	MG	2A	3336	1/1	0.91	0.17	52,52,52,52	0
57	MG	2A	3337	1/1	0.91	0.13	41,41,41,41	0
57	MG	2A	3338	1/1	0.91	0.23	36,36,36,36	0
57	MG	2a	1664	1/1	0.91	0.27	59,59,59,59	0
57	MG	1A	3322	1/1	0.91	0.22	41,41,41,41	0
57	MG	1A	3523	1/1	0.91	0.12	43,43,43,43	0
57	MG	1A	3261	1/1	0.91	0.09	31,31,31,31	0
57	MG	1a	3536	1/1	0.91	0.16	66,66,66,66	0
57	MG	2A	3647	1/1	0.91	0.15	58,58,58,58	0
57	MG	1A	3623	1/1	0.91	0.12	35,35,35,35	0
57	MG	2a	1672	1/1	0.91	0.38	49,49,49,49	0
57	MG	2a	1673	1/1	0.91	0.24	59,59,59,59	0
57	MG	1A	3869	1/1	0.91	0.12	38,38,38,38	0
57	MG	1A	3333	1/1	0.91	0.09	49,49,49,49	0
57	MG	1A	3535	1/1	0.91	0.18	41,41,41,41	0
57	MG	2A	3350	1/1	0.91	0.14	49,49,49,49	0
57	MG	1a	3543	1/1	0.91	0.12	61,61,61,61	0
57	MG	2A	3658	1/1	0.91	0.20	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	3548	1/1	0.91	0.32	47,47,47,47	0
57	MG	2A	3353	1/1	0.91	0.10	54,54,54,54	0
57	MG	1B	239	1/1	0.91	0.07	25,25,25,25	0
57	MG	2a	1693	1/1	0.91	0.26	53,53,53,53	0
57	MG	1A	3632	1/1	0.91	0.11	25,25,25,25	0
57	MG	2A	3670	1/1	0.91	0.19	34,34,34,34	0
57	MG	2A	3675	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3360	1/1	0.91	0.10	45,45,45,45	0
57	MG	1a	3553	1/1	0.91	0.15	34,34,34,34	0
57	MG	1A	3038	1/1	0.91	0.16	45,45,45,45	0
57	MG	1A	3888	1/1	0.91	0.14	31,31,31,31	0
57	MG	2A	3367	1/1	0.91	0.19	35,35,35,35	0
57	MG	2A	3683	1/1	0.91	0.14	42,42,42,42	0
57	MG	2A	3145	1/1	0.91	0.10	39,39,39,39	0
57	MG	1A	3547	1/1	0.91	0.24	30,30,30,30	0
57	MG	2a	1721	1/1	0.91	0.14	37,37,37,37	0
57	MG	2A	3373	1/1	0.91	0.20	41,41,41,41	0
57	MG	2A	3150	1/1	0.91	0.09	50,50,50,50	0
57	MG	2a	1726	1/1	0.91	0.18	38,38,38,38	0
57	MG	1A	3638	1/1	0.91	0.09	16,16,16,16	0
57	MG	2A	3386	1/1	0.91	0.22	52,52,52,52	0
57	MG	1A	3646	1/1	0.91	0.07	9,9,9,9	0
57	MG	1A	3275	1/1	0.91	0.39	32,32,32,32	0
57	MG	1a	3565	1/1	0.91	0.13	62,62,62,62	0
57	MG	1a	3566	1/1	0.91	0.12	40,40,40,40	0
57	MG	2A	3707	1/1	0.91	0.12	53,53,53,53	0
57	MG	2a	1745	1/1	0.91	0.08	48,48,48,48	0
57	MG	2A	3395	1/1	0.91	0.25	44,44,44,44	0
57	MG	1A	3072	1/1	0.91	0.21	50,50,50,50	0
57	MG	2A	3164	1/1	0.91	0.19	53,53,53,53	0
57	MG	1F	313	1/1	0.91	0.22	26,26,26,26	0
57	MG	2A	3407	1/1	0.91	0.42	65,65,65,65	0
57	MG	1A	3566	1/1	0.91	0.15	50,50,50,50	0
57	MG	1a	3708	1/1	0.91	0.10	51,51,51,51	0
57	MG	1A	3792	1/1	0.91	0.07	11,11,11,11	0
57	MG	1A	3222	1/1	0.91	0.10	32,32,32,32	0
57	MG	1O	204	1/1	0.91	0.06	41,41,41,41	0
57	MG	2A	3732	1/1	0.91	0.19	44,44,44,44	0
57	MG	1A	3182	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3420	1/1	0.91	0.17	58,58,58,58	0
57	MG	2A	3182	1/1	0.91	0.09	41,41,41,41	0
57	MG	2A	3187	1/1	0.91	0.15	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1Q	206	1/1	0.91	0.15	36,36,36,36	0
57	MG	2A	3191	1/1	0.91	0.09	47,47,47,47	0
57	MG	2A	3194	1/1	0.91	0.07	47,47,47,47	0
57	MG	1a	3718	1/1	0.91	0.12	49,49,49,49	0
57	MG	2A	3442	1/1	0.91	0.17	49,49,49,49	0
57	MG	1S	202	1/1	0.91	0.12	36,36,36,36	0
57	MG	2A	3204	1/1	0.91	0.16	40,40,40,40	0
57	MG	2a	1776	1/1	0.91	0.13	54,54,54,54	0
57	MG	1a	3589	1/1	0.91	0.26	39,39,39,39	0
57	MG	2A	3208	1/1	0.91	0.13	34,34,34,34	0
57	MG	2A	3759	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3484	1/1	0.91	0.11	42,42,42,42	0
57	MG	2A	3463	1/1	0.91	0.33	42,42,42,42	0
57	MG	1b	301	1/1	0.91	0.09	68,68,68,68	0
57	MG	1A	3002	1/1	0.91	0.09	29,29,29,29	0
57	MG	2A	3215	1/1	0.91	0.17	52,52,52,52	0
57	MG	1e	201	1/1	0.91	0.14	39,39,39,39	0
57	MG	2A	3793	1/1	0.91	0.17	49,49,49,49	0
57	MG	2A	3794	1/1	0.91	0.10	30,30,30,30	0
57	MG	1A	3494	1/1	0.91	0.15	42,42,42,42	0
57	MG	2A	3477	1/1	0.91	0.11	23,23,23,23	0
57	MG	2A	3482	1/1	0.91	0.10	13,13,13,13	0
57	MG	1A	3292	1/1	0.91	0.08	36,36,36,36	0
57	MG	1A	3688	1/1	0.91	0.17	48,48,48,48	0
59	ZN	24	501	1/1	0.91	0.10	120,120,120,120	0
57	MG	1A	3553	1/1	0.92	0.21	59,59,59,59	0
57	MG	2A	3797	1/1	0.92	0.09	35,35,35,35	0
57	MG	2A	3800	1/1	0.92	0.33	57,57,57,57	0
57	MG	1a	3549	1/1	0.92	0.20	48,48,48,48	0
57	MG	1A	3665	1/1	0.92	0.12	48,48,48,48	0
57	MG	1A	3266	1/1	0.92	0.10	32,32,32,32	0
57	MG	2A	3471	1/1	0.92	0.18	47,47,47,47	0
57	MG	2A	3213	1/1	0.92	0.09	53,53,53,53	0
57	MG	1A	3331	1/1	0.92	0.09	40,40,40,40	0
57	MG	1A	3943	1/1	0.92	0.21	40,40,40,40	0
57	MG	2A	3812	1/1	0.92	0.10	28,28,28,28	0
57	MG	2A	3218	1/1	0.92	0.19	36,36,36,36	0
57	MG	2A	3220	1/1	0.92	0.14	69,69,69,69	0
57	MG	2A	3487	1/1	0.92	0.07	44,44,44,44	0
57	MG	1A	3801	1/1	0.92	0.18	33,33,33,33	0
57	MG	1A	3093	1/1	0.92	0.08	25,25,25,25	0
57	MG	2A	3231	1/1	0.92	0.11	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3497	1/1	0.92	0.11	23,23,23,23	0
57	MG	2A	3232	1/1	0.92	0.10	42,42,42,42	0
57	MG	1A	3673	1/1	0.92	0.11	20,20,20,20	0
57	MG	1A	3677	1/1	0.92	0.08	16,16,16,16	0
57	MG	1A	3027	1/1	0.92	0.09	31,31,31,31	0
57	MG	2A	3504	1/1	0.92	0.15	37,37,37,37	0
57	MG	2A	3506	1/1	0.92	0.09	56,56,56,56	0
57	MG	1A	3813	1/1	0.92	0.21	49,49,49,49	0
57	MG	1A	3815	1/1	0.92	0.11	50,50,50,50	0
57	MG	1A	3478	1/1	0.92	0.16	38,38,38,38	0
57	MG	1A	3401	1/1	0.92	0.09	44,44,44,44	0
57	MG	1k	201	1/1	0.92	0.10	44,44,44,44	0
57	MG	1D	314	1/1	0.92	0.19	26,26,26,26	0
57	MG	1a	3573	1/1	0.92	0.22	53,53,53,53	0
57	MG	1E	305	1/1	0.92	0.23	28,28,28,28	0
57	MG	1a	3575	1/1	0.92	0.21	55,55,55,55	0
57	MG	1x	103	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3258	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	3405	1/1	0.92	0.17	29,29,29,29	0
57	MG	2A	3260	1/1	0.92	0.24	43,43,43,43	0
57	MG	2B	218	1/1	0.92	0.07	48,48,48,48	0
57	MG	1A	3483	1/1	0.92	0.30	46,46,46,46	0
57	MG	2A	3539	1/1	0.92	0.17	48,48,48,48	0
57	MG	1A	3693	1/1	0.92	0.08	35,35,35,35	0
57	MG	2A	3544	1/1	0.92	0.10	28,28,28,28	0
57	MG	1A	3583	1/1	0.92	0.08	22,22,22,22	0
57	MG	1x	110	1/1	0.92	0.14	36,36,36,36	0
57	MG	2A	3267	1/1	0.92	0.09	44,44,44,44	0
57	MG	1A	3827	1/1	0.92	0.13	8,8,8,8	0
57	MG	2E	309	1/1	0.92	0.09	49,49,49,49	0
57	MG	2E	310	1/1	0.92	0.17	26,26,26,26	0
57	MG	2A	3552	1/1	0.92	0.24	47,47,47,47	0
57	MG	1a	3585	1/1	0.92	0.28	52,52,52,52	0
57	MG	1A	3408	1/1	0.92	0.13	33,33,33,33	0
57	MG	1A	3485	1/1	0.92	0.22	49,49,49,49	0
57	MG	2F	306	1/1	0.92	0.10	34,34,34,34	0
57	MG	1A	3707	1/1	0.92	0.08	35,35,35,35	0
57	MG	1A	3710	1/1	0.92	0.10	31,31,31,31	0
57	MG	2A	3567	1/1	0.92	0.15	43,43,43,43	0
57	MG	1A	3711	1/1	0.92	0.11	32,32,32,32	0
57	MG	1A	3988	1/1	0.92	0.09	17,17,17,17	0
57	MG	1N	203	1/1	0.92	0.10	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2T	202	1/1	0.92	0.14	57,57,57,57	0
57	MG	2A	3023	1/1	0.92	0.18	49,49,49,49	0
57	MG	1O	201	1/1	0.92	0.06	54,54,54,54	0
57	MG	1A	3841	1/1	0.92	0.12	36,36,36,36	0
57	MG	2A	3283	1/1	0.92	0.13	50,50,50,50	0
57	MG	2A	3285	1/1	0.92	0.07	47,47,47,47	0
57	MG	2A	3286	1/1	0.92	0.19	42,42,42,42	0
57	MG	25	102	1/1	0.92	0.13	43,43,43,43	0
57	MG	2A	3287	1/1	0.92	0.16	49,49,49,49	0
57	MG	1A	3488	1/1	0.92	0.32	45,45,45,45	0
57	MG	27	102	1/1	0.92	0.15	44,44,44,44	0
57	MG	27	103	1/1	0.92	0.13	39,39,39,39	0
57	MG	1a	3600	1/1	0.92	0.23	29,29,29,29	0
57	MG	2A	3291	1/1	0.92	0.15	54,54,54,54	0
57	MG	2A	3037	1/1	0.92	0.08	38,38,38,38	0
57	MG	2A	3596	1/1	0.92	0.16	22,22,22,22	0
57	MG	2A	3599	1/1	0.92	0.10	25,25,25,25	0
57	MG	2A	3601	1/1	0.92	0.11	29,29,29,29	0
57	MG	1A	3336	1/1	0.92	0.12	33,33,33,33	0
57	MG	2a	1615	1/1	0.92	0.13	41,41,41,41	0
57	MG	1A	4006	1/1	0.92	0.13	41,41,41,41	0
57	MG	2A	3047	1/1	0.92	0.20	33,33,33,33	0
57	MG	1a	3603	1/1	0.92	0.17	53,53,53,53	0
57	MG	1A	3493	1/1	0.92	0.08	32,32,32,32	0
57	MG	2A	3300	1/1	0.92	0.17	44,44,44,44	0
57	MG	1A	3853	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3276	1/1	0.92	0.24	26,26,26,26	0
57	MG	2A	3064	1/1	0.92	0.21	28,28,28,28	0
57	MG	2A	3065	1/1	0.92	0.21	33,33,33,33	0
57	MG	1A	4014	1/1	0.92	0.07	37,37,37,37	0
57	MG	2A	3312	1/1	0.92	0.08	36,36,36,36	0
57	MG	1A	3428	1/1	0.92	0.19	41,41,41,41	0
57	MG	1A	3738	1/1	0.92	0.10	14,14,14,14	0
57	MG	2a	1647	1/1	0.92	0.17	49,49,49,49	0
57	MG	2A	3317	1/1	0.92	0.31	56,56,56,56	0
57	MG	2A	3080	1/1	0.92	0.22	46,46,46,46	0
57	MG	1A	3865	1/1	0.92	0.14	14,14,14,14	0
57	MG	1a	3614	1/1	0.92	0.28	61,61,61,61	0
57	MG	1V	207	1/1	0.92	0.14	47,47,47,47	0
57	MG	2a	1658	1/1	0.92	0.20	46,46,46,46	0
57	MG	2A	3088	1/1	0.92	0.12	35,35,35,35	0
57	MG	1a	3616	1/1	0.92	0.14	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3634	1/1	0.92	0.12	34,34,34,34	0
57	MG	2A	3330	1/1	0.92	0.10	38,38,38,38	0
57	MG	1a	3617	1/1	0.92	0.18	50,50,50,50	0
57	MG	1A	3597	1/1	0.92	0.10	27,27,27,27	0
57	MG	2a	1666	1/1	0.92	0.17	43,43,43,43	0
57	MG	2A	3333	1/1	0.92	0.11	47,47,47,47	0
57	MG	1a	3621	1/1	0.92	0.19	48,48,48,48	0
57	MG	1a	3622	1/1	0.92	0.10	59,59,59,59	0
57	MG	1A	3098	1/1	0.92	0.07	33,33,33,33	0
57	MG	1Y	201	1/1	0.92	0.13	35,35,35,35	0
57	MG	1A	4025	1/1	0.92	0.10	11,11,11,11	0
57	MG	1A	3209	1/1	0.92	0.18	26,26,26,26	0
57	MG	2A	3103	1/1	0.92	0.21	46,46,46,46	0
57	MG	2A	3105	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	3870	1/1	0.92	0.12	18,18,18,18	0
57	MG	10	102	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3752	1/1	0.92	0.15	22,22,22,22	0
57	MG	1A	3872	1/1	0.92	0.11	42,42,42,42	0
57	MG	1a	3635	1/1	0.92	0.15	45,45,45,45	0
57	MG	2A	3661	1/1	0.92	0.12	63,63,63,63	0
57	MG	2A	3115	1/1	0.92	0.22	40,40,40,40	0
57	MG	1A	3213	1/1	0.92	0.09	38,38,38,38	0
57	MG	1A	3875	1/1	0.92	0.12	41,41,41,41	0
57	MG	2A	3119	1/1	0.92	0.10	42,42,42,42	0
57	MG	2a	1696	1/1	0.92	0.26	49,49,49,49	0
57	MG	2A	3354	1/1	0.92	0.07	51,51,51,51	0
57	MG	1A	3290	1/1	0.92	0.08	42,42,42,42	0
57	MG	1A	3883	1/1	0.92	0.33	29,29,29,29	0
57	MG	2A	3678	1/1	0.92	0.20	43,43,43,43	0
57	MG	15	3202	1/1	0.92	0.17	31,31,31,31	0
57	MG	1A	3440	1/1	0.92	0.15	45,45,45,45	0
57	MG	1A	4048	1/1	0.92	0.12	33,33,33,33	0
57	MG	1A	4050	1/1	0.92	0.09	44,44,44,44	0
57	MG	1A	3612	1/1	0.92	0.18	6,6,6,6	0
57	MG	1A	3074	1/1	0.92	0.06	19,19,19,19	0
57	MG	1A	3112	1/1	0.92	0.23	29,29,29,29	0
57	MG	2A	3371	1/1	0.92	0.17	37,37,37,37	0
57	MG	1a	3504	1/1	0.92	0.13	47,47,47,47	0
57	MG	2A	3380	1/1	0.92	0.20	31,31,31,31	0
