



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 12:32 PM UTC

PDB ID : 9D0J / pdb_00009d0j
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with BT-33, mRNA, deacylated A-site tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.50Å resolution
Authors : Aleksandrova, E.V.; Tresco, B.I.C.; Wu, K.J.Y.; Ramkissoon, A.; Purdy, M.; See, D.N.Y.; Liu, R.Y.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2024-08-07
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

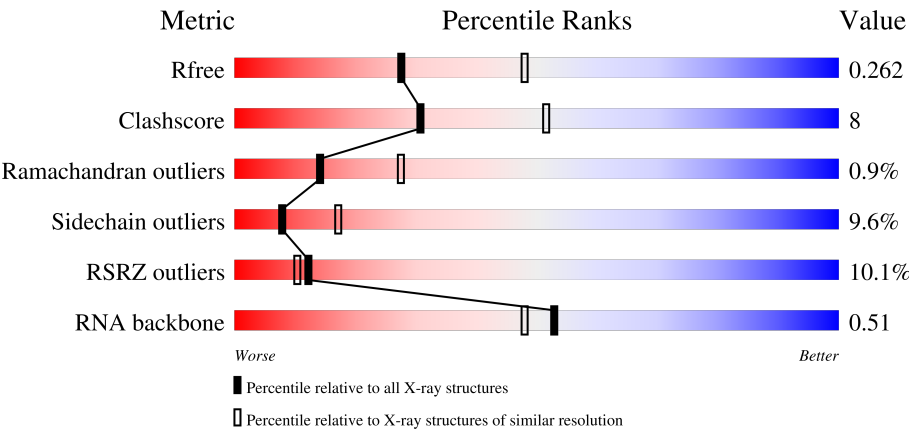
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 67% 25% 6% .
1	2A	2915	4% 59% 31% 6% .
2	1B	121	72% 26% ..
2	2B	121	2% 56% 32% 11% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
15	1T	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
27	25	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
52	2u	27	

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3386	-	-	-	X
56	MG	1A	3391	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299293 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	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	79	Total	C	N	O	S	0	0	0
			620	383	131	105	1			

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0	0
			1530	685	274	498	71	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	69	Total	C	N	O	P	S	0	0	0
			1482	662	267	482	69	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1059	Total	Mg	0	0
			1059	1059		
56	1B	39	Total	Mg	0	0
			39	39		
56	1D	12	Total	Mg	0	0
			12	12		
56	1E	16	Total	Mg	0	0
			16	16		
56	1F	14	Total	Mg	0	0
			14	14		
56	1G	4	Total	Mg	0	0
			4	4		
56	1I	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1N	6	Total 6	Mg 6	0	0
56	1O	6	Total 6	Mg 6	0	0
56	1P	6	Total 6	Mg 6	0	0
56	1Q	7	Total 7	Mg 7	0	0
56	1R	3	Total 3	Mg 3	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	7	Total 7	Mg 7	0	0
56	1V	6	Total 6	Mg 6	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1X	6	Total 6	Mg 6	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	7	Total 7	Mg 7	0	0
56	11	5	Total 5	Mg 5	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	2	Total 2	Mg 2	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	8	Total 8	Mg 8	0	0
56	16	3	Total 3	Mg 3	0	0
56	17	5	Total 5	Mg 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	18	4	Total 4 Mg 4	0	0
56	19	1	Total 1 Mg 1	0	0
56	1a	198	Total 198 Mg 198	0	0
56	1b	1	Total 1 Mg 1	0	0
56	1d	1	Total 1 Mg 1	0	0
56	1e	2	Total 2 Mg 2	0	0
56	1f	2	Total 2 Mg 2	0	0
56	1l	2	Total 2 Mg 2	0	0
56	1m	2	Total 2 Mg 2	0	0
56	1n	2	Total 2 Mg 2	0	0
56	1t	1	Total 1 Mg 1	0	0
56	1u	1	Total 1 Mg 1	0	0
56	1w	4	Total 4 Mg 4	0	0
56	1x	12	Total 12 Mg 12	0	0
56	2A	782	Total 782 Mg 782	0	0
56	2B	18	Total 18 Mg 18	0	0
56	2D	8	Total 8 Mg 8	0	0
56	2E	9	Total 9 Mg 9	0	0
56	2F	6	Total 6 Mg 6	0	0
56	2G	1	Total 1 Mg 1	0	0
56	2N	1	Total 1 Mg 1	0	0

Continued on next page...

Continued from previous page...

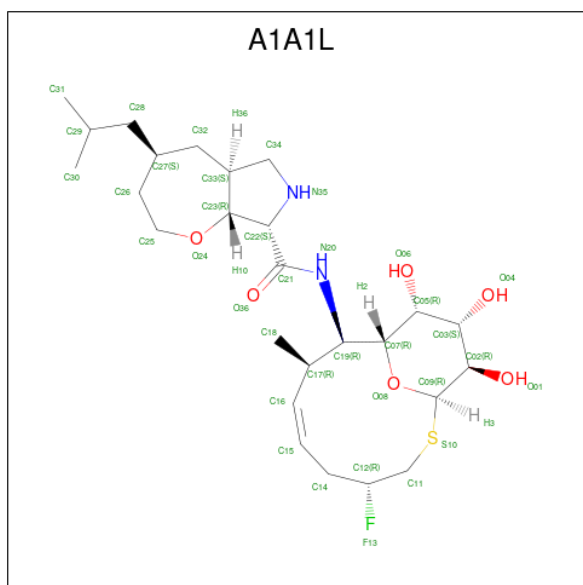
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2O	2	Total 2	Mg 2	0	0
56	2P	2	Total 2	Mg 2	0	0
56	2Q	2	Total 2	Mg 2	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2T	5	Total 5	Mg 5	0	0
56	2U	1	Total 1	Mg 1	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	1	Total 1	Mg 1	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	2Z	2	Total 2	Mg 2	0	0
56	20	1	Total 1	Mg 1	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	5	Total 5	Mg 5	0	0
56	27	4	Total 4	Mg 4	0	0
56	28	2	Total 2	Mg 2	0	0
56	2a	202	Total 202	Mg 202	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2j	1	Total	Mg	0	0
			1	1		
56	2k	1	Total	Mg	0	0
			1	1		
56	2l	5	Total	Mg	0	0
			5	5		
56	2q	2	Total	Mg	0	0
			2	2		
56	2r	2	Total	Mg	0	0
			2	2		
56	2t	2	Total	Mg	0	0
			2	2		
56	2v	1	Total	Mg	0	0
			1	1		
56	2w	3	Total	Mg	0	0
			3	3		
56	2x	6	Total	Mg	0	0
			6	6		

- Molecule 57 is (4S,5aS,8S,8aR)-N-[(1R,4R,6Z,8R,9R,10R,11R,12S,13R)-4-fluoro-11,12,13-trihydroxy-8-methyl-14-oxa-2-thiabicyclo[8.3.1]tetradec-6-en-9-yl]-4-(2-methylpropyl)octahydro-2H-oxepino[2,3-c]pyrrole-8-carboxamide (non-preferred name) (CCD ID: A1A1L) (formula: C₂₆H₄₃FN₂O₆S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
57	1A	1	Total	C	F	N	O	S	0	0
			36	26	1	2	6	1		

Continued on next page...

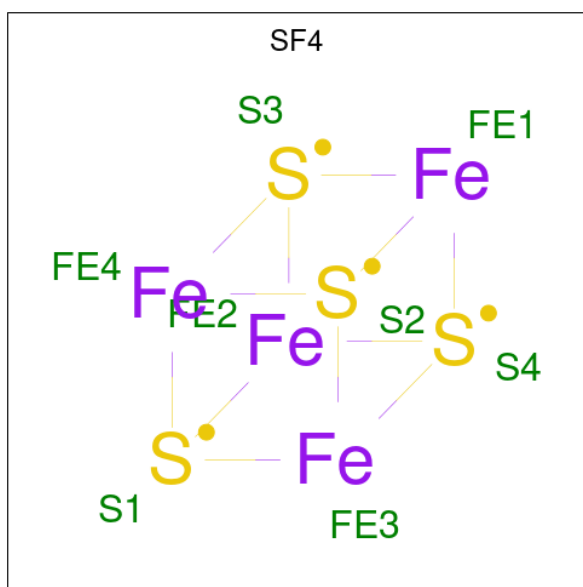
Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
57	2A	1	Total	C	F	N	O	S	0	0
			36	26	1	2	6	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	2Y	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1902	Total	O	0	0
			1902	1902		
61	1B	59	Total	O	0	0
			59	59		
61	1D	27	Total	O	0	0
			27	27		
61	1E	31	Total	O	0	0
			31	31		
61	1F	20	Total	O	0	0
			20	20		
61	1G	2	Total	O	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1H	2	Total	O	0	0
			2	2		
61	1N	6	Total	O	0	0
			6	6		
61	1O	6	Total	O	0	0
			6	6		
61	1P	18	Total	O	0	0
			18	18		
61	1Q	8	Total	O	0	0
			8	8		
61	1R	11	Total	O	0	0
			11	11		
61	1S	5	Total	O	0	0
			5	5		
61	1T	7	Total	O	0	0
			7	7		
61	1U	15	Total	O	0	0
			15	15		
61	1V	8	Total	O	0	0
			8	8		
61	1W	8	Total	O	0	0
			8	8		
61	1X	7	Total	O	0	0
			7	7		
61	1Y	3	Total	O	0	0
			3	3		
61	1Z	1	Total	O	0	0
			1	1		
61	10	8	Total	O	0	0
			8	8		
61	11	7	Total	O	0	0
			7	7		
61	12	4	Total	O	0	0
			4	4		
61	13	4	Total	O	0	0
			4	4		
61	14	1	Total	O	0	0
			1	1		
61	15	7	Total	O	0	0
			7	7		
61	16	1	Total	O	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	17	8	Total 8	O 8	0	0
61	18	13	Total 13	O 13	0	0
61	1a	298	Total 298	O 298	0	0
61	1b	1	Total 1	O 1	0	0
61	1l	5	Total 5	O 5	0	0
61	1m	1	Total 1	O 1	0	0
61	1o	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1t	1	Total 1	O 1	0	0
61	1v	5	Total 5	O 5	0	0
61	1w	4	Total 4	O 4	0	0
61	1x	9	Total 9	O 9	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	1002	Total 1002	O 1002	0	0
61	2B	16	Total 16	O 16	0	0
61	2D	23	Total 23	O 23	0	0
61	2E	16	Total 16	O 16	0	0
61	2F	14	Total 14	O 14	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	9	Total 9	O 9	0	0
61	2Q	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

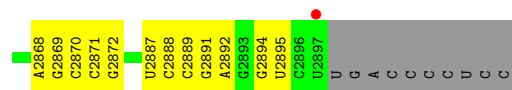
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2R	3	Total 3	O 3	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	3	Total 3	O 3	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	2	Total 2	O 2	0	0
61	2X	3	Total 3	O 3	0	0
61	20	2	Total 2	O 2	0	0
61	21	3	Total 3	O 3	0	0
61	23	3	Total 3	O 3	0	0
61	25	2	Total 2	O 2	0	0
61	27	4	Total 4	O 4	0	0
61	28	3	Total 3	O 3	0	0
61	29	1	Total 1	O 1	0	0
61	2a	168	Total 168	O 168	0	0
61	2e	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	3	Total 3	O 3	0	0
61	2p	1	Total 1	O 1	0	0
61	2t	1	Total 1	O 1	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	1	Total 1	O 1	0	0

Continued on next page...

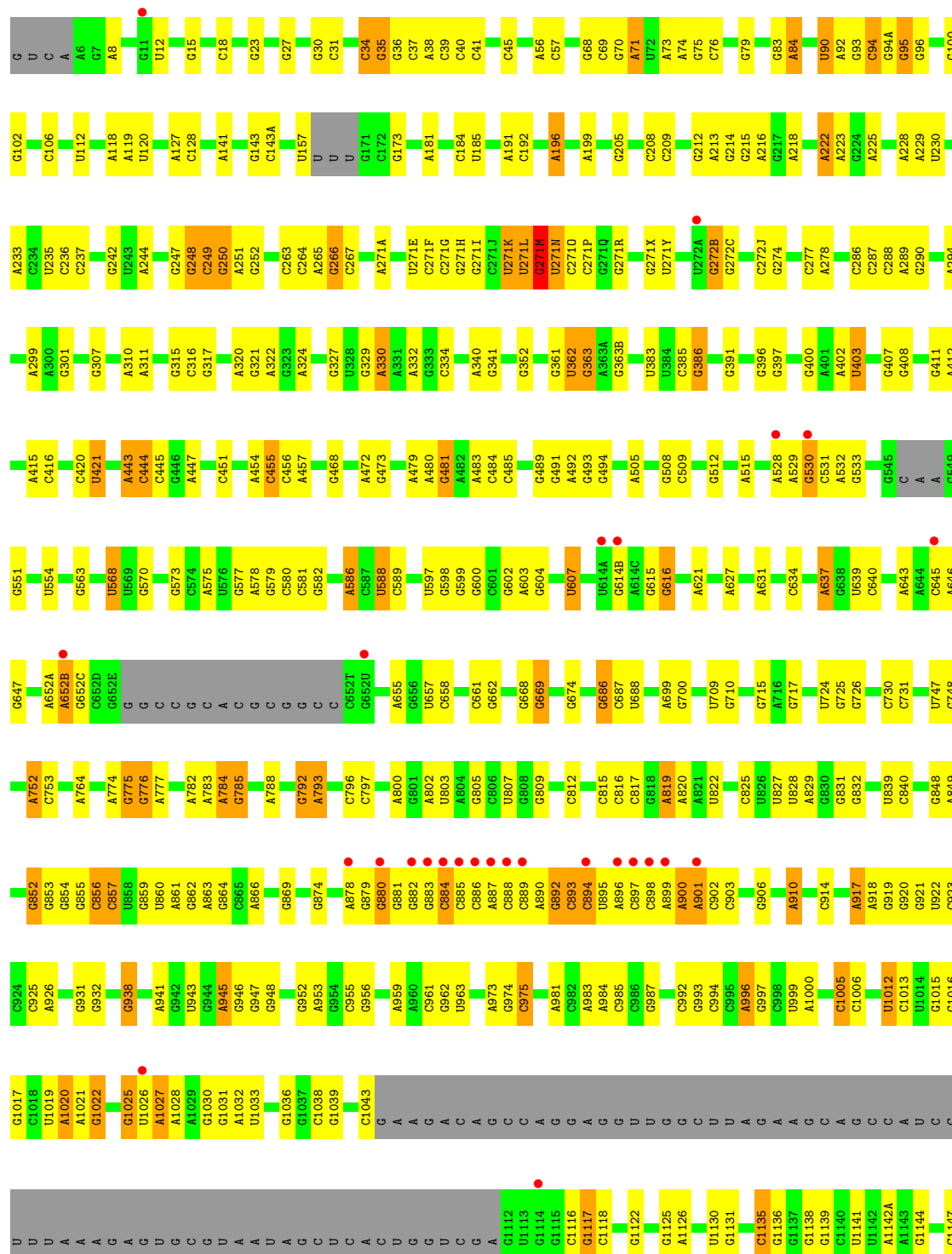
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2x	4	Total	O	0	0
			4	4		

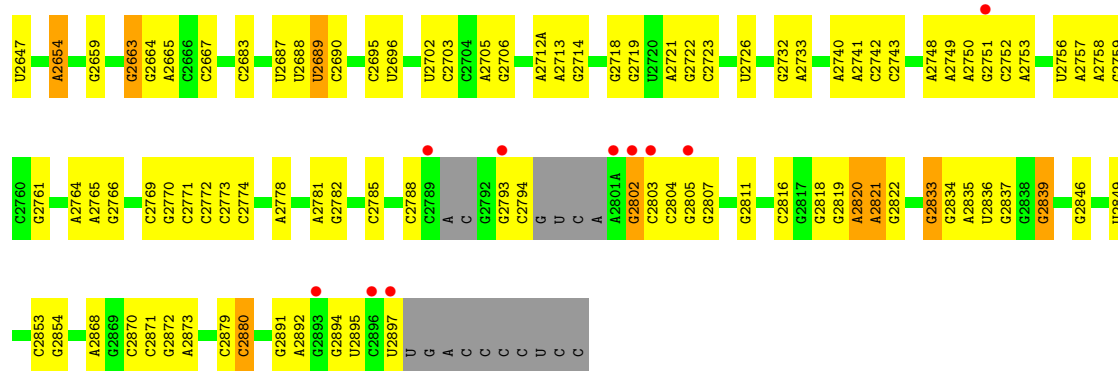
U754	C2628	A2476	C2350	U2233	C2145	C2065	U1951	A1803	G1674	A1509B		C1202	C1100
C2755	A2629	C2477	G2351	G2234	C2146	C2066	U1952	C1804	C1686	G1510	A1393	G1203	U1101
U2756	G2630	A2478	A2352	G2235	G2147	C2067	A1953	U1805	C1687	C1511	U1394	G1223	C1102
A2757	G2631			G2236	G2148	U2068	G1954	A1810	U1688	C1512	U1395	G1226	A1103
A2758		C2499	C2355	G2238	G2149	C2069	U1955	G1811	U1689	C1513	U1396	A1226	C1104
A2765	C2646	G2502		G2239	U2150	G2070	C1962	A1812	U1693	U1518	C1399	G1243	U1105
G2766	U2647	A2503	C2359	U2243	G2152	A2071	U1963	G1813	U1696	G1519		U1243	G1107
U2649	C2648	G2504	A2360	U2244	G2153		C1967	G1814	G1696	A1405	U1405	U1243	U1108
C2771	U2650	G2505	A2361		G2154	U2086	U1968	A1815	U1700	A1406	U1253	G1266	C1109
C2772				C2248	G2155	G2087	G1969	A1816	A1701	A1528A	C1407	G1266	A1111
A2778	A2654	G2512	A2366	G2251	G2157		A1970	G1817	G1702	G1532	G1416	U1271	U1112
		G2513	G2375		A2158	G2093	A1971	G1828	G1703	G	C1417	U1272	U1113
A2781	G2663	U2514	A2376	A2268	G2159	C2094	A1972	A1829	G1709	U	G1418	U1273	G1114
	A2665	G2515	A2377		G2160	G2095	A1972	A1830	C1710	A	U1267	U1278	G1115
C2787	C2666	C2517	A2378	G2271	G2161	U2096		G1839	C1710	C	U1420	C1289	C1116
C2788	C2667	A2518	G2379		G2162		A1986	C1843	G1721	G1537	G1421	C1290	G1117
C2789				G2277	C2163	U2099	U1991	U1847	A1722	U1540	A1427	U1300	G1125
A2790	G2674	U2522	G2383	A2276	G2164	G2100	G1992	A1847	A1722	G1541	C1428	U1301	C1135
C2791		G2529	G2384	G2279	G2165	G2101	U1993	U1851	G1739	G1542	G1429	U1302	C1136
G2792	A2679		C2385	G2280	U2167	U2102		C1852	G1740	A1558	C1430	C1289	G1137
G2793		G2535			G2168	C2108	G1996		A1741		U1431	C1290	G1138
C2794	C2683		U2390	C2283	A2169	U2109	G1997	C1745A	C1745A	A1566	C1432	C1300	G1139
			G2396	C2285	A2170	G2110	G1998	G1750	G1750	A1567	A1439	U1300	U1401
U2687	U2688	G2550	G2396	C2286	G2171	G2111	G1999	G1750	G1750	G1568	G1440	U1301	U1410
U2688	U2689	C2551	U2406	A2287	U2172	G2112		G1750	G1750	G1569	G1441	U1302	U1411
C2690	G2552	G2514	G2407		A2173	U2113	G2012	G1753	G1753	A1570	G1442	G1303	A1142A
	U2554		G2414	A2298	C2174	A2013	G2013	G1756	G1756	U1578		C1315	A1143
A2693		A2564		G2299	C2175	G2115	A2014			A1579	A1445		G1144
C2694		A2565	C2417		A2176	G2116		A1889		A1580		C1321	C1153
C2701	U2701	A2566	A2422	A2305	U2180	A2117	G2021	A1890	A1762	G1581	G1448	G1321	G1154
C2702	C2703	G2567	U2423	C2306	G2183	U2118	U2022	G1899	G1763		A1449	G1332	A1155
C2703		C2568	G2424	G2308	C2184	G2120	G2023	A1900	G1764	A1584	G1450	G1332	A1156
G2706			A2425	A2311	C2185	G2121	G2029	G1906	A1773	A1586		G1338	
A2712A	A2713	G2572	A2426	U2312	G2186	U2122	A2030	U1911	U1778	A1587	A1452	U1352	U1165
G2714		G2578	C2427	C2313	G2187	G2123	A2031	A1912	U1779	C1588	U1453	U1352	C1166
	C2591		G2428	G2319	C2188	G2125	A2032	A1915	A1780	C1589	A1383	U1354	U1167
G2717	G2592	G2592	G2429	G2320	U2189	A2126	A2033	U1916	C1781	G1593	C1467	G1355	
			U2431	G2321	G2190	G2127	C2043	A1917	C1782	G1594	C1468		G1170
A2721		A2602	A2435	G2325	G2192	C2128	G2049	U1918	A1784	A1603	G1482	A1389	G1171
G2722	C2723	U2605	A2439	C2326	G2193	U2130	C2050	A1919	A1785	C1607	C1493	A1380	A1174
		G2608	C2440	A2327		U2132	A2051	A1608	A1786	A1609	A1494	G1364	U1175
U2726	U2727	U2609	C2441	A2328	U2203	G2133	G2052	C1920	C1790	A1610	G1500	A1379	G1176
A2733		G2610	G2445	A2329	G2205	A2135	C2055	G1929	A1791	A1610	C1501	C1370	A1177
G2747	U2748	C2612	G2446	G2331	G2206	A2136	G2056	A1641	U1794	A1641	C1502	G1371	C1178
U2749		U2615	G2447	G2334	G2207	C2137	A2057	G1642	C1795	G1642	C1503	U1372	C1179
	A2749	C2616	A2448	A2335	U2218	C2138	A2058	G1647	U1796	G1647	C1504	U1372	G1183
	C2853	C2617	A2336	A2336	G2219	C2139	A2059	C1648	C1797	C1648	C1505	A1379	G1187
G2854		G2627	G2344	U2344	G2224	G2141	G2061	G1789	G1789	C1800	A1507	G1381	
C2855			U2347	C2347	A2225	C2142	A2062	C1801	C1801	C1670	A1508	G1381	G1191
A2860					C2226	U2144	C2064	A1802	A1802		C1509	A1384	C1201



- Molecule 1: 23S Ribosomal RNA

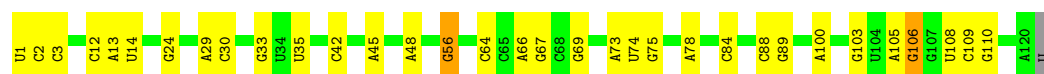


G1526	U2406	G2422	G2148	C2085	C1967	C1852	A1762	A1609	A1494	G1260	A1148
G2529	G2407	G2242	G2149	G2089	G1968	U1884	G1763	A1610	A1495	C1261	G1149
G2537	G2408	U2244	U2150	G2151	A1969	G1885	G1764	A1616	A1496	A1262	C1150
C2538	G2410	C2248	G2152	U2079	A1970	C1866	G1769	G1622	A1507	G1265	C1153
C2539	A2425	G2251	G2153	U2086	A1971	A1876	A1773	G1626	A1508	A1266	A1155
C2540	A2426	G2251	G2154	G2087	A1972	G1877	U1777	U1639	A1509	C1270	G1169
A2541	G2427	C2258	G2155	U2096	G1984	A1889	U1778	U1639	A1509A	A1271	G1170
A2542	G2428	C2258	G2156	C2097	A1980	A1890	U1779	C1640	U1514	A1272	G1171
G2543	G2429	U2262	G2157	U2098	A1981	A1891	A1780	C1647	U1515	U1273	G
G2544	A2430	U2262	G2158	U2099	U1991	G1896	G1781	G1648	U1518	A	A
U2552	U2431	A2268	G2160	U2102	G1992	G1896	G1782	C1648	U1519	U	U
G2553	A2435	A2268	G2161	C2103	U1993	G1899	A1783	G1653	G1536	A1278	G
U2554	A2436	A2273	G2162	C2103	C1996	G1899	A1784	A1654	A	A1284	A
C2558	A2439	A2274	G2163	G2104	G1997	A1900	A1785	A1654	C1530	A1287	C1178
C2559	G2440	C2275	G2165	C2105	G1998	A1901	A1786	A1668	C1531	C1417	C1179
U2566	U2441	G2276	G2166	G2106	C1999	C1902	U1790	G1667	C1532	G1418	C1180
G2567	G2447	A2278	U2167	C2107	G2002	G1906	C1790	A1664	U	U1292	C1181
C2573	U2448	G2282	G2168	U2108	U2002	U1911	A1791	A1664	A	C1299	G1186
C2573	U2449	G2282	A2170	G2109	G2010	U1911	U1794	G1666	C1536	U1300	G1187
U2580	A2450	C2283	A2171	G2110	G2011	U1912	U1795	G1667	C1536	A1301	G1188
G2576	A2453	C2285	U2172	G2111	G2012	A1913	U1796	G1668	C1536	A1302	G1189
A2577	G2457	A2286	A2173	U2113	A2014	C1914	C1797	A1669	C1536	G1303	G1189
G2578	G2468	A2287	G2175	A2114	A2014	U1915	U1798	C1670	C1536	G1303	G1189
C2579	A2469	C2288	C2176	G2115	A2014	A1916	G1799	G1674	C1536	U1299	G1189
U2580	G2472	G2289	C2177	A2116	A2020	U1917	C1800	G1674	C1536	U1313	G1196
A2589	G2472	G2290	C2178	A2117	A2021	C1920	G1801	U1688	C1536	C1314	G1196
G2592	C2475	U2291	G2179	U2118	U2022	A1802	A1802	A1689	C1536	G1325	A1204
A2602	A2476	C2292	U2180	G2120	G2023	C1924	C1804	U1693	C1536	A1342	A1210
G2603	G2484	C2295	G2181	U2122	G2027	A1927	A1812	G1696	C1536	A1345	U1211
U2604	G2485	C2296	G2182	U2123	U2028	A1928	G1813	G1697	C1536	G1346	G1212
U2605	G2488	C2297	G2183	G2124	G2029	G1929	G1814	A1698	C1536	A1349	A1220
U2609	G2489	G2299	G2184	G2125	A2030	G1930	G1815	G1699	C1536	U1352	G1226
U2611	U2491	G2300	U2189	G2127	A2031	U1931	G1816	A1567	C1536	A1353	G1227
C2612	U2492	G2300	G2190	C2128	G2032	A1932	G1817	A1569	C1536	A1354	G1227
C2617	U2493	G2303	G2192	C2129	A2033	G1933	C1829	A1460	C1536	G1355	G1236
G2625	G2502	A2305	A2198	U2130	C2040	A1936	A1829	C1467	C1536	G1359	G1239
A2629	A2503	C2306	A2199	U2132	A2042	A1938	C1830	C1468	C1536	A1360	U1240
G2630	U2504	G2307	U2203	G2133	C2043	U1939	G1831	A1469	C1536	A1360	A1241
U2631	G2505	G2308	C2205	A2134	G2049	C1942	U1833	A1471	C1536	G1364	A1242
G2631	U2506	A2310	G2206	A2135	C2050	G1946	G1835	A1472	C1536	A1365	G1243
G2634	C2507	A2311	G2207	C2136	A2051	C1947	A1741	G1473	C1536	A1366	G1244
G2634	G2516	U2312	A2208	C2137	C2055	U1946	G1837	C1474	C1536	A1367	A1247
U2635	C2517	C2313	U2218	C2138	G2056	C1947	C1838	C1743	C1536	C1370	A1263
U2636	U2518	G2314	A2225	C2139	G2056	A1952	G1839	C1744	C1536	G1478	A1263
U2637	G2520	C2315	C2142	C2140	A2059	U1955	C1843	C1754	C1536	G1478	A1263
G2639	G2524	G2316	C2143	C2141	C2060	C1988	A1847	G1755	C1536	U1371	A1254
G2646	G2525	G2317	U2144	C2142	G2061	C1988	A1848	G1756	C1536	A1372	U1255
		G2318	C2145	C2143	A2062	C1962	U1757	G1757	C1536	A1379	G1256
		G2319	C2146	G2147	C2064	U1963	U1851	G1758	C1536	A1379	G1257
		G2320	G2147	G2147	C2064	U1963	U1851	G1758	C1536	A1380	G1257



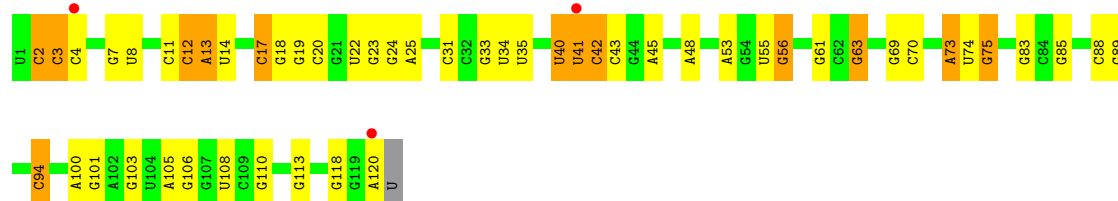
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 72% 26% ..



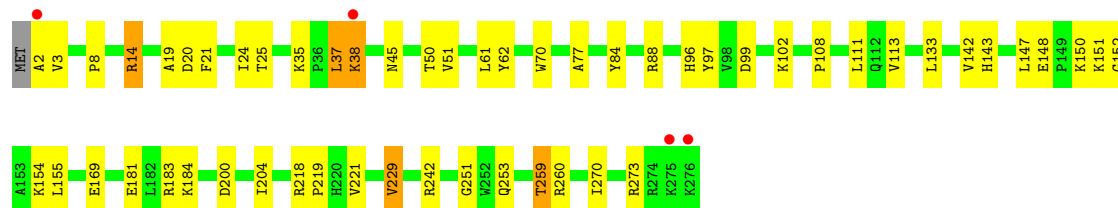
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 56% 32% 11% .



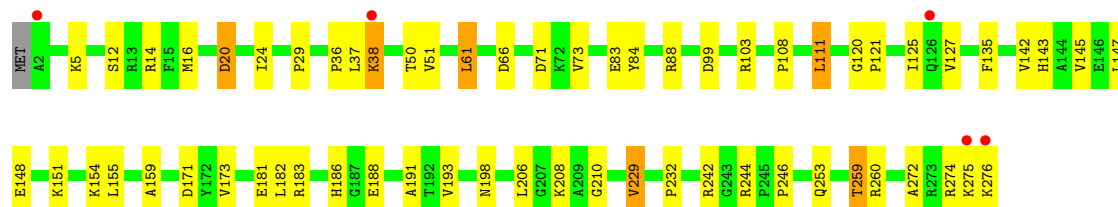
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 80% 18% .

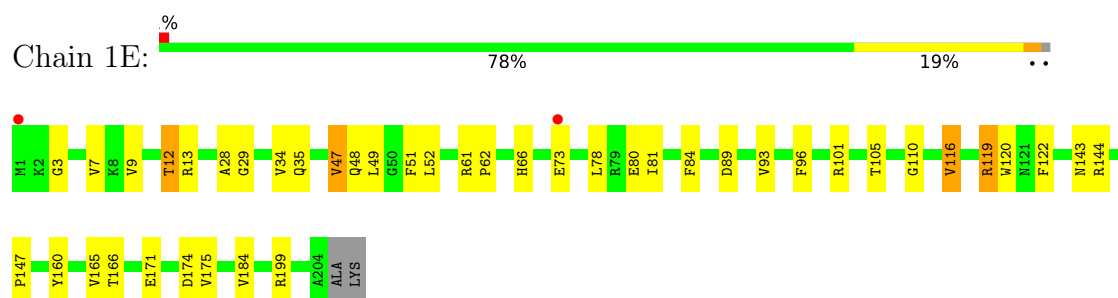


• Molecule 3: 50S ribosomal protein L2

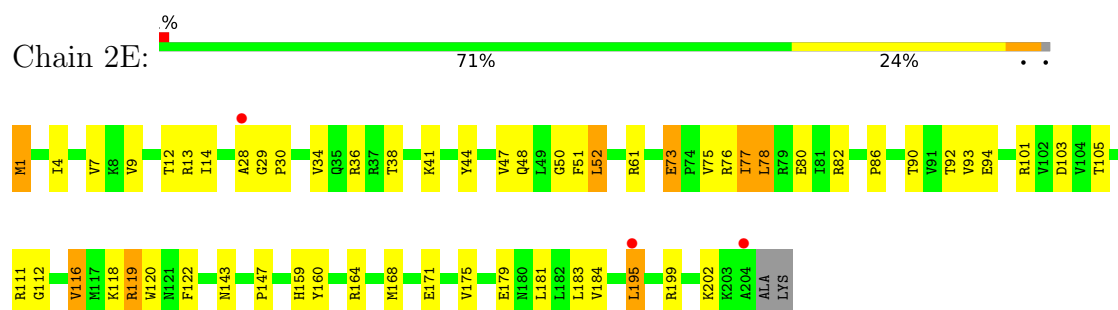
Chain 2D: 77% 20% .



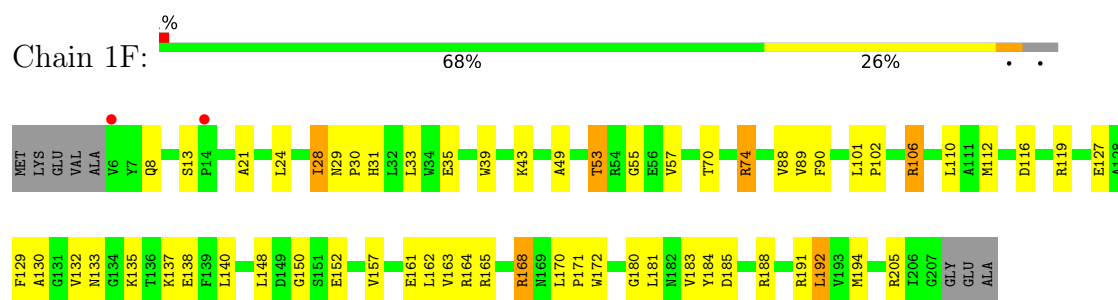
- Molecule 4: 50S ribosomal protein L3



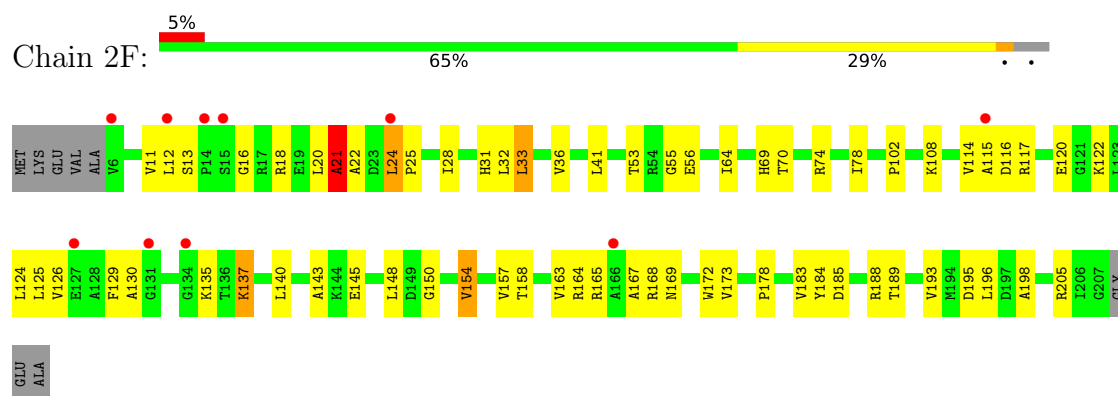
- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

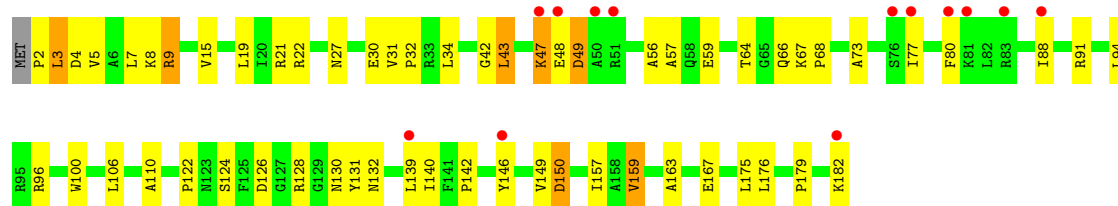


- Molecule 5: 50S ribosomal protein L4

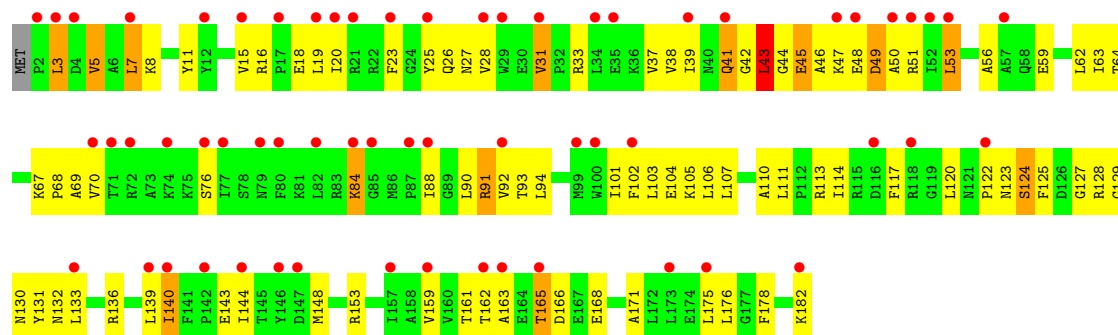


- Molecule 6: 50S ribosomal protein L5

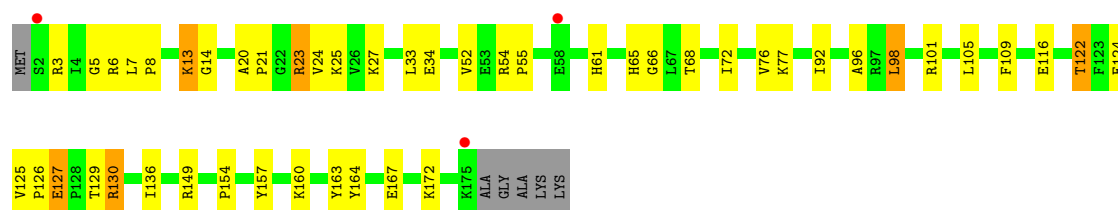
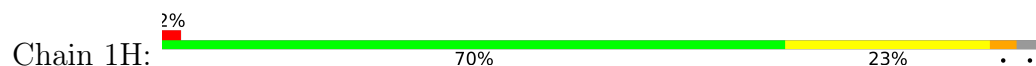




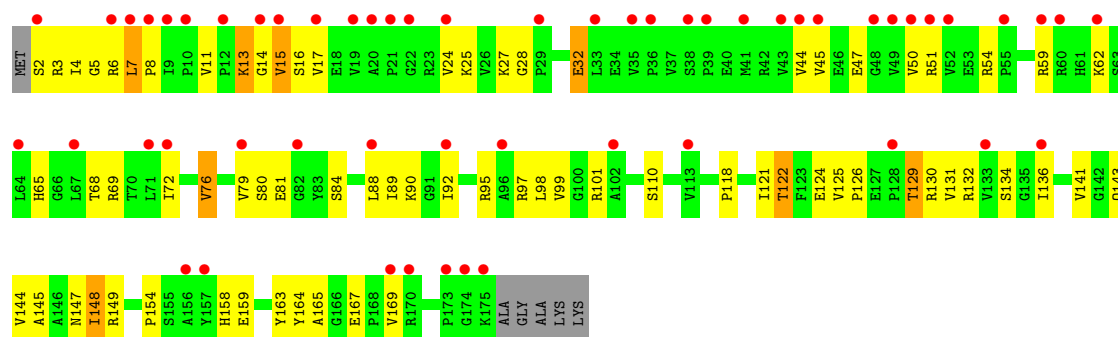
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