57	MG	2A	3696	1/1	0.92	0.20	46,46,46,46	0
57	MG	2A	3698	1/1	0.92	0.12	30,30,30,30	0
57	MG	2A	3381	1/1	0.92	0.30	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1733	1/1	0.92	0.16	47,47,47,47	0
57	MG	1A	3359	1/1	0.92	0.07	41,41,41,41	0
57	MG	1A	3775	1/1	0.92	0.11	40,40,40,40	0
57	MG	1a	3508	1/1	0.92	0.27	59,59,59,59	0
57	MG	1a	3670	1/1	0.92	0.09	59,59,59,59	0
57	MG	1a	3671	1/1	0.92	0.13	44,44,44,44	0
57	MG	2A	3389	1/1	0.92	0.18	35,35,35,35	0
57	MG	1a	3510	1/1	0.92	0.22	44,44,44,44	0
57	MG	1A	3113	1/1	0.92	0.26	37,37,37,37	0
57	MG	1a	3513	1/1	0.92	0.08	62,62,62,62	0
57	MG	1A	4073	1/1	0.92	0.10	32,32,32,32	0
57	MG	1A	4074	1/1	0.92	0.15	48,48,48,48	0
57	MG	1A	3116	1/1	0.92	0.16	30,30,30,30	0
57	MG	1A	3901	1/1	0.92	0.09	27,27,27,27	0
57	MG	1A	3783	1/1	0.92	0.12	34,34,34,34	0
57	MG	1A	3052	1/1	0.92	0.08	36,36,36,36	0
57	MG	1a	3525	1/1	0.92	0.21	39,39,39,39	0
57	MG	1a	3527	1/1	0.92	0.17	46,46,46,46	0
57	MG	2A	3176	1/1	0.92	0.14	44,44,44,44	0
57	MG	2a	1765	1/1	0.92	0.19	55,55,55,55	0
57	MG	1A	3129	1/1	0.92	0.14	26,26,26,26	0
57	MG	1a	3690	1/1	0.92	0.08	31,31,31,31	0
57	MG	1a	3529	1/1	0.92	0.15	41,41,41,41	0
57	MG	1A	3786	1/1	0.92	0.15	45,45,45,45	0
57	MG	2a	1771	1/1	0.92	0.13	40,40,40,40	0
57	MG	2A	3432	1/1	0.92	0.20	55,55,55,55	0
57	MG	1A	3453	1/1	0.92	0.18	38,38,38,38	0
57	MG	2A	3750	1/1	0.92	0.13	47,47,47,47	0
57	MG	1A	3525	1/1	0.92	0.11	53,53,53,53	0
57	MG	1A	3089	1/1	0.92	0.11	49,49,49,49	0
57	MG	2A	3755	1/1	0.92	0.12	32,32,32,32	0
57	MG	2A	3193	1/1	0.92	0.08	47,47,47,47	0
57	MG	1A	3924	1/1	0.92	0.09	44,44,44,44	0
57	MG	2A	3196	1/1	0.92	0.09	46,46,46,46	0
57	MG	1A	3380	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3764	1/1	0.92	0.10	42,42,42,42	0
57	MG	2A	3450	1/1	0.92	0.17	38,38,38,38	0
57	MG	2A	3768	1/1	0.92	0.08	51,51,51,51	0
57	MG	2A	3770	1/1	0.92	0.16	59,59,59,59	0
57	MG	2q	201	1/1	0.92	0.07	55,55,55,55	0
57	MG	2A	3771	1/1	0.92	0.07	42,42,42,42	0
57	MG	2A	3774	1/1	0.92	0.10	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3452	1/1	0.92	0.09	50,50,50,50	0
57	MG	1A	3200	1/1	0.92	0.11	26,26,26,26	0
57	MG	1A	3141	1/1	0.92	0.10	41,41,41,41	0
57	MG	1a	3544	1/1	0.92	0.22	52,52,52,52	0
57	MG	2A	3792	1/1	0.92	0.15	31,31,31,31	0
57	MG	2A	3460	1/1	0.92	0.15	36,36,36,36	0
57	MG	1A	3351	1/1	0.93	0.07	38,38,38,38	0
57	MG	2A	3779	1/1	0.93	0.11	30,30,30,30	0
57	MG	2A	3781	1/1	0.93	0.15	51,51,51,51	0
57	MG	2A	3782	1/1	0.93	0.12	55,55,55,55	0
57	MG	1A	3812	1/1	0.93	0.06	26,26,26,26	0
57	MG	2A	3784	1/1	0.93	0.12	22,22,22,22	0
57	MG	1A	3268	1/1	0.93	0.17	28,28,28,28	0
57	MG	2A	3192	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3353	1/1	0.93	0.19	44,44,44,44	0
57	MG	2A	3455	1/1	0.93	0.17	39,39,39,39	0
57	MG	1A	3354	1/1	0.93	0.16	47,47,47,47	0
57	MG	2A	3798	1/1	0.93	0.10	38,38,38,38	0
57	MG	1a	3688	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3198	1/1	0.93	0.13	48,48,48,48	0
57	MG	2A	3461	1/1	0.93	0.23	47,47,47,47	0
57	MG	1A	3463	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3166	1/1	0.93	0.28	32,32,32,32	0
57	MG	2A	3202	1/1	0.93	0.11	42,42,42,42	0
57	MG	1A	3270	1/1	0.93	0.19	46,46,46,46	0
57	MG	1A	3629	1/1	0.93	0.10	33,33,33,33	0
57	MG	2A	3474	1/1	0.93	0.16	38,38,38,38	0
57	MG	2A	3206	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3077	1/1	0.93	0.12	43,43,43,43	0
57	MG	1A	3826	1/1	0.93	0.07	36,36,36,36	0
57	MG	2A	3479	1/1	0.93	0.07	50,50,50,50	0
57	MG	2A	3481	1/1	0.93	0.11	41,41,41,41	0
57	MG	1A	3475	1/1	0.93	0.07	41,41,41,41	0
57	MG	1a	3698	1/1	0.93	0.07	53,53,53,53	0
57	MG	1A	3476	1/1	0.93	0.07	41,41,41,41	0
57	MG	1A	3830	1/1	0.93	0.13	41,41,41,41	0
57	MG	2A	3489	1/1	0.93	0.14	34,34,34,34	0
57	MG	1A	3831	1/1	0.93	0.31	21,21,21,21	0
57	MG	2A	3491	1/1	0.93	0.08	34,34,34,34	0
57	MG	1a	3524	1/1	0.93	0.14	47,47,47,47	0
57	MG	1A	3360	1/1	0.93	0.09	31,31,31,31	0
57	MG	2A	3498	1/1	0.93	0.18	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3221	1/1	0.93	0.15	41,41,41,41	0
57	MG	2B	201	1/1	0.93	0.08	58,58,58,58	0
57	MG	1a	3526	1/1	0.93	0.16	35,35,35,35	0
57	MG	2A	3226	1/1	0.93	0.12	43,43,43,43	0
57	MG	1A	3835	1/1	0.93	0.10	33,33,33,33	0
57	MG	1a	3711	1/1	0.93	0.09	51,51,51,51	0
57	MG	1A	3174	1/1	0.93	0.09	25,25,25,25	0
57	MG	2B	209	1/1	0.93	0.18	40,40,40,40	0
57	MG	1A	3363	1/1	0.93	0.18	42,42,42,42	0
57	MG	1A	3364	1/1	0.93	0.09	30,30,30,30	0
57	MG	2A	3237	1/1	0.93	0.13	47,47,47,47	0
57	MG	2B	213	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3840	1/1	0.93	0.05	23,23,23,23	0
57	MG	1A	3482	1/1	0.93	0.13	37,37,37,37	0
57	MG	1A	4058	1/1	0.93	0.12	13,13,13,13	0
57	MG	1a	3539	1/1	0.93	0.36	54,54,54,54	0
57	MG	1A	3210	1/1	0.93	0.26	24,24,24,24	0
57	MG	1A	3212	1/1	0.93	0.12	34,34,34,34	0
57	MG	1A	4068	1/1	0.93	0.13	40,40,40,40	0
57	MG	1A	3049	1/1	0.93	0.12	14,14,14,14	0
57	MG	1A	4071	1/1	0.93	0.21	46,46,46,46	0
57	MG	1A	3852	1/1	0.93	0.07	30,30,30,30	0
57	MG	2E	307	1/1	0.93	0.12	36,36,36,36	0
57	MG	1A	3215	1/1	0.93	0.26	29,29,29,29	0
57	MG	1A	3181	1/1	0.93	0.06	43,43,43,43	0
57	MG	1n	101	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3542	1/1	0.93	0.10	33,33,33,33	0
57	MG	1A	3221	1/1	0.93	0.20	45,45,45,45	0
57	MG	1A	3671	1/1	0.93	0.15	15,15,15,15	0
57	MG	1A	3047	1/1	0.93	0.13	22,22,22,22	0
57	MG	1A	3296	1/1	0.93	0.23	21,21,21,21	0
57	MG	2F	307	1/1	0.93	0.25	42,42,42,42	0
57	MG	1A	3497	1/1	0.93	0.07	48,48,48,48	0
57	MG	1A	3298	1/1	0.93	0.07	18,18,18,18	0
57	MG	1a	3561	1/1	0.93	0.10	50,50,50,50	0
57	MG	1B	205	1/1	0.93	0.28	50,50,50,50	0
57	MG	1A	3227	1/1	0.93	0.24	21,21,21,21	0
57	MG	1A	3389	1/1	0.93	0.10	36,36,36,36	0
57	MG	2A	3274	1/1	0.93	0.16	51,51,51,51	0
57	MG	1A	3183	1/1	0.93	0.08	23,23,23,23	0
57	MG	2U	203	1/1	0.93	0.14	41,41,41,41	0
57	MG	1A	3394	1/1	0.93	0.12	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2V	201	1/1	0.93	0.27	42,42,42,42	0
57	MG	1A	3509	1/1	0.93	0.16	31,31,31,31	0
57	MG	2A	3006	1/1	0.93	0.14	45,45,45,45	0
57	MG	2W	202	1/1	0.93	0.16	43,43,43,43	0
57	MG	2W	203	1/1	0.93	0.14	46,46,46,46	0
57	MG	1A	3397	1/1	0.93	0.16	37,37,37,37	0
57	MG	1A	3700	1/1	0.93	0.10	41,41,41,41	0
57	MG	1A	3702	1/1	0.93	0.08	31,31,31,31	0
57	MG	1A	3398	1/1	0.93	0.08	39,39,39,39	0
57	MG	1A	3311	1/1	0.93	0.18	42,42,42,42	0
57	MG	1A	3517	1/1	0.93	0.17	25,25,25,25	0
57	MG	1A	3402	1/1	0.93	0.10	38,38,38,38	0
57	MG	2A	3588	1/1	0.93	0.11	17,17,17,17	0
57	MG	28	102	1/1	0.93	0.19	39,39,39,39	0
57	MG	2a	1601	1/1	0.93	0.21	45,45,45,45	0
57	MG	2A	3028	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3231	1/1	0.93	0.28	43,43,43,43	0
57	MG	2a	1605	1/1	0.93	0.16	49,49,49,49	0
57	MG	1A	3714	1/1	0.93	0.13	31,31,31,31	0
57	MG	1A	3406	1/1	0.93	0.07	32,32,32,32	0
57	MG	1A	3235	1/1	0.93	0.12	31,31,31,31	0
57	MG	1A	3243	1/1	0.93	0.10	34,34,34,34	0
57	MG	2A	3041	1/1	0.93	0.21	36,36,36,36	0
57	MG	1A	3727	1/1	0.93	0.16	38,38,38,38	0
57	MG	1A	3410	1/1	0.93	0.25	46,46,46,46	0
57	MG	2a	1622	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3729	1/1	0.93	0.10	30,30,30,30	0
57	MG	2a	1624	1/1	0.93	0.15	50,50,50,50	0
57	MG	1D	313	1/1	0.93	0.20	36,36,36,36	0
57	MG	2A	3053	1/1	0.93	0.08	36,36,36,36	0
57	MG	2A	3302	1/1	0.93	0.22	47,47,47,47	0
57	MG	2A	3054	1/1	0.93	0.13	38,38,38,38	0
57	MG	2A	3613	1/1	0.93	0.21	46,46,46,46	0
57	MG	2A	3055	1/1	0.93	0.14	58,58,58,58	0
57	MG	2A	3308	1/1	0.93	0.07	56,56,56,56	0
57	MG	1A	3731	1/1	0.93	0.09	32,32,32,32	0
57	MG	1A	3411	1/1	0.93	0.15	29,29,29,29	0
57	MG	2A	3062	1/1	0.93	0.24	38,38,38,38	0
57	MG	1A	3529	1/1	0.93	0.10	42,42,42,42	0
57	MG	1E	307	1/1	0.93	0.09	36,36,36,36	0
57	MG	1A	3530	1/1	0.93	0.28	27,27,27,27	0
57	MG	2a	1650	1/1	0.93	0.16	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3072	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3073	1/1	0.93	0.08	45,45,45,45	0
57	MG	2A	3074	1/1	0.93	0.16	40,40,40,40	0
57	MG	1E	313	1/1	0.93	0.13	46,46,46,46	0
57	MG	1F	303	1/1	0.93	0.17	14,14,14,14	0
57	MG	2a	1660	1/1	0.93	0.34	50,50,50,50	0
57	MG	1A	3532	1/1	0.93	0.09	18,18,18,18	0
57	MG	2A	3328	1/1	0.93	0.08	31,31,31,31	0
57	MG	1A	3413	1/1	0.93	0.09	21,21,21,21	0
57	MG	1F	309	1/1	0.93	0.04	15,15,15,15	0
57	MG	1A	3745	1/1	0.93	0.10	11,11,11,11	0
57	MG	1A	3186	1/1	0.93	0.06	41,41,41,41	0
57	MG	1A	3540	1/1	0.93	0.30	27,27,27,27	0
57	MG	1A	3940	1/1	0.93	0.14	39,39,39,39	0
57	MG	1a	3610	1/1	0.93	0.23	43,43,43,43	0
57	MG	2A	3092	1/1	0.93	0.20	48,48,48,48	0
57	MG	1a	3611	1/1	0.93	0.09	41,41,41,41	0
57	MG	1F	314	1/1	0.93	0.09	33,33,33,33	0
57	MG	1A	3415	1/1	0.93	0.29	43,43,43,43	0
57	MG	2a	1676	1/1	0.93	0.22	37,37,37,37	0
57	MG	2A	3342	1/1	0.93	0.10	50,50,50,50	0
57	MG	2A	3096	1/1	0.93	0.15	20,20,20,20	0
57	MG	1G	204	1/1	0.93	0.08	57,57,57,57	0
57	MG	1A	3417	1/1	0.93	0.08	58,58,58,58	0
57	MG	2a	1686	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	3558	1/1	0.93	0.25	42,42,42,42	0
57	MG	1A	3559	1/1	0.93	0.25	28,28,28,28	0
57	MG	1A	3424	1/1	0.93	0.10	20,20,20,20	0
57	MG	2A	3662	1/1	0.93	0.12	65,65,65,65	0
57	MG	2A	3106	1/1	0.93	0.28	52,52,52,52	0
57	MG	1A	3150	1/1	0.93	0.09	30,30,30,30	0
57	MG	1A	3948	1/1	0.93	0.16	42,42,42,42	0
57	MG	1A	3099	1/1	0.93	0.14	48,48,48,48	0
57	MG	2A	3674	1/1	0.93	0.09	26,26,26,26	0
57	MG	2a	1699	1/1	0.93	0.21	37,37,37,37	0
57	MG	1R	205	1/1	0.93	0.13	22,22,22,22	0
57	MG	2A	3113	1/1	0.93	0.12	46,46,46,46	0
57	MG	1a	3626	1/1	0.93	0.13	43,43,43,43	0
57	MG	2A	3359	1/1	0.93	0.07	53,53,53,53	0
57	MG	1A	3950	1/1	0.93	0.16	32,32,32,32	0
57	MG	1A	3567	1/1	0.93	0.10	26,26,26,26	0
57	MG	1a	3629	1/1	0.93	0.13	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3332	1/1	0.93	0.20	46,46,46,46	0
57	MG	2A	3684	1/1	0.93	0.11	24,24,24,24	0
57	MG	2a	1720	1/1	0.93	0.25	42,42,42,42	0
57	MG	1A	3569	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3196	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3126	1/1	0.93	0.11	46,46,46,46	0
57	MG	2a	1725	1/1	0.93	0.16	66,66,66,66	0
57	MG	2A	3691	1/1	0.93	0.20	59,59,59,59	0
57	MG	1a	3634	1/1	0.93	0.33	38,38,38,38	0
57	MG	1A	3436	1/1	0.93	0.16	45,45,45,45	0