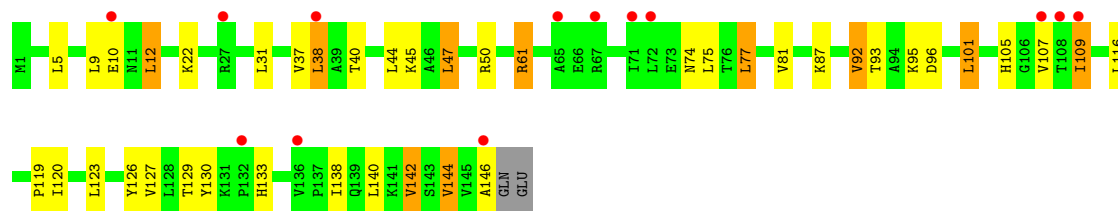


• Molecule 7: 50S ribosomal protein L6

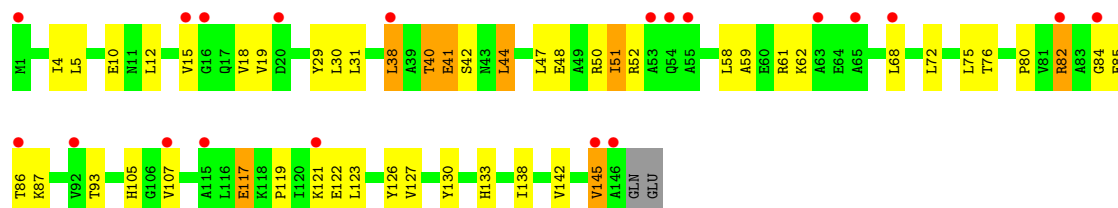


• Molecule 8: 50S ribosomal protein L9

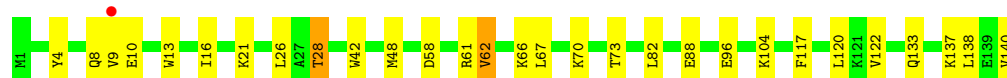
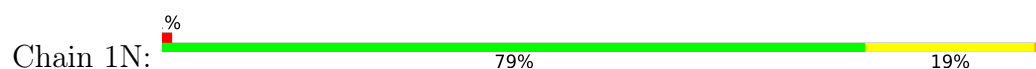




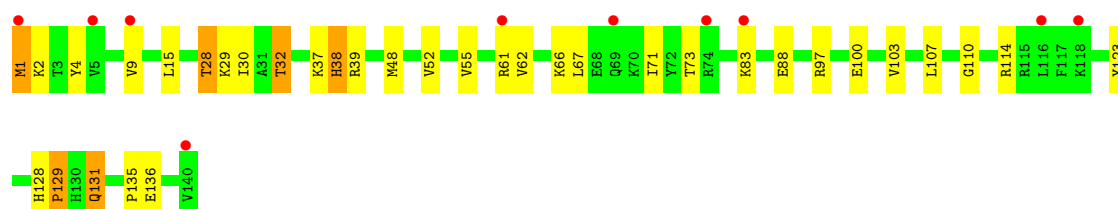
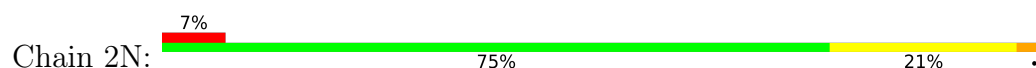
• Molecule 8: 50S ribosomal protein L9



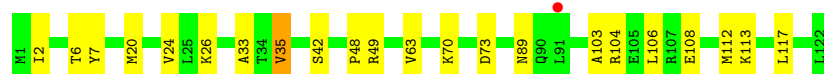
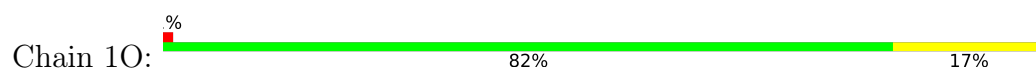
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13



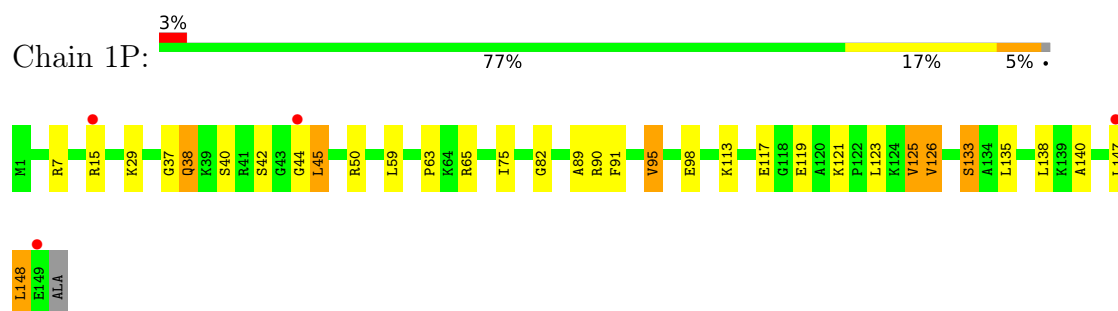
• Molecule 10: 50S ribosomal protein L14



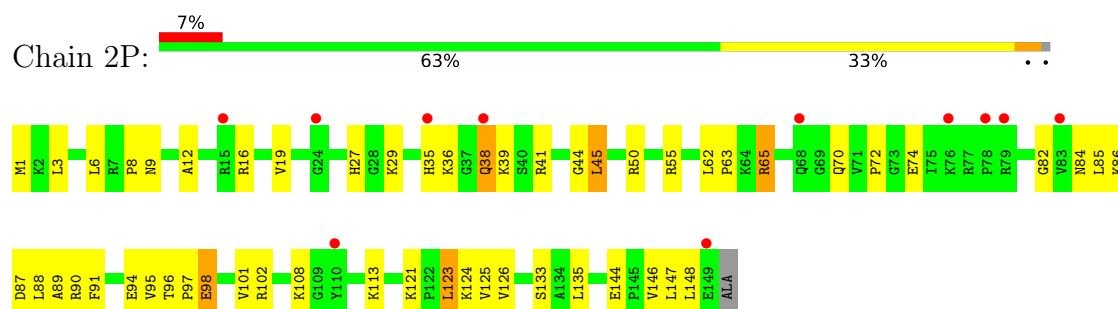
• Molecule 10: 50S ribosomal protein L14



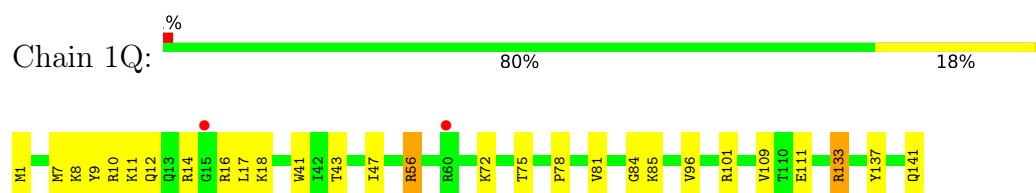
- Molecule 11: 50S ribosomal protein L15



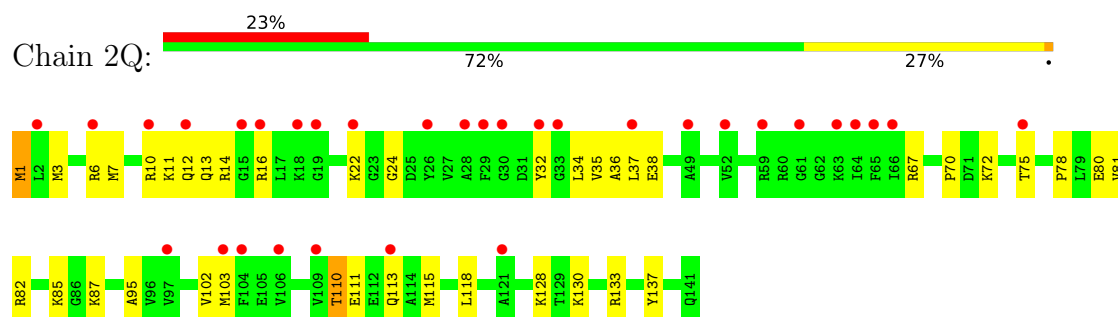
- Molecule 11: 50S ribosomal protein L15



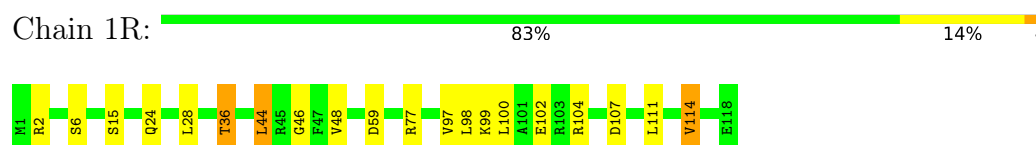
- Molecule 12: 50S ribosomal protein L16



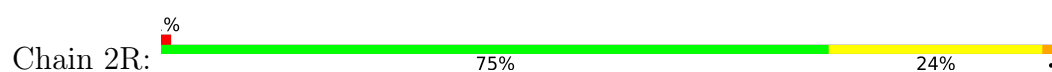
- Molecule 12: 50S ribosomal protein L16



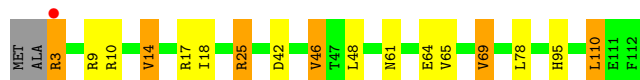
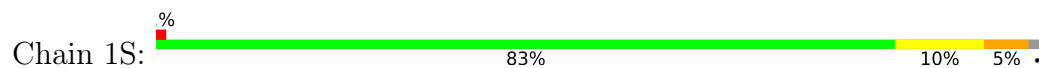
- Molecule 13: 50S ribosomal protein L17



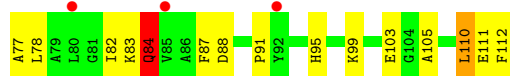
- Molecule 13: 50S ribosomal protein L17



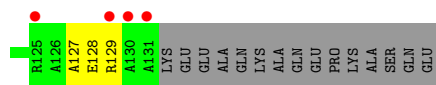
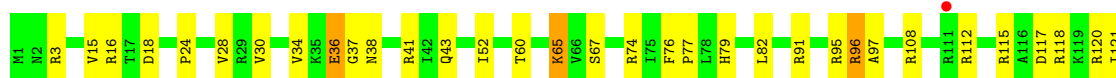
• Molecule 14: 50S ribosomal protein L18



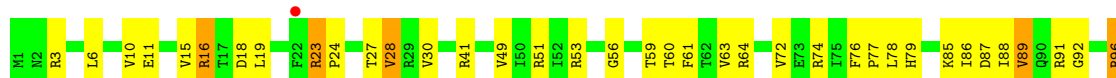
• Molecule 14: 50S ribosomal protein L18



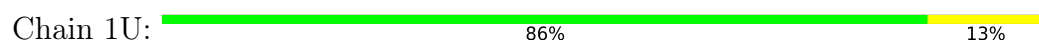
• Molecule 15: 50S ribosomal protein L19



• Molecule 15: 50S ribosomal protein L19

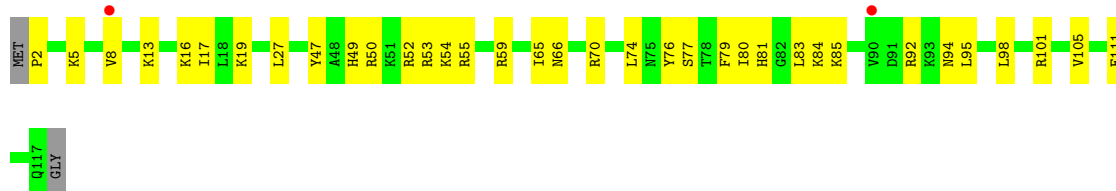


• Molecule 16: 50S ribosomal protein L20

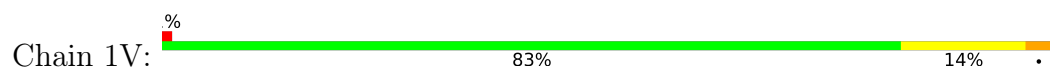




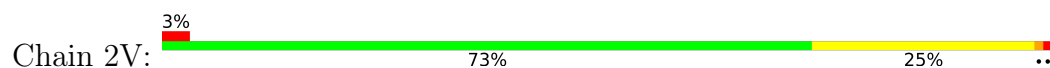
- Molecule 16: 50S ribosomal protein L20



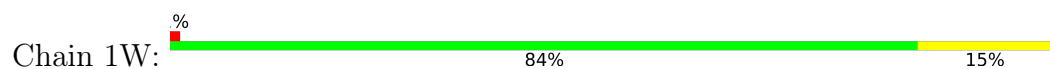
- Molecule 17: 50S ribosomal protein L21



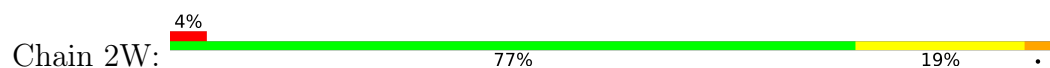
- Molecule 17: 50S ribosomal protein L21



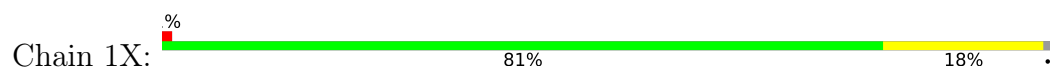
- Molecule 18: 50S ribosomal protein L22



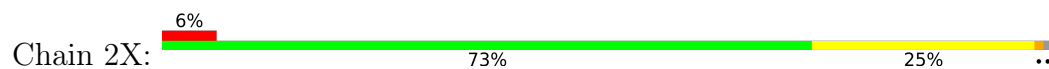
- Molecule 18: 50S ribosomal protein L22



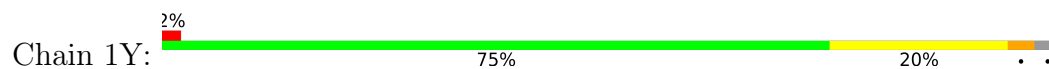
- Molecule 19: 50S ribosomal protein L23



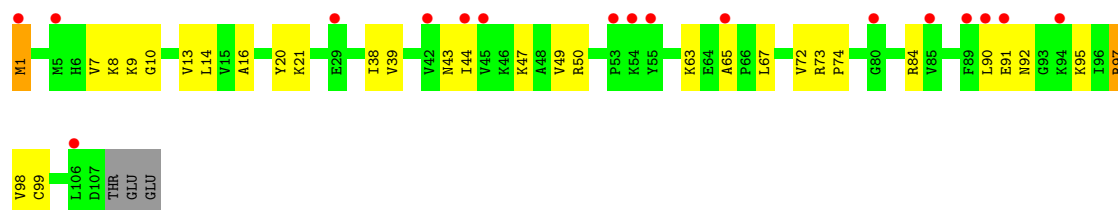
- Molecule 19: 50S ribosomal protein L23



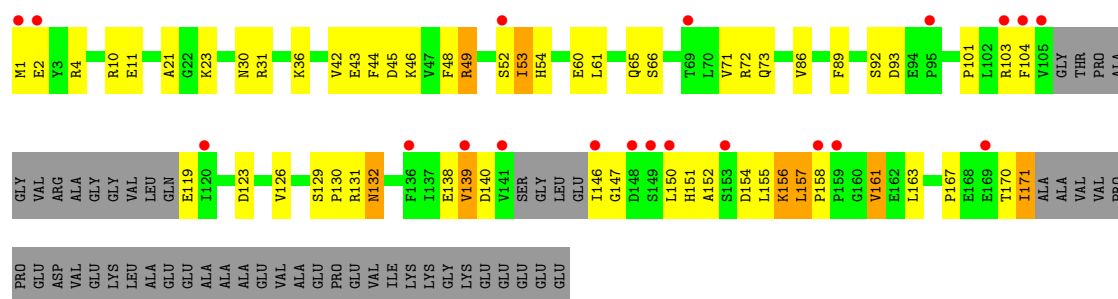
- Molecule 20: 50S ribosomal protein L24



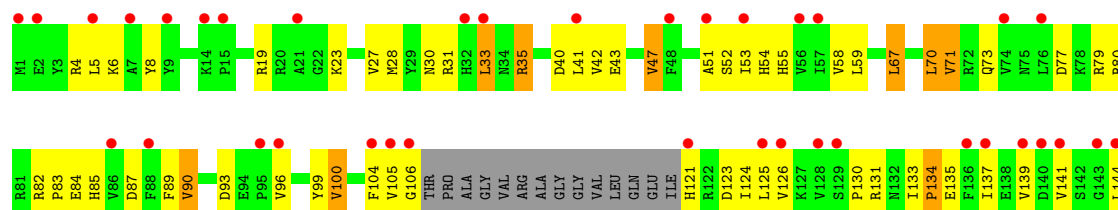
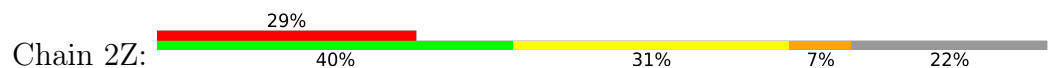
- Molecule 20: 50S ribosomal protein L24

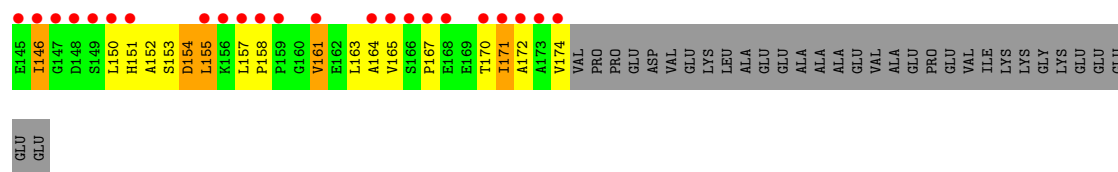


- Molecule 21: 50S ribosomal protein L25

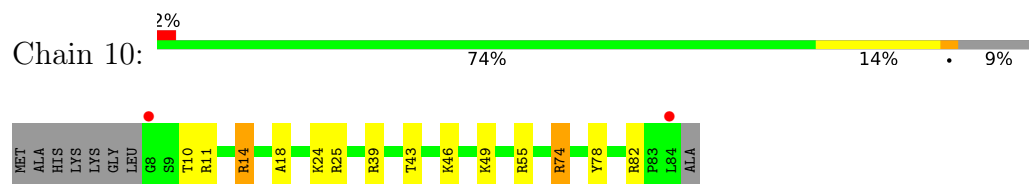


- Molecule 21: 50S ribosomal protein L25

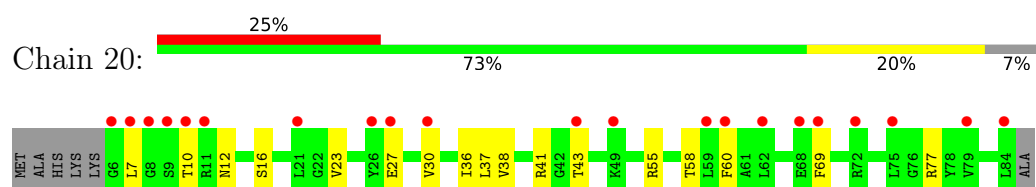




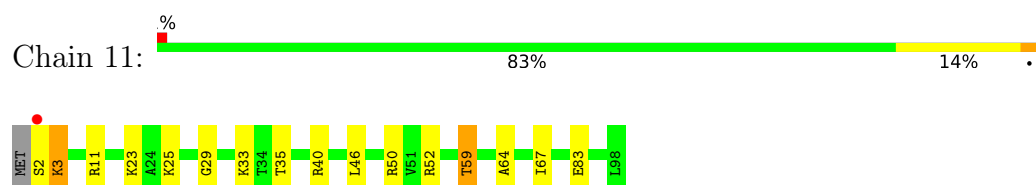
- Molecule 22: 50S ribosomal protein L27



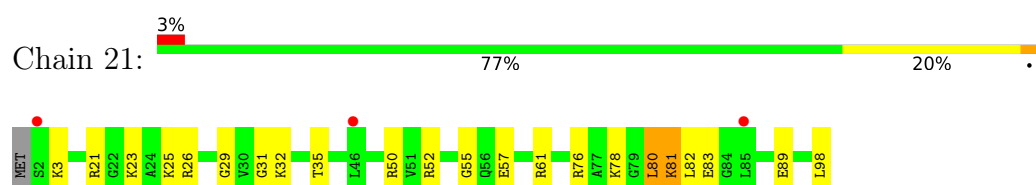
- Molecule 22: 50S ribosomal protein L27



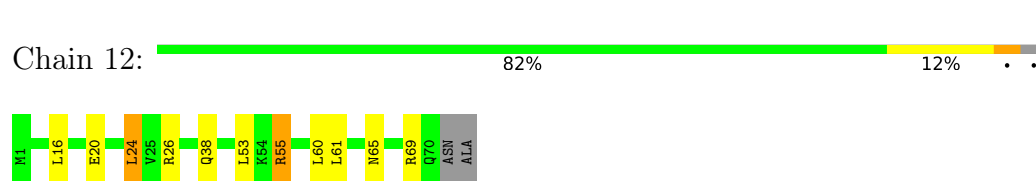
- Molecule 23: 50S ribosomal protein L28



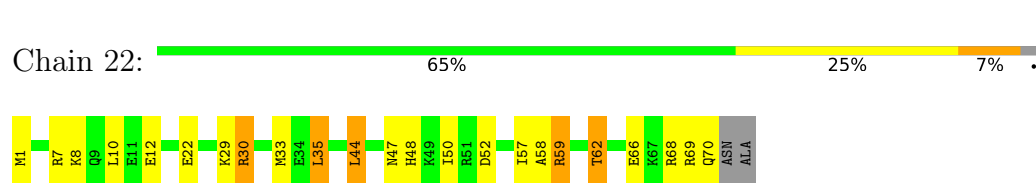
- Molecule 23: 50S ribosomal protein L28



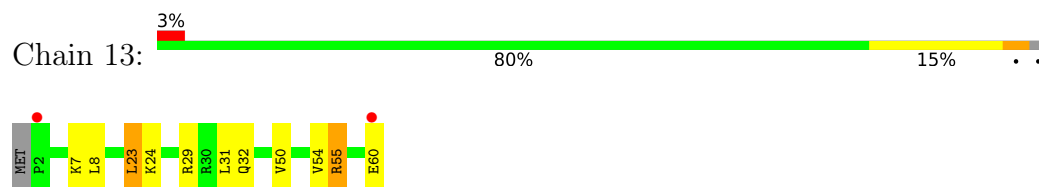
- Molecule 24: 50S ribosomal protein L29



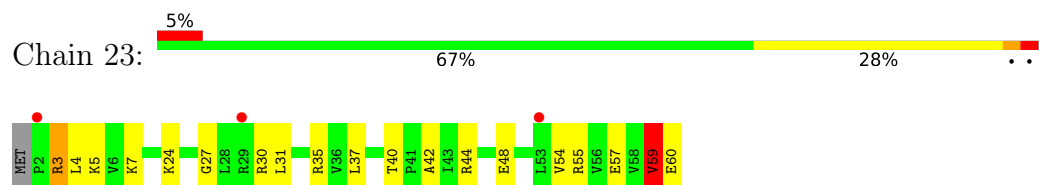
- Molecule 24: 50S ribosomal protein L29



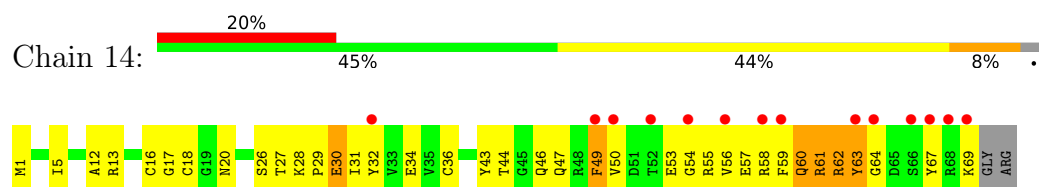
- Molecule 25: 50S ribosomal protein L30



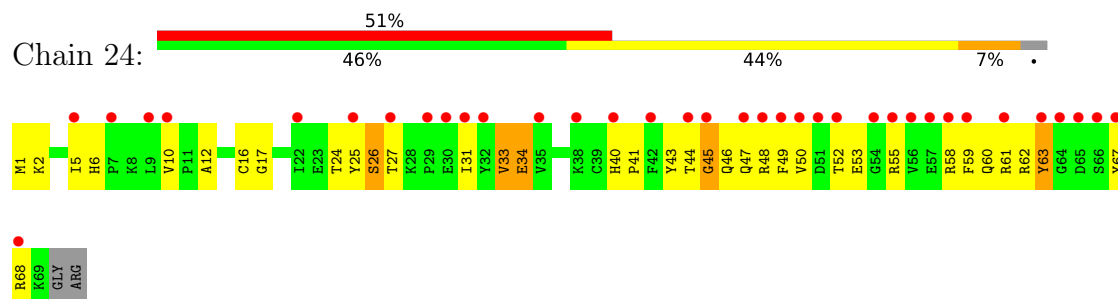
- Molecule 25: 50S ribosomal protein L30



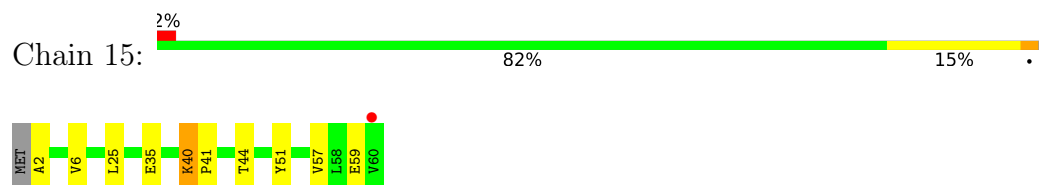
- Molecule 26: 50S ribosomal protein L31



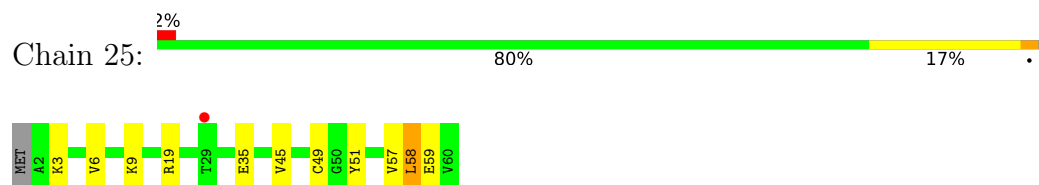
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

Chain 16:  63% 33% ..



- Molecule 28: 50S ribosomal protein L33

Chain 26:  4% 72% 24% ..



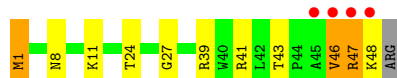
- Molecule 29: 50S ribosomal protein L34

Chain 17:  6% 80% 14% ..



- Molecule 29: 50S ribosomal protein L34

Chain 27:  8% 76% 16% 6% .



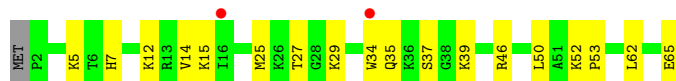
- Molecule 30: 50S ribosomal protein L35

Chain 18:  72% 25% ..



- Molecule 30: 50S ribosomal protein L35

Chain 28:  3% 71% 28% .

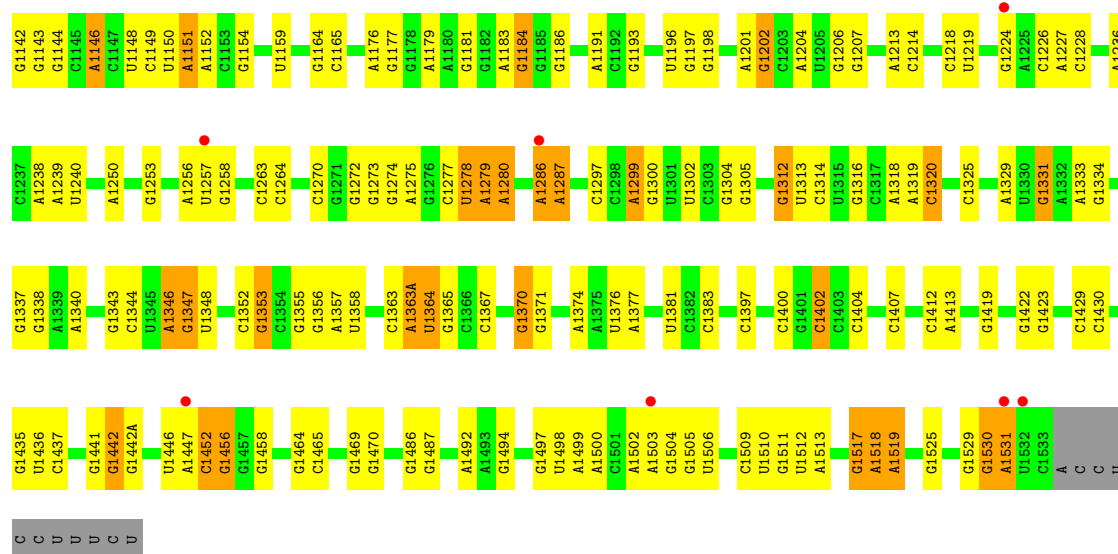


- Molecule 31: 50S ribosomal protein L36

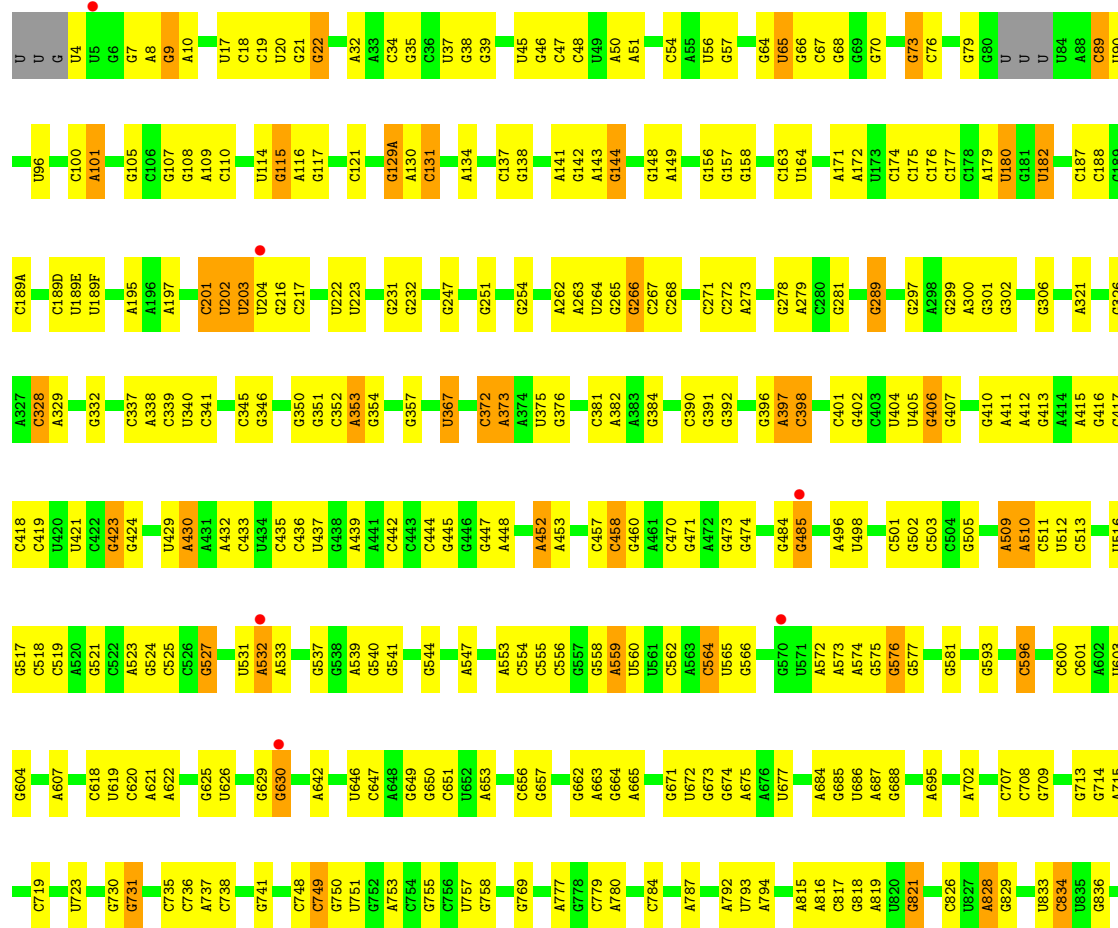
Chain 19:  84% 16%

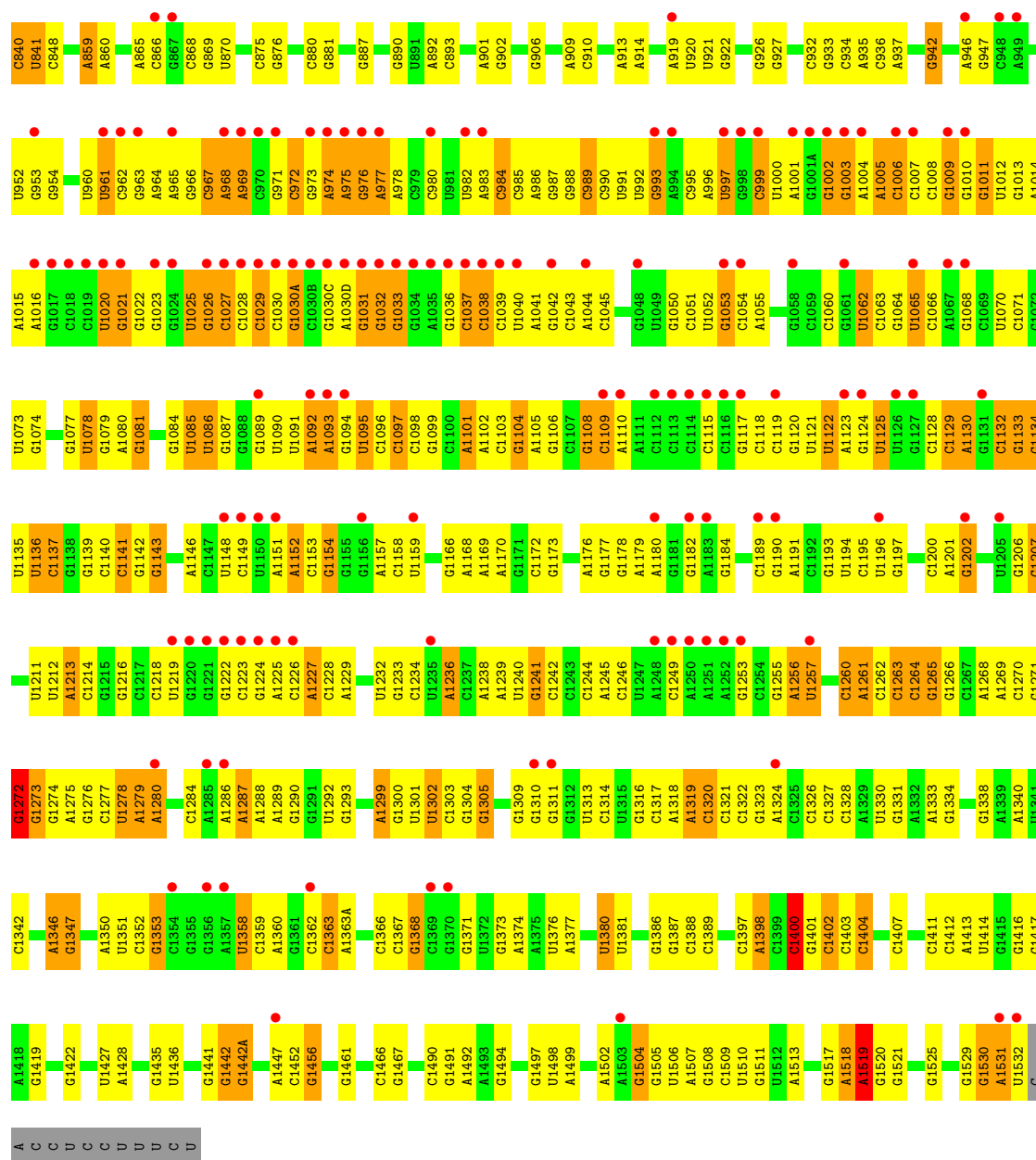


- Molecule 31: 50S ribosomal protein L36



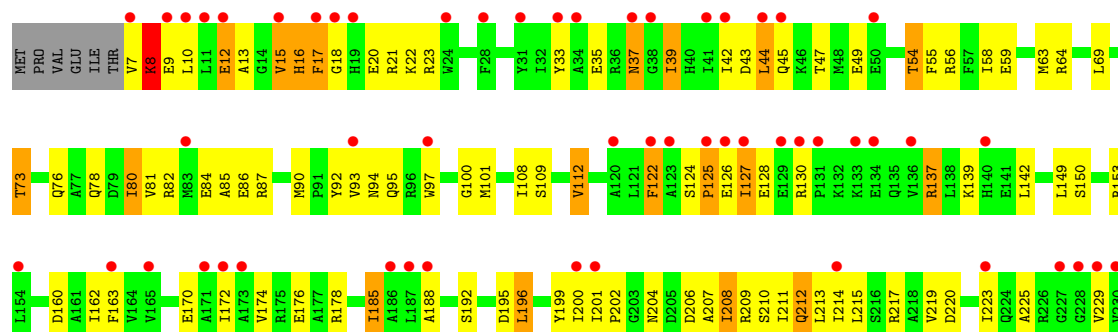
• Molecule 32: 16S Ribosomal RNA

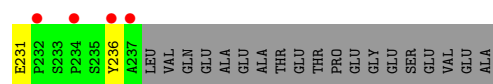




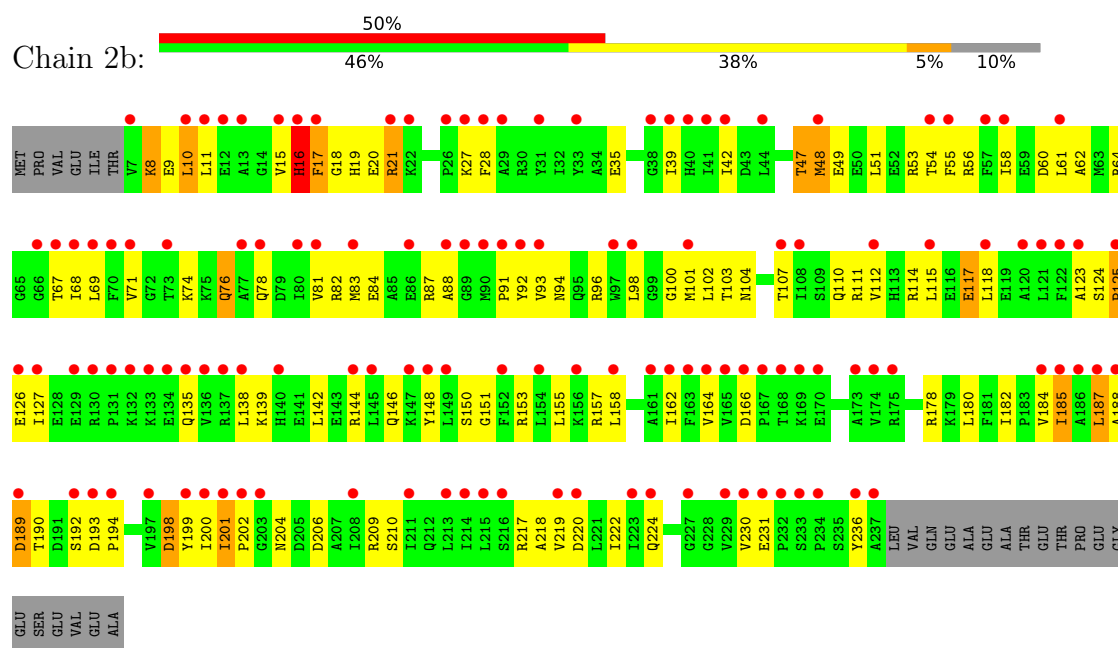
• Molecule 33: 30S ribosomal protein S2

Chain 1b: 23% 50% 32% 7% 10%

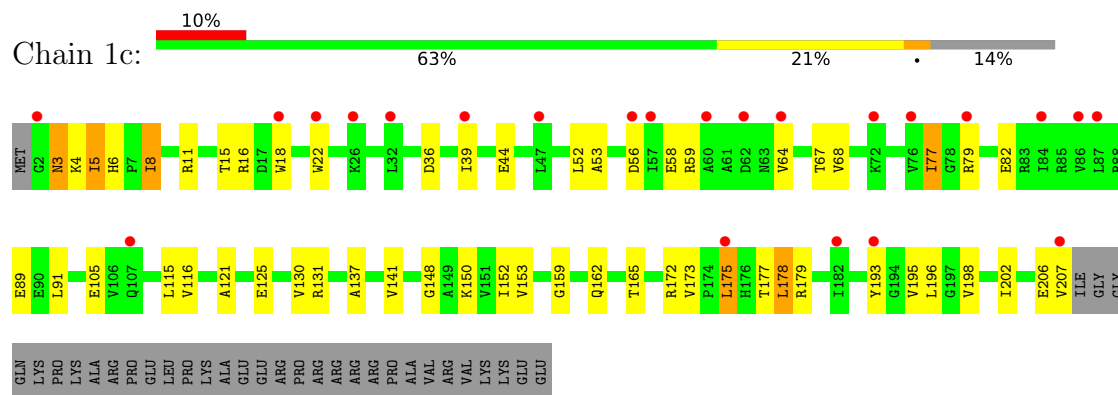




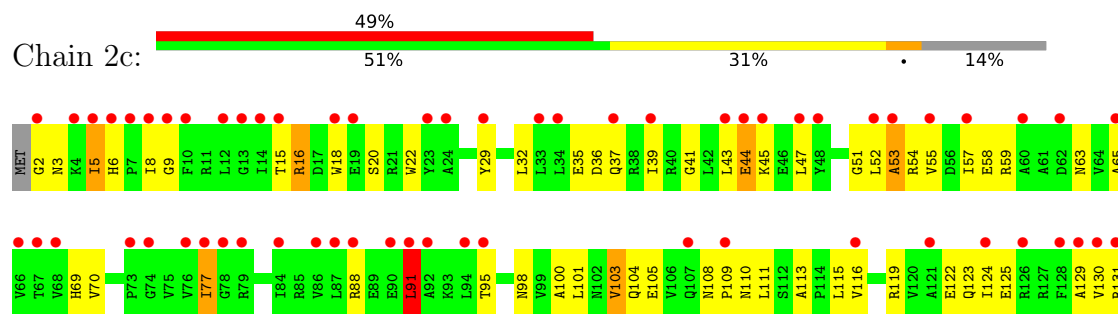
• Molecule 33: 30S ribosomal protein S2

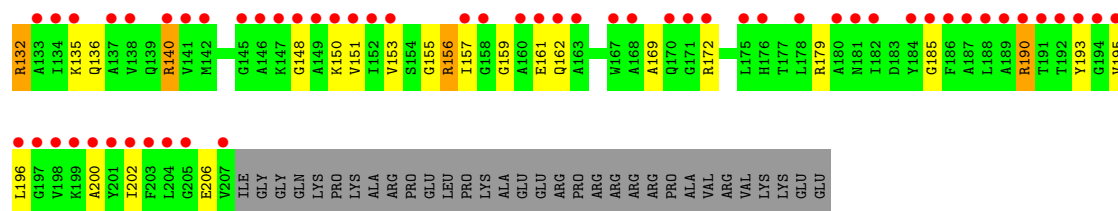


• Molecule 34: 30S ribosomal protein S3

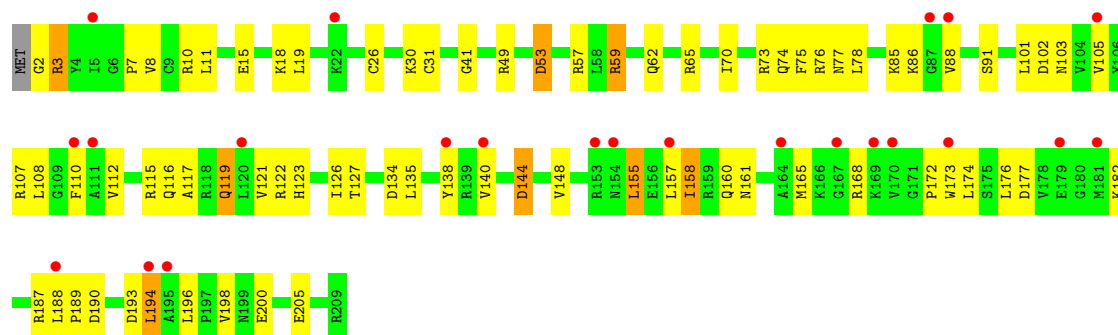


• Molecule 34: 30S ribosomal protein S3

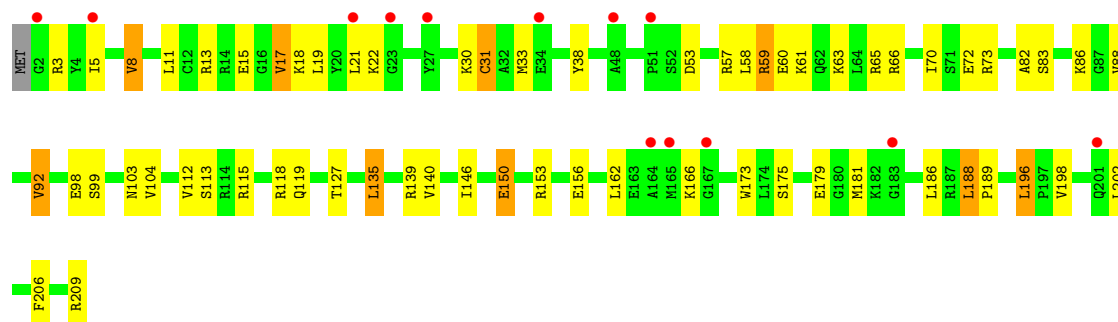




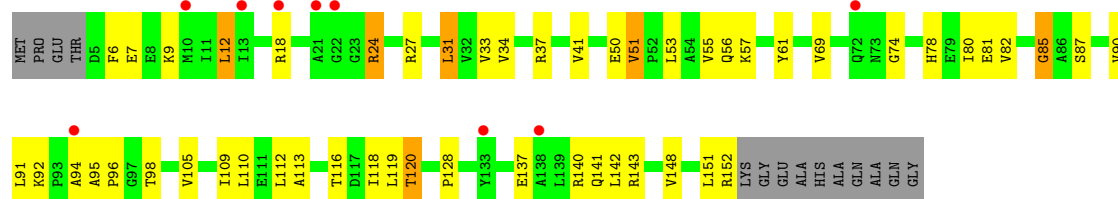
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4