57	MG	2A	3377	1/1	0.93	0.14	50,50,50,50	0
57	MG	2A	3695	1/1	0.93	0.08	45,45,45,45	0
57	MG	2A	3378	1/1	0.93	0.27	46,46,46,46	0
57	MG	2a	1734	1/1	0.93	0.22	46,46,46,46	0
57	MG	2a	1735	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3959	1/1	0.93	0.07	43,43,43,43	0
57	MG	2a	1737	1/1	0.93	0.18	38,38,38,38	0
57	MG	2a	1739	1/1	0.93	0.15	43,43,43,43	0
57	MG	1a	3637	1/1	0.93	0.14	44,44,44,44	0
57	MG	2a	1742	1/1	0.93	0.17	48,48,48,48	0
57	MG	2A	3702	1/1	0.93	0.10	28,28,28,28	0
57	MG	2a	1744	1/1	0.93	0.29	45,45,45,45	0
57	MG	1V	202	1/1	0.93	0.10	37,37,37,37	0
57	MG	2A	3384	1/1	0.93	0.21	41,41,41,41	0
57	MG	1a	3639	1/1	0.93	0.25	49,49,49,49	0
57	MG	1A	3438	1/1	0.93	0.11	32,32,32,32	0
57	MG	1A	3579	1/1	0.93	0.10	14,14,14,14	0
57	MG	1A	3963	1/1	0.93	0.08	9,9,9,9	0
57	MG	1A	3965	1/1	0.93	0.09	20,20,20,20	0
57	MG	1a	3648	1/1	0.93	0.15	46,46,46,46	0
57	MG	1A	3966	1/1	0.93	0.06	73,73,73,73	0
57	MG	2A	3394	1/1	0.93	0.20	41,41,41,41	0
57	MG	2A	3720	1/1	0.93	0.07	41,41,41,41	0
57	MG	2A	3721	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3334	1/1	0.93	0.08	22,22,22,22	0
57	MG	1A	3789	1/1	0.93	0.51	22,22,22,22	0
57	MG	2A	3398	1/1	0.93	0.07	33,33,33,33	0
57	MG	2A	3154	1/1	0.93	0.16	42,42,42,42	0
57	MG	2A	3404	1/1	0.93	0.20	41,41,41,41	0
57	MG	1A	3581	1/1	0.93	0.13	16,16,16,16	0
57	MG	2A	3406	1/1	0.93	0.18	40,40,40,40	0
57	MG	2A	3736	1/1	0.93	0.08	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3092	1/1	0.93	0.15	45,45,45,45	0
57	MG	1a	3658	1/1	0.93	0.14	46,46,46,46	0
57	MG	2A	3741	1/1	0.93	0.08	39,39,39,39	0
57	MG	2A	3409	1/1	0.93	0.12	45,45,45,45	0
57	MG	10	105	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3744	1/1	0.93	0.08	33,33,33,33	0
57	MG	2A	3411	1/1	0.93	0.14	52,52,52,52	0
57	MG	1A	3253	1/1	0.93	0.07	24,24,24,24	0
57	MG	2d	301	1/1	0.93	0.25	45,45,45,45	0
57	MG	2A	3415	1/1	0.93	0.15	44,44,44,44	0
57	MG	1A	3444	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	3340	1/1	0.93	0.19	33,33,33,33	0
57	MG	1A	3254	1/1	0.93	0.12	38,38,38,38	0
57	MG	1A	3259	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	3448	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3426	1/1	0.93	0.07	53,53,53,53	0
57	MG	1A	3160	1/1	0.93	0.27	16,16,16,16	0
57	MG	1A	3346	1/1	0.93	0.20	59,59,59,59	0
57	MG	1A	3805	1/1	0.93	0.12	59,59,59,59	0
57	MG	2A	3434	1/1	0.93	0.13	49,49,49,49	0
57	MG	1A	3347	1/1	0.93	0.12	27,27,27,27	0
57	MG	1A	3111	1/1	0.93	0.06	24,24,24,24	0
57	MG	2A	3183	1/1	0.93	0.08	47,47,47,47	0
57	MG	2A	3186	1/1	0.93	0.19	50,50,50,50	0
57	MG	2A	3443	1/1	0.93	0.29	52,52,52,52	0
57	MG	17	105	1/1	0.94	0.06	41,41,41,41	0
57	MG	18	101	1/1	0.94	0.24	47,47,47,47	0
57	MG	18	102	1/1	0.94	0.11	27,27,27,27	0
57	MG	2A	3087	1/1	0.94	0.14	45,45,45,45	0
57	MG	1A	3013	1/1	0.94	0.12	17,17,17,17	0
57	MG	1a	3643	1/1	0.94	0.11	26,26,26,26	0
57	MG	1A	4057	1/1	0.94	0.09	28,28,28,28	0
57	MG	2A	3543	1/1	0.94	0.09	24,24,24,24	0
57	MG	1A	3617	1/1	0.94	0.06	24,24,24,24	0
57	MG	1A	4060	1/1	0.94	0.08	38,38,38,38	0
57	MG	2B	204	1/1	0.94	0.18	50,50,50,50	0
57	MG	2A	3547	1/1	0.94	0.16	44,44,44,44	0
57	MG	1a	3505	1/1	0.94	0.13	46,46,46,46	0
57	MG	1A	4062	1/1	0.94	0.11	36,36,36,36	0
57	MG	1A	3776	1/1	0.94	0.08	10,10,10,10	0
57	MG	1A	3094	1/1	0.94	0.08	31,31,31,31	0
57	MG	1A	3893	1/1	0.94	0.15	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3898	1/1	0.94	0.09	43,43,43,43	0
57	MG	2A	3556	1/1	0.94	0.11	22,22,22,22	0
57	MG	2B	214	1/1	0.94	0.15	40,40,40,40	0
57	MG	2A	3100	1/1	0.94	0.11	44,44,44,44	0
57	MG	2A	3563	1/1	0.94	0.07	38,38,38,38	0
57	MG	1A	3625	1/1	0.94	0.09	46,46,46,46	0
57	MG	2D	301	1/1	0.94	0.14	35,35,35,35	0
57	MG	2A	3306	1/1	0.94	0.08	33,33,33,33	0
57	MG	1A	3781	1/1	0.94	0.10	29,29,29,29	0
57	MG	1a	3663	1/1	0.94	0.06	51,51,51,51	0
57	MG	1A	3188	1/1	0.94	0.37	23,23,23,23	0
57	MG	1A	3190	1/1	0.94	0.09	29,29,29,29	0
57	MG	2A	3572	1/1	0.94	0.11	36,36,36,36	0
57	MG	2A	3313	1/1	0.94	0.17	42,42,42,42	0
57	MG	1a	3669	1/1	0.94	0.19	50,50,50,50	0
57	MG	1a	3519	1/1	0.94	0.06	37,37,37,37	0
57	MG	2A	3580	1/1	0.94	0.13	22,22,22,22	0
57	MG	1A	3909	1/1	0.94	0.12	26,26,26,26	0
57	MG	2A	3318	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3111	1/1	0.94	0.18	38,38,38,38	0
57	MG	2A	3320	1/1	0.94	0.07	41,41,41,41	0
57	MG	1A	3913	1/1	0.94	0.10	47,47,47,47	0
57	MG	1A	3118	1/1	0.94	0.31	36,36,36,36	0
57	MG	1a	3674	1/1	0.94	0.26	45,45,45,45	0
57	MG	1A	3156	1/1	0.94	0.17	32,32,32,32	0
57	MG	1A	3521	1/1	0.94	0.15	30,30,30,30	0
57	MG	1A	3388	1/1	0.94	0.30	32,32,32,32	0
57	MG	2A	3329	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3280	1/1	0.94	0.10	37,37,37,37	0
57	MG	1A	3642	1/1	0.94	0.09	29,29,29,29	0
57	MG	2A	3605	1/1	0.94	0.17	48,48,48,48	0
57	MG	2T	204	1/1	0.94	0.12	48,48,48,48	0
57	MG	2A	3124	1/1	0.94	0.15	37,37,37,37	0
57	MG	1A	3390	1/1	0.94	0.06	33,33,33,33	0
57	MG	1A	3926	1/1	0.94	0.06	48,48,48,48	0
57	MG	2A	3130	1/1	0.94	0.19	53,53,53,53	0
57	MG	1A	3391	1/1	0.94	0.09	38,38,38,38	0
57	MG	2A	3133	1/1	0.94	0.20	24,24,24,24	0
57	MG	2A	3135	1/1	0.94	0.23	48,48,48,48	0
57	MG	1A	3342	1/1	0.94	0.14	43,43,43,43	0
57	MG	1a	3687	1/1	0.94	0.15	34,34,34,34	0
57	MG	2A	3620	1/1	0.94	0.28	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3138	1/1	0.94	0.16	26,26,26,26	0
57	MG	1A	3932	1/1	0.94	0.05	24,24,24,24	0
57	MG	1A	3232	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3395	1/1	0.94	0.10	37,37,37,37	0
57	MG	2A	3625	1/1	0.94	0.20	37,37,37,37	0
57	MG	1A	3663	1/1	0.94	0.12	6,6,6,6	0
57	MG	1A	3533	1/1	0.94	0.26	29,29,29,29	0
57	MG	1A	3534	1/1	0.94	0.18	21,21,21,21	0
57	MG	1A	3802	1/1	0.94	0.16	45,45,45,45	0
57	MG	1A	3396	1/1	0.94	0.20	24,24,24,24	0
57	MG	2A	3149	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	3021	1/1	0.94	0.17	31,31,31,31	0
57	MG	2a	1608	1/1	0.94	0.14	56,56,56,56	0
57	MG	1A	3462	1/1	0.94	0.08	38,38,38,38	0
57	MG	1A	3064	1/1	0.94	0.10	37,37,37,37	0
57	MG	2a	1612	1/1	0.94	0.21	36,36,36,36	0
57	MG	2A	3356	1/1	0.94	0.11	50,50,50,50	0
57	MG	2A	3156	1/1	0.94	0.14	37,37,37,37	0
57	MG	2A	3358	1/1	0.94	0.19	59,59,59,59	0
57	MG	1A	3552	1/1	0.94	0.13	26,26,26,26	0
57	MG	2a	1621	1/1	0.94	0.07	36,36,36,36	0
57	MG	1a	3554	1/1	0.94	0.13	55,55,55,55	0
57	MG	1a	3706	1/1	0.94	0.06	60,60,60,60	0
57	MG	1A	3678	1/1	0.94	0.09	17,17,17,17	0
57	MG	1A	3679	1/1	0.94	0.10	49,49,49,49	0
57	MG	2a	1626	1/1	0.94	0.13	45,45,45,45	0
57	MG	1a	3709	1/1	0.94	0.15	53,53,53,53	0
57	MG	2A	3167	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3650	1/1	0.94	0.13	41,41,41,41	0
57	MG	1a	3558	1/1	0.94	0.32	62,62,62,62	0
57	MG	2A	3652	1/1	0.94	0.06	37,37,37,37	0
57	MG	1D	301	1/1	0.94	0.18	24,24,24,24	0
57	MG	1D	302	1/1	0.94	0.08	25,25,25,25	0
57	MG	2a	1637	1/1	0.94	0.34	49,49,49,49	0
57	MG	2a	1640	1/1	0.94	0.26	39,39,39,39	0
57	MG	2A	3375	1/1	0.94	0.19	24,24,24,24	0
57	MG	2a	1644	1/1	0.94	0.29	40,40,40,40	0
57	MG	1D	305	1/1	0.94	0.15	30,30,30,30	0
57	MG	2A	3175	1/1	0.94	0.07	48,48,48,48	0
57	MG	2A	3379	1/1	0.94	0.24	35,35,35,35	0
57	MG	1D	309	1/1	0.94	0.13	28,28,28,28	0
57	MG	1A	3682	1/1	0.94	0.10	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3285	1/1	0.94	0.10	33,33,33,33	0
57	MG	2a	1652	1/1	0.94	0.13	40,40,40,40	0
57	MG	2A	3179	1/1	0.94	0.09	53,53,53,53	0
57	MG	1A	3469	1/1	0.94	0.13	28,28,28,28	0
57	MG	2a	1657	1/1	0.94	0.20	33,33,33,33	0
57	MG	1A	3289	1/1	0.94	0.14	40,40,40,40	0
57	MG	1A	3561	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3471	1/1	0.94	0.17	51,51,51,51	0
57	MG	1A	3404	1/1	0.94	0.19	41,41,41,41	0
57	MG	1A	3694	1/1	0.94	0.06	10,10,10,10	0
57	MG	2A	3190	1/1	0.94	0.12	39,39,39,39	0
57	MG	2A	3393	1/1	0.94	0.16	46,46,46,46	0
57	MG	1A	3348	1/1	0.94	0.07	41,41,41,41	0
57	MG	1A	3135	1/1	0.94	0.35	26,26,26,26	0
57	MG	1A	3044	1/1	0.94	0.07	19,19,19,19	0
57	MG	2A	3397	1/1	0.94	0.16	42,42,42,42	0
57	MG	1A	3169	1/1	0.94	0.09	36,36,36,36	0
57	MG	2A	3401	1/1	0.94	0.08	38,38,38,38	0
57	MG	2A	3195	1/1	0.94	0.10	24,24,24,24	0
57	MG	1A	3140	1/1	0.94	0.10	35,35,35,35	0
57	MG	1p	101	1/1	0.94	0.14	44,44,44,44	0
57	MG	2a	1674	1/1	0.94	0.24	55,55,55,55	0
57	MG	2a	1675	1/1	0.94	0.18	57,57,57,57	0
57	MG	1A	3055	1/1	0.94	0.20	35,35,35,35	0
57	MG	2A	3200	1/1	0.94	0.10	68,68,68,68	0
57	MG	1A	3412	1/1	0.94	0.08	30,30,30,30	0
57	MG	2a	1679	1/1	0.94	0.12	45,45,45,45	0
57	MG	1a	3588	1/1	0.94	0.06	45,45,45,45	0
57	MG	1A	3975	1/1	0.94	0.06	38,38,38,38	0
57	MG	1A	3578	1/1	0.94	0.10	36,36,36,36	0
57	MG	2a	1687	1/1	0.94	0.29	43,43,43,43	0
57	MG	1A	3252	1/1	0.94	0.13	52,52,52,52	0
57	MG	1A	3091	1/1	0.94	0.12	37,37,37,37	0
57	MG	1A	3984	1/1	0.94	0.09	23,23,23,23	0
57	MG	1x	109	1/1	0.94	0.16	39,39,39,39	0
57	MG	2A	3706	1/1	0.94	0.12	64,64,64,64	0
57	MG	2A	3211	1/1	0.94	0.29	38,38,38,38	0
57	MG	1A	3358	1/1	0.94	0.09	35,35,35,35	0
57	MG	2A	3710	1/1	0.94	0.16	46,46,46,46	0
57	MG	1A	3842	1/1	0.94	0.16	31,31,31,31	0
57	MG	2a	1697	1/1	0.94	0.26	55,55,55,55	0
57	MG	1x	113	1/1	0.94	0.16	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3428	1/1	0.94	0.15	35,35,35,35	0
57	MG	2a	1704	1/1	0.94	0.16	51,51,51,51	0
57	MG	1N	206	1/1	0.94	0.09	32,32,32,32	0
57	MG	2a	1709	1/1	0.94	0.22	44,44,44,44	0
57	MG	2A	3003	1/1	0.94	0.25	38,38,38,38	0
57	MG	2A	3219	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3992	1/1	0.94	0.12	25,25,25,25	0
57	MG	1A	3994	1/1	0.94	0.05	29,29,29,29	0
57	MG	2A	3725	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3727	1/1	0.94	0.17	25,25,25,25	0
57	MG	2A	3437	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3438	1/1	0.94	0.34	43,43,43,43	0
57	MG	2A	3439	1/1	0.94	0.15	48,48,48,48	0
57	MG	2A	3731	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3222	1/1	0.94	0.12	29,29,29,29	0
57	MG	1P	202	1/1	0.94	0.51	21,21,21,21	0
57	MG	1A	3995	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3997	1/1	0.94	0.12	50,50,50,50	0
57	MG	2a	1729	1/1	0.94	0.16	58,58,58,58	0
57	MG	2A	3229	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	3843	1/1	0.94	0.08	26,26,26,26	0