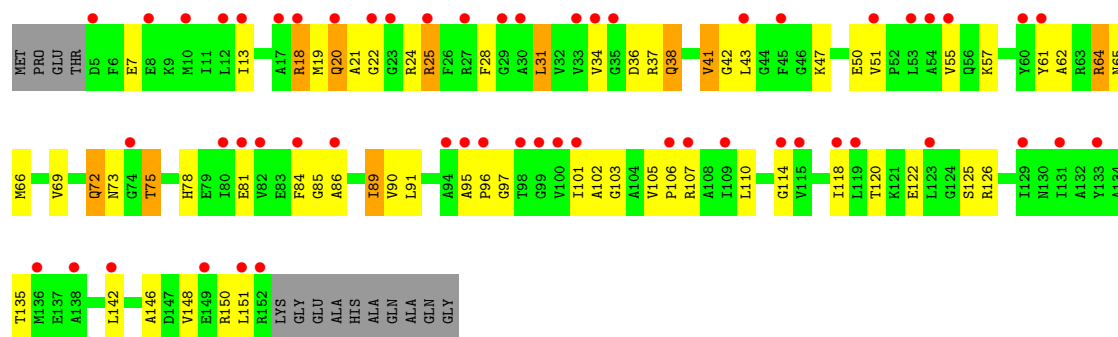


• Molecule 36: 30S ribosomal protein S5

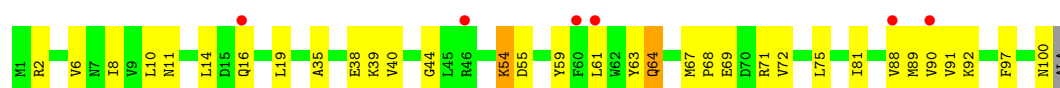


• Molecule 36: 30S ribosomal protein S5

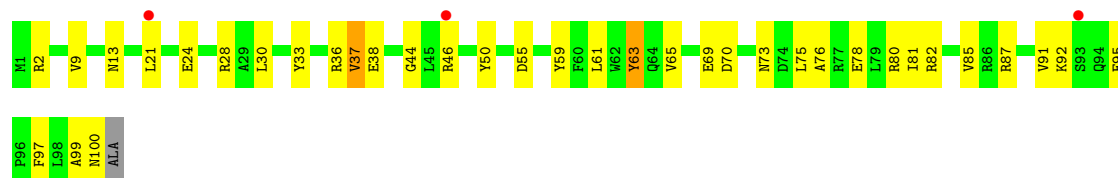




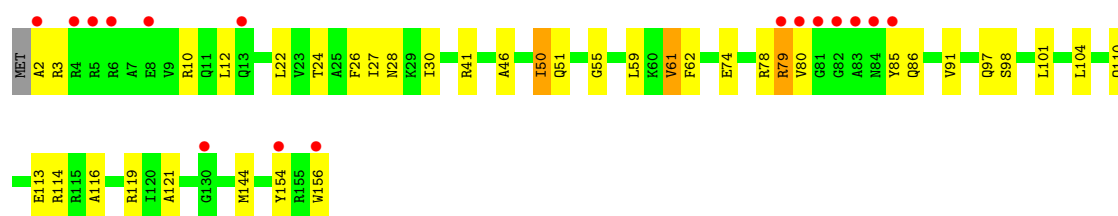
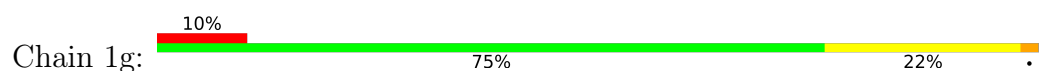
• Molecule 37: 30S ribosomal protein S6



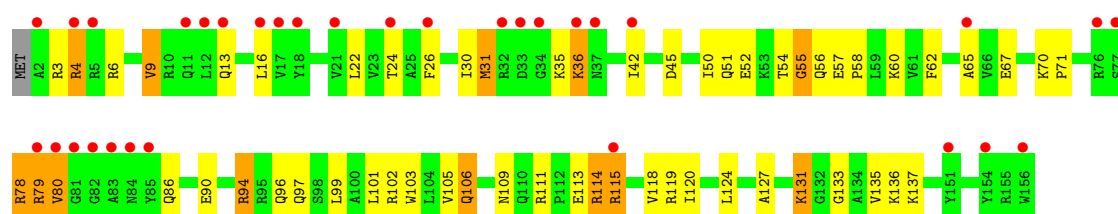
• Molecule 37: 30S ribosomal protein S6



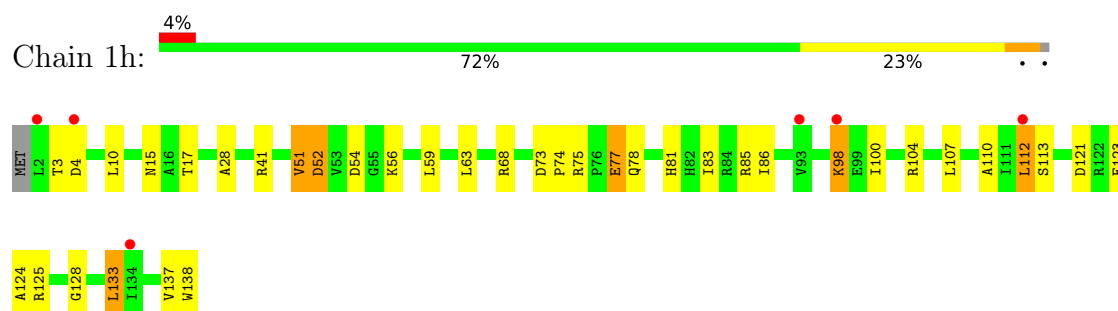
• Molecule 38: 30S ribosomal protein S7



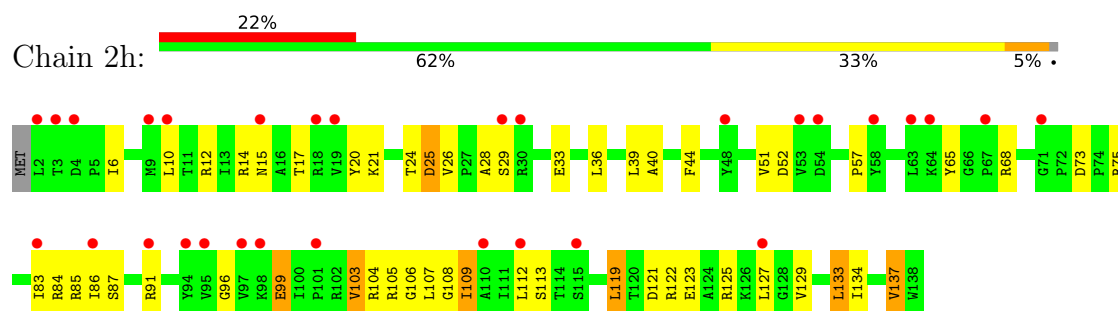
• Molecule 38: 30S ribosomal protein S7



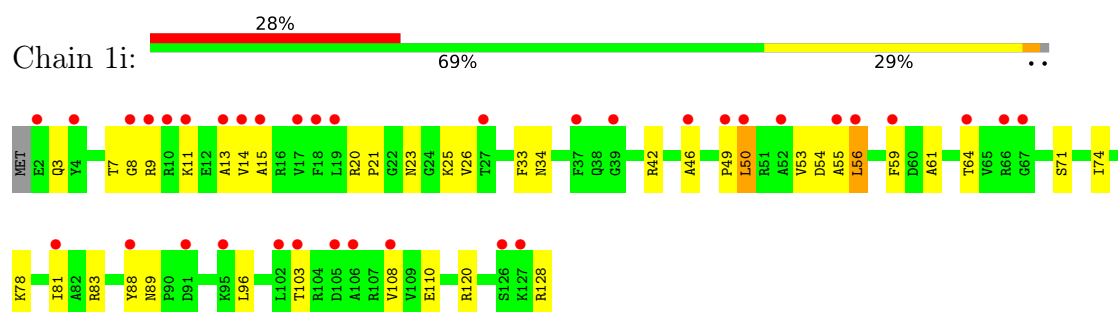
- Molecule 39: 30S ribosomal protein S8



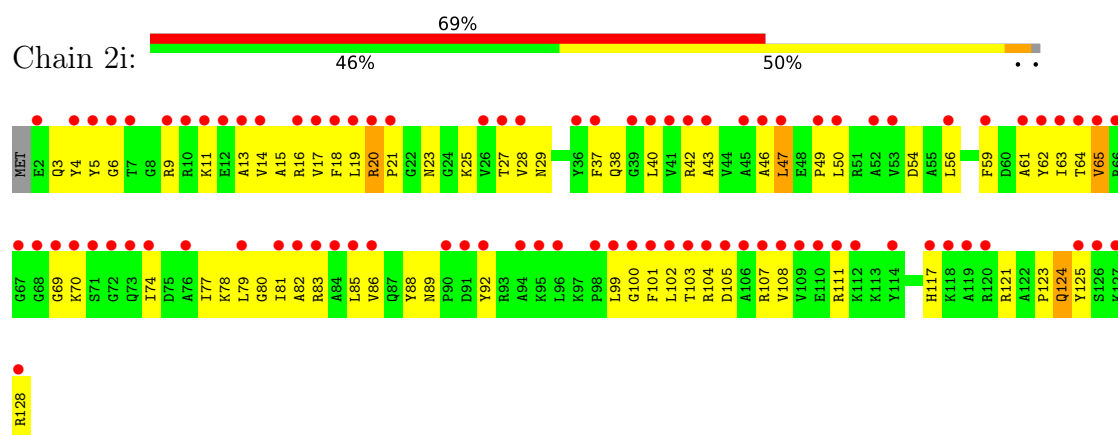
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

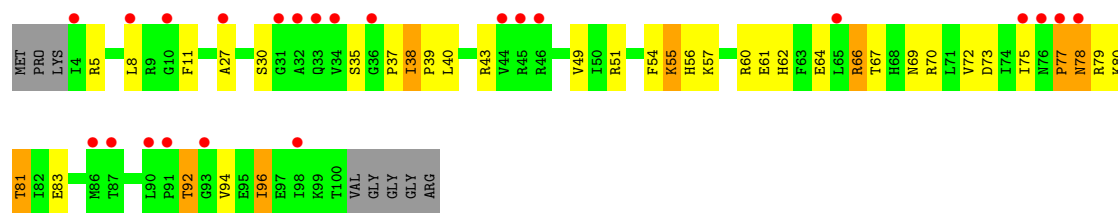


- Molecule 40: 30S ribosomal protein S9

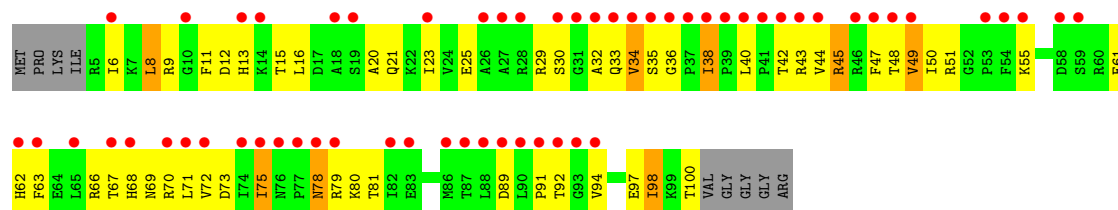
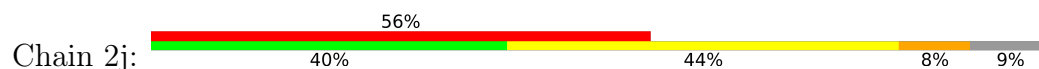


- Molecule 41: 30S ribosomal protein S10

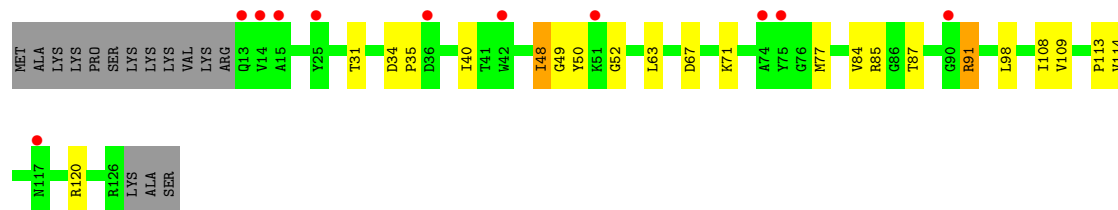




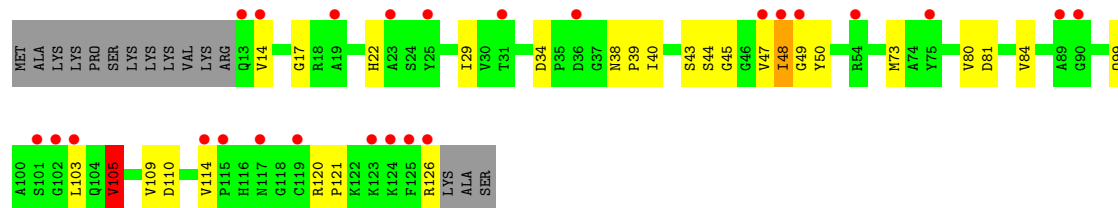
• Molecule 41: 30S ribosomal protein S10



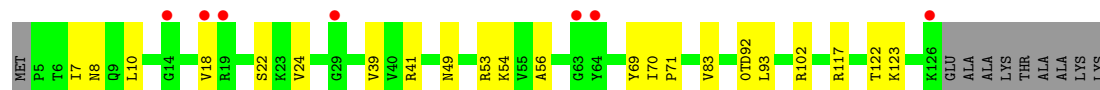
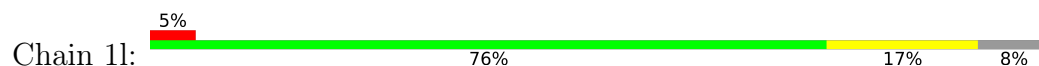
• Molecule 42: 30S ribosomal protein S11



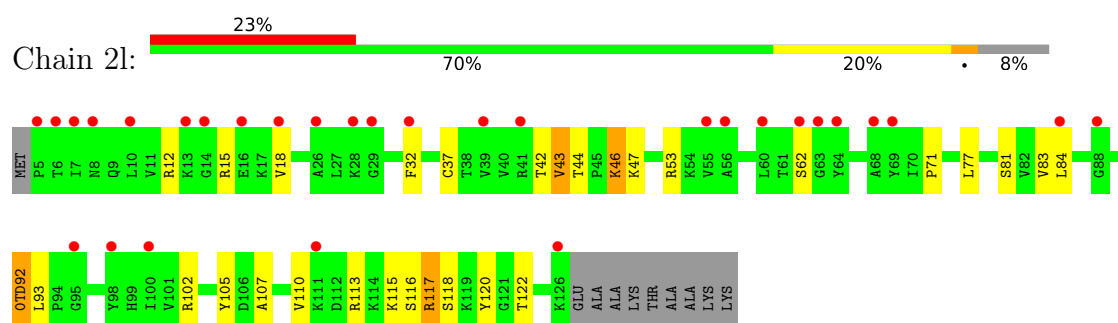
• Molecule 42: 30S ribosomal protein S11



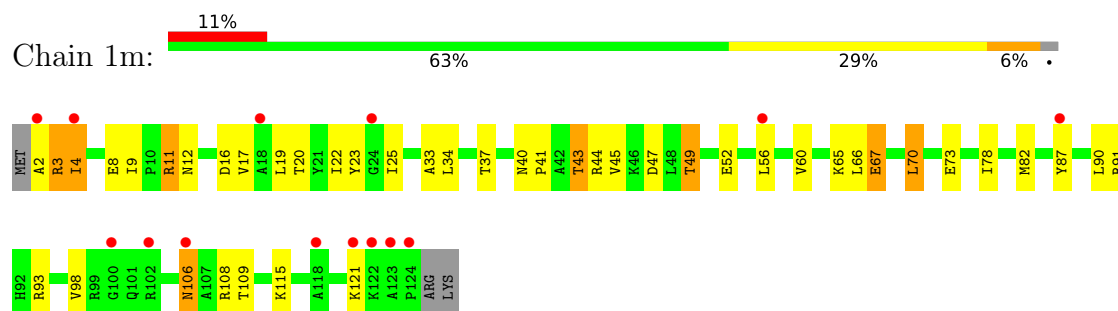
• Molecule 43: 30S ribosomal protein S12



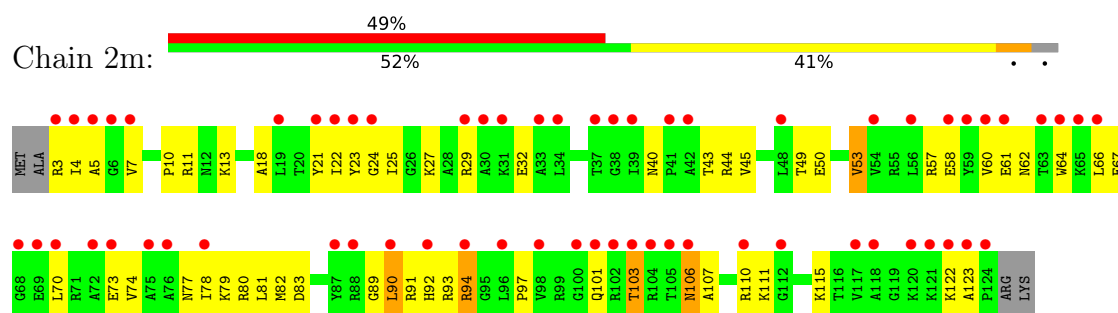
• Molecule 43: 30S ribosomal protein S12



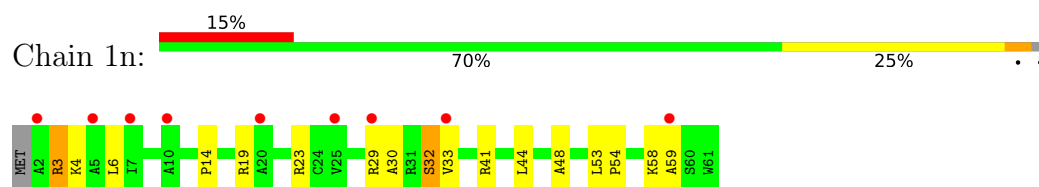
- Molecule 44: 30S ribosomal protein S13



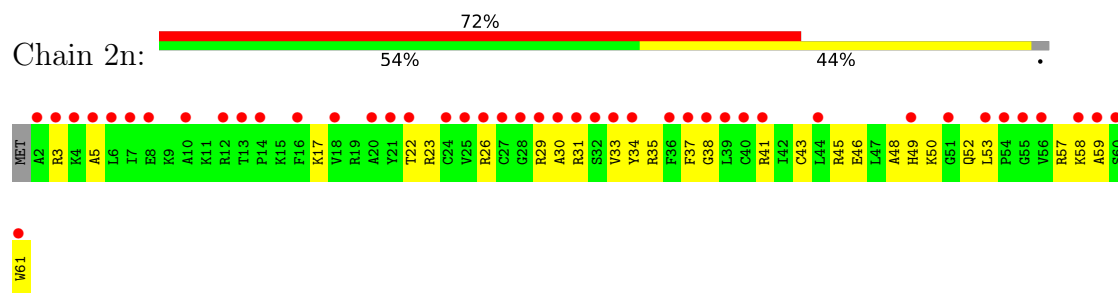
- Molecule 44: 30S ribosomal protein S13



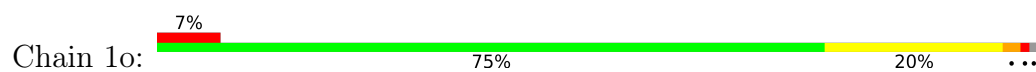
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



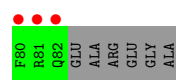
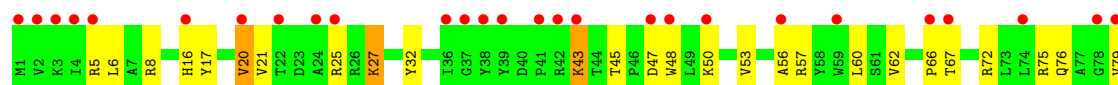
- Molecule 46: 30S ribosomal protein S15



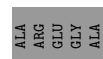
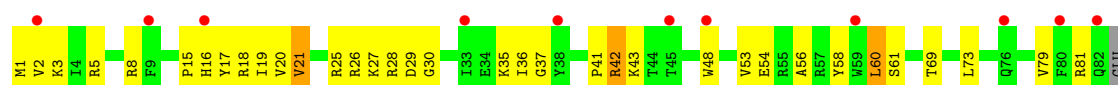
• Molecule 46: 30S ribosomal protein S15



• Molecule 47: 30S ribosomal protein S16



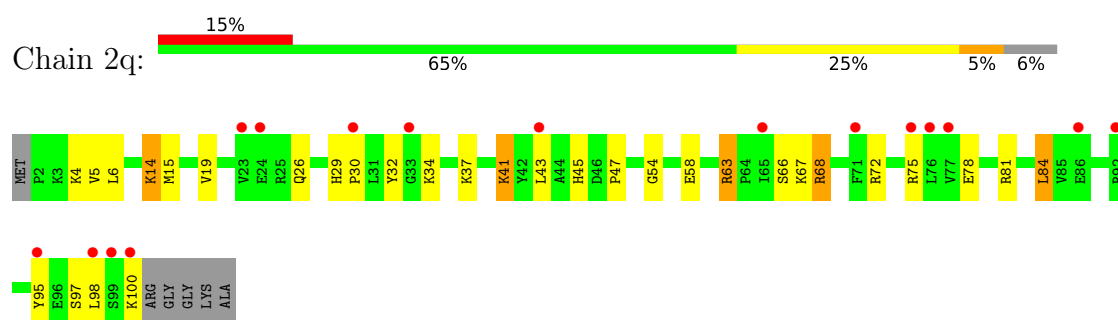
• Molecule 47: 30S ribosomal protein S16



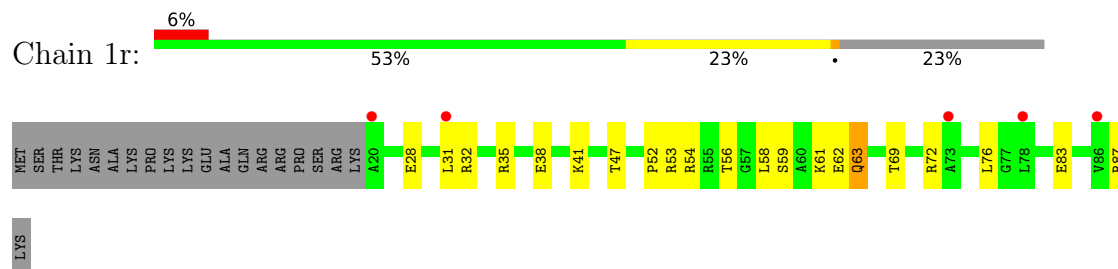
• Molecule 48: 30S ribosomal protein S17



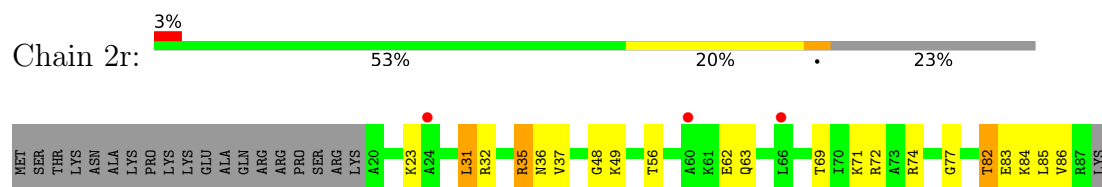
• Molecule 48: 30S ribosomal protein S17



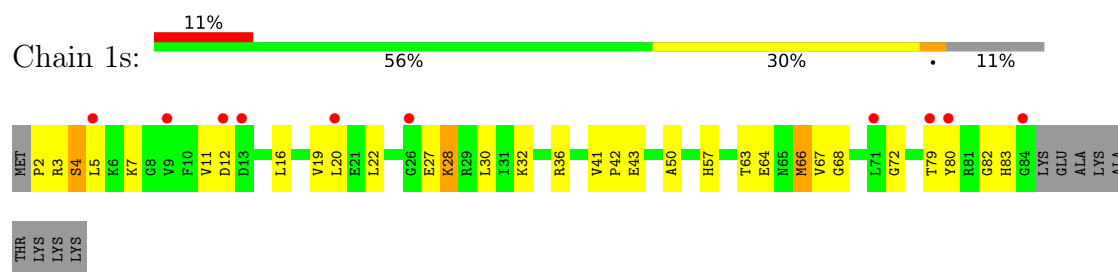
- Molecule 49: 30S ribosomal protein S18



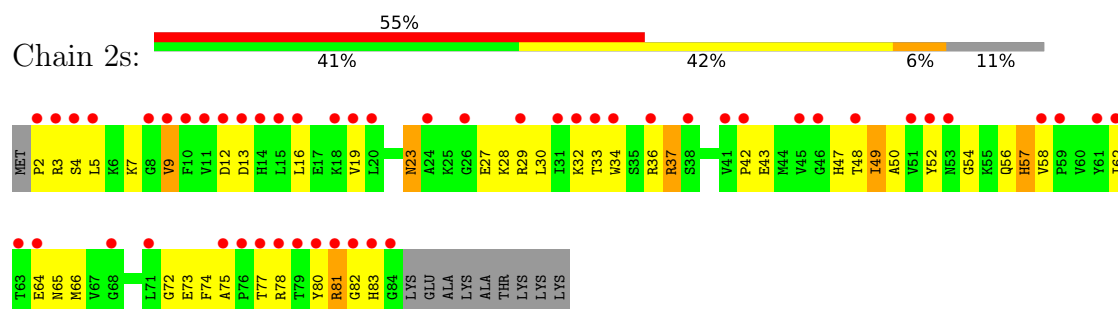
- Molecule 49: 30S ribosomal protein S18



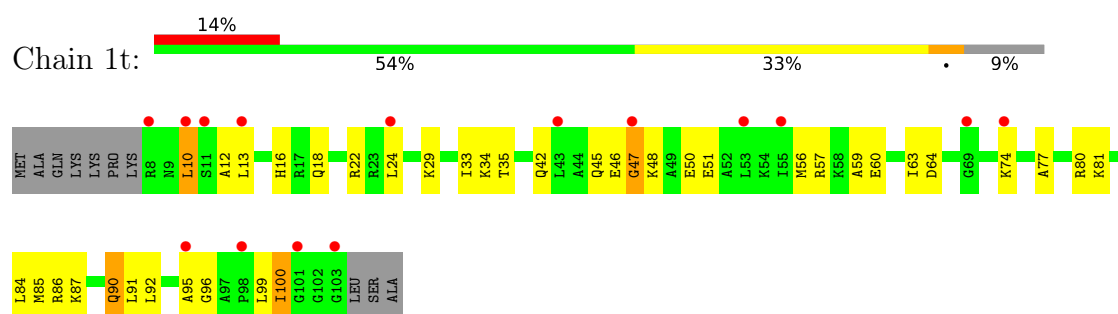
- Molecule 50: 30S ribosomal protein S19



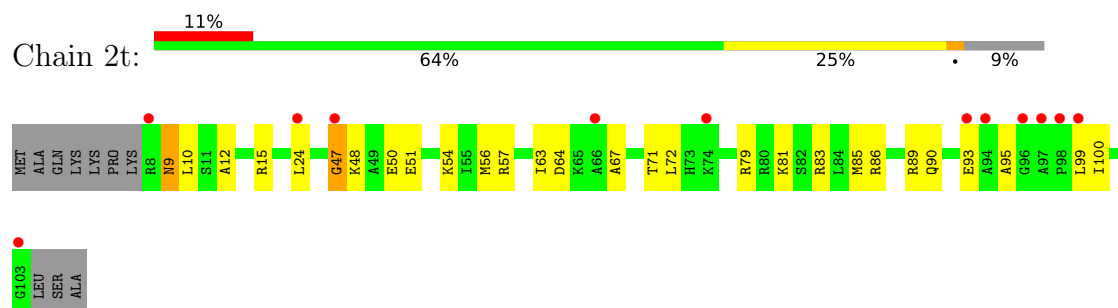
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20



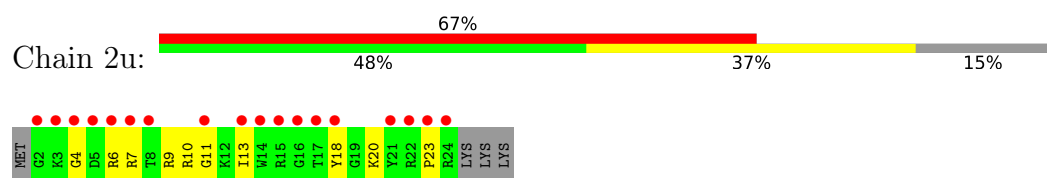
- Molecule 51: 30S ribosomal protein S20



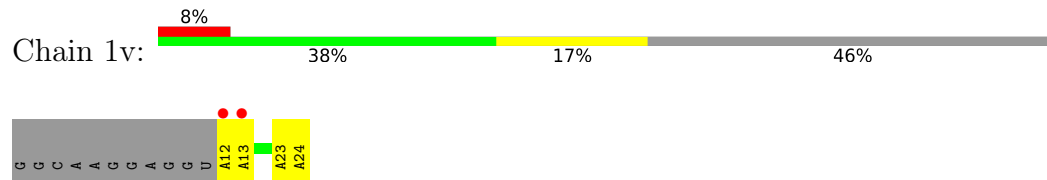
- Molecule 52: 30S ribosomal protein Thx



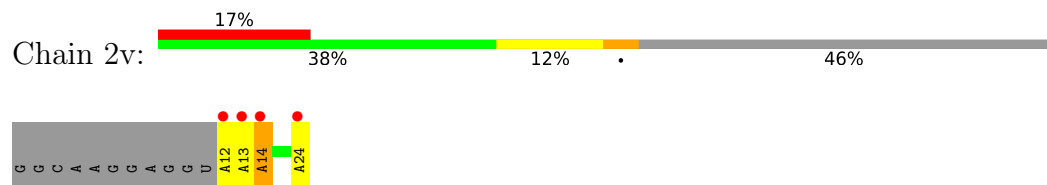
- Molecule 52: 30S ribosomal protein Thx



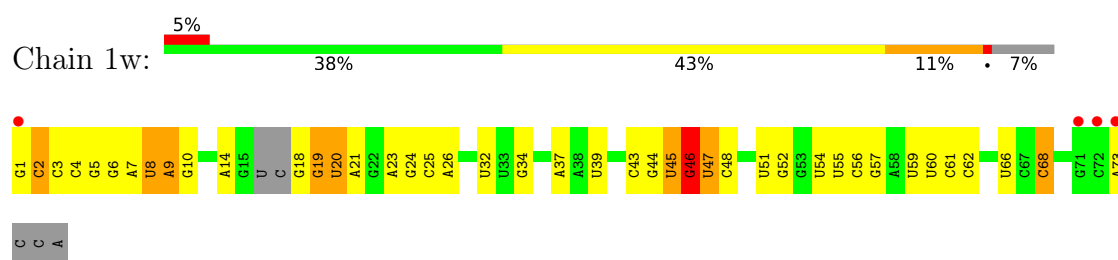
- Molecule 53: MF-mRNA



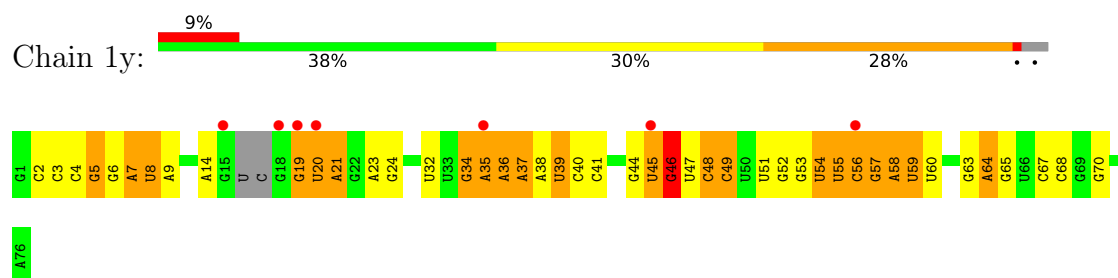
- Molecule 53: MF-mRNA



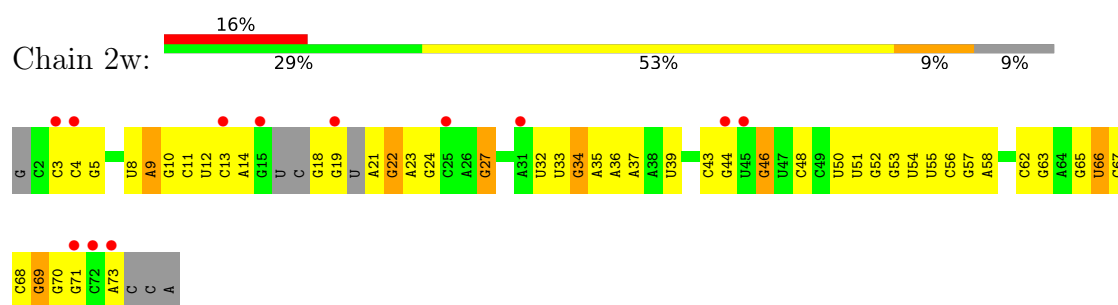
- Molecule 54: A-site and E-site Deacylated tRNAphe



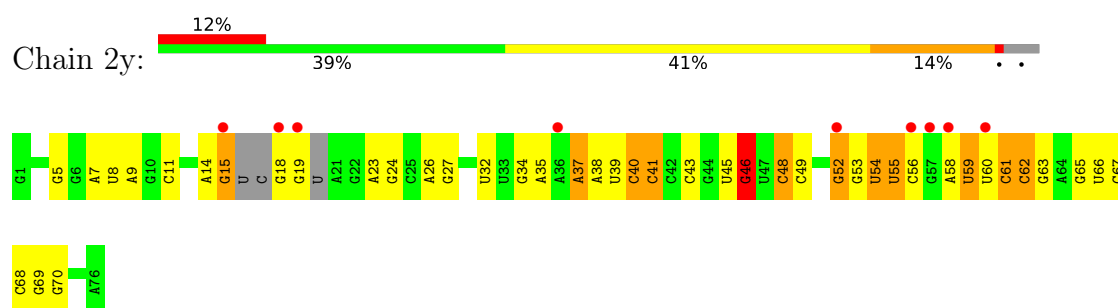
• Molecule 54: A-site and E-site Deacylated tRNA^{phe}



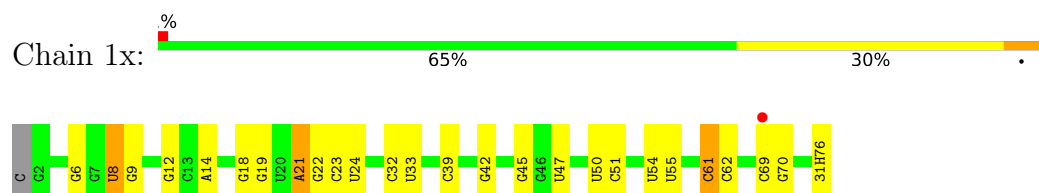
• Molecule 54: A-site and E-site Deacylated tRNA^{phe}



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

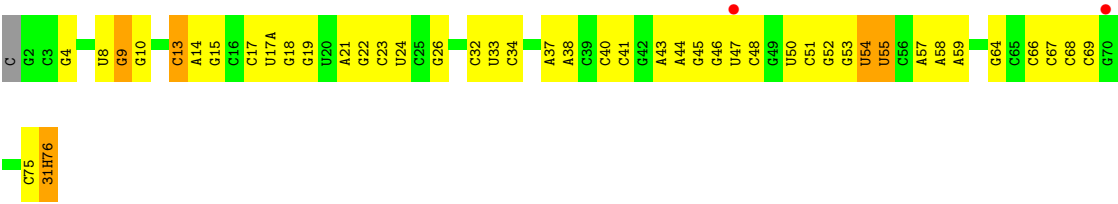


• Molecule 55: P-site Aminoacylated fMet-tRNA^{met}



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.26Å 449.69Å 619.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.86 – 2.50 121.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (121.86-2.50) 99.3 (121.86-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.218 , 0.260 0.220 , 0.262	Depositor DCC
R_{free} test set	98989 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	299293	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, PSU, OMC, M2G, OMG, MG, MA6, 5MU, ZN, MIA, A1A1L, 31H, 4SU, OMU, 2MA, 0TD, UR3, SF4, K, 4OC, 5MC, G7M