57	MG	1A	3145	1/1	0.94	0.11	25,25,25,25	0
57	MG	2A	3233	1/1	0.94	0.17	41,41,41,41	0
57	MG	1A	3418	1/1	0.94	0.15	27,27,27,27	0
57	MG	1A	3420	1/1	0.94	0.10	29,29,29,29	0
57	MG	2A	3456	1/1	0.94	0.27	46,46,46,46	0
57	MG	1A	3849	1/1	0.94	0.15	11,11,11,11	0
57	MG	1A	3851	1/1	0.94	0.11	19,19,19,19	0
57	MG	1A	3309	1/1	0.94	0.14	39,39,39,39	0
57	MG	2A	3751	1/1	0.94	0.23	63,63,63,63	0
57	MG	2A	3240	1/1	0.94	0.17	41,41,41,41	0
57	MG	1A	3495	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	3426	1/1	0.94	0.14	35,35,35,35	0
57	MG	2a	1746	1/1	0.94	0.23	49,49,49,49	0
57	MG	2A	3036	1/1	0.94	0.15	33,33,33,33	0
57	MG	1A	3737	1/1	0.94	0.09	9,9,9,9	0
57	MG	2A	3248	1/1	0.94	0.17	43,43,43,43	0
57	MG	2A	3473	1/1	0.94	0.13	38,38,38,38	0
57	MG	2A	3762	1/1	0.94	0.11	56,56,56,56	0
57	MG	1A	3861	1/1	0.94	0.11	12,12,12,12	0
57	MG	2A	3765	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3040	1/1	0.94	0.17	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1758	1/1	0.94	0.20	47,47,47,47	0
57	MG	1A	3255	1/1	0.94	0.20	52,52,52,52	0
57	MG	2A	3042	1/1	0.94	0.23	56,56,56,56	0
57	MG	2A	3045	1/1	0.94	0.11	38,38,38,38	0
57	MG	2A	3257	1/1	0.94	0.21	45,45,45,45	0
57	MG	1W	204	1/1	0.94	0.17	28,28,28,28	0
57	MG	1A	3595	1/1	0.94	0.12	31,31,31,31	0
57	MG	2A	3485	1/1	0.94	0.11	29,29,29,29	0
57	MG	1A	4023	1/1	0.94	0.12	16,16,16,16	0
57	MG	2A	3261	1/1	0.94	0.14	44,44,44,44	0
57	MG	2A	3050	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	3740	1/1	0.94	0.10	21,21,21,21	0
57	MG	1A	3256	1/1	0.94	0.25	57,57,57,57	0
57	MG	1A	3258	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3433	1/1	0.94	0.26	54,54,54,54	0
57	MG	10	103	1/1	0.94	0.13	52,52,52,52	0
57	MG	1A	3601	1/1	0.94	0.07	29,29,29,29	0
57	MG	2A	3270	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3271	1/1	0.94	0.10	53,53,53,53	0
57	MG	1A	3058	1/1	0.94	0.12	32,32,32,32	0
57	MG	1A	3873	1/1	0.94	0.13	39,39,39,39	0
57	MG	1A	3505	1/1	0.94	0.21	25,25,25,25	0
57	MG	1A	3506	1/1	0.94	0.27	30,30,30,30	0
57	MG	1A	4041	1/1	0.94	0.07	29,29,29,29	0
57	MG	1A	3877	1/1	0.94	0.08	35,35,35,35	0
57	MG	2A	3809	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3319	1/1	0.94	0.13	32,32,32,32	0
57	MG	1A	3216	1/1	0.94	0.11	30,30,30,30	0
57	MG	1A	3263	1/1	0.94	0.21	37,37,37,37	0
57	MG	2A	3516	1/1	0.94	0.11	31,31,31,31	0
57	MG	2A	3517	1/1	0.94	0.08	33,33,33,33	0
57	MG	1A	3771	1/1	0.94	0.08	22,22,22,22	0
57	MG	2A	3520	1/1	0.94	0.07	25,25,25,25	0
57	MG	2A	3081	1/1	0.94	0.22	61,61,61,61	0
57	MG	2A	3526	1/1	0.94	0.10	35,35,35,35	0
57	MG	2A	3082	1/1	0.94	0.05	42,42,42,42	0
57	MG	2A	3284	1/1	0.94	0.12	41,41,41,41	0
57	MG	18	105	1/1	0.95	0.09	30,30,30,30	0
57	MG	2A	3462	1/1	0.95	0.18	50,50,50,50	0
57	MG	1A	3154	1/1	0.95	0.21	22,22,22,22	0
57	MG	1a	3713	1/1	0.95	0.06	42,42,42,42	0
57	MG	2A	3465	1/1	0.95	0.07	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3067	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3105	1/1	0.95	0.18	23,23,23,23	0
57	MG	1A	4024	1/1	0.95	0.08	19,19,19,19	0
57	MG	2A	3224	1/1	0.95	0.14	46,46,46,46	0
57	MG	2A	3225	1/1	0.95	0.04	45,45,45,45	0
57	MG	1A	3681	1/1	0.95	0.14	42,42,42,42	0
57	MG	2A	3227	1/1	0.95	0.12	42,42,42,42	0
57	MG	1A	4026	1/1	0.95	0.10	28,28,28,28	0
57	MG	2A	3478	1/1	0.95	0.14	38,38,38,38	0
57	MG	1A	3441	1/1	0.95	0.13	22,22,22,22	0
57	MG	2A	3230	1/1	0.95	0.22	57,57,57,57	0
57	MG	1A	4028	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3683	1/1	0.95	0.07	30,30,30,30	0
57	MG	2A	3814	1/1	0.95	0.06	37,37,37,37	0
57	MG	1a	3512	1/1	0.95	0.13	12,12,12,12	0
57	MG	2A	3486	1/1	0.95	0.09	47,47,47,47	0
57	MG	2A	3818	1/1	0.95	0.15	31,31,31,31	0
57	MG	1A	3684	1/1	0.95	0.14	45,45,45,45	0
57	MG	1A	3286	1/1	0.95	0.20	47,47,47,47	0
57	MG	1a	3516	1/1	0.95	0.08	67,67,67,67	0
57	MG	1A	4035	1/1	0.95	0.06	36,36,36,36	0
57	MG	1A	3846	1/1	0.95	0.19	24,24,24,24	0
57	MG	2A	3825	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3287	1/1	0.95	0.17	21,21,21,21	0
57	MG	2A	3241	1/1	0.95	0.13	30,30,30,30	0
57	MG	2A	3242	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3106	1/1	0.95	0.15	13,13,13,13	0
57	MG	2A	3244	1/1	0.95	0.11	52,52,52,52	0
57	MG	1t	201	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3161	1/1	0.95	0.09	43,43,43,43	0
57	MG	1a	3522	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3366	1/1	0.95	0.09	29,29,29,29	0
57	MG	1A	3548	1/1	0.95	0.09	26,26,26,26	0
57	MG	2A	3250	1/1	0.95	0.16	39,39,39,39	0
57	MG	2A	3251	1/1	0.95	0.16	41,41,41,41	0
57	MG	2B	205	1/1	0.95	0.12	55,55,55,55	0
57	MG	1x	104	1/1	0.95	0.30	38,38,38,38	0
57	MG	1A	4045	1/1	0.95	0.07	26,26,26,26	0
57	MG	1A	4046	1/1	0.95	0.06	25,25,25,25	0
57	MG	1A	3162	1/1	0.95	0.20	43,43,43,43	0
57	MG	1A	3695	1/1	0.95	0.18	46,46,46,46	0
57	MG	1A	4051	1/1	0.95	0.12	12,12,12,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3163	1/1	0.95	0.08	32,32,32,32	0
57	MG	2A	3522	1/1	0.95	0.11	28,28,28,28	0
57	MG	1A	3555	1/1	0.95	0.15	42,42,42,42	0
57	MG	1A	3556	1/1	0.95	0.08	51,51,51,51	0
57	MG	1A	3370	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3293	1/1	0.95	0.09	24,24,24,24	0
57	MG	1A	3452	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3532	1/1	0.95	0.18	53,53,53,53	0
57	MG	1A	3373	1/1	0.95	0.05	37,37,37,37	0
57	MG	2A	3534	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3375	1/1	0.95	0.21	12,12,12,12	0
57	MG	2A	3009	1/1	0.95	0.08	30,30,30,30	0
57	MG	1A	3455	1/1	0.95	0.09	22,22,22,22	0
57	MG	1A	3715	1/1	0.95	0.08	8,8,8,8	0
57	MG	2E	306	1/1	0.95	0.12	24,24,24,24	0
57	MG	1a	3545	1/1	0.95	0.13	58,58,58,58	0
57	MG	1a	3546	1/1	0.95	0.24	39,39,39,39	0
57	MG	1a	3547	1/1	0.95	0.17	58,58,58,58	0
57	MG	2A	3545	1/1	0.95	0.16	28,28,28,28	0
57	MG	1A	3716	1/1	0.95	0.10	17,17,17,17	0
57	MG	1A	4070	1/1	0.95	0.16	45,45,45,45	0
57	MG	2A	3027	1/1	0.95	0.20	34,34,34,34	0
57	MG	1A	3718	1/1	0.95	0.05	11,11,11,11	0
57	MG	2A	3550	1/1	0.95	0.08	13,13,13,13	0
57	MG	2A	3029	1/1	0.95	0.19	31,31,31,31	0
57	MG	1A	3223	1/1	0.95	0.23	28,28,28,28	0
57	MG	1A	3457	1/1	0.95	0.17	29,29,29,29	0
57	MG	2Q	202	1/1	0.95	0.17	37,37,37,37	0
57	MG	2A	3032	1/1	0.95	0.06	40,40,40,40	0
57	MG	1A	3880	1/1	0.95	0.15	27,27,27,27	0
57	MG	1A	3224	1/1	0.95	0.12	41,41,41,41	0
57	MG	1A	3226	1/1	0.95	0.14	24,24,24,24	0
57	MG	1A	4078	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	4079	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3887	1/1	0.95	0.13	21,21,21,21	0
57	MG	1A	3300	1/1	0.95	0.15	34,34,34,34	0
57	MG	2A	3569	1/1	0.95	0.14	53,53,53,53	0
57	MG	2A	3289	1/1	0.95	0.23	49,49,49,49	0
57	MG	2A	3043	1/1	0.95	0.13	38,38,38,38	0
57	MG	2A	3044	1/1	0.95	0.15	47,47,47,47	0
57	MG	1A	3301	1/1	0.95	0.22	40,40,40,40	0
57	MG	2A	3293	1/1	0.95	0.08	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	202	1/1	0.95	0.11	32,32,32,32	0
57	MG	1A	3730	1/1	0.95	0.08	9,9,9,9	0
57	MG	21	102	1/1	0.95	0.12	39,39,39,39	0
57	MG	23	101	1/1	0.95	0.15	47,47,47,47	0
57	MG	1A	3576	1/1	0.95	0.12	48,48,48,48	0
57	MG	1A	3577	1/1	0.95	0.10	18,18,18,18	0
57	MG	1A	3304	1/1	0.95	0.17	35,35,35,35	0
57	MG	1A	3895	1/1	0.95	0.16	26,26,26,26	0
57	MG	1a	3571	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3897	1/1	0.95	0.08	43,43,43,43	0
57	MG	1B	211	1/1	0.95	0.12	32,32,32,32	0
57	MG	2A	3592	1/1	0.95	0.08	23,23,23,23	0
57	MG	1A	3040	1/1	0.95	0.18	20,20,20,20	0
57	MG	1B	216	1/1	0.95	0.07	29,29,29,29	0
57	MG	2a	1604	1/1	0.95	0.18	44,44,44,44	0
57	MG	2A	3307	1/1	0.95	0.09	61,61,61,61	0
57	MG	2A	3598	1/1	0.95	0.14	48,48,48,48	0
57	MG	1A	3387	1/1	0.95	0.08	29,29,29,29	0
57	MG	2A	3600	1/1	0.95	0.15	29,29,29,29	0
57	MG	2A	3309	1/1	0.95	0.17	40,40,40,40	0
57	MG	1B	220	1/1	0.95	0.09	27,27,27,27	0
57	MG	2a	1613	1/1	0.95	0.21	44,44,44,44	0
57	MG	1B	221	1/1	0.95	0.08	23,23,23,23	0
57	MG	1a	3582	1/1	0.95	0.21	36,36,36,36	0
57	MG	2a	1616	1/1	0.95	0.09	45,45,45,45	0
57	MG	1a	3583	1/1	0.95	0.10	33,33,33,33	0
57	MG	1A	3043	1/1	0.95	0.07	22,22,22,22	0
57	MG	1A	3582	1/1	0.95	0.08	37,37,37,37	0
57	MG	1a	3586	1/1	0.95	0.14	59,59,59,59	0
57	MG	2A	3079	1/1	0.95	0.08	44,44,44,44	0
57	MG	1a	3587	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3614	1/1	0.95	0.17	37,37,37,37	0
57	MG	1A	3902	1/1	0.95	0.10	27,27,27,27	0
57	MG	2A	3617	1/1	0.95	0.17	46,46,46,46	0
57	MG	2a	1629	1/1	0.95	0.12	39,39,39,39	0
57	MG	2A	3618	1/1	0.95	0.20	46,46,46,46	0
57	MG	1B	225	1/1	0.95	0.15	50,50,50,50	0
57	MG	1B	226	1/1	0.95	0.10	41,41,41,41	0
57	MG	2A	3323	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3308	1/1	0.95	0.13	27,27,27,27	0
57	MG	1A	3474	1/1	0.95	0.23	34,34,34,34	0
57	MG	1A	3750	1/1	0.95	0.08	10,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1638	1/1	0.95	0.22	37,37,37,37	0
57	MG	2A	3327	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3015	1/1	0.95	0.19	28,28,28,28	0
57	MG	1A	3755	1/1	0.95	0.05	11,11,11,11	0
57	MG	1B	234	1/1	0.95	0.08	54,54,54,54	0
57	MG	1A	3310	1/1	0.95	0.05	28,28,28,28	0
57	MG	1A	3168	1/1	0.95	0.16	27,27,27,27	0
57	MG	1A	3046	1/1	0.95	0.11	27,27,27,27	0
57	MG	1A	3920	1/1	0.95	0.11	48,48,48,48	0
57	MG	1A	3922	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3764	1/1	0.95	0.09	38,38,38,38	0
57	MG	2a	1654	1/1	0.95	0.28	31,31,31,31	0
57	MG	1A	3114	1/1	0.95	0.20	24,24,24,24	0
57	MG	2A	3636	1/1	0.95	0.10	50,50,50,50	0
57	MG	1D	303	1/1	0.95	0.22	31,31,31,31	0
57	MG	1A	3766	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3594	1/1	0.95	0.07	18,18,18,18	0
57	MG	1A	3929	1/1	0.95	0.11	44,44,44,44	0
57	MG	1A	3085	1/1	0.95	0.20	26,26,26,26	0
57	MG	2A	3344	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3318	1/1	0.95	0.09	38,38,38,38	0
57	MG	1A	3245	1/1	0.95	0.21	32,32,32,32	0
57	MG	1A	3774	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3935	1/1	0.95	0.09	16,16,16,16	0
57	MG	1A	3179	1/1	0.95	0.17	29,29,29,29	0
57	MG	1A	3937	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3324	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	3602	1/1	0.95	0.08	9,9,9,9	0
57	MG	1A	3403	1/1	0.95	0.13	48,48,48,48	0
57	MG	1F	307	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3490	1/1	0.95	0.16	32,32,32,32	0
57	MG	2A	3659	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3782	1/1	0.95	0.06	27,27,27,27	0
57	MG	1A	3608	1/1	0.95	0.07	20,20,20,20	0
57	MG	1A	3609	1/1	0.95	0.09	21,21,21,21	0
57	MG	1A	3180	1/1	0.95	0.10	30,30,30,30	0
57	MG	2A	3664	1/1	0.95	0.07	53,53,53,53	0
57	MG	2a	1680	1/1	0.95	0.20	41,41,41,41	0
57	MG	2A	3666	1/1	0.95	0.14	44,44,44,44	0
57	MG	2a	1682	1/1	0.95	0.27	46,46,46,46	0
57	MG	2A	3667	1/1	0.95	0.11	19,19,19,19	0
57	MG	2a	1684	1/1	0.95	0.25	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3327	1/1	0.95	0.22	40,40,40,40	0
57	MG	1G	201	1/1	0.95	0.12	30,30,30,30	0
57	MG	2A	3129	1/1	0.95	0.09	37,37,37,37	0
57	MG	1G	202	1/1	0.95	0.13	40,40,40,40	0
57	MG	1A	3117	1/1	0.95	0.16	28,28,28,28	0
57	MG	2A	3368	1/1	0.95	0.26	37,37,37,37	0
57	MG	1A	3407	1/1	0.95	0.12	46,46,46,46	0
57	MG	1a	3633	1/1	0.95	0.24	36,36,36,36	0
57	MG	1G	205	1/1	0.95	0.10	40,40,40,40	0
57	MG	1H	201	1/1	0.95	0.17	39,39,39,39	0
57	MG	2A	3374	1/1	0.95	0.15	33,33,33,33	0
57	MG	1A	3016	1/1	0.95	0.24	32,32,32,32	0
57	MG	2a	1698	1/1	0.95	0.19	42,42,42,42	0
57	MG	2A	3376	1/1	0.95	0.07	29,29,29,29	0
57	MG	1A	3615	1/1	0.95	0.12	14,14,14,14	0
57	MG	2a	1701	1/1	0.95	0.18	46,46,46,46	0
57	MG	1N	202	1/1	0.95	0.14	29,29,29,29	0
57	MG	2a	1705	1/1	0.95	0.15	43,43,43,43	0
57	MG	1A	3616	1/1	0.95	0.07	18,18,18,18	0
57	MG	2a	1707	1/1	0.95	0.15	27,27,27,27	0
57	MG	2a	1708	1/1	0.95	0.11	41,41,41,41	0
57	MG	1A	3019	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	3618	1/1	0.95	0.07	14,14,14,14	0
57	MG	2A	3382	1/1	0.95	0.11	46,46,46,46	0
57	MG	1O	203	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	3185	1/1	0.95	0.16	23,23,23,23	0
57	MG	1A	3796	1/1	0.95	0.08	27,27,27,27	0
57	MG	2A	3148	1/1	0.95	0.29	49,49,49,49	0
57	MG	2a	1718	1/1	0.95	0.11	42,42,42,42	0
57	MG	2A	3699	1/1	0.95	0.10	56,56,56,56	0
57	MG	1A	3127	1/1	0.95	0.13	46,46,46,46	0
57	MG	2A	3701	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3051	1/1	0.95	0.10	32,32,32,32	0
57	MG	1R	201	1/1	0.95	0.09	40,40,40,40	0
57	MG	1R	202	1/1	0.95	0.13	22,22,22,22	0
57	MG	1A	3799	1/1	0.95	0.07	38,38,38,38	0
57	MG	2a	1727	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3132	1/1	0.95	0.07	20,20,20,20	0
57	MG	1A	3004	1/1	0.95	0.08	11,11,11,11	0
57	MG	1T	201	1/1	0.95	0.19	38,38,38,38	0
57	MG	1A	3971	1/1	0.95	0.15	43,43,43,43	0
57	MG	1A	3023	1/1	0.95	0.13	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3712	1/1	0.95	0.08	20,20,20,20	0
57	MG	1A	3633	1/1	0.95	0.08	9,9,9,9	0
57	MG	2A	3165	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3717	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3402	1/1	0.95	0.17	29,29,29,29	0
57	MG	2a	1738	1/1	0.95	0.14	37,37,37,37	0
57	MG	1a	3665	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3974	1/1	0.95	0.11	36,36,36,36	0
57	MG	1A	3634	1/1	0.95	0.07	14,14,14,14	0
57	MG	2A	3722	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3195	1/1	0.95	0.10	28,28,28,28	0
57	MG	1A	3262	1/1	0.95	0.13	35,35,35,35	0
57	MG	1A	3980	1/1	0.95	0.08	14,14,14,14	0
57	MG	1A	3419	1/1	0.95	0.19	28,28,28,28	0
57	MG	2a	1748	1/1	0.95	0.18	43,43,43,43	0
57	MG	2a	1749	1/1	0.95	0.13	61,61,61,61	0
57	MG	1W	201	1/1	0.95	0.13	24,24,24,24	0
57	MG	1A	3983	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3009	1/1	0.95	0.05	12,12,12,12	0
57	MG	2A	3413	1/1	0.95	0.16	41,41,41,41	0
57	MG	1A	3643	1/1	0.95	0.08	24,24,24,24	0
57	MG	1a	3678	1/1	0.95	0.09	34,34,34,34	0
57	MG	1A	3012	1/1	0.95	0.11	18,18,18,18	0
57	MG	2A	3738	1/1	0.95	0.10	58,58,58,58	0
57	MG	1A	3647	1/1	0.95	0.12	10,10,10,10	0
57	MG	1A	3516	1/1	0.95	0.09	11,11,11,11	0
57	MG	1A	3001	1/1	0.95	0.07	20,20,20,20	0
57	MG	1A	3202	1/1	0.95	0.08	11,11,11,11	0
57	MG	2A	3427	1/1	0.95	0.20	42,42,42,42	0
57	MG	1A	3661	1/1	0.95	0.10	16,16,16,16	0
57	MG	1A	3429	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3431	1/1	0.95	0.08	30,30,30,30	0
57	MG	1A	3095	1/1	0.95	0.15	11,11,11,11	0
57	MG	10	108	1/1	0.95	0.09	25,25,25,25	0
57	MG	1A	4005	1/1	0.95	0.06	33,33,33,33	0
57	MG	1A	3431	1/1	0.95	0.09	32,32,32,32	0
57	MG	1A	3666	1/1	0.95	0.07	10,10,10,10	0
57	MG	1A	4008	1/1	0.95	0.07	30,30,30,30	0
57	MG	2A	3756	1/1	0.95	0.12	45,45,45,45	0
57	MG	1a	3694	1/1	0.95	0.12	36,36,36,36	0
57	MG	13	103	1/1	0.95	0.07	32,32,32,32	0
57	MG	13	104	1/1	0.95	0.09	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3760	1/1	0.95	0.10	39,39,39,39	0
57	MG	1A	3096	1/1	0.95	0.09	26,26,26,26	0
57	MG	2d	302	1/1	0.95	0.13	48,48,48,48	0
57	MG	15	3208	1/1	0.95	0.11	20,20,20,20	0
57	MG	2A	3763	1/1	0.95	0.10	45,45,45,45	0
57	MG	1a	3700	1/1	0.95	0.13	28,28,28,28	0
57	MG	1A	3147	1/1	0.95	0.13	18,18,18,18	0
57	MG	2A	3447	1/1	0.95	0.20	40,40,40,40	0
57	MG	2A	3449	1/1	0.95	0.11	37,37,37,37	0
57	MG	2k	201	1/1	0.95	0.14	45,45,45,45	0
57	MG	1A	4011	1/1	0.95	0.08	17,17,17,17	0
57	MG	2A	3451	1/1	0.95	0.16	46,46,46,46	0
57	MG	16	103	1/1	0.95	0.12	39,39,39,39	0
57	MG	2t	201	1/1	0.95	0.27	48,48,48,48	0
57	MG	2A	3775	1/1	0.95	0.10	23,23,23,23	0
57	MG	1A	3014	1/1	0.95	0.06	17,17,17,17	0
57	MG	1A	4017	1/1	0.95	0.11	41,41,41,41	0
57	MG	1A	3834	1/1	0.95	0.07	33,33,33,33	0
57	MG	2x	107	1/1	0.95	0.14	60,60,60,60	0
57	MG	1A	3066	1/1	0.95	0.08	25,25,25,25	0
57	MG	2A	3216	1/1	0.95	0.23	39,39,39,39	0
57	MG	1A	3528	1/1	0.95	0.08	28,28,28,28	0
57	MG	2A	3170	1/1	0.96	0.21	38,38,38,38	0
57	MG	1A	3329	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3203	1/1	0.96	0.06	18,18,18,18	0
57	MG	2A	3363	1/1	0.96	0.13	28,28,28,28	0
57	MG	1A	3385	1/1	0.96	0.16	17,17,17,17	0
57	MG	1a	3537	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3032	1/1	0.96	0.18	22,22,22,22	0
57	MG	1A	3712	1/1	0.96	0.05	35,35,35,35	0
57	MG	1a	3714	1/1	0.96	0.25	47,47,47,47	0
57	MG	1A	3288	1/1	0.96	0.08	30,30,30,30	0
57	MG	2A	3372	1/1	0.96	0.27	32,32,32,32	0
57	MG	1A	3968	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3512	1/1	0.96	0.19	28,28,28,28	0
57	MG	2A	3185	1/1	0.96	0.24	45,45,45,45	0
57	MG	1A	3143	1/1	0.96	0.33	22,22,22,22	0
57	MG	1A	3717	1/1	0.96	0.09	16,16,16,16	0
57	MG	1A	3839	1/1	0.96	0.08	22,22,22,22	0
57	MG	1A	3603	1/1	0.96	0.09	18,18,18,18	0
57	MG	2O	203	1/1	0.96	0.08	44,44,44,44	0
57	MG	2P	201	1/1	0.96	0.09	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3053	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3041	1/1	0.96	0.17	19,19,19,19	0
57	MG	1A	3337	1/1	0.96	0.16	33,33,33,33	0
57	MG	1D	310	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3057	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3341	1/1	0.96	0.29	33,33,33,33	0
57	MG	2T	203	1/1	0.96	0.12	24,24,24,24	0
57	MG	1A	3120	1/1	0.96	0.14	28,28,28,28	0
57	MG	1E	304	1/1	0.96	0.13	14,14,14,14	0
57	MG	2U	202	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3294	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	3121	1/1	0.96	0.35	23,23,23,23	0
57	MG	1A	3122	1/1	0.96	0.28	23,23,23,23	0
57	MG	2A	3391	1/1	0.96	0.26	40,40,40,40	0
57	MG	1E	310	1/1	0.96	0.12	11,11,11,11	0
57	MG	1A	3736	1/1	0.96	0.09	25,25,25,25	0
57	MG	1x	102	1/1	0.96	0.05	37,37,37,37	0
57	MG	2A	3207	1/1	0.96	0.24	45,45,45,45	0
57	MG	2A	3639	1/1	0.96	0.06	34,34,34,34	0
57	MG	21	101	1/1	0.96	0.41	38,38,38,38	0
57	MG	1A	3990	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3991	1/1	0.96	0.09	20,20,20,20	0
57	MG	25	101	1/1	0.96	0.16	29,29,29,29	0
57	MG	1A	3526	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	3993	1/1	0.96	0.09	29,29,29,29	0
57	MG	1F	306	1/1	0.96	0.09	26,26,26,26	0
57	MG	1A	3399	1/1	0.96	0.17	34,34,34,34	0
57	MG	2A	3214	1/1	0.96	0.09	28,28,28,28	0
57	MG	1F	308	1/1	0.96	0.05	16,16,16,16	0
57	MG	1A	3855	1/1	0.96	0.04	11,11,11,11	0
57	MG	28	103	1/1	0.96	0.09	26,26,26,26	0
57	MG	1a	3572	1/1	0.96	0.14	46,46,46,46	0
57	MG	1A	3124	1/1	0.96	0.34	28,28,28,28	0
57	MG	1A	3299	1/1	0.96	0.12	16,16,16,16	0
57	MG	1A	3862	1/1	0.96	0.07	21,21,21,21	0
57	MG	1A	4003	1/1	0.96	0.13	48,48,48,48	0
57	MG	1A	3620	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3621	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3744	1/1	0.96	0.07	44,44,44,44	0
57	MG	1a	3581	1/1	0.96	0.13	39,39,39,39	0
57	MG	2A	3417	1/1	0.96	0.10	38,38,38,38	0
57	MG	2A	3013	1/1	0.96	0.10	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3257	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3531	1/1	0.96	0.18	23,23,23,23	0
57	MG	2A	3665	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3751	1/1	0.96	0.06	10,10,10,10	0
57	MG	2A	3422	1/1	0.96	0.11	35,35,35,35	0
57	MG	2a	1620	1/1	0.96	0.20	47,47,47,47	0
57	MG	1A	3627	1/1	0.96	0.07	21,21,21,21	0
57	MG	1A	3753	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	4013	1/1	0.96	0.04	32,32,32,32	0
57	MG	2A	3671	1/1	0.96	0.08	37,37,37,37	0
57	MG	2A	3026	1/1	0.96	0.06	26,26,26,26	0
57	MG	2A	3234	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3628	1/1	0.96	0.09	27,27,27,27	0
57	MG	1A	4016	1/1	0.96	0.10	44,44,44,44	0
57	MG	1N	204	1/1	0.96	0.05	29,29,29,29	0
57	MG	1N	205	1/1	0.96	0.15	25,25,25,25	0
57	MG	2a	1632	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3349	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3461	1/1	0.96	0.27	27,27,27,27	0
57	MG	1O	202	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3876	1/1	0.96	0.23	36,36,36,36	0
57	MG	1A	3761	1/1	0.96	0.07	33,33,33,33	0
57	MG	1P	201	1/1	0.96	0.21	14,14,14,14	0
57	MG	2a	1639	1/1	0.96	0.13	39,39,39,39	0
57	MG	1A	3126	1/1	0.96	0.11	24,24,24,24	0
57	MG	1A	3302	1/1	0.96	0.04	23,23,23,23	0
57	MG	2a	1642	1/1	0.96	0.15	63,63,63,63	0
57	MG	2a	1643	1/1	0.96	0.13	43,43,43,43	0
57	MG	1Q	202	1/1	0.96	0.11	28,28,28,28	0
57	MG	1Q	203	1/1	0.96	0.08	38,38,38,38	0
57	MG	2a	1646	1/1	0.96	0.14	28,28,28,28	0
57	MG	2A	3448	1/1	0.96	0.17	39,39,39,39	0
57	MG	1Q	204	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3881	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3882	1/1	0.96	0.20	21,21,21,21	0