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	0.47	3/107720 (0.0%)
1	2A	0.21	0/67295	0.40	3/105042 (0.0%)
2	1B	0.22	0/2882	0.39	0/4494
2	2B	0.19	0/2879	0.37	0/4487
3	1D	0.27	0/2186	0.51	0/2944
3	2D	0.23	0/2186	0.46	0/2944
4	1E	0.29	0/1592	0.52	0/2149
4	2E	0.20	0/1592	0.45	0/2149
5	1F	0.27	0/1618	0.50	0/2191
5	2F	0.20	0/1614	0.46	2/2186 (0.1%)
6	1G	0.20	0/1448	0.46	1/1957 (0.1%)
6	2G	0.19	0/1453	0.43	0/1963
7	1H	0.22	0/1356	0.41	0/1834
7	2H	0.18	0/1356	0.36	0/1834
8	1I	0.18	0/1112	0.40	0/1514
8	2I	0.18	0/1079	0.41	0/1475
9	1N	0.25	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.39	0/1543
10	1O	0.26	0/943	0.46	0/1269
10	2O	0.20	0/943	0.45	0/1269
11	1P	0.27	0/1152	0.56	0/1533
11	2P	0.20	0/1152	0.47	0/1533
12	1Q	0.28	0/1143	0.47	0/1527
12	2Q	0.20	0/1143	0.43	0/1527
13	1R	0.28	0/982	0.50	0/1312
13	2R	0.19	0/982	0.43	0/1312
14	1S	0.21	0/883	0.48	0/1176
14	2S	0.20	0/880	0.43	0/1172
15	1T	0.25	0/1105	0.48	0/1477
15	2T	0.20	0/1097	0.43	0/1468
16	1U	0.27	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.21	0/977	0.42	0/1301
17	1V	0.27	0/782	0.51	0/1049
17	2V	0.18	0/782	0.40	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.22	0/897	0.42	0/1205
19	1X	0.26	0/764	0.51	0/1025
19	2X	0.21	0/764	0.57	3/1025 (0.3%)
20	1Y	0.23	0/819	0.49	0/1095
20	2Y	0.20	0/819	0.43	0/1095
21	1Z	0.22	0/1267	0.47	0/1717
21	2Z	0.22	0/1299	0.43	0/1763
22	10	0.26	0/616	0.49	0/821
22	20	0.19	0/628	0.44	0/837
23	11	0.25	0/762	0.44	0/1014
23	21	0.23	0/762	0.40	0/1014
24	12	0.24	0/590	0.43	0/781
24	22	0.18	0/590	0.37	0/781
25	13	0.27	0/474	0.46	0/635
25	23	0.19	0/469	0.43	0/630
26	14	0.28	0/565	0.54	0/761
26	24	0.26	0/545	0.46	0/737
27	15	0.26	0/469	0.49	0/635
27	25	0.22	0/469	0.41	0/635
28	16	0.26	0/460	0.47	0/613
28	26	0.21	0/456	0.46	0/608
29	17	0.30	0/426	0.57	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.25	0/525	0.45	0/691
30	28	0.24	0/525	0.41	0/691
31	19	0.25	0/310	0.51	0/407
31	29	0.19	0/310	0.43	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.20	0/35886	0.38	3/56005 (0.0%)
33	1b	0.21	0/1881	0.48	0/2542
33	2b	0.23	0/1860	0.49	0/2518
34	1c	0.19	0/1572	0.39	0/2126
34	2c	0.23	0/1566	0.44	0/2119
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.19	0/1704	0.44	0/2284
36	1e	0.21	0/1145	0.47	0/1543
36	2e	0.21	0/1149	0.47	0/1548
37	1f	0.20	0/823	0.38	0/1115
37	2f	0.18	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1250	0.39	0/1679
38	2g	0.20	0/1254	0.43	0/1683
39	1h	0.18	0/1108	0.41	0/1494
39	2h	0.20	0/1108	0.42	0/1494
40	1i	0.20	0/1002	0.49	0/1346
40	2i	0.23	0/997	0.46	0/1343
41	1j	0.20	0/722	0.44	0/982
41	2j	0.22	0/727	0.48	0/988
42	1k	0.19	0/844	0.44	0/1145
42	2k	0.19	0/848	0.39	0/1149
43	1l	0.20	0/937	0.42	0/1260
43	2l	0.19	0/937	0.42	0/1260
44	1m	0.20	0/969	0.47	0/1302
44	2m	0.21	0/961	0.46	0/1291
45	1n	0.18	0/501	0.44	0/664
45	2n	0.22	0/501	0.46	0/664
46	1o	0.19	0/739	0.37	0/985
46	2o	0.18	0/739	0.37	0/985
47	1p	0.20	0/697	0.48	0/939
47	2p	0.18	0/693	0.43	0/935
48	1q	0.19	0/836	0.41	0/1117
48	2q	0.18	0/836	0.43	0/1117
49	1r	0.19	0/560	0.40	0/746
49	2r	0.17	0/560	0.42	0/746
50	1s	0.20	0/667	0.47	0/900
50	2s	0.25	0/661	0.59	0/893
51	1t	0.18	0/730	0.45	0/965
51	2t	0.20	0/729	0.43	0/965
52	1u	0.18	0/203	0.42	0/266
52	2u	0.22	0/203	0.44	0/266
53	1v	0.22	0/310	0.39	0/480
53	2v	0.20	0/310	0.36	0/480
54	1w	0.28	1/1537 (0.1%)	0.39	0/2390
54	1y	0.28	2/1606 (0.1%)	0.41	0/2497
54	2w	0.32	2/1487 (0.1%)	0.42	0/2311
54	2y	0.29	2/1583 (0.1%)	0.41	0/2459
55	1x	0.26	0/1700	0.41	0/2650
55	2x	0.24	0/1700	0.39	0/2650
All	All	0.23	7/316420 (0.0%)	0.43	15/473729 (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
3	2D	0	1
33	1b	0	1
51	1t	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	46	G7M	O3'-P	5.43	1.61	1.56
54	1y	8	4SU	O3'-P	5.26	1.61	1.56
54	2w	46	G7M	O3'-P	5.26	1.61	1.56
54	1w	46	G7M	O3'-P	5.25	1.61	1.56
54	2y	8	4SU	O3'-P	5.18	1.61	1.56
54	2w	8	4SU	O3'-P	5.17	1.61	1.56
54	1y	46	G7M	O3'-P	5.13	1.61	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2X	94	GLY	CA-C-N	6.91	134.14	121.70
19	2X	94	GLY	C-N-CA	6.91	134.14	121.70
1	1A	1992	G	C2'-C3'-O3'	6.88	119.83	109.50
1	2A	1992	G	C2'-C3'-O3'	6.12	118.68	109.50
6	1G	96	ARG	CB-CA-C	-5.92	109.73	116.54
1	2A	271(M)	G	OP1-P-O3'	5.87	118.11	105.20
32	2a	1272	G	N1-C2-N2	-5.75	98.94	116.20
1	2A	271(M)	G	P-O3'-C3'	5.67	126.51	119.70
19	2X	93	GLU	N-CA-C	-5.55	106.83	113.21
5	2F	21	ALA	CA-C-N	5.31	131.26	121.70
5	2F	21	ALA	C-N-CA	5.31	131.26	121.70
32	2a	1263	C	N1-C2-O2	5.28	134.73	118.90
32	2a	1272	G	N3-C2-N2	5.20	135.51	119.90
1	1A	512	G	O4'-C1'-N9	5.16	115.94	108.20
1	1A	2629	A	C2'-C3'-O3'	5.01	117.01	109.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	122	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
51	1t	99	LEU	Peptide
3	2D	274	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31196	538	0
1	2A	60322	0	30428	632	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	36	0
3	1D	2136	0	2218	38	0
3	2D	2136	0	2218	47	0
4	1E	1559	0	1618	26	0
4	2E	1559	0	1618	36	0
5	1F	1583	0	1625	36	0
5	2F	1579	0	1619	47	0
6	1G	1423	0	1436	35	0
6	2G	1428	0	1438	59	0
7	1H	1330	0	1407	25	0
7	2H	1330	0	1407	46	0
8	1I	1097	0	1140	30	0
8	2I	1064	0	1082	25	0
9	1N	1117	0	1184	17	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	14	0
10	2O	933	0	996	25	0
11	1P	1135	0	1212	33	0
11	2P	1135	0	1212	39	0
12	1Q	1122	0	1179	16	0
12	2Q	1122	0	1179	29	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	15	0
14	2S	870	0	923	28	0
15	1T	1091	0	1151	24	0
15	2T	1083	0	1136	35	0
16	1U	959	0	1019	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	2U	959	0	1019	23	0
17	1V	771	0	830	9	0
17	2V	771	0	830	13	0
18	1W	886	0	940	9	0
18	2W	886	0	940	15	0
19	1X	750	0	814	13	0
19	2X	750	0	814	22	0
20	1Y	806	0	881	13	0
20	2Y	806	0	881	14	0
21	1Z	1240	0	1240	34	0
21	2Z	1271	0	1273	54	0
22	10	608	0	622	11	0
22	20	620	0	636	15	0
23	11	755	0	826	12	0
23	21	755	0	826	20	0
24	12	588	0	643	7	0
24	22	588	0	643	15	0
25	13	469	0	518	9	0
25	23	464	0	514	12	0
26	14	552	0	533	25	0
26	24	532	0	503	25	0
27	15	455	0	465	6	0
27	25	455	0	465	8	0
28	16	453	0	473	11	0
28	26	449	0	469	6	0
29	17	418	0	467	7	0
29	27	418	0	467	9	0
30	18	517	0	582	15	0
30	28	517	0	582	14	0
31	19	307	0	335	4	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	386	0
32	2a	32327	0	16338	514	0
33	1b	1846	0	1867	61	0
33	2b	1825	0	1828	79	0
34	1c	1548	0	1535	31	0
34	2c	1542	0	1517	62	0
35	1d	1655	0	1672	47	0
35	2d	1674	0	1714	42	0
36	1e	1129	0	1185	33	0
36	2e	1133	0	1191	42	0
37	1f	810	0	804	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	2f	816	0	808	23	0
38	1g	1231	0	1238	21	0
38	2g	1235	0	1249	37	0
39	1h	1088	0	1126	28	0
39	2h	1088	0	1126	34	0
40	1i	983	0	986	19	0
40	2i	978	0	966	50	0
41	1j	709	0	650	29	0
41	2j	714	0	672	42	0
42	1k	829	0	825	12	0
42	2k	833	0	834	14	0
43	1l	932	0	981	12	0
43	2l	932	0	981	19	0
44	1m	958	0	1002	27	0
44	2m	950	0	988	50	0
45	1n	492	0	529	12	0
45	2n	492	0	529	26	0
46	1o	728	0	760	10	0
46	2o	728	0	760	21	0
47	1p	681	0	697	20	0
47	2p	677	0	686	26	0
48	1q	823	0	891	18	0
48	2q	823	0	891	17	0
49	1r	555	0	618	17	0
49	2r	555	0	618	18	0
50	1s	652	0	662	23	0
50	2s	646	0	644	37	0
51	1t	728	0	798	25	0
51	2t	727	0	796	18	0
52	1u	199	0	208	8	0
52	2u	199	0	208	8	0
53	1v	277	0	140	4	0
53	2v	277	0	140	3	0
54	1w	1530	0	785	20	0
54	1y	1585	0	803	29	0
54	2w	1482	0	754	22	0
54	2y	1565	0	793	21	0
55	1x	1635	0	839	9	0
55	2x	1635	0	839	21	0
56	10	7	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	13	2	0	0	0	0
56	14	1	0	0	0	0
56	15	8	0	0	0	0
56	16	3	0	0	0	0
56	17	5	0	0	0	0
56	18	4	0	0	0	0
56	19	1	0	0	0	0
56	1A	1059	0	0	0	0
56	1B	39	0	0	0	0
56	1D	12	0	0	0	0
56	1E	16	0	0	0	0
56	1F	14	0	0	0	0
56	1G	4	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	6	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	7	0	0	0	0
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	7	0	0	0	0
56	1V	6	0	0	0	0
56	1W	6	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	198	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1l	2	0	0	0	0
56	1m	2	0	0	0	0
56	1n	2	0	0	0	0
56	1t	1	0	0	0	0
56	1u	1	0	0	0	0
56	1w	4	0	0	0	0
56	1x	12	0	0	0	0
56	20	1	0	0	0	0
56	21	1	0	0	0	0
56	23	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	25	5	0	0	0	0
56	27	4	0	0	0	0
56	28	2	0	0	0	0
56	2A	782	0	0	0	0
56	2B	18	0	0	0	0
56	2D	8	0	0	0	0
56	2E	9	0	0	0	0
56	2F	6	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	2	0	0	0	0
56	2R	2	0	0	0	0
56	2T	5	0	0	0	0
56	2U	1	0	0	0	0
56	2V	2	0	0	0	0
56	2W	1	0	0	0	0
56	2X	2	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	2	0	0	0	0
56	2a	202	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	5	0	0	0	0
56	2q	2	0	0	0	0
56	2r	2	0	0	0	0
56	2t	2	0	0	0	0
56	2v	1	0	0	0	0
56	2w	3	0	0	0	0
56	2x	6	0	0	0	0
57	1A	36	0	0	1	0
57	2A	36	0	0	1	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	1	0
59	2d	8	0	0	1	0
60	2x	1	0	0	0	0
61	10	8	0	0	0	0
61	11	7	0	0	0	0
61	12	4	0	0	1	0
61	13	4	0	0	0	0
61	14	1	0	0	0	0
61	15	7	0	0	0	0
61	16	1	0	0	0	0
61	17	8	0	0	0	0
61	18	13	0	0	0	0
61	1A	1902	0	0	65	0
61	1B	59	0	0	0	0
61	1D	27	0	0	0	0
61	1E	31	0	0	1	0
61	1F	20	0	0	1	0
61	1G	2	0	0	0	0
61	1H	2	0	0	0	0
61	1N	6	0	0	0	0
61	1O	6	0	0	0	0
61	1P	18	0	0	2	0
61	1Q	8	0	0	0	0
61	1R	11	0	0	2	0
61	1S	5	0	0	0	0
61	1T	7	0	0	0	0
61	1U	15	0	0	0	0
61	1V	8	0	0	0	0
61	1W	8	0	0	0	0
61	1X	7	0	0	0	0
61	1Y	3	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	298	0	0	18	0
61	1b	1	0	0	0	0
61	1l	5	0	0	0	0
61	1m	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	1o	1	0	0	0	0
61	1q	2	0	0	0	0
61	1t	1	0	0	0	0
61	1v	5	0	0	0	0
61	1w	4	0	0	0	0
61	1x	9	0	0	1	0
61	1y	1	0	0	0	0
61	20	2	0	0	0	0
61	21	3	0	0	0	0
61	23	3	0	0	0	0
61	25	2	0	0	0	0
61	27	4	0	0	0	0
61	28	3	0	0	0	0
61	29	1	0	0	0	0
61	2A	1002	0	0	68	0
61	2B	16	0	0	1	0
61	2D	23	0	0	1	0
61	2E	16	0	0	0	0
61	2F	14	0	0	0	0
61	2O	1	0	0	0	0
61	2P	9	0	0	1	0
61	2Q	1	0	0	0	0
61	2R	3	0	0	0	0
61	2T	6	0	0	0	0
61	2U	3	0	0	0	0
61	2V	1	0	0	0	0
61	2W	2	0	0	1	0
61	2X	3	0	0	0	0
61	2a	168	0	0	14	0
61	2e	1	0	0	0	0
61	2j	2	0	0	1	0
61	2l	3	0	0	0	0
61	2p	1	0	0	0	0
61	2t	1	0	0	0	0
61	2v	1	0	0	0	0
61	2w	1	0	0	0	0
61	2x	4	0	0	0	0
All	All	299293	0	196554	3999	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 (3999) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.23	1.36
1:1A:1082:U:O4	1:1A:1086:A:N1	1.94	1.00
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.27	0.98
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.44	0.97
20:1Y:92:ASN:HD21	20:1Y:94:LYS:HG2	1.33	0.90
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.54	0.90
1:1A:1062:G:H1	1:1A:1077:A:H61	1.14	0.90
38:2g:9:VAL:HG23	38:2g:94:ARG:HH21	1.37	0.90
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.53	0.89
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.54	0.89
1:1A:2499:C:OP1	61:1A:4101:HOH:O	1.88	0.89
32:1a:1505:G:OP2	61:1a:1801:HOH:O	1.91	0.88
1:1A:2427:C:OP1	61:1A:4102:HOH:O	1.90	0.88
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.22	0.87
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.08	0.86
1:2A:2589:A:OP1	61:2A:3803:HOH:O	1.92	0.86
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.24	0.86
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.42	0.85
1:1A:2136:C:N3	1:1A:2155:G:C2	2.44	0.85
33:2b:178:ARG:HH22	39:2h:68:ARG:HH22	1.23	0.85
1:2A:1204:A:H2	1:2A:1241:A:H62	1.23	0.84
32:2a:1025:U:H3	32:2a:1036:G:H1	1.25	0.84
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.24	0.84
29:17:24:THR:HG22	29:17:27:GLY:H	1.42	0.84
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.10	0.83
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.60	0.83
32:1a:1027:C:C2	32:1a:1034:G:N2	2.45	0.83
32:1a:664:G:H22	32:1a:741:G:H1	1.24	0.83
1:2A:1604:C:OP2	61:2A:3804:HOH:O	1.97	0.82
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.24	0.82
1:1A:1013:C:OP2	61:1A:4103:HOH:O	1.98	0.81
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.12	0.81
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.62	0.81
32:2a:1029:C:C4	32:2a:1032:G:N1	2.47	0.81
1:2A:2138:C:H42	1:2A:2153:G:H1	1.26	0.81
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.14	0.80
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.12	0.80
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.15	0.80
1:2A:1354:A:H5''	3:2D:38:LYS:HD3	1.63	0.80
32:1a:975:A:H4'	32:1a:976:G:H5''	1.61	0.80
36:1e:78:HIS:HD2	39:1h:104:ARG:HD2	1.46	0.80
32:1a:1441:G:H5''	32:1a:1442:G:H5'	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.45	0.80
1:1A:1669:A:OP2	61:1A:4104:HOH:O	2.00	0.80
1:1A:1014:U:OP2	61:1A:4103:HOH:O	2.00	0.79
1:1A:1082:U:N3	1:1A:1086:A:N6	2.06	0.79
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.65	0.79
32:2a:1272:G:N2	32:2a:1273:G:N7	2.29	0.79
1:1A:1332:G:OP1	61:1A:4105:HOH:O	2.00	0.79
32:2a:299:G:O6	61:2a:1902:HOH:O	2.01	0.79
1:1A:1603:A:OP1	61:1A:4106:HOH:O	2.00	0.79
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.16	0.79
1:2A:1689:A:H62	1:2A:1698:A:H2	1.31	0.78
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.15	0.78
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.15	0.78
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.65	0.78
1:1A:2550:G:OP1	61:1A:4104:HOH:O	2.01	0.78
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.66	0.78
1:2A:948:G:OP1	61:2A:3805:HOH:O	2.02	0.78
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.16	0.78
44:2m:40:ASN:HD22	44:2m:43:THR:HG23	1.48	0.78
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.17	0.78
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.66	0.77
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.67	0.77
1:2A:878:A:N6	1:2A:899:A:O2'	2.17	0.77
1:1A:1271:G:OP2	61:1A:4108:HOH:O	2.02	0.77
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.30	0.77
26:24:53:GLU:HG2	26:24:55:ARG:H	1.49	0.77
1:1A:1452:A:OP2	61:1A:4107:HOH:O	2.02	0.77
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.18	0.77
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.67	0.77
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.03	0.76
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.18	0.76
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.67	0.76
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.67	0.76
1:1A:11:G:H2'	1:1A:12:U:H5'	1.66	0.76
32:2a:544:G:OP1	35:2d:59:ARG:NH2	2.18	0.76
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.49	0.76
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.66	0.76
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.66	0.76
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.67	0.76
32:2a:1271:G:N2	32:2a:1272:G:N7	2.34	0.76
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:289:G:OP2	61:2a:1903:HOH:O	2.04	0.76
1:1A:1890:A:OP2	61:1A:4109:HOH:O	2.04	0.75
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.50	0.75
22:10:11:ARG:O	22:10:14:ARG:NH2	2.17	0.75
1:2A:1670:C:OP1	61:2A:3806:HOH:O	2.03	0.75
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.68	0.75
32:2a:953:G:H5'	32:2a:965:A:H61	1.48	0.75
32:1a:1377:A:HO2'	38:1g:2:ALA:N	1.84	0.75
33:1b:21:ARG:HB3	33:1b:39:ILE:HD12	1.69	0.75
1:2A:783:A:OP2	61:2A:3803:HOH:O	2.03	0.75
1:2A:1568:G:N7	61:2A:3835:HOH:O	2.19	0.75
1:2A:1648:C:OP1	61:2A:3807:HOH:O	2.03	0.75
1:2A:2061:G:OP2	61:2A:3808:HOH:O	2.04	0.75
2:2B:20:C:N4	2:2B:63:G:O6	2.18	0.75
26:14:55:ARG:H	26:14:56:VAL:HA	1.52	0.75
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.69	0.75
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.18	0.75
1:1A:376:C:OP1	61:1A:4111:HOH:O	2.05	0.75
17:2V:1:MET:HE2	17:2V:43:GLU:HB2	1.69	0.75
1:1A:773:U:OP1	61:1A:4110:HOH:O	2.04	0.74
32:2a:1086:U:H3	32:2a:1099:G:H22	1.34	0.74
1:1A:1647:G:OP1	61:1A:4108:HOH:O	2.02	0.74
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.69	0.74
44:2m:82:MET:HE2	44:2m:92:HIS:HB3	1.68	0.74
26:14:55:ARG:N	26:14:56:VAL:HA	2.03	0.74
32:2a:664:G:H22	32:2a:741:G:H1	1.36	0.74
1:2A:1647:G:OP1	61:2A:3807:HOH:O	2.05	0.74
21:2Z:154:ASP:OD1	21:2Z:154:ASP:N	2.20	0.74
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.21	0.74
32:1a:574:A:OP2	61:1a:1802:HOH:O	2.06	0.74
1:2A:2625:G:O6	61:2A:3810:HOH:O	2.05	0.74
32:2a:986:A:N3	50:2s:52:TYR:OH	2.20	0.74
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.20	0.73
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.67	0.73
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.70	0.73
1:2A:570:G:O6	61:2A:3809:HOH:O	2.05	0.73
1:1A:1865:G:OP1	61:1A:4112:HOH:O	2.05	0.73
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.71	0.73
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.67	0.73
5:1F:89:VAL:O	61:1F:401:HOH:O	2.05	0.73
32:1a:1025:U:O2	32:1a:1036:G:O6	2.06	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.70	0.73
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.70	0.73
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.69	0.73
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.71	0.73
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.68	0.73
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.70	0.73
32:2a:278:G:OP2	48:2q:41:LYS:NZ	2.20	0.73
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.71	0.73
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.21	0.73
41:2j:49:VAL:HG13	41:2j:61:GLU:HB3	1.69	0.73
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.22	0.72
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.22	0.72
51:1t:86:ARG:O	51:1t:90:GLN:NE2	2.23	0.72
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.54	0.72
54:2y:18:G:N2	54:2y:55:PSU:N3	2.35	0.72
1:1A:467:G:OP1	29:17:33:ARG:NH1	2.22	0.72
1:1A:826:U:OP1	61:1A:4102:HOH:O	2.07	0.72
1:1A:880:G:H1	1:1A:898:C:H42	1.38	0.72
34:1c:52:LEU:HD13	34:1c:68:VAL:HG13	1.72	0.72
1:1A:2100:G:H1	1:1A:2189:U:H3	1.38	0.72
11:2P:94:GLU:HG3	11:2P:124:LYS:HE2	1.72	0.72
1:1A:2552:OMU:OP2	61:1A:4113:HOH:O	2.07	0.71
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.71	0.71
44:1m:49:THR:HB	44:1m:52:GLU:H	1.54	0.71
34:2c:63:ASN:HB3	34:2c:98:ASN:HD22	1.53	0.71
32:1a:875:C:H1'	39:1h:15:ASN:HD21	1.55	0.71
1:1A:1468:C:OP1	61:1A:4114:HOH:O	2.07	0.71
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.72	0.71
55:1x:12:G:OP2	61:1x:201:HOH:O	2.07	0.71
1:2A:2637:U:H5''	4:2E:82:ARG:HH12	1.55	0.71
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.72	0.71
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.53	0.71
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.20	0.71
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.72	0.71
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.23	0.71
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.73	0.71
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.37	0.71
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.22	0.71
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.24	0.71
32:2a:1316:G:H22	32:2a:1319:A:H5''	1.54	0.71
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.72	0.71
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.23	0.71
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.73	0.71
1:2A:792:G:O6	61:2A:3811:HOH:O	2.06	0.71
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.55	0.71
47:1p:53:VAL:HG13	47:1p:79:VAL:HG13	1.73	0.70
54:1w:26:A:H61	54:1w:44:G:H1	1.38	0.70
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.26	0.70
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.09	0.70
1:2A:2099:U:H3	1:2A:2190:G:H1	1.38	0.70
32:2a:997:U:H3	32:2a:1044:A:H61	1.39	0.70
46:2o:7:GLU:OE1	46:2o:38:ARG:NH2	2.23	0.70
1:2A:2524:G:N7	61:2A:3860:HOH:O	2.24	0.70
1:2A:2502:G:OP2	61:2A:3808:HOH:O	2.10	0.70
32:2a:558:G:OP1	61:2a:1902:HOH:O	2.09	0.70
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.24	0.70
1:1A:1993:U:OP2	61:1A:4115:HOH:O	2.10	0.70
1:2A:2524:G:O6	61:2A:3812:HOH:O	2.08	0.70
1:2A:2592:G:OP1	61:2A:3815:HOH:O	2.10	0.70
26:24:16:CYS:HA	26:24:33:VAL:HG12	1.71	0.70
1:2A:975:C:OP1	61:2A:3816:HOH:O	2.10	0.70
1:2A:1395:A:OP1	61:2A:3804:HOH:O	2.10	0.70
1:1A:1670:C:OP2	61:1A:4104:HOH:O	2.09	0.70
33:2b:189:ASP:N	33:2b:189:ASP:OD1	2.23	0.70
1:2A:248:G:OP1	61:2A:3813:HOH:O	2.09	0.70
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.73	0.69
15:1T:65:LYS:HE2	15:1T:67:SER:HB2	1.74	0.69
1:1A:2448:A:OP1	61:1A:4101:HOH:O	2.09	0.69
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.73	0.69
34:1c:150:LYS:HE2	34:1c:152:ILE:HD11	1.73	0.69
1:1A:1060:U:H3	1:1A:1088:A:H8	1.37	0.69
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.24	0.69
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.26	0.69
32:2a:673:G:H2'	32:2a:674:G:C8	2.27	0.69
32:1a:1108:G:O6	61:1a:1803:HOH:O	2.09	0.69
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.74	0.69
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.26	0.69
32:2a:1108:G:O6	61:2a:1904:HOH:O	2.08	0.69
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.74	0.69
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.74	0.69
44:2m:122:LYS:HD3	44:2m:123:ALA:H	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.26	0.69
32:1a:1086:U:H3	32:1a:1099:G:H22	1.40	0.69
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.40	0.69
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.75	0.69
1:1A:1354:A:H5''	3:1D:38:LYS:HE3	1.75	0.69
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.25	0.69
7:2H:90:LYS:HD2	7:2H:159:GLU:HG2	1.75	0.69
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.75	0.69
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.09	0.69
1:1A:1023:U:OP2	61:1A:4117:HOH:O	2.11	0.68
32:1a:1352:C:OP1	52:1u:3:LYS:NZ	2.23	0.68
1:2A:1271:G:OP2	61:2A:3807:HOH:O	2.10	0.68
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.28	0.68
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.75	0.68
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.38	0.68
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.26	0.68
32:2a:266:G:H5''	32:2a:268:C:H41	1.56	0.68
44:2m:5:ALA:HB3	44:2m:22:ILE:HD12	1.74	0.68
1:1A:1381:G:N7	61:1A:4157:HOH:O	2.26	0.68
1:1A:2447:G:OP2	61:1A:4116:HOH:O	2.10	0.68
1:2A:321:G:OP1	5:2F:135:LYS:NZ	2.25	0.68
32:2a:1029:C:N3	32:2a:1032:G:N2	2.42	0.68
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.27	0.68
1:2A:1938:A:OP2	61:2A:3819:HOH:O	2.12	0.68
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.59	0.68
4:2E:119:ARG:HD3	4:2E:160:TYR:HB2	1.75	0.68
8:2I:59:ALA:HA	8:2I:62:LYS:HB2	1.73	0.68
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.26	0.68
33:2b:15:VAL:HG13	33:2b:209:ARG:HB3	1.76	0.68
4:1E:110:GLY:O	61:1R:301:HOH:O	2.11	0.68
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.74	0.68
19:2X:72:LYS:NZ	19:2X:75:ASP:OD1	2.26	0.68
35:2d:61:LYS:NZ	35:2d:72:GLU:OE1	2.27	0.68
40:2i:23:ASN:HD21	40:2i:25:LYS:HE2	1.59	0.68
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.26	0.68
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.24	0.68
32:1a:78:G:O6	32:1a:92:C:N4	2.27	0.68
32:2a:130:A:H5'	48:2q:63:ARG:HE	1.59	0.68
32:2a:1228:C:OP1	44:2m:115:LYS:NZ	2.22	0.68
32:2a:1317:C:O2	50:2s:37:ARG:NH2	2.27	0.68
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:662:G:H2'	32:2a:663:A:C8	2.30	0.67
35:1d:107:ARG:HH21	35:1d:194:LEU:HD21	1.59	0.67
1:2A:1299:G:N7	61:2A:3876:HOH:O	2.28	0.67
11:2P:35:HIS:O	61:2P:301:HOH:O	2.12	0.67
1:1A:1315:C:OP2	61:1A:4105:HOH:O	2.11	0.67
47:1p:53:VAL:HG22	47:1p:79:VAL:HG22	1.75	0.67
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.12	0.67
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.76	0.67
32:2a:651:C:N4	32:2a:753:A:OP2	2.27	0.67
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.28	0.67
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.27	0.67
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.42	0.67
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.59	0.67
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.59	0.67
1:1A:2794:C:H42	1:1A:2802:G:H22	1.42	0.67
32:1a:980:C:OP1	61:1a:1804:HOH:O	2.12	0.67
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.28	0.67
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.77	0.67
1:1A:763:G:OP1	61:1A:4120:HOH:O	2.13	0.67
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.75	0.67
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.77	0.67
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.76	0.67
1:2A:568:U:O4	61:2A:3814:HOH:O	2.10	0.67
1:2A:1342:A:OP2	61:2A:3818:HOH:O	2.11	0.67
1:2A:2138:C:N4	1:2A:2153:G:H1	1.92	0.67
7:2H:25:LYS:HE2	7:2H:27:LYS:HE3	1.76	0.67
32:1a:557:G:OP1	61:1a:1805:HOH:O	2.13	0.67
1:2A:271(H):G:H5'	23:21:81:LYS:HZ2	1.60	0.67
32:2a:1302:U:OP2	44:2m:21:TYR:OH	2.06	0.67
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.29	0.67
5:2F:116:ASP:OD2	11:2P:1:MET:N	2.27	0.67
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.76	0.67
54:1y:8:4SU:H4'	54:1y:48:C:H4'	1.77	0.67
41:2j:44:VAL:HG13	41:2j:66:ARG:HB3	1.75	0.67
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.27	0.67
1:2A:397:G:N7	61:2A:3867:HOH:O	2.26	0.66
1:1A:2226:C:OP2	61:1A:4122:HOH:O	2.13	0.66
32:1a:892:A:OP2	61:1a:1806:HOH:O	2.13	0.66
1:2A:962:G:OP1	61:2A:3805:HOH:O	2.13	0.66
6:1G:15:VAL:HG21	6:1G:176:LEU:HD23	1.75	0.66
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.10	0.66
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.76	0.66
19:1X:60:ARG:HH22	29:17:47:ARG:HH12	1.41	0.66
32:1a:642:A:N3	39:1h:113:SER:OG	2.29	0.66
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.77	0.66
38:2g:78:ARG:HH21	38:2g:79:ARG:HE	1.42	0.66
26:14:13:ARG:HB3	26:14:30:GLU:HG3	1.76	0.66
32:1a:757:U:H2'	32:1a:758:G:O4'	1.95	0.66
1:2A:1742:G:O6	61:2A:3817:HOH:O	2.11	0.66
6:2G:46:ALA:HB2	6:2G:53:LEU:HD23	1.78	0.66
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.75	0.66
34:2c:69:HIS:HA	34:2c:104:GLN:HB3	1.78	0.66
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.76	0.66
1:1A:884:C:H42	1:1A:892:G:H1	1.43	0.66
32:1a:1136:U:H5''	32:1a:1137:C:N3	2.11	0.66
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.78	0.66
21:2Z:105:VAL:N	21:2Z:139:VAL:O	2.28	0.66
32:2a:117:G:OP2	61:2a:1903:HOH:O	2.13	0.66
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.76	0.66
49:2r:31:LEU:HD23	49:2r:31:LEU:H	1.60	0.66
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.78	0.66
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.11	0.66
1:1A:248:G:OP1	61:1A:4118:HOH:O	2.12	0.66
32:1a:953:G:H5'	32:1a:965:A:H61	1.60	0.66
1:2A:1253:A:OP1	61:2A:3822:HOH:O	2.14	0.66
7:2H:3:ARG:HG3	7:2H:6:ARG:HH21	1.61	0.66
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.11	0.65
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.11	0.65
32:2a:1521:G:N3	61:2a:1911:HOH:O	2.28	0.65
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.30	0.65
38:2g:22:LEU:HG	38:2g:62:PHE:HE2	1.59	0.65
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.77	0.65
26:14:16:CYS:SG	26:14:17:GLY:N	2.69	0.65
32:1a:677:U:H3	32:1a:713:G:H22	1.45	0.65
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.76	0.65
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.29	0.65
50:2s:64:GLU:OE2	50:2s:65:ASN:ND2	2.29	0.65
14:2S:105:ALA:HB1	14:2S:110:LEU:HD23	1.78	0.65
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	1.78	0.65
33:1b:78:GLN:NE2	33:1b:94:ASN:O	2.29	0.65
33:1b:122:PHE:HE2	33:1b:139:LYS:HB2	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:59:ARG:HH12	35:1d:62:GLN:HB2	1.61	0.65
2:2B:3:C:H2'	2:2B:4:C:C6	2.31	0.65
32:2a:402:G:N7	61:2a:1912:HOH:O	2.28	0.65
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.31	0.65
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.79	0.65
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.25	0.65
32:2a:1029:C:N4	32:2a:1032:G:N1	2.44	0.65
3:1D:37:LEU:HD12	3:1D:62:TYR:HB2	1.78	0.65
33:2b:91:PRO:HG2	33:2b:155:LEU:HD13	1.79	0.65
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.29	0.65
1:2A:1313:U:OP1	61:2A:3824:HOH:O	2.15	0.65
44:2m:57:ARG:O	44:2m:61:GLU:HB2	1.97	0.65
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.30	0.65
1:2A:1604:C:OP1	61:2A:3821:HOH:O	2.13	0.65
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.30	0.65
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.22	0.65
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.32	0.65
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.79	0.65
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.62	0.64
1:1A:249:C:O2	30:18:12:LYS:NZ	2.28	0.64
1:1A:530:G:N1	1:1A:2023:G:OP1	2.23	0.64
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.30	0.64
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.29	0.64
19:2X:94:GLY:CA	19:2X:95:LEU:HB2	2.27	0.64
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.32	0.64
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.80	0.64
33:1b:125:PRO:HB2	33:1b:128:GLU:H	1.62	0.64
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.80	0.64
1:2A:637:A:OP1	11:2P:133:SER:OG	2.13	0.64
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.15	0.64
32:1a:165:C:H2'	32:1a:166:G:H8	1.62	0.64
38:2g:70:LYS:HD3	38:2g:96:GLN:HB3	1.79	0.64
41:2j:47:PHE:N	41:2j:63:PHE:O	2.28	0.64
1:1A:2136:C:C2	1:1A:2155:G:N2	2.65	0.64
1:2A:2576:G:OP1	61:2A:3823:HOH:O	2.14	0.64
32:2a:642:A:N3	39:2h:113:SER:OG	2.31	0.64
1:2A:2577:A:OP1	61:2A:3823:HOH:O	2.15	0.64
1:1A:2344:U:OP1	28:16:37:ARG:NH1	2.31	0.64
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.61	0.64
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.78	0.64
21:2Z:104:PHE:HA	21:2Z:139:VAL:HB	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:92:TYR:N	33:2b:151:GLY:O	2.24	0.64
47:2p:28:ARG:NH1	47:2p:29:ASP:OD1	2.31	0.64
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.31	0.64
32:1a:67:C:H2'	32:1a:68:G:C8	2.33	0.64
32:1a:116:A:OP1	61:1a:1807:HOH:O	2.14	0.64
1:2A:1830:C:OP2	61:2A:3825:HOH:O	2.15	0.64
26:24:44:THR:O	26:24:46:GLN:N	2.30	0.64
29:27:24:THR:HB	29:27:27:GLY:H	1.62	0.64
32:2a:254:G:OP1	48:2q:66:SER:OG	2.16	0.64
32:2a:1128:C:O2'	32:2a:1129:C:OP1	2.15	0.64
32:2a:1136:U:OP2	32:2a:1137:C:N4	2.31	0.64
1:1A:880:G:H2'	1:1A:881:G:H8	1.61	0.64
4:1E:119:ARG:HG3	4:1E:160:TYR:HB2	1.80	0.64
1:2A:892:G:H2'	1:2A:893:C:H4'	1.80	0.64
1:2A:2453:A:N7	61:2A:3886:HOH:O	2.30	0.64
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.23	0.64
32:2a:444:C:H2'	32:2a:445:G:H8	1.62	0.64
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.80	0.64
1:1A:897:C:N3	1:1A:898:C:N4	2.45	0.64
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.31	0.64
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.80	0.64
32:1a:405:U:O4	35:1d:2:GLY:N	2.30	0.63
33:1b:12:GLU:HB2	33:1b:213:LEU:HD21	1.80	0.63
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.79	0.63
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.79	0.63
1:1A:1203:G:O6	61:1A:4119:HOH:O	2.12	0.63
24:22:29:LYS:HE2	24:22:57:ILE:HG21	1.80	0.63
32:2a:17:U:H2'	32:2a:18:C:C6	2.33	0.63
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.63	0.63
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.31	0.63
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.32	0.63
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.79	0.63
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.32	0.63
1:2A:1394:U:OP1	61:2A:3821:HOH:O	2.16	0.63
40:2i:11:LYS:HA	40:2i:108:VAL:HG12	1.80	0.63
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.63	0.63
54:2y:11:C:H42	54:2y:24:G:H1	1.46	0.63
32:1a:945:G:OP1	61:1a:1808:HOH:O	2.16	0.63
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.32	0.63
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.64	0.63
32:2a:1133:G:H1	32:2a:1141:C:H42	1.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.21	0.63
1:2A:2127:G:H1	1:2A:2160:G:H1	1.46	0.63
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.81	0.63
37:2f:37:VAL:HA	37:2f:65:VAL:HG12	1.81	0.63
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.81	0.63
7:2H:80:SER:OG	7:2H:81:GLU:OE1	2.17	0.63
42:1k:85:ARG:HD3	42:1k:113:PRO:HD3	1.81	0.63
1:2A:1346:G:OP2	61:2A:3826:HOH:O	2.15	0.63
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.63	0.63
1:1A:1143:A:OP2	61:1A:4124:HOH:O	2.16	0.63
12:2Q:111:GLU:OE1	12:2Q:133:ARG:NH2	2.32	0.63
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.81	0.63
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.63	0.62
21:1Z:93:ASP:HB3	21:1Z:131:ARG:HH22	1.63	0.62
44:2m:25:ILE:HD11	44:2m:60:VAL:HG11	1.81	0.62
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.81	0.62
32:2a:1225:A:OP1	44:2m:103:THR:OG1	2.16	0.62
1:1A:226:G:H21	1:1A:228:A:H62	1.48	0.62
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.31	0.62
32:2a:975:A:H4'	32:2a:976:G:H5''	1.80	0.62
1:1A:818:G:O6	61:1A:4123:HOH:O	2.14	0.62
1:2A:947:G:O6	61:2A:3827:HOH:O	2.16	0.62
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.32	0.62
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.29	0.62
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.81	0.62
32:2a:890:G:O2'	32:2a:906:G:O6	2.17	0.62
32:2a:1003:G:N2	32:2a:1025:U:O4	2.32	0.62
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.32	0.62
11:2P:124:LYS:HG3	11:2P:144:GLU:HB3	1.82	0.62
19:2X:31:HIS:HD2	19:2X:33:LYS:H	1.45	0.62
26:24:16:CYS:SG	26:24:17:GLY:N	2.73	0.62
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.33	0.62
38:2g:54:THR:O	38:2g:56:GLN:N	2.33	0.62
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.80	0.62
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.34	0.62
50:2s:33:THR:H	50:2s:57:HIS:HE1	1.46	0.62
1:2A:1371:G:O6	61:2A:3820:HOH:O	2.13	0.62
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.18	0.62
33:2b:185:ILE:HB	33:2b:199:TYR:HB2	1.82	0.62
34:2c:88:ARG:HA	34:2c:91:LEU:HB2	1.81	0.62
54:2w:18:G:O2'	54:2w:57:G:N2	2.27	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1500:A:OP2	61:1a:1809:HOH:O	2.16	0.62
1:2A:2317:C:N4	1:2A:2318:G:O6	2.33	0.62
5:2F:13:SER:OG	5:2F:16:GLY:O	2.17	0.62
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.82	0.62
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.32	0.62
38:2g:105:VAL:O	38:2g:109:ASN:ND2	2.31	0.62
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.82	0.62
32:1a:1278:U:H5'	32:1a:1279:A:O4'	1.99	0.62
21:2Z:150:LEU:HB2	21:2Z:171:ILE:HD11	1.82	0.62
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.64	0.62
51:2t:50:GLU:HB2	51:2t:99:LEU:HD12	1.82	0.62
1:1A:654:A:OP2	61:1A:4126:HOH:O	2.16	0.61
1:1A:1702:G:N7	61:1A:4180:HOH:O	2.31	0.61
6:1G:122:PRO:HG3	6:1G:182:LYS:H	1.62	0.61
40:1i:3:GLN:HE21	40:1i:20:ARG:CZ	2.14	0.61
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.82	0.61
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.33	0.61
1:2A:2143:C:H42	1:2A:2148:G:H1	1.46	0.61
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.81	0.61
11:1P:38:GLN:O	11:1P:40:SER:N	2.29	0.61
1:2A:852:G:H2'	1:2A:853:G:H8	1.64	0.61
1:2A:2125:G:N3	1:2A:2173:A:N6	2.48	0.61
32:2a:148:G:H2'	32:2a:149:A:H8	1.63	0.61
38:2g:16:LEU:HD22	40:2i:42:ARG:HA	1.82	0.61
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.82	0.61
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.81	0.61
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.82	0.61
26:24:40:HIS:HD2	26:24:41:PRO:HD2	1.65	0.61
32:2a:407:G:H5''	35:2d:115:ARG:HB3	1.82	0.61
7:1H:101:ARG:HH22	7:1H:122:THR:HA	1.66	0.61
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	1.99	0.61
21:2Z:100:VAL:HG21	21:2Z:134:PRO:HG2	1.81	0.61
32:2a:1239:A:H62	32:2a:1299:A:H62	1.48	0.61
42:2k:73:MET:HG2	42:2k:103:LEU:HD21	1.80	0.61
4:1E:29:GLY:HA3	61:1E:5006:HOH:O	1.99	0.61
21:1Z:156:LYS:HD2	21:1Z:158:PRO:HD3	1.82	0.61
6:2G:63:ILE:HD11	6:2G:144:ILE:HG13	1.82	0.61
38:2g:113:GLU:HG3	38:2g:118:VAL:HG12	1.82	0.61
49:2r:56:THR:HG21	49:2r:63:GLN:HE22	1.66	0.61
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.81	0.61
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2N:15:LEU:N	9:2N:136:GLU:O	2.33	0.61
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.81	0.61
1:1A:2141:G:O6	1:1A:2150:U:O2	2.19	0.61
1:1A:2612:C:OP2	27:15:2:ALA:N	2.34	0.61
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.35	0.61
54:1y:63:G:H2'	54:1y:64:A:O4'	2.01	0.61
7:2H:98:LEU:HD11	7:2H:124:GLU:HA	1.83	0.61
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.32	0.61
1:2A:586:A:N1	1:2A:809:G:O2'	2.32	0.61
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.83	0.61
18:2W:88:ARG:HB2	18:2W:92:ARG:HG2	1.82	0.61
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.65	0.61
32:2a:1129:C:H5'	40:2i:16:ARG:HH22	1.66	0.61
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.34	0.61
54:2w:27:G:H1	54:2w:43:C:H42	1.47	0.61
54:2y:14:A:O2'	54:2y:15:G:OP1	2.17	0.61
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.33	0.61
1:1A:2702:U:OP2	61:1A:4125:HOH:O	2.16	0.61
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.34	0.61
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.36	0.61
32:1a:1337:G:N7	61:1a:1830:HOH:O	2.30	0.61
44:1m:87:TYR:HA	44:1m:90:LEU:HD12	1.82	0.61
1:2A:249:C:O2	30:28:12:LYS:NZ	2.33	0.61
1:2A:880:G:N2	1:2A:898:C:O2	2.33	0.61
2:2B:22:U:H3	2:2B:61:G:H1	1.49	0.61
44:2m:13:LYS:O	44:2m:45:VAL:N	2.26	0.61
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	1.83	0.60
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.32	0.60
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.83	0.60
32:2a:876:G:O5'	39:2h:14:ARG:NH1	2.35	0.60
1:1A:2817:G:OP1	13:1R:99:LYS:NZ	2.31	0.60
33:1b:15:VAL:HB	33:1b:209:ARG:HG3	1.83	0.60
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.83	0.60
32:2a:376:G:H5''	47:2p:5:ARG:HB2	1.82	0.60
1:1A:295:G:H4'	20:1Y:1:MET:HE3	1.82	0.60
1:1A:668:G:N7	61:1A:4183:HOH:O	2.32	0.60
32:1a:405:U:H5''	32:1a:495:A:H2	1.66	0.60
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.37	0.60
1:2A:307:G:N1	1:2A:310:A:OP2	2.34	0.60
1:2A:890:A:H2'	1:2A:892:G:H8	1.66	0.60
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.14	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:149:ARG:NH1	7:2H:167:GLU:OE1	2.33	0.60
32:2a:1055:A:N7	32:2a:1200:C:N4	2.48	0.60
42:2k:121:PRO:HG2	42:2k:126:ARG:HG2	1.84	0.60
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.37	0.60
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.74	0.60
34:1c:11:ARG:NH2	34:1c:177:THR:O	2.35	0.60
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.83	0.60
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.82	0.60
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.35	0.60
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.34	0.60
15:2T:24:PRO:HA	15:2T:49:VAL:HG12	1.82	0.60
26:24:67:TYR:HD2	50:2s:9:VAL:HB	1.66	0.60
32:2a:596:C:OP2	61:2a:1906:HOH:O	2.16	0.60
32:2a:662:G:O2'	32:2a:836:G:OP1	2.19	0.60
32:2a:1073:U:O2'	33:2b:104:ASN:OD1	2.19	0.60
32:2a:1104:G:O3'	33:2b:111:ARG:NH2	2.34	0.60
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.37	0.60
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.01	0.60
1:1A:2136:C:N4	1:1A:2155:G:C6	2.70	0.60
32:1a:278:G:OP2	48:1q:92:ARG:NH2	2.34	0.60
34:1c:58:GLU:HB3	41:1j:92:THR:HG21	1.82	0.60
1:2A:1021:A:H62	1:2A:1141:U:H3	1.50	0.60
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.31	0.60
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.36	0.60
48:2q:45:HIS:CD2	48:2q:47:PRO:HG3	2.36	0.60
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.37	0.60
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.34	0.60
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.01	0.60
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.37	0.60
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.82	0.60
39:2h:84:ARG:NH1	39:2h:85:ARG:O	2.35	0.60
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.01	0.60
1:2A:468:G:N7	29:27:39:ARG:NH2	2.49	0.60
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.30	0.60
1:2A:881:G:C2	1:2A:882:G:H1'	2.36	0.60
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.37	0.60
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.50	0.60
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.83	0.60
33:2b:58:ILE:HA	33:2b:61:LEU:HB3	1.84	0.60
1:1A:1053:C:H42	1:1A:1106:G:H1	1.49	0.60
1:1A:2102:U:H3	1:1A:2187:G:H1	1.50	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1499:A:OP2	61:1a:1801:HOH:O	2.17	0.60
1:2A:796:C:H2'	1:2A:797:C:C6	2.36	0.60
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.37	0.60
26:14:61:ARG:HD3	50:1s:67:VAL:HG12	1.84	0.60
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.65	0.60
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.65	0.60
32:2a:273:A:N7	61:2a:1917:HOH:O	2.31	0.60
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.37	0.60
1:1A:1176:G:H21	1:1A:1178:C:P	2.25	0.60
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.83	0.60
19:1X:92:LEU:O	19:1X:94:GLY:N	2.35	0.60
32:1a:560:U:O2'	32:1a:561:U:OP2	2.18	0.60
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.82	0.60
32:2a:1417:G:O6	61:2a:1905:HOH:O	2.15	0.60
33:2b:198:ASP:N	33:2b:198:ASP:OD1	2.33	0.60
1:1A:1648:C:OP1	61:1A:4108:HOH:O	2.17	0.59
11:1P:44:GLY:O	11:1P:45:LEU:HB2	2.01	0.59
47:1p:60:LEU:HD11	47:1p:66:PRO:HD3	1.84	0.59
1:2A:332:A:O2'	1:2A:334:C:OP2	2.20	0.59
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.35	0.59
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.35	0.59
7:2H:125:VAL:HG22	7:2H:131:VAL:HG22	1.84	0.59
26:24:24:THR:OG1	26:24:25:TYR:N	2.34	0.59
32:2a:984:C:H2'	32:2a:985:C:C6	2.37	0.59
35:2d:18:LYS:NZ	35:2d:31:CYS:SG	2.75	0.59
44:2m:78:ILE:HA	44:2m:81:LEU:HD12	1.83	0.59
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.83	0.59
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.37	0.59
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.83	0.59
34:1c:131:ARG:NH2	36:1e:50:GLU:OE2	2.35	0.59
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.49	0.59
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.19	0.59
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.84	0.59
32:2a:222:U:H2'	32:2a:223:U:C6	2.37	0.59
54:2w:9:A:H8	54:2w:11:C:H41	1.48	0.59
1:1A:2428:G:OP1	61:1A:4102:HOH:O	2.16	0.59
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.84	0.59
32:1a:1036:G:H5''	32:1a:1037:C:C5	2.37	0.59
1:2A:1891:G:O6	61:2A:3828:HOH:O	2.16	0.59
12:2Q:75:THR:HG21	12:2Q:87:LYS:HE3	1.84	0.59
40:2i:29:ASN:OD1	40:2i:65:VAL:N	2.34	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.84	0.59
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.84	0.59
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	1.84	0.59
32:2a:719:C:H42	49:2r:71:LYS:HE2	1.68	0.59
32:2a:1190:G:O2'	34:2c:3:ASN:HB2	2.03	0.59
32:2a:1328:C:O2'	44:2m:29:ARG:NH2	2.31	0.59
41:2j:21:GLN:HE22	41:2j:25:GLU:HG2	1.66	0.59
41:2j:40:LEU:HB2	41:2j:69:ASN:HB3	1.82	0.59
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.18	0.59
1:2A:362:U:O2'	1:2A:363:G:H5''	2.02	0.59
7:2H:76:VAL:HA	7:2H:79:VAL:HG22	1.85	0.59
25:23:40:THR:HG22	25:23:42:ALA:H	1.67	0.59
1:1A:1075:C:H2'	1:1A:1076:C:H2'	1.84	0.59
1:2A:860:U:H1'	1:2A:2268:A:H5'	1.85	0.59
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.84	0.59
1:1A:878:A:N6	1:1A:899:A:O2'	2.35	0.59
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.00	0.59
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.38	0.59
1:1A:528:A:O2'	1:1A:529:A:H5'	2.03	0.59
32:1a:473:G:OP2	47:1p:75:ARG:NH1	2.35	0.59
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.26	0.59
1:2A:2207:G:H3'	1:2A:2208:A:H5''	1.84	0.59
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.83	0.59
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.36	0.59
33:2b:96:ARG:HG2	33:2b:98:LEU:HD12	1.85	0.59
48:2q:81:ARG:HH21	48:2q:84:LEU:HD21	1.66	0.59
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.84	0.59
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.18	0.59
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.85	0.59
14:2S:11:LYS:HG3	14:2S:91:PRO:HB3	1.84	0.59
23:21:83:GLU:OE1	23:21:83:GLU:N	2.36	0.59
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.36	0.59
1:2A:890:A:H2'	1:2A:892:G:C8	2.38	0.59
1:2A:1993:U:OP2	61:2A:3829:HOH:O	2.17	0.59
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.38	0.59
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.36	0.59
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.03	0.59
32:2a:1060:C:OP1	45:2n:45:ARG:NH2	2.35	0.59
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.67	0.59
35:2d:150:GLU:H	35:2d:150:GLU:CD	2.10	0.59
4:1E:47:VAL:HG22	4:1E:84:PHE:O	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1239:A:H62	32:1a:1299:A:H62	1.52	0.58
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.33	0.58
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.49	0.58
1:2A:906:G:O2'	12:2Q:67:ARG:NH2	2.28	0.58
32:2a:1004:A:C8	32:2a:1005:A:H4'	2.37	0.58
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.38	0.58
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.37	0.58
48:1q:67:LYS:HA	48:1q:70:ARG:HH12	1.68	0.58
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.84	0.58
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.03	0.58
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.31	0.58
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.51	0.58
33:2b:16:HIS:HB2	33:2b:204:ASN:HD22	1.68	0.58
1:2A:2049:G:N7	61:2A:3898:HOH:O	2.32	0.58
5:2F:137:LYS:HA	5:2F:140:LEU:HD12	1.84	0.58
11:2P:8:PRO:HB2	11:2P:12:ALA:HB3	1.85	0.58
32:2a:1272:G:N2	32:2a:1273:G:C5	2.71	0.58
34:2c:69:HIS:CD2	34:2c:104:GLN:HG2	2.38	0.58
35:2d:175:SER:HB3	35:2d:186:LEU:HD21	1.84	0.58
1:1A:1054:A:H61	1:1A:1105:U:H3	1.52	0.58
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.68	0.58
32:1a:1325:C:OP1	52:1u:15:ARG:NH1	2.35	0.58
1:2A:307:G:H21	1:2A:330:A:H62	1.50	0.58
14:2S:84:GLN:H	14:2S:111:GLU:HB2	1.69	0.58
32:2a:947:G:H1	32:2a:1234:C:H42	1.49	0.58
7:2H:88:LEU:HD11	7:2H:165:ALA:HA	1.84	0.58
32:2a:1239:A:H62	32:2a:1299:A:N6	2.02	0.58
32:2a:1316:G:H5''	45:2n:17:LYS:HE3	1.84	0.58
51:1t:34:LYS:HE3	51:1t:80:ARG:HH22	1.68	0.58
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.69	0.58
5:2F:148:LEU:HD11	5:2F:193:VAL:HG21	1.85	0.58
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.04	0.58
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.19	0.58
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.36	0.58
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	1.84	0.58
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.86	0.58
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.85	0.58
1:2A:568:U:H5'	1:2A:945:A:N1	2.18	0.58
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.85	0.58
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	1.85	0.58
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1263:C:N3	32:2a:1272:G:O6	2.36	0.58
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.86	0.58
51:1t:42:GLN:NE2	51:1t:46:GLU:OE2	2.36	0.58
1:2A:839:U:H2'	1:2A:840:C:C6	2.38	0.58
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.68	0.58
37:2f:36:ARG:NH2	37:2f:38:GLU:OE2	2.37	0.58
8:1I:75:LEU:HD22	8:1I:105:HIS:HD2	1.69	0.58
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.85	0.58
34:2c:18:TRP:HH2	45:2n:57:ARG:HD3	1.69	0.58
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.86	0.57
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.39	0.57
1:2A:400:G:N7	61:2A:3899:HOH:O	2.32	0.57
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.39	0.57
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.37	0.57
4:2E:30:PRO:HB3	4:2E:92:THR:HG22	1.86	0.57
32:2a:920:U:H2'	32:2a:921:U:C6	2.39	0.57
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.68	0.57
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.38	0.57
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.39	0.57
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	1.85	0.57
26:24:46:GLN:C	26:24:48:ARG:H	2.11	0.57
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.37	0.57
32:2a:984:C:H2'	32:2a:985:C:H6	1.68	0.57
32:2a:1264:C:N4	32:2a:1265:G:O6	2.36	0.57
32:2a:1400:5MC:N4	55:2x:34:C:H1'	2.19	0.57
41:2j:42:THR:HG23	41:2j:68:HIS:HA	1.87	0.57
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.69	0.57
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.04	0.57
21:2Z:6:LYS:HE3	21:2Z:8:TYR:HE2	1.69	0.57
26:24:58:ARG:HH21	44:2m:80:ARG:HH22	1.52	0.57
33:2b:47:THR:O	33:2b:51:LEU:N	2.36	0.57
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.86	0.57
38:2g:22:LEU:HG	38:2g:62:PHE:CE2	2.39	0.57
1:1A:2830:G:N7	61:1A:4192:HOH:O	2.32	0.57
19:1X:11:PRO:HB3	19:1X:92:LEU:HD21	1.87	0.57
32:1a:567:G:N3	61:1a:1835:HOH:O	2.31	0.57
40:1i:53:VAL:O	40:1i:55:ALA:N	2.37	0.57
1:2A:27:G:N2	1:2A:512:G:H1'	2.20	0.57
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.51	0.57
18:1W:1:MET:HE3	18:1W:2:GLU:H	1.70	0.57
32:1a:1035:A:H2'	32:1a:1036:G:H21	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:44:GLU:HA	34:1c:52:LEU:HD23	1.85	0.57
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.40	0.57
36:2e:36:ASP:O	36:2e:38:GLN:N	2.35	0.57
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.19	0.57
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.68	0.57
9:1N:42:TRP:HA	9:1N:48:MET:HE1	1.86	0.57
20:1Y:92:ASN:ND2	20:1Y:94:LYS:HG2	2.13	0.57
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.38	0.57
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.68	0.57
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.87	0.57
38:2g:133:GLY:O	38:2g:137:LYS:N	2.30	0.57
50:2s:33:THR:H	50:2s:57:HIS:CE1	2.22	0.57
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.04	0.57
8:1I:37:VAL:HG13	8:1I:38:LEU:HD23	1.85	0.57
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.87	0.57
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.86	0.57
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.40	0.57
12:2Q:110:THR:HB	12:2Q:113:GLN:H	1.69	0.57
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.18	0.57
34:2c:179:ARG:NH1	34:2c:206:GLU:OE1	2.38	0.57
54:2y:34:G:H2'	54:2y:35:A:C8	2.40	0.57
12:1Q:16:ARG:HG2	12:1Q:18:LYS:HE3	1.87	0.57
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.39	0.57
32:2a:677:U:H3	32:2a:713:G:H22	1.50	0.57
32:2a:826:C:O2	39:2h:15:ASN:ND2	2.37	0.57
33:2b:185:ILE:HG22	33:2b:199:TYR:HD2	1.70	0.57
44:2m:79:LYS:NZ	44:2m:83:ASP:OD2	2.36	0.57
48:2q:95:TYR:HA	48:2q:98:LEU:HD12	1.87	0.57
50:2s:52:TYR:HD1	50:2s:57:HIS:HD2	1.53	0.57
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.87	0.57
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.87	0.57
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.86	0.57
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.87	0.57
32:2a:148:G:H2'	32:2a:149:A:C8	2.40	0.57
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.70	0.57
33:2b:178:ARG:NH2	39:2h:68:ARG:HH22	1.99	0.57
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.40	0.56
27:15:40:LYS:NZ	27:15:44:THR:O	2.34	0.56
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	1.87	0.56
19:2X:60:ARG:HH12	29:27:47:ARG:HH22	1.53	0.56
32:2a:1227:A:OP2	44:2m:111:LYS:HD3	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:3:ARG:N	44:2m:7:VAL:O	2.38	0.56
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.20	0.56
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.86	0.56
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.87	0.56
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.04	0.56
1:2A:2124:G:O6	1:2A:2125:G:N2	2.35	0.56
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.05	0.56
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.39	0.56
33:2b:74:LYS:HD2	33:2b:166:ASP:HB2	1.86	0.56
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.69	0.56
1:1A:1039:G:H1	1:1A:1116:C:H42	1.53	0.56
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.30	0.56
32:1a:92:C:H2'	32:1a:93:G:H8	1.70	0.56
40:1i:9:ARG:HG2	40:1i:14:VAL:HG12	1.86	0.56
1:2A:271(H):G:H5'	23:21:81:LYS:NZ	2.20	0.56
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.40	0.56
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.06	0.56
32:2a:35:G:O2'	43:2l:118:SER:O	2.19	0.56
32:2a:444:C:H2'	32:2a:445:G:C8	2.40	0.56
33:2b:104:ASN:OD1	33:2b:107:THR:OG1	2.23	0.56
36:2e:102:ALA:O	36:2e:107:ARG:NH2	2.39	0.56
40:2i:17:VAL:HG11	40:2i:81:ILE:HA	1.87	0.56
50:2s:13:ASP:HA	50:2s:16:LEU:HB3	1.87	0.56
1:1A:184:C:H2'	1:1A:185:U:C6	2.40	0.56
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.41	0.56
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.40	0.56
55:1x:8:4SU:O2	55:1x:21:A:H2	1.87	0.56
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.39	0.56
26:14:54:GLY:N	26:14:55:ARG:HA	2.20	0.56
33:1b:174:VAL:O	33:1b:178:ARG:HG2	2.05	0.56
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.40	0.56
1:2A:652(A):A:H3'	1:2A:652(B):A:H5''	1.87	0.56
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.37	0.56
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.88	0.56
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.40	0.56
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.88	0.56
41:2j:6:ILE:HG12	41:2j:98:ILE:HD11	1.88	0.56
21:1Z:132:ASN:N	21:1Z:132:ASN:OD1	2.38	0.56
32:1a:1239:A:H62	32:1a:1299:A:N6	2.03	0.56
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.23	0.56
14:2S:30:ARG:HB2	14:2S:35:ILE:HD12	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:560:U:H5'	32:2a:566:G:N2	2.20	0.56
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.21	0.56
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.27	0.56
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.87	0.56
7:1H:127:GLU:HG3	7:1H:130:ARG:HB2	1.87	0.56
11:1P:126:VAL:HG12	11:1P:148:LEU:HD13	1.88	0.56
32:1a:356:A:N3	32:1a:368:U:O2'	2.33	0.56
32:1a:373:A:H2'	32:1a:374:A:H8	1.69	0.56
32:1a:1198:G:OP1	61:1a:1811:HOH:O	2.18	0.56
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.88	0.56
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.88	0.56
7:2H:8:PRO:HG3	7:2H:51:ARG:HD3	1.87	0.56
26:24:26:SER:OG	26:24:27:THR:N	2.36	0.56
32:2a:564:C:HO2'	39:2h:91:ARG:HH12	1.49	0.56
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.19	0.56
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.05	0.56
41:2j:98:ILE:O	61:2j:301:HOH:O	2.18	0.56
1:1A:123:G:OP2	61:1A:4128:HOH:O	2.18	0.56
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.87	0.56
1:1A:2336:A:H61	22:10:43:THR:HG22	1.71	0.56
32:1a:38:G:H22	32:1a:397:A:H5''	1.70	0.56
32:1a:456:C:H2'	32:1a:457:C:C6	2.41	0.56
32:1a:828:A:H2'	32:1a:829:G:O4'	2.05	0.56
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.36	0.56
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.21	0.56
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.88	0.56
32:2a:1012:U:H2'	32:2a:1013:G:C8	2.41	0.56
33:2b:81:VAL:HB	33:2b:94:ASN:HD21	1.71	0.56
43:2l:117:ARG:HB3	43:2l:122:THR:HB	1.87	0.56
32:1a:159:G:N2	32:1a:162:A:OP2	2.39	0.56
32:2a:1216:G:H5''	45:2n:5:ALA:HB2	1.87	0.56
32:2a:1271:G:C2	32:2a:1272:G:N7	2.74	0.56
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.14	0.56
33:2b:158:LEU:HD23	33:2b:182:ILE:HD11	1.88	0.56
1:1A:55:G:O2'	1:1A:127:A:N1	2.37	0.56
9:1N:21:LYS:NZ	9:1N:140:VAL:OXT	2.35	0.56
15:1T:127:ALA:C	15:1T:129:ARG:H	2.13	0.56
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.14	0.56
32:1a:1500:A:OP1	61:1a:1810:HOH:O	2.16	0.56
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.88	0.56
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:668:G:H5'	1:2A:669:G:OP2	2.05	0.56
33:2b:219:VAL:HA	33:2b:222:ILE:HG12	1.88	0.56
1:1A:1063:G:H2'	1:1A:1064:C:H5	1.71	0.55
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.70	0.55
20:1Y:20:TYR:HB3	20:1Y:23:ARG:HG3	1.88	0.55
32:1a:222:U:H2'	32:1a:223:U:C6	2.41	0.55
32:1a:510:A:OP2	35:1d:49:ARG:NH1	2.38	0.55
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.41	0.55
34:1c:36:ASP:OD1	34:1c:59:ARG:NH2	2.37	0.55
19:2X:60:ARG:HH12	29:27:47:ARG:NH2	2.03	0.55
32:2a:1029:C:N4	32:2a:1032:G:C6	2.74	0.55
32:2a:1125:U:OP1	41:2j:35:SER:OG	2.21	0.55
34:2c:22:TRP:CH2	34:2c:32:LEU:HB3	2.40	0.55
54:2w:21:A:O2'	54:2w:22:G:OP1	2.23	0.55
1:1A:1139:G:OP2	9:1N:70:LYS:NZ	2.37	0.55
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.39	0.55
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.39	0.55
51:1t:45:GLN:HB2	51:1t:91:LEU:HD13	1.88	0.55
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	1.87	0.55
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.04	0.55
7:1H:96:ALA:HB2	7:1H:105:LEU:HD23	1.87	0.55
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.07	0.55
37:1f:11:ASN:HB3	37:1f:14:LEU:HG	1.88	0.55
1:2A:2127:G:H22	1:2A:2160:G:H22	1.53	0.55
32:2a:452:A:HO2'	32:2a:453:A:H8	1.54	0.55
32:2a:1274:G:N2	32:2a:1275:A:N7	2.54	0.55
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.87	0.55
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.39	0.55
1:1A:2128:C:N3	1:1A:2160:G:N2	2.54	0.55
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.87	0.55
8:1I:77:LEU:HG	8:1I:101:LEU:HD22	1.88	0.55
26:14:18:CYS:SG	26:14:20:ASN:HB2	2.47	0.55
37:1f:6:VAL:HG13	37:1f:90:VAL:HG22	1.88	0.55
54:1w:26:A:N6	54:1w:44:G:H1	2.04	0.55
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.42	0.55
5:2F:33:LEU:HB3	11:2P:6:LEU:HD21	1.87	0.55
55:2x:4:G:H1	55:2x:69:C:H42	1.54	0.55
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.18	0.55
1:1A:2096:U:H3	1:1A:2193:G:H1	1.55	0.55
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.41	0.55
32:1a:1025:U:C2	32:1a:1036:G:O6	2.60	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:854:G:H2'	1:2A:855:G:H8	1.71	0.55
32:2a:1342:C:H4'	40:2i:125:TYR:HB3	1.88	0.55
34:2c:77:ILE:HG23	34:2c:103:VAL:HG21	1.89	0.55
14:1S:61:ASN:HB3	14:1S:64:GLU:HB2	1.87	0.55
22:10:24:LYS:O	22:10:25:ARG:NH1	2.36	0.55
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.42	0.55
1:2A:582:G:OP2	61:2A:3830:HOH:O	2.17	0.55
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.32	0.55
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.22	0.55
28:26:35:GLU:HG3	28:26:50:ARG:HD3	1.87	0.55
32:2a:64:G:H4'	32:2a:65:U:H3'	1.89	0.55
32:2a:978:A:O2'	32:2a:1322:C:N3	2.33	0.55
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.70	0.55
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.42	0.55
32:2a:1366:C:OP1	40:2i:117:HIS:NE2	2.38	0.55
33:2b:19:HIS:HB2	33:2b:204:ASN:HB2	1.88	0.55
7:1H:101:ARG:NH2	7:1H:122:THR:OG1	2.40	0.55
26:14:58:ARG:O	26:14:61:ARG:N	2.40	0.55
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.89	0.55
33:1b:15:VAL:HG11	33:1b:213:LEU:HD22	1.88	0.55
48:1q:88:TYR:HD2	48:1q:89:LEU:HD23	1.71	0.55
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.23	0.55
1:2A:2663:G:H3'	1:2A:2664:G:H8	1.72	0.55
7:2H:24:VAL:HG21	7:2H:72:ILE:HD12	1.89	0.55
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.07	0.55
21:2Z:155:LEU:HB2	21:2Z:157:LEU:HD12	1.89	0.55
34:2c:47:LEU:O	34:2c:51:GLY:N	2.35	0.55
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.40	0.55
32:1a:583:A:N6	32:1a:758:G:O2'	2.37	0.55
1:2A:893:C:H5'	1:2A:894:C:C5	2.41	0.55
1:2A:1791:A:H5'	3:2D:206:LEU:HD12	1.87	0.55
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.42	0.55
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.88	0.55
32:2a:999:C:H42	32:2a:1042:G:H1	1.55	0.55
32:2a:1089:G:H1	32:2a:1096:C:H42	1.54	0.55
35:2d:3:ARG:HH12	35:2d:5:ILE:HG13	1.72	0.55
44:2m:60:VAL:HG13	44:2m:64:TRP:HE3	1.72	0.55
32:1a:396:G:O2'	32:1a:398:C:OP1	2.20	0.55
32:1a:736:C:H2'	32:1a:737:A:C8	2.42	0.55
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.21	0.55
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.07	0.55
1:2A:800:A:H8	1:2A:800:A:OP1	1.89	0.55
21:2Z:70:LEU:HD12	21:2Z:71:VAL:H	1.72	0.55
32:2a:646:U:H2'	32:2a:647:C:C6	2.42	0.55
32:2a:913:A:OP1	43:2l:46:LYS:NZ	2.40	0.55
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.37	0.55
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.42	0.55
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.87	0.55
32:1a:486:U:H2'	32:1a:487:A:H8	1.71	0.55
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.72	0.55
39:1h:86:ILE:HD12	39:1h:133:LEU:HD22	1.87	0.55
49:1r:56:THR:HG21	49:1r:63:GLN:HE22	1.72	0.55
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.42	0.55
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.72	0.55
32:2a:1095:U:OP2	61:2a:1904:HOH:O	2.18	0.55
44:2m:94:ARG:HH21	50:2s:81:ARG:HA	1.71	0.55
54:2w:34:G:H2'	54:2w:35:A:C8	2.42	0.55
1:1A:897:C:H5'	54:1w:56:C:OP1	2.07	0.54
27:15:35:GLU:HG3	27:15:51:TYR:CD1	2.42	0.54
41:1j:64:GLU:OE2	41:1j:66:ARG:NE	2.31	0.54
1:2A:93:G:H2'	1:2A:94:C:C6	2.41	0.54
32:2a:1314:C:N4	50:2s:2:PRO:O	2.39	0.54
44:2m:107:ALA:HB3	44:2m:111:LYS:HE2	1.88	0.54
1:1A:1058:G:N2	1:1A:1080:C:N3	2.53	0.54
1:1A:2140:C:H42	1:1A:2150:U:H3	1.55	0.54
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.42	0.54
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.71	0.54
19:2X:94:GLY:HA3	19:2X:95:LEU:HB2	1.88	0.54
32:2a:972:C:O2'	41:2j:55:LYS:O	2.25	0.54
34:2c:41:GLY:O	34:2c:45:LYS:NZ	2.40	0.54
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.07	0.54
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.90	0.54
6:2G:111:LEU:HD21	6:2G:120:LEU:HD21	1.87	0.54
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.89	0.54
1:1A:9:U:H3	1:1A:2629:A:H2	1.55	0.54
1:1A:11:G:C2'	1:1A:12:U:H5'	2.35	0.54
1:1A:602:G:O2'	1:1A:655:A:N6	2.40	0.54
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.07	0.54
32:1a:573:A:OP2	61:1a:1802:HOH:O	2.18	0.54
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.43	0.54
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:247:G:H4'	1:2A:386:G:C5	2.42	0.54
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.43	0.54
1:2A:1183:G:H5''	25:23:30:ARG:NH2	2.22	0.54
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.42	0.54
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.90	0.54
1:1A:576:U:H2'	1:1A:577:G:C8	2.43	0.54
1:1A:2049:G:N7	61:1A:4194:HOH:O	2.33	0.54
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.43	0.54
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.06	0.54
12:1Q:12:GLN:NE2	12:1Q:72:LYS:HG3	2.23	0.54
32:1a:401:C:P	35:1d:73:ARG:HH21	2.30	0.54
2:2B:14:U:OP2	2:2B:70:C:O2'	2.22	0.54
4:2E:9:VAL:HG13	15:2T:3:ARG:HG2	1.89	0.54
25:23:35:ARG:HG2	25:23:37:LEU:HD21	1.89	0.54
1:1A:192:C:OP1	61:1A:4130:HOH:O	2.18	0.54
1:1A:2128:C:N4	1:1A:2160:G:H1	2.05	0.54
1:1A:2361:A:OP1	30:18:27:THR:OG1	2.19	0.54
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.73	0.54
32:1a:316:G:OP2	32:1a:351:G:O2'	2.23	0.54
32:1a:1273:G:H3'	32:1a:1274:G:H8	1.73	0.54
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.40	0.54
1:2A:643:A:N1	1:2A:2369:A:O2'	2.37	0.54
1:2A:2362:G:N3	61:2A:3900:HOH:O	2.33	0.54
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.89	0.54
26:24:40:HIS:CD2	26:24:41:PRO:HD2	2.43	0.54
31:29:7:VAL:HG12	31:29:34:GLN:HB3	1.88	0.54
40:2i:82:ALA:HA	40:2i:85:LEU:HD12	1.90	0.54
1:1A:1057:A:N6	1:1A:1087:G:OP2	2.37	0.54
1:1A:1439:A:OP1	61:1A:4114:HOH:O	2.18	0.54
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	1.89	0.54
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.07	0.54
1:2A:884:C:H3'	1:2A:885:C:H6	1.73	0.54
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.43	0.54
7:2H:68:THR:O	7:2H:72:ILE:HG12	2.07	0.54
32:2a:56:U:H2'	32:2a:57:G:C8	2.42	0.54
32:2a:757:U:H2'	32:2a:758:G:O4'	2.08	0.54
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.22	0.54
37:2f:99:ALA:HB1	49:2r:23:LYS:NZ	2.23	0.54
1:1A:1058:G:N1	1:1A:1080:C:N4	2.55	0.54
1:1A:2131:G:H5''	1:1A:2132:U:H3'	1.88	0.54
32:1a:920:U:H2'	32:1a:921:U:C6	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.23	0.54
42:1k:84:VAL:HG11	42:1k:91:ARG:HD2	1.90	0.54
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.88	0.54
1:2A:1533:G:N2	1:2A:1536:C:O2	2.31	0.54
1:2A:1603:A:OP1	61:2A:3804:HOH:O	2.19	0.54
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.07	0.54
4:2E:77:ILE:HD13	4:2E:195:LEU:HD22	1.90	0.54
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.89	0.54
19:2X:92:LEU:C	19:2X:94:GLY:H	2.16	0.54
32:2a:297:G:N2	32:2a:300:A:OP2	2.40	0.54
34:2c:35:GLU:O	34:2c:39:ILE:HG13	2.07	0.54
36:2e:81:GLU:HG2	36:2e:90:VAL:HG13	1.89	0.54
38:2g:111:ARG:NH1	38:2g:113:GLU:OE2	2.39	0.54
44:2m:23:TYR:HE2	44:2m:70:LEU:HD22	1.71	0.54
54:2y:61:C:H2'	54:2y:62:C:C6	2.43	0.54
6:1G:4:ASP:OD1	6:1G:9:ARG:NH1	2.41	0.54
21:1Z:10:ARG:HG3	21:1Z:36:LYS:HB3	1.89	0.54
32:1a:1179:A:H4'	40:1i:103:THR:HA	1.90	0.54
1:2A:662:G:H5''	11:2P:16:ARG:HG2	1.90	0.54
5:2F:24:LEU:HD21	5:2F:114:VAL:HG12	1.90	0.54
7:2H:15:VAL:HG12	7:2H:28:GLY:HA3	1.90	0.54
32:2a:1290:G:OP1	38:2g:35:LYS:NZ	2.41	0.54
41:2j:8:LEU:HD11	41:2j:20:ALA:HB2	1.90	0.54
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.08	0.54
1:1A:1156:A:OP1	16:1U:55:ARG:NH1	2.40	0.54
1:1A:2821:A:OP2	61:1R:301:HOH:O	2.19	0.54
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.43	0.54
1:2A:963:U:OP2	61:2A:3805:HOH:O	2.17	0.54
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.41	0.54
39:2h:106:GLY:O	39:2h:122:ARG:NH2	2.38	0.54
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.34	0.53
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.08	0.53
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.41	0.53
2:1B:42:C:OP1	6:1G:67:LYS:NZ	2.40	0.53
4:1E:7:VAL:HG23	4:1E:51:PHE:HE2	1.72	0.53
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.90	0.53
32:1a:184:G:H2'	32:1a:185:A:H8	1.74	0.53
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.41	0.53
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.72	0.53
10:2O:19:ILE:HG22	10:2O:43:VAL:HA	1.89	0.53
11:2P:98:GLU:OE1	11:2P:102:ARG:NH1	2.40	0.53