57	MG	1A	3303	1/1	0.96	0.09	30,30,30,30	0
57	MG	2A	3048	1/1	0.96	0.11	22,22,22,22	0
57	MG	2A	3454	1/1	0.96	0.12	41,41,41,41	0
57	MG	1A	3539	1/1	0.96	0.19	48,48,48,48	0
57	MG	1A	3466	1/1	0.96	0.16	26,26,26,26	0
57	MG	1A	3544	1/1	0.96	0.11	20,20,20,20	0
57	MG	1A	3467	1/1	0.96	0.09	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3639	1/1	0.96	0.05	13,13,13,13	0
57	MG	1A	3640	1/1	0.96	0.06	9,9,9,9	0
57	MG	1A	3158	1/1	0.96	0.19	12,12,12,12	0
57	MG	2A	3262	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3549	1/1	0.96	0.07	23,23,23,23	0
57	MG	2A	3060	1/1	0.96	0.14	40,40,40,40	0
57	MG	2A	3713	1/1	0.96	0.15	32,32,32,32	0
57	MG	2A	3061	1/1	0.96	0.18	41,41,41,41	0
57	MG	1U	205	1/1	0.96	0.24	26,26,26,26	0
57	MG	2A	3716	1/1	0.96	0.08	35,35,35,35	0
57	MG	2A	3470	1/1	0.96	0.05	41,41,41,41	0
57	MG	1U	206	1/1	0.96	0.15	28,28,28,28	0
57	MG	2A	3472	1/1	0.96	0.18	49,49,49,49	0
57	MG	1U	210	1/1	0.96	0.14	17,17,17,17	0
57	MG	2A	3067	1/1	0.96	0.07	39,39,39,39	0
57	MG	1a	3619	1/1	0.96	0.20	37,37,37,37	0
57	MG	1A	3551	1/1	0.96	0.09	26,26,26,26	0
57	MG	1A	3896	1/1	0.96	0.11	40,40,40,40	0
57	MG	2A	3726	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	4039	1/1	0.96	0.12	30,30,30,30	0
57	MG	1V	204	1/1	0.96	0.16	21,21,21,21	0
57	MG	2A	3480	1/1	0.96	0.10	27,27,27,27	0
57	MG	1A	3048	1/1	0.96	0.09	25,25,25,25	0
57	MG	2A	3077	1/1	0.96	0.16	42,42,42,42	0
57	MG	1A	3649	1/1	0.96	0.07	9,9,9,9	0
57	MG	1A	3107	1/1	0.96	0.07	18,18,18,18	0
57	MG	1A	4044	1/1	0.96	0.06	26,26,26,26	0
57	MG	1W	205	1/1	0.96	0.09	12,12,12,12	0
57	MG	1X	103	1/1	0.96	0.17	29,29,29,29	0
57	MG	1A	3554	1/1	0.96	0.14	25,25,25,25	0
57	MG	2A	3085	1/1	0.96	0.28	31,31,31,31	0
57	MG	1A	3193	1/1	0.96	0.23	29,29,29,29	0
57	MG	2A	3492	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3658	1/1	0.96	0.19	50,50,50,50	0
57	MG	2A	3495	1/1	0.96	0.14	31,31,31,31	0
57	MG	2A	3745	1/1	0.96	0.17	43,43,43,43	0
57	MG	2A	3496	1/1	0.96	0.09	29,29,29,29	0
57	MG	1Y	203	1/1	0.96	0.29	35,35,35,35	0
57	MG	1A	3904	1/1	0.96	0.06	27,27,27,27	0
57	MG	2A	3749	1/1	0.96	0.11	43,43,43,43	0
57	MG	1A	3265	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3557	1/1	0.96	0.05	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1702	1/1	0.96	0.18	35,35,35,35	0
57	MG	2A	3501	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3753	1/1	0.96	0.15	42,42,42,42	0
57	MG	1A	3911	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3076	1/1	0.96	0.11	18,18,18,18	0
57	MG	1A	3010	1/1	0.96	0.07	30,30,30,30	0
57	MG	2A	3505	1/1	0.96	0.14	36,36,36,36	0
57	MG	1A	3312	1/1	0.96	0.20	46,46,46,46	0
57	MG	1A	3362	1/1	0.96	0.13	43,43,43,43	0
57	MG	1a	3644	1/1	0.96	0.15	24,24,24,24	0
57	MG	1A	4061	1/1	0.96	0.08	53,53,53,53	0
57	MG	2a	1715	1/1	0.96	0.20	45,45,45,45	0
57	MG	2A	3510	1/1	0.96	0.12	40,40,40,40	0
57	MG	1A	3313	1/1	0.96	0.13	16,16,16,16	0
57	MG	2A	3513	1/1	0.96	0.12	25,25,25,25	0
57	MG	1A	4063	1/1	0.96	0.07	37,37,37,37	0
57	MG	13	101	1/1	0.96	0.15	25,25,25,25	0
57	MG	2A	3767	1/1	0.96	0.11	33,33,33,33	0
57	MG	2a	1722	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3136	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	4065	1/1	0.96	0.06	25,25,25,25	0
57	MG	1A	4066	1/1	0.96	0.14	28,28,28,28	0
57	MG	1a	3656	1/1	0.96	0.10	39,39,39,39	0
57	MG	2A	3305	1/1	0.96	0.21	53,53,53,53	0
57	MG	1A	3481	1/1	0.96	0.09	37,37,37,37	0
57	MG	2A	3777	1/1	0.96	0.13	28,28,28,28	0
57	MG	15	3204	1/1	0.96	0.13	30,30,30,30	0
57	MG	15	3205	1/1	0.96	0.15	27,27,27,27	0
57	MG	2A	3112	1/1	0.96	0.16	20,20,20,20	0
57	MG	1A	3921	1/1	0.96	0.08	35,35,35,35	0
57	MG	1a	3661	1/1	0.96	0.16	44,44,44,44	0
57	MG	1A	3230	1/1	0.96	0.07	29,29,29,29	0
57	MG	2A	3786	1/1	0.96	0.09	36,36,36,36	0
57	MG	2A	3787	1/1	0.96	0.08	24,24,24,24	0
57	MG	16	101	1/1	0.96	0.12	30,30,30,30	0
57	MG	2A	3791	1/1	0.96	0.05	38,38,38,38	0
57	MG	1A	3674	1/1	0.96	0.05	10,10,10,10	0
57	MG	2A	3315	1/1	0.96	0.18	31,31,31,31	0
57	MG	2A	3538	1/1	0.96	0.12	29,29,29,29	0
57	MG	2A	3795	1/1	0.96	0.11	22,22,22,22	0
57	MG	2A	3796	1/1	0.96	0.07	26,26,26,26	0
57	MG	1a	3666	1/1	0.96	0.06	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3540	1/1	0.96	0.07	31,31,31,31	0
57	MG	2A	3121	1/1	0.96	0.07	34,34,34,34	0
57	MG	1a	3667	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3421	1/1	0.96	0.13	28,28,28,28	0
57	MG	1A	3422	1/1	0.96	0.14	26,26,26,26	0
57	MG	1A	3927	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3572	1/1	0.96	0.10	37,37,37,37	0
57	MG	1A	3680	1/1	0.96	0.11	25,25,25,25	0
57	MG	1A	3197	1/1	0.96	0.04	25,25,25,25	0
57	MG	1A	3487	1/1	0.96	0.15	18,18,18,18	0
57	MG	2A	3132	1/1	0.96	0.16	36,36,36,36	0
57	MG	1A	3425	1/1	0.96	0.06	40,40,40,40	0
57	MG	1a	3502	1/1	0.96	0.17	39,39,39,39	0
57	MG	1A	3806	1/1	0.96	0.12	26,26,26,26	0
57	MG	1A	3198	1/1	0.96	0.19	8,8,8,8	0
57	MG	1A	4085	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3427	1/1	0.96	0.07	37,37,37,37	0
57	MG	2A	3559	1/1	0.96	0.09	38,38,38,38	0
57	MG	2a	1766	1/1	0.96	0.13	38,38,38,38	0
57	MG	2A	3561	1/1	0.96	0.11	18,18,18,18	0
57	MG	1A	3809	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3233	1/1	0.96	0.17	17,17,17,17	0
57	MG	1A	3320	1/1	0.96	0.08	29,29,29,29	0
57	MG	2A	3826	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3372	1/1	0.96	0.10	34,34,34,34	0
57	MG	1A	3814	1/1	0.96	0.08	23,23,23,23	0
57	MG	1A	3079	1/1	0.96	0.24	25,25,25,25	0
57	MG	1A	3945	1/1	0.96	0.14	47,47,47,47	0
57	MG	1A	3241	1/1	0.96	0.08	27,27,27,27	0
57	MG	1B	212	1/1	0.96	0.09	33,33,33,33	0
57	MG	1B	213	1/1	0.96	0.14	23,23,23,23	0
57	MG	2A	3152	1/1	0.96	0.35	51,51,51,51	0
57	MG	2A	3576	1/1	0.96	0.09	38,38,38,38	0
57	MG	2e	201	1/1	0.96	0.05	51,51,51,51	0
57	MG	1A	3025	1/1	0.96	0.25	53,53,53,53	0
57	MG	2A	3578	1/1	0.96	0.21	39,39,39,39	0
57	MG	2A	3579	1/1	0.96	0.07	12,12,12,12	0
57	MG	1A	3326	1/1	0.96	0.06	35,35,35,35	0
57	MG	2A	3155	1/1	0.96	0.31	53,53,53,53	0
57	MG	2A	3583	1/1	0.96	0.12	26,26,26,26	0
57	MG	1A	3820	1/1	0.96	0.08	30,30,30,30	0
57	MG	2l	201	1/1	0.96	0.12	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3062	1/1	0.96	0.20	29,29,29,29	0
57	MG	1A	3502	1/1	0.96	0.13	47,47,47,47	0
57	MG	2q	202	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3823	1/1	0.96	0.07	9,9,9,9	0
57	MG	1A	3953	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3701	1/1	0.96	0.11	18,18,18,18	0
57	MG	2v	102	1/1	0.96	0.09	45,45,45,45	0
57	MG	1A	3437	1/1	0.96	0.14	24,24,24,24	0
57	MG	2x	102	1/1	0.96	0.15	44,44,44,44	0
57	MG	1a	3703	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3166	1/1	0.96	0.13	24,24,24,24	0
57	MG	2x	106	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	3956	1/1	0.96	0.13	43,43,43,43	0
57	MG	2A	3597	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3328	1/1	0.96	0.19	27,27,27,27	0
57	MG	1a	3530	1/1	0.96	0.22	45,45,45,45	0
57	MG	1A	3762	1/1	0.97	0.08	7,7,7,7	0
57	MG	1A	3102	1/1	0.97	0.18	29,29,29,29	0
57	MG	2A	3197	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3641	1/1	0.97	0.07	16,16,16,16	0
57	MG	2O	202	1/1	0.97	0.11	43,43,43,43	0
57	MG	1A	3472	1/1	0.97	0.20	21,21,21,21	0
57	MG	1A	3103	1/1	0.97	0.10	21,21,21,21	0
57	MG	1A	3767	1/1	0.97	0.07	9,9,9,9	0
57	MG	2A	3399	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3236	1/1	0.97	0.09	18,18,18,18	0
57	MG	2A	3203	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3237	1/1	0.97	0.09	19,19,19,19	0
57	MG	1A	3104	1/1	0.97	0.35	29,29,29,29	0
57	MG	1A	3297	1/1	0.97	0.16	32,32,32,32	0
57	MG	1x	112	1/1	0.97	0.09	31,31,31,31	0
57	MG	1A	3652	1/1	0.97	0.05	36,36,36,36	0
57	MG	1a	3576	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	4029	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	4030	1/1	0.97	0.08	10,10,10,10	0
57	MG	1A	3242	1/1	0.97	0.05	26,26,26,26	0
57	MG	1O	205	1/1	0.97	0.04	29,29,29,29	0
57	MG	2A	3007	1/1	0.97	0.07	31,31,31,31	0
57	MG	2A	3645	1/1	0.97	0.09	36,36,36,36	0
57	MG	1A	3655	1/1	0.97	0.06	11,11,11,11	0
57	MG	2A	3010	1/1	0.97	0.07	30,30,30,30	0
57	MG	1A	4033	1/1	0.97	0.10	11,11,11,11	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3037	1/1	0.97	0.24	22,22,22,22	0
57	MG	1Q	201	1/1	0.97	0.14	19,19,19,19	0
57	MG	1A	3005	1/1	0.97	0.08	29,29,29,29	0
57	MG	2A	3017	1/1	0.97	0.21	48,48,48,48	0
57	MG	2A	3018	1/1	0.97	0.06	29,29,29,29	0
57	MG	2A	3424	1/1	0.97	0.06	40,40,40,40	0
57	MG	25	104	1/1	0.97	0.05	43,43,43,43	0
57	MG	2A	3425	1/1	0.97	0.09	36,36,36,36	0
57	MG	2A	3657	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3416	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3021	1/1	0.97	0.25	33,33,33,33	0
57	MG	1A	3563	1/1	0.97	0.08	13,13,13,13	0
57	MG	2A	3429	1/1	0.97	0.08	58,58,58,58	0
57	MG	1A	3192	1/1	0.97	0.29	14,14,14,14	0
57	MG	1A	3664	1/1	0.97	0.07	12,12,12,12	0
57	MG	2A	3025	1/1	0.97	0.14	36,36,36,36	0
57	MG	1A	3144	1/1	0.97	0.14	17,17,17,17	0
57	MG	1A	3024	1/1	0.97	0.27	28,28,28,28	0
57	MG	2a	1606	1/1	0.97	0.11	23,23,23,23	0
57	MG	2A	3435	1/1	0.97	0.06	31,31,31,31	0
57	MG	1S	201	1/1	0.97	0.06	34,34,34,34	0
57	MG	2a	1609	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3905	1/1	0.97	0.06	25,25,25,25	0
57	MG	1A	3108	1/1	0.97	0.11	18,18,18,18	0
57	MG	1A	3305	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3250	1/1	0.97	0.10	44,44,44,44	0
57	MG	1A	4047	1/1	0.97	0.05	25,25,25,25	0
57	MG	2A	3034	1/1	0.97	0.07	37,37,37,37	0
57	MG	2A	3035	1/1	0.97	0.25	34,34,34,34	0
57	MG	1A	3790	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3489	1/1	0.97	0.16	23,23,23,23	0
57	MG	2a	1619	1/1	0.97	0.12	36,36,36,36	0
57	MG	2A	3446	1/1	0.97	0.09	45,45,45,45	0
57	MG	2A	3038	1/1	0.97	0.25	24,24,24,24	0
57	MG	1A	3423	1/1	0.97	0.16	25,25,25,25	0
57	MG	1A	3109	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3675	1/1	0.97	0.11	6,6,6,6	0
57	MG	1A	3676	1/1	0.97	0.05	32,32,32,32	0
57	MG	2A	3688	1/1	0.97	0.10	39,39,39,39	0
57	MG	2a	1627	1/1	0.97	0.15	42,42,42,42	0
57	MG	1A	3148	1/1	0.97	0.15	30,30,30,30	0
57	MG	1A	3365	1/1	0.97	0.10	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3149	1/1	0.97	0.10	32,32,32,32	0
57	MG	1V	206	1/1	0.97	0.12	24,24,24,24	0
57	MG	1A	3054	1/1	0.97	0.12	19,19,19,19	0
57	MG	2A	3457	1/1	0.97	0.08	30,30,30,30	0
57	MG	1A	3006	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3925	1/1	0.97	0.15	34,34,34,34	0
57	MG	1a	3612	1/1	0.97	0.15	47,47,47,47	0
57	MG	1W	202	1/1	0.97	0.08	30,30,30,30	0
57	MG	1A	3369	1/1	0.97	0.20	16,16,16,16	0
57	MG	1A	3083	1/1	0.97	0.11	13,13,13,13	0
57	MG	1A	3084	1/1	0.97	0.23	28,28,28,28	0
57	MG	1A	3585	1/1	0.97	0.09	47,47,47,47	0
57	MG	1A	3930	1/1	0.97	0.07	30,30,30,30	0
57	MG	2A	3058	1/1	0.97	0.14	31,31,31,31	0
57	MG	2A	3059	1/1	0.97	0.15	32,32,32,32	0
57	MG	2A	3708	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3501	1/1	0.97	0.14	44,44,44,44	0
57	MG	1a	3620	1/1	0.97	0.21	24,24,24,24	0
57	MG	1A	3587	1/1	0.97	0.07	19,19,19,19	0
57	MG	2A	3063	1/1	0.97	0.10	26,26,26,26	0
57	MG	1Z	301	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3689	1/1	0.97	0.10	19,19,19,19	0
57	MG	2A	3066	1/1	0.97	0.04	36,36,36,36	0
57	MG	1Z	303	1/1	0.97	0.07	39,39,39,39	0
57	MG	2A	3068	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3026	1/1	0.97	0.09	11,11,11,11	0
57	MG	2A	3070	1/1	0.97	0.04	25,25,25,25	0
57	MG	2A	3071	1/1	0.97	0.09	19,19,19,19	0
57	MG	1A	3205	1/1	0.97	0.08	21,21,21,21	0
57	MG	1A	3435	1/1	0.97	0.11	31,31,31,31	0
57	MG	10	104	1/1	0.97	0.18	39,39,39,39	0
57	MG	1A	3011	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3938	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3939	1/1	0.97	0.07	14,14,14,14	0
57	MG	2A	3078	1/1	0.97	0.17	36,36,36,36	0
57	MG	1A	3376	1/1	0.97	0.14	14,14,14,14	0
57	MG	1A	4080	1/1	0.97	0.11	39,39,39,39	0
57	MG	1A	3696	1/1	0.97	0.08	33,33,33,33	0
57	MG	2A	3494	1/1	0.97	0.11	42,42,42,42	0
57	MG	11	103	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3816	1/1	0.97	0.06	42,42,42,42	0
57	MG	2A	3735	1/1	0.97	0.14	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3697	1/1	0.97	0.15	37,37,37,37	0
57	MG	2A	3737	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3508	1/1	0.97	0.23	34,34,34,34	0
57	MG	1A	3699	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	3059	1/1	0.97	0.08	25,25,25,25	0
57	MG	15	3201	1/1	0.97	0.37	27,27,27,27	0
57	MG	1B	204	1/1	0.97	0.09	33,33,33,33	0
57	MG	15	3203	1/1	0.97	0.35	17,17,17,17	0
57	MG	1A	3378	1/1	0.97	0.42	29,29,29,29	0
57	MG	1B	206	1/1	0.97	0.06	34,34,34,34	0
57	MG	15	3206	1/1	0.97	0.14	31,31,31,31	0
57	MG	2A	3297	1/1	0.97	0.10	63,63,63,63	0
57	MG	2a	1685	1/1	0.97	0.12	42,42,42,42	0
57	MG	15	3207	1/1	0.97	0.17	24,24,24,24	0
57	MG	1a	3650	1/1	0.97	0.15	44,44,44,44	0
57	MG	1A	3379	1/1	0.97	0.22	27,27,27,27	0
57	MG	2A	3097	1/1	0.97	0.14	45,45,45,45	0
57	MG	1A	3007	1/1	0.97	0.04	16,16,16,16	0
57	MG	1A	3824	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3513	1/1	0.97	0.12	34,34,34,34	0
57	MG	1A	3264	1/1	0.97	0.09	26,26,26,26	0
57	MG	17	102	1/1	0.97	0.06	20,20,20,20	0
57	MG	2A	3518	1/1	0.97	0.11	18,18,18,18	0
57	MG	2A	3104	1/1	0.97	0.15	28,28,28,28	0
57	MG	1A	3708	1/1	0.97	0.07	18,18,18,18	0
57	MG	2A	3521	1/1	0.97	0.08	22,22,22,22	0
57	MG	17	104	1/1	0.97	0.12	25,25,25,25	0
57	MG	2A	3523	1/1	0.97	0.07	25,25,25,25	0
57	MG	1A	3828	1/1	0.97	0.11	12,12,12,12	0
57	MG	1a	3662	1/1	0.97	0.11	33,33,33,33	0
57	MG	1A	3045	1/1	0.97	0.10	21,21,21,21	0
57	MG	1B	215	1/1	0.97	0.12	37,37,37,37	0
57	MG	1A	3323	1/1	0.97	0.12	26,26,26,26	0
57	MG	2A	3531	1/1	0.97	0.08	21,21,21,21	0
57	MG	1A	3606	1/1	0.97	0.07	16,16,16,16	0
57	MG	18	106	1/1	0.97	0.10	52,52,52,52	0
57	MG	2A	3772	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3773	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3713	1/1	0.97	0.07	42,42,42,42	0
57	MG	1a	3501	1/1	0.97	0.10	40,40,40,40	0
57	MG	2A	3116	1/1	0.97	0.10	41,41,41,41	0
57	MG	2A	3537	1/1	0.97	0.09	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3833	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3211	1/1	0.97	0.16	29,29,29,29	0
57	MG	2A	3780	1/1	0.97	0.08	18,18,18,18	0
57	MG	1A	3962	1/1	0.97	0.07	17,17,17,17	0
57	MG	2A	3120	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3267	1/1	0.97	0.07	23,23,23,23	0
57	MG	1A	3030	1/1	0.97	0.20	21,21,21,21	0
57	MG	1A	3008	1/1	0.97	0.05	6,6,6,6	0
57	MG	1A	3065	1/1	0.97	0.10	15,15,15,15	0
57	MG	1a	3509	1/1	0.97	0.07	55,55,55,55	0
57	MG	2A	3790	1/1	0.97	0.10	31,31,31,31	0
57	MG	1B	228	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3033	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3330	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3125	1/1	0.97	0.07	47,47,47,47	0
57	MG	1a	3514	1/1	0.97	0.17	48,48,48,48	0
57	MG	1a	3683	1/1	0.97	0.05	61,61,61,61	0
57	MG	2A	3553	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3725	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3392	1/1	0.97	0.17	31,31,31,31	0
57	MG	1a	3686	1/1	0.97	0.18	61,61,61,61	0
57	MG	1A	3279	1/1	0.97	0.14	32,32,32,32	0
57	MG	1A	3035	1/1	0.97	0.07	8,8,8,8	0
57	MG	1A	3281	1/1	0.97	0.12	30,30,30,30	0
57	MG	2a	1741	1/1	0.97	0.31	46,46,46,46	0
57	MG	2A	3562	1/1	0.97	0.07	30,30,30,30	0
57	MG	2A	3341	1/1	0.97	0.04	34,34,34,34	0
57	MG	2A	3564	1/1	0.97	0.16	32,32,32,32	0
57	MG	1A	3847	1/1	0.97	0.26	19,19,19,19	0
57	MG	1A	3170	1/1	0.97	0.04	29,29,29,29	0
57	MG	1A	3732	1/1	0.97	0.12	23,23,23,23	0
57	MG	1A	3850	1/1	0.97	0.09	26,26,26,26	0
57	MG	1A	3172	1/1	0.97	0.26	25,25,25,25	0
57	MG	1A	3986	1/1	0.97	0.06	10,10,10,10	0
57	MG	2A	3147	1/1	0.97	0.12	32,32,32,32	0
57	MG	1D	307	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3735	1/1	0.97	0.06	11,11,11,11	0
57	MG	1A	3622	1/1	0.97	0.06	25,25,25,25	0
57	MG	2A	3822	1/1	0.97	0.12	41,41,41,41	0
57	MG	2a	1756	1/1	0.97	0.21	39,39,39,39	0
57	MG	2A	3575	1/1	0.97	0.12	29,29,29,29	0
57	MG	1A	3068	1/1	0.97	0.14	10,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1D	312	1/1	0.97	0.12	16,16,16,16	0
57	MG	1A	3624	1/1	0.97	0.09	46,46,46,46	0
57	MG	1a	3532	1/1	0.97	0.29	42,42,42,42	0
57	MG	1a	3704	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3857	1/1	0.97	0.11	11,11,11,11	0
57	MG	2A	3582	1/1	0.97	0.06	29,29,29,29	0
57	MG	1a	3534	1/1	0.97	0.12	17,17,17,17	0
57	MG	2A	3832	1/1	0.97	0.06	47,47,47,47	0
57	MG	1a	3535	1/1	0.97	0.13	42,42,42,42	0
57	MG	1E	302	1/1	0.97	0.11	23,23,23,23	0
57	MG	1A	3225	1/1	0.97	0.13	17,17,17,17	0
57	MG	1A	3860	1/1	0.97	0.07	30,30,30,30	0
57	MG	2A	3589	1/1	0.97	0.05	19,19,19,19	0
57	MG	1A	3626	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3741	1/1	0.97	0.07	19,19,19,19	0
57	MG	2A	3366	1/1	0.97	0.17	30,30,30,30	0
57	MG	1E	309	1/1	0.97	0.03	28,28,28,28	0
57	MG	1A	3998	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3595	1/1	0.97	0.14	42,42,42,42	0
57	MG	1A	3069	1/1	0.97	0.05	5,5,5,5	0
57	MG	1A	4000	1/1	0.97	0.05	37,37,37,37	0
57	MG	1F	302	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	4001	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3536	1/1	0.97	0.18	27,27,27,27	0
57	MG	1A	3130	1/1	0.97	0.28	18,18,18,18	0
57	MG	1A	3465	1/1	0.97	0.17	44,44,44,44	0
57	MG	2A	3603	1/1	0.97	0.12	30,30,30,30	0
57	MG	2A	3604	1/1	0.97	0.13	26,26,26,26	0
57	MG	1A	3070	1/1	0.97	0.15	23,23,23,23	0
57	MG	2D	302	1/1	0.97	0.12	17,17,17,17	0
57	MG	1A	3543	1/1	0.97	0.17	26,26,26,26	0
57	MG	1A	3134	1/1	0.97	0.07	23,23,23,23	0
57	MG	2A	3181	1/1	0.97	0.21	41,41,41,41	0
57	MG	1A	3545	1/1	0.97	0.23	34,34,34,34	0
57	MG	1A	3754	1/1	0.97	0.09	38,38,38,38	0
57	MG	2A	3184	1/1	0.97	0.05	33,33,33,33	0
57	MG	2A	3612	1/1	0.97	0.08	40,40,40,40	0
57	MG	1a	3556	1/1	0.97	0.14	41,41,41,41	0
57	MG	1A	3468	1/1	0.97	0.05	35,35,35,35	0
57	MG	1m	3001	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3050	1/1	0.97	0.14	12,12,12,12	0
57	MG	1A	3758	1/1	0.97	0.05	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2x	105	1/1	0.97	0.14	47,47,47,47	0
57	MG	1A	3100	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3878	1/1	0.97	0.10	19,19,19,19	0
57	MG	2F	303	1/1	0.97	0.10	39,39,39,39	0
57	MG	1a	3562	1/1	0.97	0.07	62,62,62,62	0
57	MG	1A	3550	1/1	0.97	0.10	22,22,22,22	0
59	ZN	2n	501	1/1	0.97	0.04	89,89,89,89	0
60	SF4	1d	302	8/8	0.97	0.05	56,62,66,68	0
57	MG	1E	303	1/1	0.98	0.08	17,17,17,17	0
57	MG	1A	3274	1/1	0.98	0.12	16,16,16,16	0
57	MG	2A	3151	1/1	0.98	0.07	50,50,50,50	0
57	MG	1A	3486	1/1	0.98	0.28	11,11,11,11	0
57	MG	1A	3746	1/1	0.98	0.08	10,10,10,10	0
57	MG	2A	3011	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	3748	1/1	0.98	0.05	41,41,41,41	0
57	MG	1E	308	1/1	0.98	0.11	11,11,11,11	0
57	MG	2A	3157	1/1	0.98	0.16	21,21,21,21	0
57	MG	1A	3667	1/1	0.98	0.07	33,33,33,33	0
57	MG	1A	3240	1/1	0.98	0.23	23,23,23,23	0
57	MG	2A	3016	1/1	0.98	0.13	25,25,25,25	0
57	MG	2A	3616	1/1	0.98	0.05	35,35,35,35	0
57	MG	2A	3785	1/1	0.98	0.09	42,42,42,42	0
57	MG	2A	3161	1/1	0.98	0.10	45,45,45,45	0
57	MG	1A	3598	1/1	0.98	0.10	9,9,9,9	0
57	MG	2A	3788	1/1	0.98	0.10	27,27,27,27	0
57	MG	1E	312	1/1	0.98	0.27	32,32,32,32	0
57	MG	1A	3670	1/1	0.98	0.07	11,11,11,11	0
57	MG	1F	301	1/1	0.98	0.13	30,30,30,30	0
57	MG	2a	1653	1/1	0.98	0.12	32,32,32,32	0
57	MG	1A	3599	1/1	0.98	0.07	26,26,26,26	0
57	MG	1A	3208	1/1	0.98	0.06	22,22,22,22	0
57	MG	1A	3277	1/1	0.98	0.19	19,19,19,19	0
57	MG	2A	3466	1/1	0.98	0.17	28,28,28,28	0
57	MG	1A	3443	1/1	0.98	0.14	25,25,25,25	0
57	MG	2A	3468	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3491	1/1	0.98	0.15	24,24,24,24	0
57	MG	1A	4042	1/1	0.98	0.04	7,7,7,7	0
57	MG	2A	3801	1/1	0.98	0.09	43,43,43,43	0
57	MG	2A	3173	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	3760	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3604	1/1	0.98	0.06	8,8,8,8	0
57	MG	1A	3278	1/1	0.98	0.29	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3546	1/1	0.98	0.11	22,22,22,22	0
57	MG	2A	3807	1/1	0.98	0.05	24,24,24,24	0
57	MG	1a	3641	1/1	0.98	0.10	54,54,54,54	0
57	MG	1A	3400	1/1	0.98	0.06	41,41,41,41	0
57	MG	2A	3637	1/1	0.98	0.10	54,54,54,54	0
57	MG	2A	3811	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3357	1/1	0.98	0.05	31,31,31,31	0