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	1.90	0.53
32:2a:751:U:H4'	46:2o:24:SER:HA	1.90	0.53
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	1.89	0.53
42:2k:48:ILE:O	42:2k:50:TYR:N	2.35	0.53
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.43	0.53
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.90	0.53
33:1b:87:ARG:NH2	33:1b:220:ASP:OD1	2.29	0.53
49:1r:31:LEU:HD23	49:1r:31:LEU:H	1.72	0.53
1:2A:455:C:N3	1:2A:472:A:H2'	2.23	0.53
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.05	0.53
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.41	0.53
41:2j:13:HIS:HB3	41:2j:68:HIS:CE1	2.43	0.53
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.73	0.53
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.89	0.53
34:1c:8:ILE:HD12	34:1c:16:ARG:HG3	1.90	0.53
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.91	0.53
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.43	0.53
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.90	0.53
7:2H:3:ARG:HH12	7:2H:5:GLY:H	1.55	0.53
32:2a:1360:A:H8	32:2a:1360:A:OP1	1.91	0.53
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.90	0.53
39:2h:36:LEU:O	39:2h:40:ALA:N	2.42	0.53
1:1A:2171:A:O2'	1:1A:2172:U:H5''	2.09	0.53
1:1A:2336:A:H61	22:10:43:THR:CG2	2.21	0.53
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.91	0.53
32:1a:79:G:H1'	32:1a:91:C:O2	2.07	0.53
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	1.91	0.53
21:2Z:106:GLY:HA3	21:2Z:141:VAL:HB	1.90	0.53
36:2e:95:ALA:O	36:2e:97:GLY:N	2.41	0.53
43:2l:43:VAL:HG12	43:2l:44:THR:H	1.72	0.53
55:2x:55:PSU:O2'	55:2x:57:A:N7	2.40	0.53
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.72	0.53
32:1a:17:U:H2'	32:1a:18:C:C6	2.44	0.53
50:1s:36:ARG:HB3	50:1s:72:GLY:HA3	1.90	0.53
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	1.90	0.53
1:2A:236:C:H2'	1:2A:237:C:H6	1.73	0.53
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.08	0.53
32:2a:735:C:H2'	32:2a:736:C:H6	1.74	0.53
32:2a:1006:C:H2'	32:2a:1007:C:O4'	2.08	0.53
35:2d:59:ARG:NH1	35:2d:59:ARG:HA	2.23	0.53
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.43	0.53
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	1.91	0.53
41:1j:57:LYS:HE2	41:1j:60:ARG:NH2	2.24	0.53
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.44	0.53
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.24	0.53
21:2Z:153:SER:HB2	21:2Z:167:PRO:HB3	1.91	0.53
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.44	0.53
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.24	0.53
51:1t:50:GLU:HA	51:1t:100:ILE:HG12	1.91	0.53
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.18	0.53
1:2A:2104:G:H1	1:2A:2185:C:H42	1.55	0.53
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.09	0.53
1:2A:2336:A:H61	22:20:43:THR:HG22	1.74	0.53
3:2D:29:PRO:HA	3:2D:83:GLU:OE1	2.09	0.53
36:2e:43:LEU:H	36:2e:65:ASN:HB3	1.73	0.53
48:2q:4:LYS:HE3	48:2q:6:LEU:HD21	1.91	0.53
54:2w:11:C:H42	54:2w:24:G:H1	1.57	0.53
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.74	0.53
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.90	0.53
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.42	0.53
32:1a:447:G:O6	32:1a:485:G:O2'	2.26	0.53
41:1j:38:ILE:HD11	41:1j:40:LEU:HD23	1.91	0.53
44:1m:19:LEU:HD11	44:1m:56:LEU:HD21	1.90	0.53
1:2A:2819:G:OP1	61:2A:3832:HOH:O	2.19	0.53
6:2G:41:GLN:O	6:2G:43:LEU:N	2.41	0.53
32:2a:1244:C:H42	32:2a:1293:G:H1	1.55	0.53
33:2b:27:LYS:NZ	33:2b:193:ASP:OD1	2.39	0.53
39:2h:33:GLU:O	39:2h:36:LEU:N	2.40	0.53
39:2h:96:GLY:N	39:2h:99:GLU:OE1	2.40	0.53
1:1A:588:U:H2'	1:1A:589:C:C6	2.43	0.53
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.43	0.53
21:1Z:126:VAL:HG11	21:1Z:161:VAL:HB	1.91	0.53
32:1a:1037:C:H2'	32:1a:1038:C:C6	2.43	0.53
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.25	0.53
24:22:44:LEU:HD23	24:22:47:ASN:HA	1.91	0.53
32:2a:1456:G:O6	51:2t:54:LYS:NZ	2.33	0.53
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	1.91	0.53
42:2k:110:ASP:HB3	49:2r:85:LEU:HB3	1.91	0.53
50:2s:27:GLU:HB3	50:2s:28:LYS:HD3	1.91	0.53
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.74	0.53
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:764:A:H5''	3:2D:210:GLY:CA	2.39	0.53
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.73	0.53
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.39	0.53
26:24:61:ARG:HG2	50:2s:42:PRO:HG3	1.91	0.53
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.44	0.53
44:2m:10:PRO:HD2	44:2m:18:ALA:HB1	1.89	0.53
1:1A:1399:C:OP1	19:1X:25:LYS:NZ	2.41	0.52
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.72	0.52
1:1A:2384:G:OP2	22:10:55:ARG:NH2	2.36	0.52
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.91	0.52
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.42	0.52
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.73	0.52
7:1H:98:LEU:HD11	7:1H:125:VAL:H	1.73	0.52
32:1a:1320:C:O2	50:1s:36:ARG:NH2	2.41	0.52
39:1h:83:ILE:HG13	39:1h:137:VAL:HG22	1.90	0.52
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.92	0.52
49:1r:52:PRO:HB2	49:1r:54:ARG:HG3	1.91	0.52
1:2A:34:C:H41	1:2A:447:A:H61	1.57	0.52
1:2A:831:G:O2'	11:2P:38:GLN:OE1	2.23	0.52
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.24	0.52
1:2A:2781:A:H5''	1:2A:2782:G:H5'	1.91	0.52
19:2X:2:LYS:NZ	19:2X:38:GLU:OE2	2.41	0.52
32:2a:372:C:O2	61:2a:1907:HOH:O	2.18	0.52
32:2a:973:G:H3'	32:2a:974:A:H5''	1.90	0.52
46:2o:39:LEU:HB3	46:2o:56:LEU:HD12	1.89	0.52
32:1a:532:A:N6	32:1a:1206:G:O2'	2.42	0.52
36:1e:80:ILE:HG22	36:1e:91:LEU:HB2	1.92	0.52
44:1m:20:THR:C	44:1m:22:ILE:H	2.18	0.52
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.90	0.52
1:2A:492:A:H2'	1:2A:493:G:O4'	2.09	0.52
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.09	0.52
1:2A:2448:A:OP1	61:2A:3809:HOH:O	2.18	0.52
19:2X:5:TYR:OH	24:22:30:ARG:NH1	2.42	0.52
26:24:45:GLY:C	26:24:47:GLN:H	2.17	0.52
34:2c:39:ILE:HG22	34:2c:43:LEU:HD11	1.91	0.52
32:1a:673:G:H2'	32:1a:674:G:C8	2.44	0.52
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.23	0.52
1:2A:271(P):C:O3'	8:2I:42:SER:OG	2.26	0.52
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.09	0.52
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.70	0.52
6:2G:165:THR:HG23	6:2G:168:GLU:HG3	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:80:PRO:HA	8:2I:145:VAL:HG12	1.92	0.52
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.92	0.52
32:2a:396:G:O2'	32:2a:398:C:OP1	2.24	0.52
33:2b:103:THR:HA	33:2b:180:LEU:HD11	1.92	0.52
50:2s:4:SER:HB3	50:2s:7:LYS:HG3	1.91	0.52
54:2w:34:G:H2'	54:2w:35:A:H8	1.75	0.52
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.42	0.52
43:1l:39:VAL:HG11	43:1l:41:ARG:NH1	2.23	0.52
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.44	0.52
1:2A:2103:C:H2'	1:2A:2104:G:C8	2.44	0.52
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.90	0.52
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.90	0.52
32:2a:1081:G:OP1	36:2e:18:ARG:HG2	2.09	0.52
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.09	0.52
33:2b:114:ARG:O	33:2b:118:LEU:N	2.27	0.52
37:2f:33:TYR:HE2	37:2f:78:GLU:HG2	1.75	0.52
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.90	0.52
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	1.92	0.52
32:2a:328:C:H4'	32:2a:329:A:H5'	1.91	0.52
32:2a:736:C:H2'	32:2a:737:A:C8	2.45	0.52
32:2a:1347:G:H22	32:2a:1373:G:H2'	1.74	0.52
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.45	0.52
41:2j:25:GLU:O	41:2j:29:ARG:HG2	2.10	0.52
1:1A:247:G:H4'	1:1A:386:G:C5	2.44	0.52
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.10	0.52
7:1H:23:ARG:NH2	7:1H:34:GLU:OE2	2.42	0.52
31:19:17:ILE:HD13	31:19:26:ILE:HD13	1.91	0.52
32:1a:458:C:H2'	32:1a:460:G:O4'	2.10	0.52
1:2A:271(G):C:O2'	23:21:81:LYS:NZ	2.33	0.52
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.44	0.52
32:2a:1060:C:H5'	45:2n:45:ARG:HH12	1.74	0.52
32:2a:1397:C:OP2	36:2e:24:ARG:NH2	2.34	0.52
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.45	0.52
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.92	0.52
54:2y:9:A:H4'	54:2y:46:G7M:H5'	1.91	0.52
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.43	0.52
32:1a:56:U:H2'	32:1a:57:G:C8	2.45	0.52
32:1a:96:U:H2'	32:1a:97:G:H8	1.75	0.52
32:1a:848:C:H2'	32:1a:849:C:C6	2.45	0.52
38:1g:46:ALA:HB1	38:1g:121:ALA:HB2	1.92	0.52
1:2A:184:C:H2'	1:2A:185:U:C6	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:11:C:OP2	2:2B:12:C:N4	2.32	0.52
2:2B:13:A:N1	2:2B:69:G:O2'	2.41	0.52
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.92	0.52
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.41	0.52
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.92	0.52
1:1A:1094:U:H1'	1:1A:1097:U:C4	2.45	0.52
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.25	0.52
32:1a:848:C:H2'	32:1a:849:C:H6	1.74	0.52
32:1a:1112:C:H1'	34:1c:179:ARG:HH11	1.75	0.52
33:1b:92:TYR:HH	33:1b:150:SER:HG	1.56	0.52
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	1.92	0.52
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.10	0.52
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.44	0.52
32:2a:1193:G:O2'	36:2e:25:ARG:NH2	2.42	0.52
34:2c:162:GLN:NE2	53:2v:24:A:O3'	2.42	0.52
1:1A:1183:G:O3'	25:13:29:ARG:NH2	2.43	0.52
2:1B:66:A:H61	2:1B:109:C:H5'	1.75	0.52
32:1a:433:C:H2'	32:1a:434:U:H6	1.74	0.52
37:1f:38:GLU:HB2	37:1f:64:GLN:HG3	1.92	0.52
54:1w:5:G:H1	54:1w:68:C:H42	1.57	0.52
1:2A:223:A:O2'	1:2A:420:C:O2	2.26	0.52
1:2A:271(M):G:H4'	1:2A:271(N):U:OP1	2.10	0.52
1:2A:2320:A:H1'	1:2A:2321:G:C2	2.45	0.52
8:2I:40:THR:OG1	8:2I:41:GLU:N	2.36	0.52
21:2Z:163:LEU:HG	21:2Z:165:VAL:HG22	1.92	0.52
1:1A:668:G:H5'	1:1A:669:G:OP2	2.10	0.52
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.22	0.52
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.92	0.52
28:16:35:GLU:OE1	28:16:50:ARG:NH2	2.43	0.52
34:1c:162:GLN:NE2	53:1v:24:A:O3'	2.35	0.52
49:1r:38:GLU:HA	49:1r:41:LYS:HE2	1.92	0.52
1:2A:715:G:O4'	46:2o:60:VAL:HG11	2.09	0.52
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.09	0.52
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.74	0.52
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.45	0.52
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.91	0.52
17:2V:40:LEU:HD11	17:2V:101:GLY:HA3	1.91	0.52
32:2a:1085:U:H3'	32:2a:1086:U:C6	2.45	0.52
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.43	0.52
34:2c:108:ASN:HB3	34:2c:111:LEU:HB2	1.92	0.52
34:2c:155:GLY:O	34:2c:157:ILE:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:6:ILE:HB	41:2j:72:VAL:HB	1.92	0.52
1:1A:1986:A:OP1	61:1A:4129:HOH:O	2.18	0.51
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.10	0.51
11:1P:59:LEU:HD11	30:18:10:ALA:HA	1.92	0.51
54:1y:51:U:H2'	54:1y:52:G:H8	1.75	0.51
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.24	0.51
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.92	0.51
32:2a:143:A:H5''	32:2a:144:G:H5'	1.92	0.51
32:2a:539:A:OP2	43:2l:115:LYS:NZ	2.32	0.51
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.45	0.51
1:2A:271(K):U:H4'	1:2A:271(L):U:OP1	2.10	0.51
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.50	0.51
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.10	0.51
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.24	0.51
8:1l:130:TYR:HB3	8:1l:138:ILE:HB	1.91	0.51
32:1a:250:A:H4'	32:1a:251:G:O5'	2.10	0.51
33:1b:112:VAL:HG12	33:1b:149:LEU:HD13	1.92	0.51
1:2A:191:A:H2'	1:2A:192:C:C6	2.44	0.51
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.91	0.51
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.41	0.51
3:2D:127:VAL:HA	3:2D:193:VAL:HG12	1.91	0.51
38:2g:57:GLU:HG3	38:2g:60:LYS:H	1.76	0.51
51:2t:63:ILE:HG21	51:2t:81:LYS:HG3	1.91	0.51
1:1A:135:G:N7	61:1A:4195:HOH:O	2.34	0.51
1:1A:272(J):C:H2'	1:1A:274:G:C8	2.38	0.51
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.93	0.51
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.11	0.51
1:1A:2124:G:H1	1:1A:2174:C:H42	1.58	0.51
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.10	0.51
32:1a:60:A:N1	32:1a:107:G:O2'	2.41	0.51
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.10	0.51
35:1d:112:VAL:H	35:1d:116:GLN:NE2	2.08	0.51
1:2A:639:U:H2'	1:2A:640:C:C6	2.46	0.51
1:2A:646:A:H2'	1:2A:647:G:O4'	2.10	0.51
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.10	0.51
32:2a:565:U:OP2	32:2a:566:G:O2'	2.22	0.51
32:2a:1029:C:C2	32:2a:1032:G:N2	2.76	0.51
38:2g:26:PHE:O	38:2g:30:ILE:HD12	2.10	0.51
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.09	0.51
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.91	0.51
54:2w:66:U:H5'	54:2w:67:C:OP2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.91	0.51
40:1i:7:THR:O	40:1i:83:ARG:NH1	2.40	0.51
54:1w:51:U:H2'	54:1w:52:G:C8	2.45	0.51
54:1y:51:U:H2'	54:1y:52:G:C8	2.45	0.51
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.26	0.51
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.35	0.51
54:2w:9:A:O2'	54:2w:10:G:N7	2.42	0.51
55:2x:58:A:H4'	55:2x:59:A:OP1	2.10	0.51
1:1A:2820:A:P	13:1R:2:ARG:HH22	2.32	0.51
3:1D:152:GLY:O	3:1D:154:LYS:HD3	2.11	0.51
32:1a:60:A:H4'	32:1a:61:G:H5'	1.93	0.51
32:1a:515:G:N7	61:1a:1841:HOH:O	2.34	0.51
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.11	0.51
36:1e:78:HIS:HE1	36:1e:142:LEU:HA	1.75	0.51
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.45	0.51
14:2S:62:LYS:HA	14:2S:65:VAL:HG22	1.93	0.51
27:25:57:VAL:HG12	27:25:58:LEU:HD13	1.93	0.51
37:2f:99:ALA:HB1	49:2r:23:LYS:HZ3	1.76	0.51
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.45	0.51
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.10	0.51
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.46	0.51
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.46	0.51
1:1A:1321:A:N1	61:1A:4203:HOH:O	2.34	0.51
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.46	0.51
1:1A:2151:G:H2'	1:1A:2152:G:C8	2.46	0.51
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.38	0.51
19:1X:1:MET:HE1	24:12:26:ARG:HH21	1.75	0.51
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.76	0.51
32:1a:110:C:H2'	32:1a:111:G:O4'	2.11	0.51
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.09	0.51
1:2A:71:A:H5''	1:2A:73:A:C8	2.46	0.51
1:2A:893:C:H2'	1:2A:894:C:N3	2.26	0.51
1:2A:921:G:O6	61:2A:3836:HOH:O	2.19	0.51
1:2A:1434:A:H61	1:2A:1558:A:H62	1.59	0.51
7:2H:149:ARG:HD3	7:2H:164:TYR:CE2	2.46	0.51
12:2Q:85:LYS:HB2	22:20:7:LEU:HD12	1.92	0.51
32:2a:593:G:N2	61:2a:1914:HOH:O	2.29	0.51
32:2a:953:G:H5'	32:2a:965:A:N6	2.23	0.51
32:2a:1212:U:H5'	32:2a:1213:A:C8	2.45	0.51
32:2a:1249:C:O4'	40:2i:70:LYS:NZ	2.43	0.51
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.93	0.51
1:1A:1079:C:H2'	1:1A:1080:C:O4'	2.11	0.51
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.44	0.51
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.46	0.51
21:1Z:151:HIS:HA	21:1Z:171:ILE:HG23	1.92	0.51
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.93	0.51
26:14:63:TYR:N	26:14:64:GLY:HA2	2.25	0.51
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.40	0.51
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.44	0.51
1:2A:2853:C:H2'	1:2A:2854:G:C8	2.46	0.51
21:2Z:23:LYS:NZ	21:2Z:40:ASP:HB2	2.25	0.51
21:2Z:53:ILE:HG22	21:2Z:71:VAL:O	2.10	0.51
28:26:23:THR:OG1	28:26:24:GLU:N	2.41	0.51
32:2a:603:U:H2'	32:2a:604:G:H8	1.75	0.51
37:2f:70:ASP:OD1	37:2f:70:ASP:N	2.44	0.51
55:2x:40:C:H2'	55:2x:41:C:H6	1.76	0.51
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.39	0.51
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.10	0.51
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.76	0.51
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.45	0.51
2:1B:66:A:H61	2:1B:108:U:H2'	1.76	0.51
5:1F:161:GLU:O	5:1F:165:ARG:HG3	2.11	0.51
15:1T:15:VAL:HG13	15:1T:79:HIS:CE1	2.46	0.51
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.45	0.51
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.92	0.51
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.26	0.51
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.26	0.51
54:1y:48:C:C2	54:1y:59:U:H1'	2.45	0.51
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.56	0.51
1:2A:361:G:O2'	1:2A:362:U:H5'	2.10	0.51
1:2A:775:G:O3'	61:2A:3837:HOH:O	2.20	0.51
6:2G:39:ILE:HD11	6:2G:102:PHE:CZ	2.46	0.51
9:2N:123:TYR:CZ	9:2N:129:PRO:HD2	2.45	0.51
32:2a:1053:G:H4'	32:2a:1054:C:H3'	1.93	0.51
32:2a:1388:C:H2'	32:2a:1389:C:C6	2.46	0.51
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.92	0.51
1:1A:568:U:H5'	1:1A:945:A:N6	2.26	0.51
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.10	0.51
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.45	0.51
1:1A:2375:G:O2'	1:1A:2377:A:N7	2.43	0.51
1:1A:2390:U:O4	61:1A:4127:HOH:O	2.18	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.26	0.51
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.76	0.51
32:1a:7:G:H5'	32:1a:298:A:O4'	2.10	0.51
1:2A:882:G:H22	1:2A:894:C:H42	1.59	0.51
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.46	0.51
1:2A:1973:G:OP1	61:2A:3834:HOH:O	2.19	0.51
1:2A:2171:A:H1'	1:2A:2172:U:C6	2.45	0.51
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.92	0.51
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.11	0.51
7:2H:54:ARG:HG2	7:2H:65:HIS:ND1	2.25	0.51
32:2a:1060:C:C5	34:2c:2:GLY:HA3	2.45	0.51
32:2a:1178:G:O2'	32:2a:1180:A:N7	2.44	0.51
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.76	0.51
34:2c:185:GLY:O	34:2c:200:ALA:N	2.41	0.51
47:2p:15:PRO:O	47:2p:16:HIS:ND1	2.44	0.51
1:1A:518:G:H2'	1:1A:519:U:C6	2.47	0.50
1:1A:1062:G:H2'	1:1A:1063:G:C8	2.45	0.50
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.11	0.50
1:1A:1991:U:H2'	1:1A:1992:G:H5''	1.93	0.50
54:1y:8:4SU:O2'	54:1y:21:A:N1	2.38	0.50
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.25	0.50
1:2A:956:G:OP2	12:2Q:14:ARG:NH1	2.40	0.50
1:2A:1805:U:O2	3:2D:50:THR:HB	2.10	0.50
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.75	0.50
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.92	0.50
2:2B:83:G:H1	2:2B:94:C:H42	1.59	0.50
9:2N:32:THR:HG22	9:2N:37:LYS:HB2	1.93	0.50
32:2a:20:U:H2'	32:2a:21:G:O4'	2.10	0.50
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.77	0.50
32:2a:1133:G:H1	32:2a:1141:C:N4	2.10	0.50
1:1A:829:A:N7	1:1A:2248:C:H5'	2.26	0.50
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.11	0.50
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.26	0.50
26:14:61:ARG:NE	26:14:61:ARG:O	2.44	0.50
32:1a:382:A:H2'	32:1a:383:A:H8	1.75	0.50
32:1a:833:U:H2'	32:1a:834:C:C6	2.46	0.50
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.92	0.50
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.93	0.50
15:2T:92:GLY:O	15:2T:120:ARG:NH2	2.44	0.50
48:2q:58:GLU:OE2	48:2q:75:ARG:NH2	2.44	0.50
1:1A:671:C:N4	61:1A:4293:HOH:O	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.45	0.50
1:1A:862:G:H2'	1:1A:863:A:O4'	2.11	0.50
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.41	0.50
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.24	0.50
32:1a:507:C:OP2	32:1a:508:C:O2'	2.22	0.50
34:1c:39:ILE:HG23	34:1c:91:LEU:HD11	1.93	0.50
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.59	0.50
51:1t:64:ASP:OD1	51:1t:81:LYS:NZ	2.38	0.50
1:2A:30:G:H2'	1:2A:31:C:C6	2.47	0.50
1:2A:1345:C:OP2	61:2A:3826:HOH:O	2.19	0.50
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.11	0.50
5:2F:148:LEU:HD13	5:2F:154:VAL:HG21	1.92	0.50
20:2Y:43:ASN:ND2	20:2Y:65:ALA:O	2.45	0.50
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.94	0.50
32:2a:107:G:H2'	32:2a:108:G:O4'	2.12	0.50
32:2a:430:A:OP2	35:2d:22:LYS:NZ	2.45	0.50
32:2a:921:U:O2	36:2e:19:MET:HB2	2.11	0.50
36:2e:37:ARG:HB3	36:2e:114:GLY:HA2	1.92	0.50
37:2f:97:PHE:HE2	49:2r:62:GLU:HG2	1.74	0.50
39:2h:28:ALA:HB3	39:2h:57:PRO:HB2	1.93	0.50
1:1A:601:C:O2'	1:1A:605:C:H5''	2.11	0.50
41:1j:62:HIS:HB3	45:1n:59:ALA:HB3	1.93	0.50
43:1l:53:ARG:HB2	43:1l:93:LEU:HD11	1.94	0.50
49:1r:56:THR:HG22	49:1r:58:LEU:HG	1.93	0.50
4:2E:119:ARG:HG2	4:2E:120:TRP:CD1	2.46	0.50
5:2F:117:ARG:HH12	11:2P:1:MET:N	2.10	0.50
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.92	0.50
32:2a:9:G:H2'	32:2a:10:A:C8	2.47	0.50
44:2m:73:GLU:O	44:2m:77:ASN:HB2	2.12	0.50
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.46	0.50
1:1A:1364:G:P	23:11:3:LYS:HG3	2.51	0.50
32:1a:67:C:H4'	32:1a:172:A:O4'	2.11	0.50
32:1a:189:G:H1	32:1a:189(K):U:H3	1.60	0.50
32:1a:1176:A:H2'	32:1a:1177:G:C8	2.47	0.50
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.94	0.50
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.30	0.50
1:2A:882:G:H22	1:2A:894:C:N4	2.09	0.50
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.27	0.50
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.94	0.50
5:2F:12:LEU:HD12	5:2F:124:LEU:HD21	1.94	0.50
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.39	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.47	0.50
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.12	0.50
38:2g:86:GLN:HE21	38:2g:86:GLN:HA	1.77	0.50
44:2m:3:ARG:HH22	44:2m:11:ARG:HG3	1.76	0.50
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.93	0.50
46:2o:56:LEU:O	46:2o:60:VAL:HG22	2.11	0.50
1:1A:1268:A:C2	1:1A:2013:A:C4	3.00	0.50
1:1A:2128:C:N4	1:1A:2160:G:N1	2.59	0.50
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.77	0.50
1:1A:2727:G:O2'	10:1O:70:LYS:NZ	2.41	0.50
4:1E:9:VAL:HG13	15:1T:3:ARG:HG2	1.93	0.50
32:1a:973:G:H3'	32:1a:974:A:H5''	1.94	0.50
54:1y:7:A:O2'	54:1y:49:C:OP2	2.24	0.50
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.11	0.50
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.47	0.50
8:2I:4:ILE:HD11	8:2I:44:LEU:HD13	1.93	0.50
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.94	0.50
32:2a:45:U:H2'	32:2a:46:G:C8	2.46	0.50
32:2a:524:G:H2'	32:2a:525:C:C6	2.47	0.50
34:2c:151:VAL:HG22	34:2c:200:ALA:HA	1.93	0.50
40:2i:100:GLY:O	40:2i:103:THR:HG22	2.12	0.50
1:1A:732:C:OP1	61:1A:4131:HOH:O	2.18	0.50
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE2	1.75	0.50
32:1a:453:A:C5	32:1a:454:C:C4	3.00	0.50
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.47	0.50
1:2A:2042:A:OP1	61:2A:3831:HOH:O	2.18	0.50
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.27	0.50
8:2I:75:LEU:HD13	8:2I:105:HIS:CD2	2.47	0.50
32:2a:1272:G:N2	32:2a:1273:G:C8	2.80	0.50
34:2c:129:ALA:HB3	34:2c:132:ARG:HE	1.77	0.50
1:1A:1183:G:H4'	25:13:29:ARG:HH22	1.76	0.50
32:1a:92:C:H2'	32:1a:93:G:C8	2.45	0.50
32:1a:165:C:H2'	32:1a:166:G:C8	2.46	0.50
32:1a:598:U:H2'	32:1a:599:C:C6	2.46	0.50
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.77	0.50
54:1y:67:C:H2'	54:1y:68:C:C6	2.46	0.50
1:2A:236:C:H2'	1:2A:237:C:C6	2.47	0.50
1:2A:581:C:H2'	1:2A:582:G:C8	2.47	0.50
1:2A:854:G:H2'	1:2A:855:G:C8	2.46	0.50
1:2A:900:A:O2'	1:2A:901:A:OP1	2.27	0.50
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.27	0.50
36:2e:110:LEU:HD13	36:2e:118:ILE:HD13	1.93	0.50
38:2g:90:GLU:OE1	38:2g:90:GLU:N	2.43	0.50
1:1A:2853:C:H2'	1:1A:2854:G:C8	2.46	0.50
8:1I:93:THR:OG1	8:1I:96:ASP:OD1	2.29	0.50
11:1P:90:ARG:HG2	11:1P:90:ARG:HH11	1.77	0.50
21:1Z:138:GLU:H	21:1Z:156:LYS:HE3	1.76	0.50
32:1a:78:G:N1	32:1a:91:C:C4	2.80	0.50
32:1a:1456:G:N2	51:1t:51:GLU:OE2	2.44	0.50
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.94	0.50
36:1e:51:VAL:O	36:1e:55:VAL:HG23	2.12	0.50
40:1i:11:LYS:C	40:1i:13:ALA:H	2.20	0.50
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.27	0.50
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.93	0.50
32:2a:419:C:OP1	32:2a:513:C:O2'	2.27	0.50
32:2a:983:A:N1	32:2a:1222:G:N2	2.60	0.50
32:2a:1065:U:H5''	32:2a:1190:G:N2	2.27	0.50
32:2a:1202:G:N2	45:2n:46:GLU:OE2	2.44	0.50
32:2a:1268:A:H2'	32:2a:1269:A:C8	2.47	0.50
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.47	0.50
42:2k:43:SER:HA	42:2k:47:VAL:HG21	1.93	0.50
51:2t:86:ARG:O	51:2t:90:GLN:HB2	2.11	0.50
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.12	0.49
1:1A:2136:C:C4	1:1A:2155:G:C2	3.00	0.49
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.12	0.49
6:1G:19:LEU:HD13	6:1G:32:PRO:HD2	1.93	0.49
32:1a:431:A:H2'	32:1a:432:A:O4'	2.12	0.49
48:1q:57:VAL:HG12	48:1q:76:LEU:HA	1.94	0.49
1:2A:784:A:H5'	1:2A:785:G:OP1	2.12	0.49
1:2A:825:C:O2	11:2P:55:ARG:NH1	2.44	0.49
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.46	0.49
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.93	0.49
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.12	0.49
1:2A:2128:C:H2'	1:2A:2129:C:O4'	2.12	0.49
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.27	0.49
1:2A:2667:C:N3	7:2H:110:SER:OG	2.40	0.49
32:2a:157:G:N2	32:2a:164:U:O2	2.39	0.49
32:2a:404:U:H2'	32:2a:405:U:C6	2.46	0.49
32:2a:1313:U:OP2	50:2s:5:LEU:HD13	2.12	0.49
33:2b:48:MET:HA	33:2b:51:LEU:HB2	1.94	0.49
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:88:C:H2'	2:1B:89:G:O4'	2.12	0.49
9:1N:73:THR:HB	9:1N:82:LEU:HD11	1.93	0.49
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.20	0.49
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.27	0.49
35:1d:53:ASP:N	35:1d:53:ASP:OD1	2.41	0.49
1:2A:242:G:C8	30:28:5:LYS:HG2	2.47	0.49
1:2A:602:G:N1	1:2A:655:A:OP2	2.40	0.49
1:2A:839:U:H2'	1:2A:840:C:H6	1.77	0.49
1:2A:1721:G:H8	1:2A:1741:A:H62	1.58	0.49
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.94	0.49
3:2D:12:SER:HB3	3:2D:208:LYS:HB3	1.94	0.49
11:2P:84:ASN:HB3	11:2P:86:LYS:HG2	1.94	0.49
30:28:34:TRP:CG	30:28:35:GLN:N	2.80	0.49
32:2a:1095:U:H2'	32:2a:1096:C:C6	2.47	0.49
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.94	0.49
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.93	0.49
32:1a:620:C:H2'	32:1a:621:A:O4'	2.13	0.49
32:1a:625:G:H2'	32:1a:626:U:C6	2.47	0.49
32:1a:1503:A:C2	53:1v:12:A:H2	2.29	0.49
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.76	0.49
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.47	0.49
1:2A:1668:A:O2'	1:2A:1674:G:N7	2.39	0.49
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.28	0.49
5:2F:116:ASP:O	5:2F:120:GLU:HG2	2.12	0.49
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.93	0.49
32:2a:436:C:H2'	32:2a:437:U:H6	1.78	0.49
32:2a:1130:A:H5''	40:2i:18:PHE:HE2	1.77	0.49
34:2c:47:LEU:HB2	34:2c:52:LEU:HD22	1.94	0.49
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	1.94	0.49
40:2i:47:LEU:O	40:2i:50:LEU:HG	2.12	0.49
45:2n:59:ALA:HB1	45:2n:61:TRP:HZ3	1.78	0.49
1:1A:593:G:H4'	30:18:4:MET:HE2	1.94	0.49
61:1A:4597:HOH:O	11:1P:44:GLY:HA3	2.13	0.49
32:1a:382:A:H2'	32:1a:383:A:C8	2.48	0.49
36:1e:85:GLY:C	36:1e:87:SER:H	2.21	0.49
49:1r:47:THR:O	49:1r:83:GLU:N	2.36	0.49
1:2A:287:C:H2'	1:2A:288:C:H6	1.77	0.49
1:2A:774:A:H2'	1:2A:774:A:N3	2.27	0.49
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.12	0.49
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.48	0.49
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:109:A:C6	32:2a:326:G:C6	3.01	0.49
32:2a:171:A:H2'	32:2a:172:A:C8	2.47	0.49
32:2a:187:C:O2'	51:2t:89:ARG:NH2	2.42	0.49
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.27	0.49
36:2e:7:GLU:OE1	36:2e:37:ARG:NH2	2.33	0.49
44:2m:40:ASN:ND2	44:2m:43:THR:HG23	2.22	0.49
1:1A:278:A:H2'	1:1A:279:C:C6	2.48	0.49
1:1A:536:A:H2'	1:1A:537:C:C6	2.48	0.49
1:1A:747:U:O2	1:1A:2014:A:H1'	2.12	0.49
5:1F:152:GLU:OE1	5:1F:191:ARG:HD2	2.13	0.49
6:1G:149:VAL:HG22	6:1G:150:ASP:H	1.78	0.49
8:1I:130:TYR:O	8:1I:138:ILE:N	2.45	0.49
32:1a:1007:C:N3	32:1a:1022:G:O6	2.45	0.49
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.13	0.49
43:1l:117:ARG:HB3	43:1l:122:THR:HB	1.93	0.49
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.41	0.49
1:2A:2002:G:OP2	13:2R:9:LYS:NZ	2.44	0.49
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.31	0.49
7:2H:27:LYS:HA	7:2H:32:GLU:HB3	1.94	0.49
24:22:1:MET:N	24:22:52:ASP:OD1	2.45	0.49
32:2a:9:G:H2'	32:2a:10:A:H8	1.76	0.49
32:2a:564:C:O2'	39:2h:91:ARG:NH1	2.27	0.49
32:2a:815:A:N7	32:2a:1509:C:O2'	2.39	0.49
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.94	0.49
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.28	0.49
39:2h:73:ASP:OD1	39:2h:75:ARG:NE	2.35	0.49
54:2y:14:A:H3'	54:2y:15:G:C8	2.48	0.49
1:1A:228:A:H8	1:1A:229:A:H5'	1.76	0.49
18:1W:2:GLU:OE2	18:1W:72:LYS:NZ	2.26	0.49
35:1d:196:LEU:O	35:1d:198:VAL:N	2.39	0.49
36:1e:152:ARG:NH2	39:1h:107:LEU:O	2.45	0.49
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.13	0.49
54:1y:38:A:H2'	54:1y:39:PSU:O4'	2.13	0.49
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.13	0.49
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.13	0.49
4:2E:7:VAL:HG23	4:2E:51:PHE:HE2	1.77	0.49
6:2G:70:VAL:HA	6:2G:90:LEU:HD23	1.95	0.49
25:23:5:LYS:NZ	25:23:57:GLU:OE2	2.39	0.49
29:27:46:VAL:HG13	29:27:48:LYS:NZ	2.28	0.49
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.13	0.49
32:1a:333:G:H4'	51:1t:16:HIS:CE1	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:715:A:H2'	32:1a:716:A:C8	2.47	0.49
32:1a:998:G:H1	32:1a:1043:C:H42	1.59	0.49
33:1b:93:VAL:HG11	33:1b:97:TRP:CD1	2.47	0.49
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.30	0.49
54:1w:46:G7M:H3'	54:1w:47:U:H5''	1.93	0.49
1:2A:597:U:H2'	1:2A:598:G:C8	2.48	0.49
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.28	0.49
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.43	0.49
32:2a:67:C:H2'	32:2a:68:G:C8	2.47	0.49
34:2c:8:ILE:HG23	34:2c:16:ARG:HG2	1.94	0.49
44:2m:90:LEU:HD23	44:2m:93:ARG:HE	1.76	0.49
1:1A:898:C:N4	1:1A:899:A:N7	2.60	0.49
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.47	0.49
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.48	0.49
34:1c:18:TRP:H	34:1c:18:TRP:HE3	1.61	0.49
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.48	0.49
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.93	0.49
1:2A:208:C:H2'	1:2A:209:C:C6	2.47	0.49
1:2A:884:C:H3'	1:2A:885:C:C6	2.47	0.49
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.47	0.49