57	MG	1A	4049	1/1	0.98	0.08	14,14,14,14	0
57	MG	1a	3645	1/1	0.98	0.08	23,23,23,23	0
57	MG	2A	3815	1/1	0.98	0.06	30,30,30,30	0
57	MG	1A	3316	1/1	0.98	0.11	17,17,17,17	0
57	MG	1A	3131	1/1	0.98	0.06	28,28,28,28	0
57	MG	2A	3483	1/1	0.98	0.11	30,30,30,30	0
57	MG	1A	3164	1/1	0.98	0.11	29,29,29,29	0
57	MG	1A	3101	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	4054	1/1	0.98	0.08	32,32,32,32	0
57	MG	1a	3652	1/1	0.98	0.08	22,22,22,22	0
57	MG	2A	3648	1/1	0.98	0.09	27,27,27,27	0
57	MG	2A	3189	1/1	0.98	0.04	26,26,26,26	0
57	MG	1A	3036	1/1	0.98	0.16	22,22,22,22	0
57	MG	1A	3772	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	3859	1/1	0.98	0.11	35,35,35,35	0
57	MG	1A	4059	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3321	1/1	0.98	0.19	31,31,31,31	0
57	MG	1A	3687	1/1	0.98	0.07	6,6,6,6	0
57	MG	1A	3189	1/1	0.98	0.17	25,25,25,25	0
57	MG	1A	3957	1/1	0.98	0.07	33,33,33,33	0
57	MG	2A	3051	1/1	0.98	0.06	56,56,56,56	0
57	MG	1A	3075	1/1	0.98	0.11	16,16,16,16	0
57	MG	1A	3248	1/1	0.98	0.19	42,42,42,42	0
57	MG	1A	3691	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3867	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3504	1/1	0.98	0.21	23,23,23,23	0
57	MG	1A	3619	1/1	0.98	0.04	15,15,15,15	0
57	MG	1A	3191	1/1	0.98	0.13	18,18,18,18	0
57	MG	1A	3560	1/1	0.98	0.04	21,21,21,21	0
57	MG	2a	1703	1/1	0.98	0.13	36,36,36,36	0
57	MG	1A	4072	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3967	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3123	1/1	0.98	0.26	21,21,21,21	0
57	MG	1A	3152	1/1	0.98	0.17	30,30,30,30	0
57	MG	1Q	205	1/1	0.98	0.06	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3672	1/1	0.98	0.08	37,37,37,37	0
57	MG	1A	3063	1/1	0.98	0.13	29,29,29,29	0
57	MG	1A	3564	1/1	0.98	0.11	20,20,20,20	0
57	MG	1A	3171	1/1	0.98	0.08	26,26,26,26	0
57	MG	2a	1713	1/1	0.98	0.20	42,42,42,42	0
57	MG	1R	203	1/1	0.98	0.15	20,20,20,20	0
57	MG	2B	217	1/1	0.98	0.22	47,47,47,47	0
57	MG	1R	204	1/1	0.98	0.14	21,21,21,21	0
57	MG	1A	3138	1/1	0.98	0.15	23,23,23,23	0
57	MG	1A	3173	1/1	0.98	0.15	19,19,19,19	0
57	MG	2D	303	1/1	0.98	0.29	32,32,32,32	0
57	MG	2A	3365	1/1	0.98	0.18	24,24,24,24	0
57	MG	1A	3374	1/1	0.98	0.24	18,18,18,18	0
57	MG	1A	4082	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	4083	1/1	0.98	0.08	31,31,31,31	0
57	MG	2A	3686	1/1	0.98	0.05	26,26,26,26	0
57	MG	1a	3552	1/1	0.98	0.09	35,35,35,35	0
57	MG	2A	3524	1/1	0.98	0.09	19,19,19,19	0
57	MG	1A	3976	1/1	0.98	0.05	24,24,24,24	0
57	MG	1A	3018	1/1	0.98	0.17	32,32,32,32	0
57	MG	2A	3527	1/1	0.98	0.06	19,19,19,19	0
57	MG	1A	3199	1/1	0.98	0.09	17,17,17,17	0
57	MG	1A	3571	1/1	0.98	0.14	7,7,7,7	0
57	MG	1A	3709	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	3982	1/1	0.98	0.06	56,56,56,56	0
57	MG	1U	207	1/1	0.98	0.16	23,23,23,23	0
57	MG	1U	208	1/1	0.98	0.29	28,28,28,28	0
57	MG	1U	209	1/1	0.98	0.13	21,21,21,21	0
57	MG	1A	3884	1/1	0.98	0.09	14,14,14,14	0
57	MG	1A	3515	1/1	0.98	0.19	27,27,27,27	0
57	MG	1A	3985	1/1	0.98	0.08	8,8,8,8	0
57	MG	1a	3697	1/1	0.98	0.06	40,40,40,40	0
57	MG	1A	3228	1/1	0.98	0.21	34,34,34,34	0
57	MG	1A	3574	1/1	0.98	0.07	10,10,10,10	0
57	MG	1V	205	1/1	0.98	0.22	20,20,20,20	0
57	MG	2Q	201	1/1	0.98	0.12	37,37,37,37	0
57	MG	1a	3568	1/1	0.98	0.14	39,39,39,39	0
57	MG	1A	3177	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3260	1/1	0.98	0.12	26,26,26,26	0
57	MG	1A	3078	1/1	0.98	0.06	17,17,17,17	0
57	MG	1A	3803	1/1	0.98	0.05	30,30,30,30	0
57	MG	1A	3338	1/1	0.98	0.19	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1W	203	1/1	0.98	0.20	20,20,20,20	0
57	MG	1A	3339	1/1	0.98	0.25	17,17,17,17	0
57	MG	1A	3522	1/1	0.98	0.07	29,29,29,29	0
57	MG	2A	3101	1/1	0.98	0.08	39,39,39,39	0
57	MG	1X	101	1/1	0.98	0.29	24,24,24,24	0
57	MG	1B	217	1/1	0.98	0.06	37,37,37,37	0
57	MG	1X	104	1/1	0.98	0.10	42,42,42,42	0
57	MG	2A	3252	1/1	0.98	0.06	46,46,46,46	0
57	MG	2A	3400	1/1	0.98	0.29	41,41,41,41	0
57	MG	1A	3996	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3724	1/1	0.98	0.06	54,54,54,54	0
57	MG	2A	3558	1/1	0.98	0.14	35,35,35,35	0
57	MG	1A	3157	1/1	0.98	0.17	19,19,19,19	0
57	MG	2A	3560	1/1	0.98	0.20	39,39,39,39	0
57	MG	1A	3720	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3645	1/1	0.98	0.09	10,10,10,10	0
57	MG	1A	3722	1/1	0.98	0.05	22,22,22,22	0
57	MG	1A	3029	1/1	0.98	0.19	18,18,18,18	0
57	MG	1A	3724	1/1	0.98	0.05	33,33,33,33	0
57	MG	1A	3903	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3128	1/1	0.98	0.09	34,34,34,34	0
57	MG	1A	3726	1/1	0.98	0.10	11,11,11,11	0
57	MG	1B	229	1/1	0.98	0.10	30,30,30,30	0
57	MG	1d	301	1/1	0.98	0.19	29,29,29,29	0
57	MG	1A	3906	1/1	0.98	0.04	6,6,6,6	0
57	MG	1A	3648	1/1	0.98	0.05	9,9,9,9	0
57	MG	1A	3584	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3910	1/1	0.98	0.04	17,17,17,17	0
57	MG	1A	3650	1/1	0.98	0.04	15,15,15,15	0
57	MG	11	101	1/1	0.98	0.26	27,27,27,27	0
57	MG	1a	3597	1/1	0.98	0.22	33,33,33,33	0
57	MG	1A	3912	1/1	0.98	0.06	22,22,22,22	0
57	MG	2A	3125	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3423	1/1	0.98	0.11	14,14,14,14	0
57	MG	1A	4012	1/1	0.98	0.06	19,19,19,19	0
57	MG	1A	3234	1/1	0.98	0.08	10,10,10,10	0
57	MG	12	102	1/1	0.98	0.16	35,35,35,35	0
57	MG	1A	3914	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3020	1/1	0.98	0.04	17,17,17,17	0
57	MG	2A	3586	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3653	1/1	0.98	0.07	10,10,10,10	0
57	MG	1A	3073	1/1	0.98	0.08	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3134	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3734	1/1	0.98	0.08	32,32,32,32	0
57	MG	1D	304	1/1	0.98	0.13	32,32,32,32	0
57	MG	1A	3184	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	3589	1/1	0.98	0.08	19,19,19,19	0
57	MG	1A	3657	1/1	0.98	0.05	10,10,10,10	0
57	MG	1A	3238	1/1	0.98	0.38	21,21,21,21	0
57	MG	1A	3659	1/1	0.98	0.04	19,19,19,19	0
57	MG	1A	3239	1/1	0.98	0.14	17,17,17,17	0
57	MG	1A	3271	1/1	0.98	0.10	24,24,24,24	0
57	MG	2A	3001	1/1	0.98	0.26	33,33,33,33	0
57	MG	1A	3272	1/1	0.98	0.15	18,18,18,18	0
57	MG	1E	301	1/1	0.98	0.29	21,21,21,21	0
59	ZN	14	501	1/1	0.98	0.06	98,98,98,98	0
59	ZN	1n	102	1/1	0.98	0.04	72,72,72,72	0
59	ZN	2Y	202	1/1	0.98	0.04	75,75,75,75	0
57	MG	2A	3769	1/1	0.98	0.07	41,41,41,41	0
59	ZN	29	501	1/1	0.98	0.04	55,55,55,55	0
57	MG	1A	3273	1/1	0.98	0.15	18,18,18,18	0
57	MG	17	101	1/1	0.98	0.05	23,23,23,23	0
57	MG	1A	3017	1/1	0.99	0.07	11,11,11,11	0
57	MG	1A	3031	1/1	0.99	0.14	18,18,18,18	0
57	MG	1A	3459	1/1	0.99	0.03	34,34,34,34	0
57	MG	1A	3042	1/1	0.99	0.10	25,25,25,25	0
57	MG	1A	3218	1/1	0.99	0.12	28,28,28,28	0
57	MG	1w	401	1/1	0.99	0.10	23,23,23,23	0
57	MG	1A	3811	1/1	0.99	0.05	28,28,28,28	0
57	MG	1A	3964	1/1	0.99	0.07	10,10,10,10	0
57	MG	1A	3777	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3885	1/1	0.99	0.04	17,17,17,17	0
57	MG	2A	3414	1/1	0.99	0.23	29,29,29,29	0
57	MG	2A	3799	1/1	0.99	0.09	18,18,18,18	0
57	MG	1A	3778	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3219	1/1	0.99	0.04	19,19,19,19	0
57	MG	2A	3172	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3660	1/1	0.99	0.06	10,10,10,10	0
57	MG	1A	3747	1/1	0.99	0.02	11,11,11,11	0
57	MG	1B	218	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3220	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	4015	1/1	0.99	0.05	27,27,27,27	0
57	MG	1A	3749	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3133	1/1	0.99	0.03	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3022	1/1	0.99	0.11	6,6,6,6	0
57	MG	1A	3894	1/1	0.99	0.07	39,39,39,39	0
57	MG	1U	201	1/1	0.99	0.17	17,17,17,17	0
57	MG	2A	3680	1/1	0.99	0.08	33,33,33,33	0
57	MG	1A	3856	1/1	0.99	0.08	16,16,16,16	0
57	MG	1U	203	1/1	0.99	0.20	16,16,16,16	0
57	MG	1A	3056	1/1	0.99	0.09	23,23,23,23	0
57	MG	1A	3978	1/1	0.99	0.07	11,11,11,11	0
57	MG	2A	3008	1/1	0.99	0.05	26,26,26,26	0
57	MG	1A	3637	1/1	0.99	0.05	23,23,23,23	0
57	MG	2A	3128	1/1	0.99	0.35	34,34,34,34	0
57	MG	1A	3071	1/1	0.99	0.19	6,6,6,6	0
57	MG	2A	3689	1/1	0.99	0.02	34,34,34,34	0
57	MG	1A	3151	1/1	0.99	0.06	15,15,15,15	0
57	MG	1A	3090	1/1	0.99	0.15	12,12,12,12	0
57	MG	1A	3757	1/1	0.99	0.04	17,17,17,17	0
57	MG	1U	211	1/1	0.99	0.13	19,19,19,19	0
57	MG	1A	3863	1/1	0.99	0.10	10,10,10,10	0
57	MG	1a	3651	1/1	0.99	0.02	27,27,27,27	0
57	MG	1V	201	1/1	0.99	0.12	15,15,15,15	0
57	MG	2A	3697	1/1	0.99	0.09	30,30,30,30	0
57	MG	1A	3003	1/1	0.99	0.04	11,11,11,11	0
57	MG	1A	3541	1/1	0.99	0.08	11,11,11,11	0
57	MG	2A	3020	1/1	0.99	0.03	17,17,17,17	0
57	MG	1A	3542	1/1	0.99	0.17	18,18,18,18	0
57	MG	1A	3644	1/1	0.99	0.06	12,12,12,12	0
57	MG	1A	3989	1/1	0.99	0.03	22,22,22,22	0
57	MG	1A	3139	1/1	0.99	0.06	9,9,9,9	0
57	MG	2A	3512	1/1	0.99	0.04	29,29,29,29	0
57	MG	17	106	1/1	0.99	0.05	26,26,26,26	0
57	MG	1A	3908	1/1	0.99	0.05	15,15,15,15	0
57	MG	1A	3081	1/1	0.99	0.08	24,24,24,24	0
57	MG	27	101	1/1	0.99	0.09	38,38,38,38	0
57	MG	18	103	1/1	0.99	0.18	24,24,24,24	0
57	MG	1A	3115	1/1	0.99	0.26	24,24,24,24	0
57	MG	1A	3082	1/1	0.99	0.08	23,23,23,23	0
57	MG	1A	3034	1/1	0.99	0.11	25,25,25,25	0
57	MG	1D	306	1/1	0.99	0.03	10,10,10,10	0
57	MG	1A	3175	1/1	0.99	0.10	17,17,17,17	0
59	ZN	1Y	204	1/1	0.99	0.03	54,54,54,54	0
57	MG	1X	102	1/1	0.99	0.09	33,33,33,33	0
59	ZN	15	3210	1/1	0.99	0.07	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	ZN	16	104	1/1	0.99	0.03	31,31,31,31	0
57	MG	1D	308	1/1	0.99	0.11	19,19,19,19	0
57	MG	1A	3768	1/1	0.99	0.03	8,8,8,8	0
57	MG	1A	3176	1/1	0.99	0.08	15,15,15,15	0
59	ZN	25	105	1/1	0.99	0.04	46,46,46,46	0
59	ZN	26	102	1/1	0.99	0.03	47,47,47,47	0
57	MG	1X	106	1/1	0.99	0.10	16,16,16,16	0
57	MG	1A	3159	1/1	0.99	0.17	19,19,19,19	0
57	MG	1A	3214	1/1	0.99	0.23	23,23,23,23	0
60	SF4	2d	303	8/8	0.99	0.04	51,58,65,70	0
59	ZN	19	102	1/1	1.00	0.03	30,30,30,30	0
57	MG	1A	3703	1/1	1.00	0.06	5,5,5,5	0
57	MG	2A	3673	1/1	1.00	0.01	19,19,19,19	0
57	MG	1A	4056	1/1	1.00	0.03	17,17,17,17	0
57	MG	1A	3704	1/1	1.00	0.02	6,6,6,6	0

6.5 Other polymers (i)

There are no such residues in this entry.