1:2A:2305:A:H1'	6:2G:136:ARG:HG2	1.94	0.49
3:2D:147:LEU:HD13	3:2D:155:LEU:HD11	1.95	0.49
7:2H:44:VAL:HG22	7:2H:51:ARG:O	2.13	0.49
19:2X:26:TYR:HB3	19:2X:92:LEU:HD23	1.95	0.49
32:2a:1041:A:H2'	32:2a:1042:G:C8	2.48	0.49
32:2a:1042:G:H2'	32:2a:1043:C:O4'	2.13	0.49
32:2a:1206:G:O2'	34:2c:193:TYR:HA	2.13	0.49
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.47	0.49
32:2a:1275:A:H2'	32:2a:1276:G:O4'	2.13	0.49
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.81	0.49
34:2c:88:ARG:HA	34:2c:91:LEU:HD13	1.95	0.49
34:2c:113:ALA:HB2	34:2c:202:ILE:HG13	1.95	0.49
51:2t:64:ASP:OD2	51:2t:81:LYS:NZ	2.41	0.49
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.37	0.49
1:1A:2125:G:N1	1:1A:2172:U:OP1	2.29	0.49
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.13	0.49
7:1H:55:PRO:HG2	7:1H:61:HIS:CE1	2.48	0.49
32:1a:1033:G:H3'	32:1a:1034:G:H8	1.77	0.49
38:1g:78:ARG:HD3	38:1g:156:TRP:CZ3	2.48	0.49
54:1y:4:C:H2'	54:1y:5:G:O4'	2.13	0.49
54:1y:36:A:H2'	54:1y:37:MIA:O4'	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:994:C:OP2	16:2U:54:LYS:NZ	2.45	0.49
1:2A:1359:A:H2	1:2A:1372:U:O4	1.96	0.49
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.94	0.49
18:2W:64:MET:HE2	18:2W:109:GLU:HG3	1.94	0.49
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.45	0.49
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH22	1.78	0.49
21:2Z:130:PRO:HA	21:2Z:133:ILE:HG13	1.95	0.49
27:25:45:VAL:HG11	27:25:58:LEU:HD22	1.95	0.49
32:2a:448:A:P	32:2a:485:G:H22	2.36	0.49
32:2a:748:C:H4'	32:2a:749:C:O5'	2.13	0.49
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.96	0.49
8:1I:109:ILE:HG23	8:1I:130:TYR:CZ	2.48	0.49
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.94	0.49
32:1a:433:C:H2'	32:1a:434:U:C6	2.48	0.49
36:1e:92:LYS:HB3	36:1e:119:LEU:HB2	1.95	0.49
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	1.95	0.49
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.95	0.49
1:2A:2135:A:OP1	1:2A:2160:G:H1'	2.13	0.49
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.48	0.49
2:2B:24:G:H4'	2:2B:25:A:C8	2.48	0.49
6:2G:123:ASN:O	6:2G:125:PHE:N	2.46	0.49
15:2T:41:ARG:NH2	32:2a:346:G:OP1	2.37	0.49
25:23:7:LYS:HB3	25:23:55:ARG:HB3	1.95	0.49
32:2a:7:G:O2'	36:2e:120:THR:O	2.31	0.49
32:2a:562:C:H1'	43:2I:15:ARG:HB3	1.95	0.49
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.47	0.49
1:1A:278:A:O2'	1:1A:279:C:OP1	2.27	0.48
1:1A:2503:2MA:H8	57:1A:4060:A1A1L:O36	2.13	0.48
17:1V:55:ALA:CA	17:1V:101:GLY:HA2	2.42	0.48
32:1a:1318:A:H5''	50:1s:3:ARG:NH1	2.28	0.48
33:1b:178:ARG:HH22	39:1h:74:PRO:HB3	1.77	0.48
37:1f:97:PHE:HB3	49:1r:32:ARG:HG3	1.95	0.48
51:1t:92:LEU:O	51:1t:96:GLY:HA2	2.13	0.48
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.46	0.48
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.13	0.48
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.13	0.48
1:2A:2343:C:O2'	1:2A:2373:G:O2'	2.25	0.48
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.45	0.48
7:2H:124:GLU:OE2	7:2H:132:ARG:HD2	2.13	0.48
11:2P:121:LYS:O	11:2P:123:LEU:N	2.45	0.48
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:4:TYR:CZ	40:2i:88:TYR:HD1	2.31	0.48
54:2y:18:G:N2	54:2y:55:PSU:C4	2.80	0.48
54:2y:48:C:C5	54:2y:59:U:H5''	2.48	0.48
1:1A:721:C:H2'	1:1A:722:A:C8	2.47	0.48
32:1a:160:A:H1'	32:1a:344:A:C5	2.49	0.48
32:1a:202:U:H3'	32:1a:203:U:C6	2.47	0.48
32:1a:568:G:O2'	32:1a:574:A:N1	2.40	0.48
32:1a:618:C:H5''	32:1a:619:U:H5''	1.93	0.48
35:1d:53:ASP:O	35:1d:57:ARG:HG3	2.12	0.48
44:1m:12:ASN:O	44:1m:44:ARG:NH1	2.46	0.48
51:1t:59:ALA:O	51:1t:63:ILE:HG13	2.13	0.48
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.78	0.48
6:2G:68:PRO:HB3	6:2G:92:VAL:HB	1.95	0.48
7:2H:7:LEU:HD23	7:2H:69:ARG:NH2	2.27	0.48
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.49	0.48
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.27	0.48
32:2a:174:C:H2'	32:2a:175:C:H6	1.78	0.48
32:2a:662:G:H2'	32:2a:663:A:H8	1.75	0.48
32:2a:909:A:H2'	32:2a:910:C:O4'	2.13	0.48
34:2c:131:ARG:HH21	34:2c:135:LYS:HE3	1.78	0.48
1:1A:579:G:H2'	1:1A:580:C:C6	2.48	0.48
1:1A:1580:A:OP2	1:1A:1580:A:H8	1.97	0.48
1:1A:2175:C:H2'	1:1A:2176:A:O4'	2.12	0.48
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.47	0.48
14:1S:46:VAL:HG12	14:1S:48:LEU:HD12	1.94	0.48
23:11:50:ARG:HG2	23:11:59:THR:CG2	2.44	0.48
28:16:9:LEU:HD13	28:16:51:GLU:HG3	1.94	0.48
32:1a:653:A:OP1	39:1h:56:LYS:NZ	2.47	0.48
32:1a:977:A:O2'	32:1a:979:C:OP2	2.30	0.48
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.48	0.48
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.49	0.48
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.48	0.48
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.94	0.48
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.95	0.48
32:2a:232:G:H1'	32:2a:262:A:N1	2.29	0.48
32:2a:1103:C:P	33:2b:96:ARG:HH22	2.36	0.48
55:2x:53:G:H3'	55:2x:54:5MU:H73	1.95	0.48
1:1A:121:G:H4'	1:1A:149:A:H5'	1.95	0.48
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.14	0.48
1:1A:2706:G:N7	61:1A:4215:HOH:O	2.35	0.48
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.95	0.48
7:1H:68:THR:O	7:1H:72:ILE:HG12	2.13	0.48
32:1a:58:C:O2'	32:1a:388:G:N7	2.36	0.48
32:1a:691:G:H2'	32:1a:692:U:C6	2.47	0.48
32:1a:935:A:O2'	32:1a:1383:C:N3	2.44	0.48
39:1h:121:ASP:OD2	39:1h:125:ARG:NH2	2.46	0.48
44:1m:65:LYS:NZ	44:1m:73:GLU:OE1	2.46	0.48
54:1y:56:C:H2'	54:1y:57:G:O4'	2.14	0.48
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.13	0.48
1:2A:955:C:OP2	12:2Q:14:ARG:HG3	2.14	0.48
1:2A:981:A:N1	1:2A:2027:G:O2'	2.46	0.48
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.47	0.48
1:2A:2184:G:H2'	1:2A:2185:C:C6	2.48	0.48
2:2B:2:C:H2'	2:2B:3:C:C6	2.49	0.48
3:2D:36:PRO:HA	3:2D:61:LEU:HD12	1.94	0.48
11:2P:62:LEU:HD11	30:28:50:LEU:HD11	1.95	0.48
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.94	0.48
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.49	0.48
32:2a:1318:A:OP1	50:2s:3:ARG:NH2	2.33	0.48
1:1A:857:C:N4	1:1A:858:U:O4	2.47	0.48
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.13	0.48
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.96	0.48
55:1x:39:C:O2'	54:1y:35:A:O2'	2.31	0.48
1:2A:1754:C:H5	15:2T:96:ARG:NH2	2.11	0.48
4:2E:119:ARG:HG2	4:2E:120:TRP:NE1	2.27	0.48
6:2G:123:ASN:C	6:2G:125:PHE:H	2.22	0.48
8:2I:29:TYR:HD2	8:2I:30:LEU:HD23	1.78	0.48
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.45	0.48
11:2P:19:VAL:HG12	11:2P:27:HIS:HB3	1.95	0.48
15:2T:127:ALA:C	15:2T:129:ARG:H	2.21	0.48
32:2a:997:U:H3	32:2a:1044:A:N6	2.08	0.48
32:2a:1074:G:O2'	33:2b:103:THR:OG1	2.32	0.48
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.37	0.48
32:2a:1309:G:O3'	44:2m:77:ASN:ND2	2.47	0.48
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.13	0.48
1:1A:2126:A:H4'	1:1A:2127:G:OP1	2.12	0.48
1:1A:2136:C:C2	1:1A:2155:G:C2	3.01	0.48
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.13	0.48
32:1a:262:A:H2'	32:1a:263:A:C8	2.49	0.48
50:1s:27:GLU:HG3	50:1s:28:LYS:HE3	1.94	0.48
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.49	0.48
12:2Q:24:GLY:HA2	12:2Q:67:ARG:NH2	2.29	0.48
16:2U:65:ILE:HD11	16:2U:95:LEU:HB3	1.95	0.48
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.30	0.48
32:2a:1228:C:H2'	32:2a:1229:A:H8	1.79	0.48
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.95	0.48
40:2i:37:PHE:HB3	40:2i:43:ALA:HB2	1.96	0.48
44:2m:18:ALA:HB3	44:2m:45:VAL:HG21	1.96	0.48
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.39	0.48
1:1A:894:C:H2'	1:1A:895:U:O4'	2.14	0.48
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.29	0.48
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.94	0.48
32:1a:867:G:O2'	32:1a:873:A:N1	2.45	0.48
33:1b:55:PHE:HA	33:1b:58:ILE:HB	1.95	0.48
1:2A:272(B):G:H2'	1:2A:272(C):G:C8	2.49	0.48
1:2A:775:G:N3	61:2A:3918:HOH:O	2.35	0.48
1:2A:1913:A:H4'	1:2A:1914:C:H5''	1.96	0.48
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.79	0.48
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	1.95	0.48
8:2I:47:LEU:O	8:2I:51:ILE:HG12	2.13	0.48
8:2I:62:LYS:HG3	8:2I:133:HIS:CE1	2.49	0.48
32:2a:457:C:H2'	32:2a:458:C:C6	2.49	0.48
32:2a:1152:A:OP1	41:2j:70:ARG:NH2	2.44	0.48
32:2a:1245:A:H61	32:2a:1292:U:H3	1.62	0.48
34:2c:131:ARG:NH2	34:2c:135:LYS:HE3	2.29	0.48
41:2j:16:LEU:HD23	41:2j:94:VAL:HG22	1.96	0.48
44:2m:101:GLN:OE1	44:2m:101:GLN:N	2.47	0.48
1:1A:899:A:H2'	1:1A:899:A:N3	2.27	0.48
1:1A:1062:G:C8	1:1A:1070:A:H4'	2.48	0.48
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.48	0.48
1:1A:2206:G:H3'	1:1A:2207:G:N7	2.29	0.48
26:14:61:ARG:NH1	50:1s:42:PRO:HD3	2.29	0.48
32:1a:946:A:H2'	32:1a:947:G:C8	2.49	0.48
32:1a:1191:A:H5''	34:1c:4:LYS:NZ	2.29	0.48
36:1e:94:ALA:HB1	36:1e:98:THR:HG21	1.95	0.48
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.96	0.48
54:1y:67:C:H2'	54:1y:68:C:H6	1.77	0.48
1:2A:1287:A:H8	13:2R:104:ARG:HD3	1.78	0.48
2:2B:42:C:O2'	6:2G:67:LYS:O	2.24	0.48
6:2G:43:LEU:C	6:2G:45:GLU:H	2.21	0.48
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:964:A:N3	32:2a:969:A:O2'	2.47	0.48
32:2a:1263:C:C4	32:2a:1272:G:O6	2.67	0.48
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.78	0.48
36:2e:72:GLN:O	36:2e:75:THR:HG22	2.14	0.48
37:2f:13:ASN:ND2	37:2f:55:ASP:OD2	2.47	0.48
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.96	0.48
43:2l:37:CYS:SG	43:2l:81:SER:HB2	2.54	0.48
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.78	0.48
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.47	0.48
33:1b:178:ARG:NH1	33:1b:196:LEU:O	2.47	0.48
37:1f:35:ALA:HA	37:1f:67:MET:HB3	1.96	0.48
45:1n:6:LEU:HB3	45:1n:23:ARG:NH2	2.28	0.48
54:1y:35:A:H5'	54:1y:36:A:OP2	2.14	0.48
1:2A:2846:G:N7	61:2A:3919:HOH:O	2.35	0.48
6:2G:165:THR:OG1	6:2G:166:ASP:N	2.47	0.48
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.14	0.48
32:2a:1122:U:N3	32:2a:1123:A:N7	2.62	0.48
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.13	0.48
50:2s:72:GLY:HA2	50:2s:75:ALA:HB3	1.95	0.48
1:1A:484:C:H2'	1:1A:485:C:C6	2.49	0.48
1:1A:2469:A:O3'	12:1Q:56:ARG:NH1	2.47	0.48
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.49	0.48
43:1l:7:ILE:HD13	43:1l:10:LEU:HD12	1.96	0.48
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	1.95	0.48
55:1x:50:U:H2'	55:1x:51:C:C6	2.49	0.48
1:2A:2116:G:N1	1:2A:2162:G:OP1	2.46	0.48
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.32	0.48
21:2Z:171:ILE:H	21:2Z:171:ILE:HG13	1.53	0.48
32:2a:1026:G:O6	32:2a:1036:G:N2	2.46	0.48
32:2a:1106:G:H5''	34:2c:172:ARG:HB3	1.96	0.48
38:2g:31:MET:HG3	38:2g:36:LYS:HA	1.95	0.48
1:1A:1062:G:O5'	1:1A:1070:A:O2'	2.30	0.47
1:1A:1063:G:H2'	1:1A:1064:C:C5	2.48	0.47
1:1A:2067:G:N7	61:1A:4217:HOH:O	2.36	0.47
3:1D:19:ALA:HB2	3:1D:204:ILE:HD11	1.96	0.47
32:1a:444:C:H2'	32:1a:445:G:H8	1.77	0.47
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.49	0.47
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.46	0.47
44:1m:2:ALA:N	44:1m:8:GLU:HB2	2.29	0.47
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.96	0.47
54:1w:51:U:H2'	54:1w:52:G:H8	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:686:G:N2	1:2A:788:A:H61	2.12	0.47
13:2R:38:VAL:HG12	13:2R:42:LYS:HD2	1.96	0.47
21:2Z:77:ASP:N	21:2Z:82:ARG:O	2.47	0.47
32:2a:603:U:H2'	32:2a:604:G:C8	2.47	0.47
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.29	0.47
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.61	0.47
34:2c:29:TYR:HE1	41:2j:11:PHE:HE2	1.61	0.47
1:1A:72:U:H5'	24:12:61:LEU:HD12	1.96	0.47
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.50	0.47
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.78	0.47
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.48	0.47
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.14	0.47
27:15:40:LYS:HE3	27:15:41:PRO:O	2.13	0.47
32:1a:300:A:H2'	32:1a:301:G:O4'	2.14	0.47
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.49	0.47
1:2A:925:C:H2'	1:2A:926:A:H8	1.79	0.47
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.49	0.47
1:2A:2771:C:H5''	4:2E:202:LYS:HD3	1.96	0.47
21:2Z:53:ILE:CD1	21:2Z:99:TYR:HB2	2.44	0.47
32:2a:157:G:H1	32:2a:164:U:H3	1.60	0.47
32:2a:685:G:C2	32:2a:686:U:C4	3.02	0.47
32:2a:936:C:H2'	32:2a:937:A:O4'	2.13	0.47
32:2a:1316:G:N2	32:2a:1319:A:H5''	2.23	0.47
32:2a:1330:U:H4'	44:2m:23:TYR:CZ	2.49	0.47
33:2b:81:VAL:HB	33:2b:94:ASN:ND2	2.29	0.47
35:2d:3:ARG:HE	35:2d:118:ARG:HD3	1.79	0.47
41:2j:30:SER:O	41:2j:81:THR:OG1	2.24	0.47
44:2m:24:GLY:HA3	44:2m:66:LEU:HD23	1.95	0.47
54:2w:33:U:N3	54:2w:36:A:OP2	2.47	0.47
1:1A:657:U:H2'	1:1A:658:C:C6	2.49	0.47
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.14	0.47
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.14	0.47
1:1A:2853:C:H2'	1:1A:2854:G:H8	1.80	0.47
2:1B:14:U:O2	2:1B:108:U:H4'	2.15	0.47
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.97	0.47
20:1Y:34:LYS:NZ	61:1Y:301:HOH:O	2.23	0.47
21:1Z:157:LEU:HD22	21:1Z:161:VAL:HG23	1.97	0.47
23:11:2:SER:HB3	23:11:46:LEU:HD12	1.97	0.47
32:1a:328:C:H4'	32:1a:329:A:H5'	1.96	0.47
35:1d:57:ARG:HD3	35:1d:205:GLU:HB3	1.95	0.47
1:2A:709:U:H2'	1:2A:710:G:C8	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.47	0.47
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.15	0.47
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.95	0.47
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.29	0.47
6:2G:15:VAL:HG13	6:2G:175:LEU:HB2	1.96	0.47
7:2H:80:SER:HG	7:2H:81:GLU:CD	2.21	0.47
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	1.96	0.47
32:2a:840:C:H4'	32:2a:841:U:OP1	2.13	0.47
32:2a:952:U:H2'	32:2a:953:G:H8	1.78	0.47
54:2y:40:C:H2'	54:2y:41:C:C6	2.48	0.47
1:1A:800:A:H8	1:1A:800:A:OP1	1.97	0.47
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.30	0.47
1:1A:2149:G:C6	1:1A:2150:U:C2	3.02	0.47
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	1.96	0.47
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.79	0.47
32:1a:142:G:H2'	32:1a:143:A:H8	1.79	0.47
32:1a:629:G:H2'	32:1a:630:G:C8	2.49	0.47
32:1a:721:G:H4'	32:1a:722:A:O4'	2.15	0.47
32:1a:1068:G:N7	32:1a:1094:G:H2'	2.29	0.47
35:1d:59:ARG:NH1	35:1d:59:ARG:HA	2.29	0.47
42:1k:48:ILE:HG21	42:1k:63:LEU:HB3	1.97	0.47
54:1y:9:A:O3'	54:1y:45:U:O2'	2.29	0.47
1:2A:893:C:H2'	1:2A:894:C:C4	2.50	0.47
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.11	0.47
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.14	0.47
29:27:8:ASN:HB3	29:27:11:LYS:HB3	1.96	0.47
32:2a:8:A:N6	35:2d:209:ARG:HB2	2.29	0.47
39:2h:39:LEU:HG	39:2h:44:PHE:HB2	1.96	0.47
39:2h:122:ARG:HG3	39:2h:125:ARG:HH21	1.79	0.47
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.23	0.47
1:1A:839:U:H2'	1:1A:840:C:C6	2.49	0.47
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.96	0.47
1:1A:2136:C:C4	1:1A:2155:G:N1	2.83	0.47
1:1A:2355:C:H1'	22:10:39:ARG:HH21	1.79	0.47
1:1A:2615:U:H2'	1:1A:2616:C:C6	2.50	0.47
32:1a:186:C:H2'	32:1a:187:C:C6	2.50	0.47
32:1a:1273:G:C2	32:1a:1274:G:H1'	2.49	0.47
33:1b:37:ASN:C	33:1b:39:ILE:H	2.22	0.47
39:1h:17:THR:O	39:1h:78:GLN:NE2	2.44	0.47
1:2A:320:A:H4'	1:2A:322:A:N7	2.30	0.47
1:2A:602:G:O2'	1:2A:655:A:N6	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1364:G:P	23:21:3:LYS:HG3	2.54	0.47
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.37	0.47
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.96	0.47
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.49	0.47
32:2a:932:C:H2'	32:2a:933:G:C8	2.50	0.47
32:2a:1026:G:H4'	32:2a:1027:C:OP2	2.14	0.47
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.44	0.47
34:2c:156:ARG:N	34:2c:196:LEU:HD22	2.29	0.47
46:2o:54:ARG:HG3	46:2o:58:MET:HE2	1.96	0.47
1:1A:721:C:H2'	1:1A:722:A:H8	1.80	0.47
1:1A:880:G:H2'	1:1A:881:G:C8	2.47	0.47
1:1A:2848:G:C8	15:1T:97:ALA:HB2	2.50	0.47
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.69	0.47
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.39	0.47
51:1t:63:ILE:HG22	51:1t:77:ALA:HB1	1.97	0.47
1:2A:212:G:H2'	1:2A:213:A:O4'	2.14	0.47
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.49	0.47
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.79	0.47
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.30	0.47
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.11	0.47
6:2G:7:LEU:HD11	6:2G:107:LEU:HD12	1.96	0.47
7:2H:89:ILE:HG22	7:2H:129:THR:HG22	1.97	0.47
15:2T:59:THR:HG23	15:2T:78:LEU:HB3	1.96	0.47
16:2U:81:HIS:HD2	16:2U:84:LYS:HD3	1.79	0.47
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.13	0.47
21:2Z:126:VAL:HB	21:2Z:161:VAL:HG23	1.96	0.47
32:2a:1148:U:H5'	40:2i:16:ARG:HD2	1.97	0.47
34:2c:39:ILE:O	34:2c:43:LEU:HG	2.14	0.47
34:2c:53:ALA:HB2	34:2c:115:LEU:CD1	2.44	0.47
34:2c:65:ALA:HA	34:2c:100:ALA:HB3	1.95	0.47
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.95	0.47
54:2y:18:G:N2	54:2y:55:PSU:HN3	2.09	0.47
1:1A:271(V):G:O6	61:1A:4133:HOH:O	2.20	0.47
1:1A:329:G:OP2	20:1Y:71:LYS:HD2	2.15	0.47
1:1A:340:A:H2'	1:1A:341:G:O4'	2.15	0.47
1:1A:888:C:H2'	1:1A:889:C:C5	2.49	0.47
1:1A:1359:A:C2	1:1A:1372:U:O4	2.67	0.47
1:1A:1500:G:H2'	1:1A:1501:C:C6	2.50	0.47
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.14	0.47
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.49	0.47
1:1A:2822:G:O2'	1:1A:2824:C:OP2	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.80	0.47
8:1I:77:LEU:HA	8:1I:77:LEU:HD23	1.74	0.47
32:1a:21:G:H2'	32:1a:22:G:C8	2.50	0.47
32:1a:184:G:H2'	32:1a:185:A:C8	2.49	0.47
32:1a:1006:C:H42	32:1a:1023:G:H1	1.62	0.47
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.50	0.47
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	1.97	0.47
36:1e:69:VAL:HG11	36:1e:113:ALA:HB1	1.97	0.47
39:1h:4:ASP:CG	39:1h:85:ARG:HH21	2.23	0.47
1:2A:910:A:N1	1:2A:2277:G:H1'	2.29	0.47
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.28	0.47
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.47	0.47
24:22:8:LYS:O	24:22:12:GLU:HG2	2.15	0.47
32:2a:509:A:O2'	32:2a:510:A:OP1	2.28	0.47
39:2h:39:LEU:HD11	39:2h:137:VAL:HG11	1.95	0.47
40:2i:9:ARG:HA	40:2i:13:ALA:O	2.15	0.47
1:1A:26:G:OP1	18:1W:80:PRO:HB3	2.15	0.47
1:1A:288:C:H2'	1:1A:289:A:H8	1.80	0.47
1:1A:900:A:H2'	1:1A:901:A:O4'	2.14	0.47
1:1A:1062:G:H8	1:1A:1070:A:H4'	1.79	0.47
1:1A:2115:G:H21	1:1A:2171:A:H61	1.63	0.47
7:1H:6:ARG:NH2	7:1H:54:ARG:HH22	2.12	0.47
11:1P:121:LYS:O	11:1P:123:LEU:N	2.48	0.47
12:1Q:78:PRO:HG2	12:1Q:81:VAL:HG11	1.97	0.47
26:14:57:GLU:HA	26:14:58:ARG:HA	1.62	0.47
32:1a:731:G:H5'	32:1a:766:A:H4'	1.96	0.47
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.79	0.47
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.96	0.47
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.29	0.47
1:2A:1665:A:H2'	1:2A:1666:G:O4'	2.15	0.47
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.15	0.47
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	1.96	0.47
11:2P:121:LYS:HE2	11:2P:123:LEU:HD11	1.95	0.47
21:2Z:52:SER:C	21:2Z:54:HIS:H	2.23	0.47
32:2a:406:G:H21	35:2d:119:GLN:NE2	2.02	0.47
32:2a:1085:U:H3'	32:2a:1086:U:C5	2.49	0.47
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.14	0.47
32:2a:1272:G:H5'	32:2a:1273:G:OP2	2.15	0.47
33:2b:8:LYS:HB3	33:2b:217:ARG:HG3	1.97	0.47
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.97	0.47
33:2b:135:GLN:O	33:2b:139:LYS:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:99:SER:HB3	35:2d:139:ARG:HG3	1.96	0.47
36:2e:89:ILE:HD12	36:2e:89:ILE:HA	1.75	0.47
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.50	0.47
55:2x:40:C:H2'	55:2x:41:C:C6	2.50	0.47
6:1G:126:ASP:N	6:1G:130:ASN:O	2.48	0.47
8:1I:81:VAL:O	8:1I:146:ALA:HA	2.14	0.47
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.13	0.47
32:1a:815:A:N7	32:1a:1509:C:O2'	2.45	0.47
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.50	0.47
1:2A:752:A:H3'	29:27:1:MET:HE1	1.97	0.47
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.30	0.47
14:2S:19:LYS:C	14:2S:21:THR:H	2.23	0.47
32:2a:523:A:H61	43:2l:92:OTD:CG	2.27	0.47
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.28	0.47
36:2e:102:ALA:HB2	36:2e:120:THR:HG21	1.97	0.47
49:2r:82:THR:OG1	49:2r:83:GLU:N	2.48	0.47
51:2t:56:MET:HE3	51:2t:85:MET:HG2	1.97	0.47
55:2x:9:G:H21	55:2x:45:G:H3'	1.80	0.47
1:1A:907:U:HO2'	12:1Q:101:ARG:HH22	1.62	0.47
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.80	0.47
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.97	0.47
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.80	0.47
11:1P:138:LEU:C	11:1P:140:ALA:H	2.23	0.47
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.30	0.47
32:1a:933:G:OP2	38:1g:3:ARG:HB2	2.15	0.47
35:1d:59:ARG:HA	35:1d:59:ARG:HH11	1.80	0.47
35:1d:148:VAL:HG21	35:1d:158:ILE:HG21	1.97	0.47
36:1e:18:ARG:HH11	36:1e:27:ARG:HH12	1.62	0.47
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	1.96	0.47
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.50	0.47
1:2A:1032:A:H2	1:2A:1122:G:H22	1.62	0.47
1:2A:2135:A:C4	1:2A:2136:C:H5	2.33	0.47
2:2B:31:C:N4	14:2S:32:LEU:HD13	2.30	0.47
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	1.97	0.47
5:2F:165:ARG:HG2	5:2F:168:ARG:NH2	2.30	0.47
10:2O:71:ARG:NE	10:2O:105:GLU:OE2	2.48	0.47
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.50	0.47
34:2c:156:ARG:H	34:2c:196:LEU:HD22	1.79	0.47
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.30	0.47
41:2j:50:ILE:O	45:2n:41:ARG:NH1	2.48	0.47
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.97	0.46
32:1a:7:G:H2'	36:1e:119:LEU:HD22	1.95	0.46
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.37	0.46
32:1a:555:C:H2'	32:1a:556:C:C6	2.50	0.46
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.15	0.46
35:1d:165:MET:SD	35:1d:168:ARG:HD2	2.55	0.46
46:1o:63:ARG:HG2	46:1o:67:LEU:HD12	1.96	0.46
51:1t:87:LYS:O	51:1t:91:LEU:HG	2.15	0.46
1:2A:34:C:N4	1:2A:447:A:H61	2.13	0.46
1:2A:2299:G:N1	1:2A:2318:G:N7	2.64	0.46
3:2D:186:HIS:CE1	3:2D:188:GLU:HG2	2.50	0.46
6:2G:125:PHE:HB3	6:2G:166:ASP:OD2	2.15	0.46
7:2H:118:PRO:HG2	7:2H:121:ILE:HG13	1.97	0.46
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.15	0.46
13:2R:104:ARG:HD2	13:2R:107:ASP:OD1	2.14	0.46
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.97	0.46
17:2V:55:ALA:HA	17:2V:101:GLY:HA2	1.96	0.46
41:2j:44:VAL:HA	41:2j:66:ARG:HA	1.97	0.46
46:2o:39:LEU:HD23	46:2o:39:LEU:HA	1.73	0.46
48:2q:14:LYS:HE3	48:2q:14:LYS:HB3	1.67	0.46
50:2s:52:TYR:CD1	50:2s:57:HIS:HD2	2.33	0.46
54:2w:50:U:H2'	54:2w:51:U:C6	2.50	0.46
54:2y:62:C:H2'	54:2y:63:G:H8	1.79	0.46
1:1A:207:A:H2'	1:1A:208:C:O4'	2.14	0.46
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.98	0.46
5:1F:8:GLN:HE22	5:1F:21:ALA:HB2	1.81	0.46
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.97	0.46
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.50	0.46
25:13:23:LEU:HD13	25:13:50:VAL:HG11	1.97	0.46
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.31	0.46
30:18:26:LYS:HG2	30:18:46:ARG:O	2.15	0.46
32:1a:116:A:H61	32:1a:313:A:H1'	1.80	0.46
33:1b:212:GLN:HG3	33:1b:213:LEU:N	2.31	0.46
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.98	0.46
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.96	0.46
44:1m:82:MET:O	44:1m:93:ARG:NH2	2.49	0.46
4:2E:48:GLN:HA	4:2E:80:GLU:HA	1.97	0.46
13:2R:36:THR:HG22	13:2R:37:THR:H	1.80	0.46
1:1A:1092:C:H2'	1:1A:1093:G:H5'	1.96	0.46
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.50	0.46
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	1.98	0.46
28:16:10:LEU:HG	28:16:54:ILE:HG13	1.98	0.46
33:1b:207:ALA:O	33:1b:211:ILE:HG13	2.16	0.46
36:1e:7:GLU:OE2	36:1e:37:ARG:NH2	2.48	0.46
37:1f:61:LEU:HD23	37:1f:63:TYR:HE2	1.81	0.46
1:2A:330:A:H2	1:2A:1210:A:O2'	1.97	0.46
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.50	0.46
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.30	0.46
2:2B:56:G:H5'	6:2G:27:ASN:ND2	2.31	0.46
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.97	0.46
22:20:37:LEU:HG	22:20:60:PHE:HA	1.98	0.46
32:2a:1502:A:H5'	32:2a:1504:G:N7	2.30	0.46
38:2g:133:GLY:HA2	38:2g:136:LYS:HB2	1.97	0.46
1:1A:299:A:OP2	61:1A:4134:HOH:O	2.21	0.46
1:1A:2701:C:H2'	1:1A:2702:U:H2'	1.98	0.46
10:1O:49:ARG:NH1	32:1a:1423:G:OP1	2.47	0.46
17:1V:1:MET:HE3	17:1V:43:GLU:HB2	1.98	0.46
24:12:55:ARG:NH1	61:12:201:HOH:O	2.26	0.46
32:1a:407:G:OP1	35:1d:115:ARG:NH2	2.49	0.46
32:1a:952:U:H2'	32:1a:953:G:C8	2.50	0.46
32:1a:972:C:O2'	41:1j:55:LYS:O	2.33	0.46
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.97	0.46
37:1f:8:ILE:HG12	37:1f:88:VAL:HG22	1.97	0.46
39:1h:124:ALA:O	39:1h:128:GLY:N	2.48	0.46
1:2A:570:G:H2'	1:2A:2030:A:C5	2.50	0.46
1:2A:764:A:H5''	3:2D:210:GLY:HA3	1.97	0.46
1:2A:894:C:O2'	1:2A:895:U:H5''	2.15	0.46
1:2A:900:A:H3'	1:2A:901:A:H8	1.80	0.46
1:2A:947:G:H2'	1:2A:948:G:C8	2.51	0.46
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.97	0.46
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.50	0.46
6:2G:49:ASP:N	6:2G:49:ASP:OD1	2.48	0.46
7:2H:101:ARG:HH12	7:2H:122:THR:HG23	1.80	0.46
21:2Z:123:ASP:N	21:2Z:123:ASP:OD1	2.49	0.46
32:2a:447:G:O6	32:2a:485:G:O2'	2.19	0.46
32:2a:779:C:H2'	32:2a:780:A:O4'	2.16	0.46
32:2a:946:A:H2'	32:2a:947:G:C8	2.50	0.46
32:2a:1264:C:H42	32:2a:1271:G:H1	1.63	0.46
42:2k:44:SER:OG	42:2k:47:VAL:HG23	2.16	0.46
44:2m:13:LYS:HA	44:2m:44:ARG:NH1	2.30	0.46
54:2y:65:G:H2'	54:2y:66:U:C6	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:613:G:N2	1:1A:614(C):A:O2'	2.49	0.46
1:1A:1912:A:HO2'	32:1a:1494:G:HO2'	1.61	0.46
1:1A:2099:U:H2'	1:1A:2100:G:C8	2.51	0.46
2:1B:2:C:H2'	2:1B:3:C:C6	2.50	0.46
6:1G:132:ASN:HA	6:1G:157:ILE:O	2.16	0.46
15:1T:36:GLU:O	15:1T:38:ASN:N	2.48	0.46
32:1a:22:G:H4'	32:1a:885:G:C8	2.50	0.46
32:1a:119:A:H4'	32:1a:120:A:C8	2.50	0.46
32:1a:447:G:H2'	32:1a:485:G:N2	2.29	0.46
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.14	0.46
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.36	0.46
36:1e:151:LEU:HD21	39:1h:77:GLU:HG2	1.98	0.46
38:1g:78:ARG:HG3	38:1g:79:ARG:H	1.79	0.46
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.15	0.46
6:2G:33:ARG:O	6:2G:161:THR:HG23	2.15	0.46
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.50	0.46
32:2a:730:G:C5	32:2a:731:G:H1'	2.51	0.46
32:2a:1090:U:H2'	32:2a:1091:U:C6	2.51	0.46
32:2a:1121:U:H2'	32:2a:1122:U:C6	2.50	0.46
33:2b:76:GLN:NE2	33:2b:76:GLN:H	2.13	0.46
1:1A:1365:A:O2'	23:11:11:ARG:NH1	2.49	0.46
1:1A:1429:G:H2'	1:1A:1430:C:H6	1.80	0.46
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.51	0.46
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.16	0.46
2:1B:66:A:N6	2:1B:109:C:H5'	2.30	0.46
3:1D:70:TRP:CE2	3:1D:150:LYS:HD3	2.50	0.46
6:1G:49:ASP:OD1	6:1G:49:ASP:N	2.49	0.46
8:1I:31:LEU:HD21	8:1I:38:LEU:HD22	1.96	0.46
28:16:12:GLU:OE1	28:16:52:VAL:HG11	2.15	0.46
32:1a:392:G:OP1	47:1p:8:ARG:NH2	2.49	0.46
32:1a:922:G:C6	32:1a:923:A:C6	3.04	0.46
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.37	0.46
32:1a:1006:C:H2'	32:1a:1007:C:C6	2.51	0.46
35:1d:18:LYS:HG2	59:1d:302:SF4:S1	2.56	0.46
1:2A:822:U:OP2	61:2A:3839:HOH:O	2.21	0.46
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.15	0.46
32:2a:865:A:H5'	32:2a:1078:U:C5	2.51	0.46
32:2a:1054:C:C5	54:2w:34:G:H1'	2.50	0.46
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.50	0.46
35:2d:188:LEU:HD12	35:2d:189:PRO:HD2	1.98	0.46
36:2e:41:VAL:O	36:2e:66:MET:HA	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.50	0.46
41:2j:78:ASN:O	41:2j:80:LYS:N	2.48	0.46
1:1A:583:G:OP2	16:1U:10:ARG:HD2	2.15	0.46
4:1E:96:PHE:O	4:1E:175:VAL:HG21	2.16	0.46
12:1Q:43:THR:O	12:1Q:47:ILE:HG13	2.16	0.46
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD11	1.97	0.46
33:1b:45:GLN:O	33:1b:49:GLU:HG3	2.16	0.46
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.98	0.46
1:2A:299:A:N1	1:2A:322:A:O2'	2.41	0.46
1:2A:530:G:C5	1:2A:2022:U:H5''	2.50	0.46
1:2A:931:G:O2'	25:23:24:LYS:HD3	2.14	0.46
1:2A:984:A:H5''	1:2A:985:C:H5	1.80	0.46
1:2A:1155:A:H5''	16:2U:55:ARG:NE	2.31	0.46
21:2Z:28:MET:HG2	21:2Z:90:VAL:HG22	1.98	0.46
26:24:12:ALA:HB3	26:24:26:SER:HB3	1.98	0.46
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.31	0.46
33:2b:53:ARG:HA	33:2b:56:ARG:NH1	2.30	0.46
34:2c:122:GLU:HA	34:2c:125:GLU:HG2	1.97	0.46
35:2d:82:ALA:HB1	35:2d:92:VAL:HG13	1.97	0.46
47:2p:36:ILE:HD12	47:2p:56:ALA:HB2	1.98	0.46
1:1A:284:U:H2'	1:1A:285:C:C6	2.51	0.46
1:1A:922:U:H2'	1:1A:923:C:C6	2.51	0.46
1:1A:1012:U:C5	9:1N:28:THR:HG21	2.51	0.46
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.50	0.46
1:1A:2429:G:OP1	61:1A:4102:HOH:O	2.20	0.46
4:1E:119:ARG:HD3	4:1E:120:TRP:CE2	2.51	0.46
21:1Z:104:PHE:CZ	21:1Z:119:GLU:HG2	2.51	0.46
32:1a:376:G:H5''	47:1p:5:ARG:HG2	1.97	0.46
32:1a:767:A:H2'	32:1a:768:A:O4'	2.15	0.46
36:1e:81:GLU:HG2	36:1e:90:VAL:HG13	1.97	0.46
1:2A:973:A:H8	1:2A:973:A:OP1	1.99	0.46
1:2A:2134:A:O2'	1:2A:2159:G:N2	2.49	0.46
1:2A:2390:U:P	30:28:35:GLN:HE22	2.39	0.46
1:2A:2579:C:OP1	61:2A:3841:HOH:O	2.21	0.46
32:2a:89:C:H2'	32:2a:90:U:O4'	2.16	0.46
32:2a:1153:C:H2'	32:2a:1154:G:C8	2.50	0.46
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	1.98	0.46
34:2c:59:ARG:HD3	34:2c:63:ASN:O	2.15	0.46
54:2w:21:A:HO2'	54:2w:22:G:P	2.38	0.46
54:2w:27:G:H1	54:2w:43:C:N4	2.13	0.46
1:1A:1069:A:H4'	1:1A:1070:A:H5''	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.98	0.46
11:1P:125:VAL:HG13	11:1P:138:LEU:HD21	1.98	0.46
32:1a:890:G:O2'	32:1a:906:G:O6	2.26	0.46
33:1b:101:MET:HA	33:1b:108:ILE:HD12	1.98	0.46
33:1b:163:PHE:CD1	33:1b:185:ILE:HG13	2.51	0.46
50:1s:20:LEU:HD21	50:1s:43:GLU:HG2	1.98	0.46
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.51	0.46
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.16	0.46
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.51	0.46
7:2H:145:ALA:HA	7:2H:148:ILE:HD12	1.97	0.46
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HB3	1.98	0.46
24:22:66:GLU:HA	24:22:69:ARG:NH1	2.31	0.46
32:2a:1178:G:N2	32:2a:1180:A:H3'	2.30	0.46
32:2a:1502:A:C8	32:2a:1505:G:N2	2.83	0.46
41:2j:47:PHE:CZ	45:2n:37:PHE:HE2	2.34	0.46
43:2l:110:VAL:HG23	43:2l:120:TYR:HB3	1.98	0.46
50:2s:32:LYS:HD2	50:2s:34:TRP:HZ3	1.81	0.46
1:1A:639:U:H2'	1:1A:640:C:C6	2.51	0.46
1:1A:793:A:OP2	1:1A:2071:A:O2'	2.32	0.46
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.51	0.46
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.14	0.46
1:1A:2052:G:H4'	4:1E:143:ASN:O	2.16	0.46
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.51	0.46
8:1I:45:LYS:HB3	8:1I:45:LYS:HE2	1.67	0.46
21:1Z:44:PHE:CZ	21:1Z:86:VAL:HG11	2.51	0.46
21:1Z:163:LEU:HD23	21:1Z:167:PRO:HG3	1.98	0.46
32:1a:219:C:H2'	32:1a:220:G:O4'	2.16	0.46
32:1a:600:C:H2'	32:1a:601:C:C6	2.51	0.46
32:1a:664:G:N2	32:1a:741:G:H1	2.02	0.46
32:1a:974:A:H8	32:1a:974:A:OP1	1.99	0.46
32:1a:1518:MA6:H93	32:1a:1519:MA6:C9	2.46	0.46
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.38	0.46
36:1e:24:ARG:H	36:1e:24:ARG:HG2	1.55	0.46
1:2A:76:C:O3'	24:22:59:ARG:HG3	2.16	0.46
1:2A:315:G:H2'	1:2A:316:C:C6	2.51	0.46
1:2A:987:G:O2'	1:2A:1000:A:N3	2.41	0.46
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.16	0.46
57:2A:3783:A1A1L:N20	57:2A:3783:A1A1L:O24	2.47	0.46
7:2H:92:ILE:H	7:2H:92:ILE:HD12	1.81	0.46
26:24:46:GLN:O	26:24:48:ARG:N	2.47	0.46
32:2a:737:A:H2'	32:2a:738:C:C6	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:881:G:P	43:2l:12:ARG:HH22	2.39	0.46
32:2a:1224:G:H1	32:2a:1363:C:N4	2.14	0.46
32:2a:1318:A:H5''	50:2s:3:ARG:NH2	2.31	0.46
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.31	0.46
38:2g:67:GLU:HA	38:2g:70:LYS:HG3	1.98	0.46
44:2m:97:PRO:HA	44:2m:110:ARG:HD3	1.98	0.46
1:1A:185:U:H4'	1:1A:218:A:H4'	1.98	0.45
1:1A:570:G:H2'	1:1A:2030:A:N7	2.31	0.45
1:1A:1070:A:N7	1:1A:1096:A:H2'	2.31	0.45
8:1I:109:ILE:HA	8:1I:109:ILE:HD13	1.75	0.45
33:1b:188:ALA:HB1	33:1b:192:SER:OG	2.16	0.45
54:1w:4:C:H2'	54:1w:5:G:C8	2.51	0.45
54:1w:56:C:H2'	54:1w:57:G:O4'	2.15	0.45
54:1y:23:A:H2'	54:1y:24:G:C8	2.51	0.45
1:2A:493:G:H2'	1:2A:494:G:O4'	2.16	0.45
1:2A:862:G:H2'	1:2A:863:A:O4'	2.16	0.45
1:2A:863:A:H2'	1:2A:864:G:H8	1.81	0.45
1:2A:1754:C:H5	15:2T:96:ARG:HH21	1.64	0.45
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.51	0.45
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.51	0.45
6:2G:171:ALA:O	6:2G:175:LEU:HG	2.15	0.45
32:2a:532:A:N6	32:2a:1206:G:O2'	2.50	0.45
32:2a:620:C:C2	35:2d:135:LEU:HG	2.51	0.45
32:2a:674:G:H2'	32:2a:675:A:H8	1.81	0.45
32:2a:1129:C:OP1	40:2i:16:ARG:NH1	2.41	0.45
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	1.98	0.45
32:2a:1310:G:H2'	32:2a:1311:G:C8	2.51	0.45
55:2x:75:C:H2'	55:2x:76:31H:H1'	1.98	0.45
1:1A:271(K):U:H1'	8:1I:50:ARG:HD2	1.97	0.45
1:1A:1058:G:H1	1:1A:1080:C:N4	2.15	0.45
1:1A:2239:G:H5'	3:1D:251:GLY:HA3	1.99	0.45
1:1A:2313:C:H4'	6:1G:91:ARG:HG3	1.98	0.45
21:1Z:103:ARG:O	21:1Z:139:VAL:HG23	2.16	0.45
32:1a:299:G:O5'	32:1a:299:G:H8	1.98	0.45
32:1a:339:C:H2'	32:1a:340:U:C6	2.51	0.45
32:1a:405:U:H5''	32:1a:495:A:C2	2.49	0.45
32:1a:1355:G:H2'	32:1a:1356:G:C8	2.51	0.45
32:1a:1377:A:O2'	38:1g:2:ALA:N	2.47	0.45
33:1b:8:LYS:HB3	33:1b:9:GLU:H	1.58	0.45
33:1b:59:GLU:HG2	33:1b:225:ALA:HB2	1.98	0.45
35:1d:194:LEU:HD13	35:1d:194:LEU:HA	1.74	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:79:ARG:HD2	38:1g:80:VAL:N	2.31	0.45
41:1j:38:ILE:O	41:1j:38:ILE:HG13	2.16	0.45
54:1y:55:PSU:N3	54:1y:58:A:OP2	2.38	0.45
1:2A:863:A:H2'	1:2A:864:G:C8	2.51	0.45
1:2A:918:A:C5	1:2A:919:G:H1'	2.51	0.45
1:2A:2318:G:H21	14:2S:3:ARG:NE	2.14	0.45
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.15	0.45
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	1.97	0.45
32:2a:1009:G:H22	32:2a:1021:G:H1'	1.82	0.45
32:2a:1327:C:H5''	52:2u:20:LYS:HB3	1.98	0.45
33:2b:92:TYR:CZ	33:2b:151:GLY:HA3	2.50	0.45
36:2e:103:GLY:O	36:2e:106:PRO:HD2	2.15	0.45
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.81	0.45
54:2y:9:A:H5'	54:2y:46:G7M:O4'	2.15	0.45
1:1A:1709:U:H2'	1:1A:1710:C:C6	2.52	0.45
1:1A:2135:A:H2'	1:1A:2135:A:N3	2.31	0.45
1:1A:2165:G:H1	1:1A:2171:A:H2'	1.82	0.45
10:1O:104:ARG:NE	15:1T:36:GLU:OE2	2.32	0.45
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.98	0.45
32:1a:613:C:H2'	32:1a:614:A:H8	1.82	0.45
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.16	0.45
32:1a:1151:A:H5''	41:1j:40:LEU:O	2.16	0.45
41:1j:27:ALA:HA	41:1j:81:THR:HG21	1.97	0.45
41:1j:54:PHE:O	41:1j:56:HIS:N	2.49	0.45
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.52	0.45
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.16	0.45
2:2B:7:G:H21	14:2S:38:GLN:NE2	2.04	0.45
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.50	0.45
10:2O:68:GLU:OE1	10:2O:78:ARG:NH1	2.48	0.45
14:2S:52:SER:HB2	14:2S:55:ALA:HB3	1.98	0.45
19:2X:95:LEU:HD23	19:2X:95:LEU:HA	1.79	0.45
32:2a:130:A:O2'	32:2a:131:C:O5'	2.30	0.45
32:2a:337:C:H2'	32:2a:338:A:C8	2.51	0.45
32:2a:866:C:H4'	32:2a:919:A:H5'	1.98	0.45
32:2a:1320:C:H1'	50:2s:73:GLU:HG3	1.98	0.45
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.31	0.45
35:2d:65:ARG:NH1	35:2d:70:ILE:O	2.48	0.45
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.51	0.45
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.49	0.45
1:1A:226:G:N2	1:1A:228:A:H62	2.12	0.45
1:1A:796:C:H2'	1:1A:797:C:C6	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:881:G:C2	1:1A:882:G:H1'	2.51	0.45
1:1A:2136:C:N4	1:1A:2155:G:N1	2.64	0.45
4:1E:34:VAL:HB	4:1E:48:GLN:HE21	1.82	0.45
7:1H:157:TYR:CE1	7:1H:172:LYS:HG3	2.52	0.45
32:1a:551:U:H2'	32:1a:552:U:C6	2.52	0.45
32:1a:736:C:H2'	32:1a:737:A:H8	1.82	0.45
32:1a:1095:U:P	32:1a:1108:G:H1	2.38	0.45
35:1d:108:LEU:HD23	35:1d:110:PHE:CZ	2.51	0.45
37:1f:64:GLN:HG3	37:1f:64:GLN:O	2.16	0.45
50:1s:63:THR:HG23	50:1s:66:MET:HE3	1.97	0.45
1:2A:1355:G:O6	61:2A:3833:HOH:O	2.19	0.45
1:2A:1607:C:H5''	1:2A:1608:A:H5'	1.99	0.45
1:2A:1913:A:C8	32:2a:1494:G:H4'	2.51	0.45
1:2A:2103:C:H2'	1:2A:2104:G:H8	1.81	0.45
5:2F:117:ARG:HH12	11:2P:1:MET:H2	1.63	0.45
10:2O:17:ARG:HD3	10:2O:17:ARG:HA	1.77	0.45
18:2W:4:LYS:HE2	18:2W:6:ILE:HD11	1.99	0.45
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.16	0.45
39:2h:25:ASP:N	39:2h:25:ASP:OD1	2.49	0.45
41:2j:15:THR:HB	41:2j:94:VAL:HG23	1.98	0.45
41:2j:36:GLY:O	41:2j:38:ILE:HD13	2.16	0.45
47:2p:27:LYS:HG3	47:2p:30:GLY:HA3	1.97	0.45
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.51	0.45
2:1B:24:G:N7	2:1B:56:G:H2'	2.31	0.45
6:1G:57:ALA:HA	6:1G:68:PRO:HG2	1.99	0.45
15:1T:117:ASP:OD2	15:1T:120:ARG:NE	2.48	0.45
32:1a:501:C:H2'	32:1a:502:G:C8	2.52	0.45
32:1a:963:G:H5'	61:1a:1932:HOH:O	2.16	0.45
33:1b:127:ILE:HD12	33:1b:130:ARG:HD3	1.99	0.45
41:1j:81:THR:C	41:1j:83:GLU:H	2.25	0.45
1:2A:922:U:H2'	1:2A:923:C:C6	2.51	0.45
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.41	0.45
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.32	0.45
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.34	0.45
9:2N:4:TYR:HB2	16:2U:101:ARG:NH1	2.31	0.45
12:2Q:32:TYR:OH	12:2Q:111:GLU:OE1	2.28	0.45
32:2a:993:G:N3	32:2a:993:G:H2'	2.31	0.45
32:2a:1064:G:OP1	32:2a:1386:G:H4'	2.16	0.45
32:2a:1347:G:HO2'	32:2a:1373:G:H1	1.65	0.45
33:2b:16:HIS:CB	33:2b:210:SER:HB2	2.45	0.45
34:2c:125:GLU:O	34:2c:190:ARG:NH2	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:66:ARG:HH12	41:2j:68:HIS:CE1	2.35	0.45
50:2s:49:ILE:HG12	50:2s:50:ALA:N	2.31	0.45
1:1A:880:G:H1	1:1A:898:C:N4	2.09	0.45
1:1A:1082:U:H3	1:1A:1086:A:H61	0.54	0.45
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.97	0.45
11:1P:95:VAL:HG22	11:1P:125:VAL:HB	1.98	0.45
17:1V:24:LYS:HE2	17:1V:24:LYS:HB3	1.80	0.45
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.82	0.45
32:1a:1228:C:OP1	44:1m:115:LYS:NZ	2.46	0.45
33:1b:200:ILE:HG22	33:1b:202:PRO:HD3	1.99	0.45
34:1c:79:ARG:O	34:1c:82:GLU:HG2	2.16	0.45
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.33	0.45
36:1e:57:LYS:HG2	36:1e:61:TYR:CE2	2.51	0.45
36:1e:137:GLU:HG3	36:1e:141:GLN:HE21	1.82	0.45
42:1k:48:ILE:O	42:1k:50:TYR:N	2.45	0.45
1:2A:817:C:O2'	1:2A:839:U:H5''	2.17	0.45
1:2A:1364:G:C8	23:21:3:LYS:HD2	2.51	0.45
18:2W:6:ILE:HG22	18:2W:8:ARG:HG3	1.98	0.45
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.16	0.45
21:2Z:150:LEU:H	21:2Z:171:ILE:HD11	1.82	0.45
23:21:35:THR:OG1	23:21:35:THR:O	2.33	0.45
23:21:50:ARG:HD2	23:21:57:GLU:OE2	2.15	0.45
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.17	0.45
32:2a:1014:A:H2'	32:2a:1015:A:C8	2.52	0.45
32:2a:1121:U:O2'	32:2a:1122:U:H5'	2.17	0.45
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.50	0.45
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.31	0.45
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.81	0.45
33:2b:58:ILE:O	33:2b:62:ALA:N	2.42	0.45
34:2c:119:ARG:O	34:2c:123:GLN:HG3	2.16	0.45
1:1A:279:C:H42	1:1A:361:G:H1	1.63	0.45
1:1A:444:C:H5''	61:1A:4900:HOH:O	2.16	0.45
1:1A:817:C:H4'	1:1A:932:G:C5	2.51	0.45
1:1A:878:A:H61	1:1A:899:A:C2'	2.28	0.45
1:1A:1054:A:H3'	1:1A:1055:G:H8	1.82	0.45
1:1A:1540:U:H2'	1:1A:1541:G:O4'	2.17	0.45
1:1A:1721:G:H1'	1:1A:1741:A:N6	2.32	0.45
1:1A:2100:G:O2'	1:1A:2101:G:H5'	2.17	0.45
1:1A:2379:G:O2'	14:1S:17:ARG:NH2	2.50	0.45
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.98	0.45
13:1R:104:ARG:HD2	13:1R:107:ASP:OD1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:16:13:CYS:SG	28:16:47:THR:HG21	2.57	0.45
32:1a:377:G:OP1	47:1p:5:ARG:HD2	2.16	0.45
32:1a:1316:G:N1	32:1a:1319:A:OP2	2.46	0.45
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.52	0.45
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.65	0.45
35:1d:121:VAL:HG22	35:1d:126:ILE:HG13	1.98	0.45
44:1m:66:LEU:HB3	44:1m:67:GLU:H	1.59	0.45
54:1y:2:C:H2'	54:1y:3:C:C6	2.51	0.45
1:2A:1036:G:P	7:2H:59:ARG:HD2	2.56	0.45
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.52	0.45
1:2A:2637:U:H5''	4:2E:82:ARG:NH1	2.28	0.45
2:2B:19:G:H2'	2:2B:20:C:O4'	2.16	0.45
4:2E:1:MET:HE3	4:2E:199:ARG:HB3	1.99	0.45
19:2X:94:GLY:N	19:2X:95:LEU:HB2	2.32	0.45
31:29:10:ILE:HD12	31:29:32:HIS:HA	1.99	0.45
32:2a:20:U:OP2	36:2e:125:SER:HB3	2.17	0.45
32:2a:375:U:OP1	47:2p:69:THR:OG1	2.26	0.45
32:2a:416:G:C5	32:2a:417:C:C4	3.05	0.45
32:2a:708:C:H2'	32:2a:709:G:H8	1.82	0.45
34:2c:129:ALA:HB3	34:2c:132:ARG:HB3	1.98	0.45
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.98	0.45
47:2p:15:PRO:HD2	47:2p:42:ARG:HD3	1.99	0.45
1:1A:818:G:H5'	1:1A:839:U:OP1	2.17	0.45
1:1A:2311:A:N1	6:1G:47:LYS:NZ	2.65	0.45
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.52	0.45
1:1A:2470:G:P	12:1Q:56:ARG:HH12	2.40	0.45
5:1F:13:SER:HB2	5:1F:127:GLU:HG3	1.99	0.45
32:1a:456:C:H2'	32:1a:457:C:H6	1.80	0.45
32:1a:857:C:H2'	32:1a:858:G:O4'	2.16	0.45
1:2A:30:G:C5	1:2A:31:C:C4	3.05	0.45
1:2A:70:G:H5''	1:2A:112:U:O2	2.17	0.45
1:2A:90:U:H1'	1:2A:92:A:C8	2.52	0.45
1:2A:340:A:H2'	1:2A:341:G:O4'	2.17	0.45
1:2A:515:A:H1'	1:2A:581:C:H1'	1.99	0.45
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.17	0.45
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.52	0.45
1:2A:1448:G:H2'	1:2A:1449:A:C8	2.52	0.45
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.52	0.45
1:2A:2242:G:OP1	61:2A:3838:HOH:O	2.20	0.45
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.31	0.45
4:2E:111:ARG:HG2	4:2E:118:LYS:HD3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:76:TYR:HH	16:2U:92:ARG:HE	1.59	0.45
26:24:48:ARG:HG3	26:24:52:THR:HG23	1.99	0.45
32:2a:373:A:H61	32:2a:391:G:H1'	1.81	0.45
32:2a:1073:U:H2'	32:2a:1074:G:C8	2.52	0.45
32:2a:1236:A:O2'	32:2a:1304:G:H4'	2.17	0.45
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.51	0.45
1:1A:604:G:P	11:1P:90:ARG:HH21	2.39	0.45
1:1A:882:G:H4'	54:1w:19:G:C6	2.52	0.45
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.17	0.45
1:1A:2279:G:O6	22:10:14:ARG:HG3	2.16	0.45
2:1B:1:U:H2'	2:1B:2:C:C6	2.52	0.45
4:1E:47:VAL:O	4:1E:80:GLU:HA	2.17	0.45
5:1F:29:ASN:H	5:1F:112:MET:HE3	1.82	0.45
8:1I:96:ASP:OD1	8:1I:96:ASP:N	2.49	0.45
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.17	0.45
30:18:23:VAL:CG1	30:18:47:LYS:HD3	2.45	0.45
32:1a:695:A:OP1	42:1k:52:GLY:HA3	2.17	0.45
32:1a:1226:C:H4'	50:1s:80:TYR:OH	2.17	0.45
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.53	0.45
35:1d:144:ASP:N	35:1d:144:ASP:OD1	2.46	0.45
37:1f:89:MET:HE3	37:1f:91:VAL:HG21	1.99	0.45
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.15	0.45
1:2A:815:C:H2'	1:2A:816:C:C6	2.52	0.45
1:2A:1257:C:O2'	61:2A:3840:HOH:O	2.21	0.45
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.51	0.45
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.17	0.45
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.44	0.45
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.39	0.45
2:2B:17:C:H2'	2:2B:18:G:O4'	2.17	0.45
2:2B:41:U:H5	6:2G:70:VAL:H	1.63	0.45
15:2T:125:ARG:HE	15:2T:125:ARG:HB3	1.59	0.45
29:27:46:VAL:HG13	29:27:48:LYS:HZ2	1.82	0.45
32:2a:73:G:H1	32:2a:96:U:H3	1.64	0.45
32:2a:114:U:O2'	32:2a:115:G:H5'	2.17	0.45
32:2a:141:A:H1'	32:2a:182:U:O2	2.17	0.45
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.82	0.45
32:1a:748:C:H4'	32:1a:749:C:O5'	2.17	0.45
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.99	0.45
44:1m:90:LEU:HD23	44:1m:93:ARG:NH1	2.31	0.45
1:2A:2659:G:OP1	7:2H:158:HIS:NE2	2.42	0.45
1:2A:2803:C:H2'	1:2A:2804:C:C6	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.52	0.45
3:2D:20:ASP:OD1	3:2D:20:ASP:N	2.44	0.45
30:28:46:ARG:HE	30:28:46:ARG:HB3	1.50	0.45
32:2a:600:C:H2'	32:2a:601:C:C6	2.52	0.45
32:2a:735:C:H2'	32:2a:736:C:C6	2.51	0.45
32:2a:833:U:H2'	32:2a:834:C:H6	1.81	0.45
32:2a:1273:G:C6	32:2a:1274:G:C4	3.05	0.45
32:2a:1321:C:O2'	50:2s:77:THR:HG21	2.16	0.45
34:2c:6:HIS:HB3	45:2n:49:HIS:CD2	2.52	0.45
36:2e:28:PHE:O	36:2e:47:LYS:HA	2.16	0.45
54:2w:43:C:H2'	54:2w:44:G:C8	2.52	0.45
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.32	0.44
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.32	0.44
5:1F:89:VAL:HG12	5:1F:90:PHE:CD2	2.52	0.44
8:1I:9:LEU:HD23	8:1I:12:LEU:HD12	1.99	0.44
32:1a:435:C:H2'	32:1a:436:C:C6	2.52	0.44
32:1a:1039:C:H2'	32:1a:1040:U:H6	1.83	0.44
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.25	0.44
38:1g:144:MET:HE2	38:1g:144:MET:HB3	1.81	0.44
39:1h:110:ALA:HB3	39:1h:121:ASP:HB3	1.99	0.44
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.17	0.44
53:1v:23:A:H4'	53:1v:24:A:H5'	2.00	0.44
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.17	0.44
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.35	0.44
13:2R:33:ARG:NH2	13:2R:115:GLU:OE1	2.47	0.44
17:2V:24:LYS:HA	17:2V:92:THR:OG1	2.16	0.44
25:23:4:LEU:HD23	25:23:4:LEU:HA	1.75	0.44
32:2a:54:C:N4	32:2a:353:A:OP2	2.40	0.44
32:2a:685:G:N1	32:2a:686:U:O4	2.50	0.44
32:2a:714:G:H2'	32:2a:715:A:C8	2.51	0.44
32:2a:841:U:H6	32:2a:841:U:P	2.41	0.44
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.82	0.44
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.17	0.44
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.17	0.44
32:2a:1508:G:H2'	32:2a:1509:C:C6	2.53	0.44
40:2i:18:PHE:O	40:2i:61:ALA:HA	2.17	0.44
16:1U:104:GLN:NE2	16:1U:105:VAL:HG23	2.32	0.44
32:1a:265:G:H5'	48:1q:64:PRO:O	2.17	0.44
32:1a:376:G:OP2	47:1p:67:THR:HG21	2.17	0.44
32:1a:435:C:H2'	32:1a:436:C:H6	1.80	0.44
32:1a:865:A:H2	32:1a:918:A:H4'	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:955:U:O2'	50:1s:83:HIS:HD2	2.00	0.44
32:1a:1067:A:N1	32:1a:1108:G:O2'	2.39	0.44
41:1j:78:ASN:O	41:1j:80:LYS:N	2.50	0.44
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.17	0.44
51:1t:10:LEU:HD22	51:1t:10:LEU:HA	1.80	0.44
1:2A:848:G:H2'	1:2A:849:A:C8	2.52	0.44
1:2A:860:U:C2	1:2A:2268:A:C8	3.05	0.44
1:2A:2218:U:N3	23:21:55:GLY:O	2.48	0.44
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.82	0.44
1:2A:2638:G:OP1	4:2E:82:ARG:NH2	2.50	0.44
3:2D:66:ASP:OD2	3:2D:103:ARG:NH1	2.44	0.44
27:25:35:GLU:HG3	27:25:51:TYR:CD1	2.52	0.44
32:2a:189(D):C:H2'	32:2a:189(E):U:O4'	2.18	0.44
32:2a:501:C:H2'	32:2a:502:G:H8	1.82	0.44
32:2a:833:U:H2'	32:2a:834:C:C6	2.52	0.44
32:2a:983:A:H3'	32:2a:983:A:N3	2.32	0.44
32:2a:1264:C:C4	32:2a:1272:G:O6	2.70	0.44
33:2b:185:ILE:HG22	33:2b:199:TYR:CD2	2.49	0.44
34:2c:9:GLY:N	45:2n:49:HIS:O	2.50	0.44
54:2y:11:C:N4	54:2y:24:G:H1	2.12	0.44
1:1A:839:U:H1'	1:1A:1191:G:H1'	2.00	0.44
1:1A:848:G:H2'	1:1A:849:A:C8	2.53	0.44
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.82	0.44
1:1A:1584:C:O2'	1:1A:1586:A:H5'	2.18	0.44
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.99	0.44
7:1H:25:LYS:HE2	7:1H:27:LYS:HE2	2.00	0.44
15:1T:16:ARG:HB3	15:1T:18:ASP:OD1	2.17	0.44
15:1T:127:ALA:C	15:1T:129:ARG:N	2.74	0.44
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.38	0.44
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.47	0.44
32:1a:448:A:OP2	32:1a:485:G:N1	2.35	0.44
33:1b:9:GLU:O	33:1b:10:LEU:HD23	2.17	0.44
54:1w:18:G:H4'	54:1w:60:U:C6	2.52	0.44
1:2A:39:C:H2'	1:2A:40:C:C6	2.52	0.44
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.17	0.44
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.32	0.44
1:2A:2749:A:O3'	7:2H:62:LYS:NZ	2.50	0.44
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.83	0.44
4:2E:4:ILE:HD11	4:2E:29:GLY:HA2	1.99	0.44
7:2H:11:VAL:HG13	7:2H:15:VAL:HG23	1.99	0.44
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:79:PHE:CZ	16:2U:83:LEU:HD11	2.52	0.44
32:2a:340:U:H2'	32:2a:341:C:C6	2.52	0.44
32:2a:576:G:OP1	61:2a:1908:HOH:O	2.20	0.44
32:2a:952:U:H2'	32:2a:953:G:C8	2.53	0.44
35:2d:88:VAL:O	35:2d:92:VAL:HG12	2.17	0.44
38:2g:114:ARG:HG3	38:2g:115:ARG:HH22	1.82	0.44
41:2j:38:ILE:HD11	41:2j:71:LEU:HD23	1.99	0.44
48:2q:26:GLN:HG2	48:2q:37:LYS:HG2	2.00	0.44
54:2w:56:C:H2'	54:2w:57:G:O4'	2.17	0.44
1:1A:428:A:H8	1:1A:428:A:OP2	2.01	0.44
1:1A:858:U:O2	1:1A:2268:A:H2'	2.17	0.44
1:1A:2360:A:H8	1:1A:2360:A:O5'	2.01	0.44
2:1B:103:G:N2	21:1Z:73:GLN:HE22	2.14	0.44
15:1T:41:ARG:NH2	15:1T:43:GLN:HE21	2.16	0.44
32:1a:28:G:O2'	32:1a:296:U:OP1	2.29	0.44
32:1a:130:A:N3	32:1a:263:A:O2'	2.47	0.44
32:1a:256:U:H2'	32:1a:257:G:O4'	2.17	0.44
32:1a:269:C:H2'	32:1a:270:A:C8	2.53	0.44
33:1b:73:THR:HG22	33:1b:95:GLN:O	2.17	0.44
33:1b:137:ARG:HB3	33:1b:137:ARG:CZ	2.47	0.44
35:1d:119:GLN:HE21	35:1d:119:GLN:HB3	1.59	0.44
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.32	0.44
48:1q:5:VAL:O	48:1q:6:LEU:HD23	2.17	0.44
49:1r:53:ARG:HH21	49:1r:59:SER:HA	1.82	0.44
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.46	0.44
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.52	0.44
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.29	0.44
1:2A:2114:A:H62	1:2A:2115:G:H21	1.65	0.44
1:2A:2130:U:O3'	1:2A:2133:G:H5'	2.18	0.44
2:2B:105:A:H5'	2:2B:106:G:OP2	2.16	0.44
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.51	0.44
14:2S:87:PHE:HB2	14:2S:112:PHE:CE1	2.52	0.44
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	1.99	0.44
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.58	0.44
32:2a:397:A:H5'	32:2a:398:C:OP1	2.17	0.44
32:2a:473:G:H2'	32:2a:474:G:H8	1.82	0.44
32:2a:1097:C:H2'	32:2a:1098:C:H6	1.82	0.44
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.35	0.44
33:2b:27:LYS:O	33:2b:194:PRO:HG2	2.18	0.44
33:2b:54:THR:HA	33:2b:199:TYR:HB3	1.99	0.44
49:2r:35:ARG:O	49:2r:37:VAL:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:2u:20:LYS:O	52:2u:23:PRO:HD3	2.17	0.44
1:1A:412:A:H8	1:1A:412:A:O5'	2.00	0.44
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.52	0.44
32:1a:1025:U:O2	32:1a:1036:G:C6	2.70	0.44
32:1a:1272:G:H2'	32:1a:1273:G:O4'	2.18	0.44
32:1a:1370:G:C2	32:1a:1371:G:C8	3.05	0.44
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.53	0.44
41:1j:30:SER:HB3	41:1j:81:THR:HG23	1.99	0.44
42:1k:108:ILE:O	49:1r:87:ARG:HG3	2.18	0.44
51:1t:56:MET:HE3	51:1t:85:MET:HG2	1.99	0.44
55:1x:45:G:H8	55:1x:45:G:O5'	2.01	0.44
1:2A:196:A:N3	1:2A:196:A:H2'	2.33	0.44
1:2A:208:C:H2'	1:2A:209:C:H6	1.82	0.44
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.18	0.44
1:2A:2287:A:C8	1:2A:2289:G:C8	3.05	0.44
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.34	0.44
5:2F:158:THR:O	5:2F:164:ARG:HD3	2.18	0.44
6:2G:120:LEU:HB3	6:2G:131:TYR:OH	2.18	0.44
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.18	0.44
32:2a:1004:A:N3	32:2a:1038:C:C2	2.86	0.44
32:2a:1525:G:OP1	42:2k:120:ARG:NH2	2.50	0.44
34:2c:136:GLN:O	34:2c:140:ARG:HG3	2.16	0.44
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.18	0.44
1:1A:191:A:H2'	1:1A:192:C:C6	2.52	0.44
1:1A:1359:A:H2	1:1A:1372:U:O4	2.00	0.44
1:1A:1406:U:H2'	1:1A:1407:C:H6	1.79	0.44
1:1A:1509(A):A:H3'	1:1A:1509(B):A:H8	1.82	0.44
2:1B:103:G:H21	21:1Z:73:GLN:NE2	2.14	0.44
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.44	0.44
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.53	0.44
26:14:62:ARG:C	26:14:63:TYR:CG	2.95	0.44
32:1a:179:A:H2'	32:1a:180:U:C6	2.52	0.44
32:1a:202:U:H3'	32:1a:203:U:C5	2.52	0.44
32:1a:925:G:H1'	32:1a:1502:A:C4	2.53	0.44
33:1b:21:ARG:O	33:1b:23:ARG:N	2.51	0.44
33:1b:56:ARG:HE	33:1b:56:ARG:HB2	1.52	0.44
41:1j:61:GLU:OE2	45:1n:58:LYS:NZ	2.48	0.44
49:1r:63:GLN:HA	49:1r:63:GLN:HE21	1.82	0.44
1:2A:883:G:N2	1:2A:895:U:H1'	2.33	0.44
1:2A:1181:C:H2'	1:2A:1182:A:C8	2.53	0.44
1:2A:1184:G:P	25:23:30:ARG:HH21	2.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1260:G:C6	1:2A:1261:C:C4	3.06	0.44
1:2A:2131:G:C8	1:2A:2133:G:C2	3.05	0.44
1:2A:2721:A:OP1	61:2A:3843:HOH:O	2.21	0.44
2:2B:2:C:H2'	2:2B:3:C:H6	1.83	0.44
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.51	0.44
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	2.00	0.44
15:2T:91:ARG:HB2	15:2T:121:ILE:HG13	2.00	0.44
21:2Z:23:LYS:HZ2	21:2Z:40:ASP:HB2	1.82	0.44
21:2Z:124:ILE:HD13	21:2Z:163:LEU:HD11	2.00	0.44
32:2a:502:G:H2'	32:2a:503:C:O4'	2.18	0.44
32:2a:947:G:H1	32:2a:1234:C:N4	2.15	0.44
32:2a:977:A:O3'	32:2a:980:C:N4	2.51	0.44
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	2.00	0.44
32:2a:1223:C:H5''	32:2a:1224:G:H5''	2.00	0.44
32:2a:1313:U:OP1	50:2s:5:LEU:HB2	2.18	0.44
35:2d:3:ARG:NH1	35:2d:5:ILE:HG13	2.32	0.44
42:2k:17:GLY:O	42:2k:80:VAL:HA	2.18	0.44
44:2m:60:VAL:HG12	44:2m:66:LEU:HD11	1.98	0.44
54:2y:18:G:N1	54:2y:55:PSU:C4	2.86	0.44
54:2y:34:G:H2'	54:2y:35:A:H8	1.82	0.44
1:1A:213:A:H2'	1:1A:214:G:O4'	2.18	0.44
1:1A:2756:U:H1'	1:1A:2757:A:H5''	2.00	0.44
8:1I:9:LEU:HD12	8:1I:9:LEU:HA	1.76	0.44
32:1a:78:G:C6	32:1a:91:C:N4	2.86	0.44
32:1a:109:A:H2'	32:1a:326:G:N2	2.31	0.44
32:1a:341:C:H2'	32:1a:342:C:C6	2.53	0.44
32:1a:576:G:O6	32:1a:880:C:O2'	2.31	0.44
32:1a:833:U:H2'	32:1a:834:C:H6	1.83	0.44
35:1d:173:TRP:CZ3	35:1d:174:LEU:HG	2.53	0.44
1:2A:699:A:H2'	1:2A:700:G:O4'	2.17	0.44
1:2A:921:G:H2'	1:2A:922:U:C6	2.52	0.44
2:2B:7:G:N2	14:2S:38:GLN:HE22	2.04	0.44
2:2B:13:A:O2'	2:2B:14:U:H3'	2.18	0.44
2:2B:103:G:N2	21:2Z:73:GLN:HE22	2.15	0.44
3:2D:253:GLN:HG3	61:2D:412:HOH:O	2.17	0.44
6:2G:69:ALA:HB3	6:2G:91:ARG:HH21	1.83	0.44
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.57	0.44
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.50	0.44
32:2a:397:A:H3'	32:2a:397:A:N3	2.32	0.44
32:2a:417:C:H2'	32:2a:418:C:H6	1.82	0.44
32:2a:1224:G:H1	32:2a:1363:C:H42	1.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1227:A:OP1	50:2s:80:TYR:OH	2.28	0.44
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.18	0.44
37:2f:100:ASN:HD21	49:2r:23:LYS:HG2	1.83	0.44
39:2h:104:ARG:HB2	39:2h:108:GLY:H	1.83	0.44
44:2m:90:LEU:HD23	44:2m:90:LEU:HA	1.87	0.44
1:1A:414:C:H2'	1:1A:415:A:C8	2.52	0.44
1:1A:614(C):A:C4	5:1F:180:GLY:HA2	2.53	0.44
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.53	0.44
1:1A:2184:G:H2'	1:1A:2185:C:C6	2.53	0.44
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.31	0.44
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.18	0.44
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.99	0.44
32:1a:952:U:H2'	32:1a:953:G:H8	1.83	0.44
32:1a:1346:A:O3'	32:1a:1347:G:H4'	2.17	0.44
35:1d:122:ARG:HD2	35:1d:122:ARG:HA	1.71	0.44
35:1d:134:ASP:OD1	35:1d:134:ASP:N	2.48	0.44
38:1g:86:GLN:HA	38:1g:86:GLN:HE21	1.82	0.44
44:1m:33:ALA:O	44:1m:37:THR:OG1	2.35	0.44
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.18	0.44
1:2A:657:U:H2'	1:2A:658:C:C6	2.52	0.44
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.33	0.44
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	2.00	0.44
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.18	0.44
16:2U:66:ASN:O	16:2U:70:ARG:HG3	2.18	0.44
32:2a:109:A:H5'	32:2a:110:C:H5	1.83	0.44
32:2a:554:C:H2'	32:2a:555:C:C6	2.53	0.44
32:2a:833:U:O2'	32:2a:834:C:H5'	2.17	0.44
32:2a:859:A:H2'	32:2a:860:A:O4'	2.18	0.44
32:2a:1360:A:OP2	45:2n:35:ARG:NH2	2.51	0.44
43:2l:117:ARG:HB2	43:2l:117:ARG:CZ	2.47	0.44
44:2m:50:GLU:O	44:2m:53:VAL:HG22	2.17	0.44
46:2o:54:ARG:NH2	46:2o:58:MET:SD	2.90	0.44
1:1A:821:A:H2'	1:1A:946:G:H5''	1.99	0.44
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.52	0.44
1:1A:1753:G:N1	1:1A:1756:G:OP2	2.51	0.44
5:1F:110:LEU:HD11	5:1F:181:LEU:HG	2.00	0.44
6:1G:32:PRO:HB3	6:1G:163:ALA:HB2	1.99	0.44
10:1O:7:TYR:HE2	10:1O:20:MET:HE3	1.82	0.44
11:1P:59:LEU:HD21	30:18:10:ALA:HB2	1.99	0.44
26:14:28:LYS:HE2	26:14:29:PRO:HD2	2.00	0.44
32:1a:232:G:H1'	32:1a:262:A:N1	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:9:A:O2'	54:1w:10:G:N7	2.51	0.44
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.53	0.44
1:2A:776:G:H4'	1:2A:777:A:O5'	2.18	0.44
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.52	0.44
1:2A:2759:G:OP2	61:2A:3842:HOH:O	2.21	0.44
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.17	0.44
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.99	0.44
32:2a:56:U:H2'	32:2a:57:G:H8	1.81	0.44
32:2a:1194:U:H2'	32:2a:1195:C:C6	2.53	0.44
32:2a:1287:A:N6	32:2a:1371:G:O4'	2.43	0.44
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.18	0.44
33:2b:74:LYS:HE2	33:2b:74:LYS:HB3	1.81	0.44
39:2h:12:ARG:HD3	39:2h:26:VAL:HG12	1.99	0.44
1:1A:196:A:H2'	1:1A:196:A:N3	2.33	0.43
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.18	0.43
1:1A:2124:G:H1	1:1A:2174:C:N4	2.15	0.43
7:1H:3:ARG:HD2	7:1H:3:ARG:HA	1.42	0.43
14:1S:110:LEU:HD12	14:1S:110:LEU:HA	1.71	0.43
25:13:24:LYS:HB2	25:13:24:LYS:HE2	1.76	0.43
32:1a:193:C:H2'	32:1a:194:C:C6	2.52	0.43
32:1a:714:G:H2'	32:1a:715:A:C8	2.53	0.43
35:1d:18:LYS:NZ	35:1d:26:CYS:O	2.34	0.43
35:1d:165:MET:HE2	35:1d:176:LEU:HD23	2.00	0.43
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.53	0.43
38:1g:51:GLN:O	38:1g:55:GLY:HA2	2.18	0.43
38:1g:97:GLN:O	38:1g:101:LEU:HG	2.18	0.43
51:1t:50:GLU:O	51:1t:100:ILE:HD11	2.18	0.43
54:1y:55:PSU:N3	54:1y:57:G:H5'	2.32	0.43
1:2A:37:C:H4'	1:2A:451:C:OP1	2.18	0.43
1:2A:289:A:H2'	1:2A:290:G:O4'	2.17	0.43
1:2A:1027:A:C6	1:2A:1126:A:C4	3.06	0.43
1:2A:2722:G:H5'	13:2R:4:LEU:HD12	1.99	0.43
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.33	0.43
32:2a:988:G:H2'	32:2a:989:C:O4'	2.18	0.43
32:2a:1097:C:H2'	32:2a:1098:C:C6	2.53	0.43
32:2a:1135:U:H4'	32:2a:1136:U:H5	1.82	0.43
40:2i:117:HIS:CE1	40:2i:123:PRO:HB3	2.53	0.43
43:2l:84:LEU:HB2	43:2l:105:TYR:CE2	2.53	0.43
47:2p:43:LYS:HA	47:2p:48:TRP:HB3	1.98	0.43
54:2w:18:G:HO2'	54:2w:57:G:H22	1.59	0.43
1:1A:548:A:H1'	1:1A:549:G:OP1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.83	0.43
1:1A:1607:C:O2	61:1A:4132:HOH:O	2.19	0.43
1:1A:1693:U:H1'	3:1D:14:ARG:NH2	2.33	0.43
1:1A:2094:G:OP1	8:1I:22:LYS:HD2	2.18	0.43
1:1A:2189:U:H5'	1:1A:2190:G:OP2	2.18	0.43
8:1I:61:ARG:HD3	8:1I:61:ARG:HA	1.77	0.43
18:1W:66:GLU:HA	18:1W:69:LEU:HD12	2.00	0.43
21:1Z:21:ALA:O	21:1Z:23:LYS:NZ	2.49	0.43
32:1a:401:C:O2'	32:1a:621:A:N3	2.45	0.43
32:1a:994:A:N1	32:1a:1047:G:H4'	2.33	0.43
32:1a:1150:U:C2'	32:1a:1151:A:H5'	2.48	0.43
32:1a:1456:G:H22	51:1t:51:GLU:CD	2.25	0.43
34:1c:178:LEU:HD13	34:1c:178:LEU:HA	1.85	0.43
47:1p:56:ALA:O	47:1p:60:LEU:HB2	2.18	0.43
1:2A:802:A:H2'	1:2A:803:U:O4'	2.19	0.43
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.18	0.43
1:2A:2833:G:H4'	1:2A:2834:G:OP2	2.18	0.43
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.18	0.43
26:24:60:GLN:O	26:24:62:ARG:NH1	2.51	0.43
32:2a:353:A:H5'	32:2a:353:A:H8	1.83	0.43
32:2a:1168:A:C6	32:2a:1169:A:C6	3.06	0.43
34:2c:124:ILE:HG21	34:2c:130:VAL:HG13	1.99	0.43
35:2d:166:LYS:NZ	35:2d:179:GLU:OE2	2.50	0.43
41:2j:12:ASP:HB3	41:2j:15:THR:OG1	2.18	0.43
41:2j:89:ASP:O	41:2j:91:PRO:HD3	2.19	0.43
48:2q:15:MET:HE1	48:2q:43:LEU:HD22	2.00	0.43
1:1A:1041:C:H42	1:1A:1114:G:H1	1.67	0.43
1:1A:1170:G:H2'	1:1A:1171:G:O4'	2.18	0.43
1:1A:1512:U:H2'	1:1A:1513:C:C6	2.53	0.43
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.17	0.43
4:1E:143:ASN:HD22	4:1E:147:PRO:CD	2.32	0.43
15:1T:36:GLU:HG2	32:1a:346:G:OP1	2.17	0.43
15:1T:60:THR:HG22	15:1T:77:PRO:HA	2.00	0.43
26:14:44:THR:O	26:14:47:GLN:HB2	2.18	0.43
33:1b:15:VAL:HG21	33:1b:213:LEU:HD23	1.99	0.43
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	2.00	0.43
48:1q:58:GLU:O	48:1q:74:LEU:N	2.42	0.43
54:1y:34:G:C2	54:1y:35:A:C4	3.07	0.43
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	2.01	0.43
6:2G:122:PRO:HG3	6:2G:182:LYS:C	2.43	0.43
12:2Q:11:LYS:HD3	12:2Q:87:LYS:HG2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:892:A:H2'	32:2a:893:C:C6	2.54	0.43
32:2a:1089:G:H1	32:2a:1096:C:N4	2.16	0.43
32:2a:1380:U:C4	38:2g:3:ARG:HG2	2.53	0.43
34:2c:29:TYR:HE1	41:2j:11:PHE:CE2	2.36	0.43
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.83	0.43
41:2j:8:LEU:HD23	41:2j:8:LEU:H	1.84	0.43
41:2j:9:ARG:NH1	41:2j:69:ASN:OD1	2.51	0.43
44:2m:49:THR:O	44:2m:53:VAL:HG13	2.18	0.43
52:2u:6:ARG:HA	52:2u:11:GLY:HA3	2.01	0.43
1:1A:774:A:N3	1:1A:774:A:H2'	2.32	0.43
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.53	0.43
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.35	0.43
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.33	0.43
1:1A:1805:U:O2	3:1D:50:THR:HB	2.18	0.43
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.81	0.43
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.18	0.43
13:1R:98:LEU:HD12	27:15:57:VAL:HG11	2.00	0.43
19:1X:26:TYR:HB3	19:1X:92:LEU:HD12	2.01	0.43
32:1a:860:A:H2'	32:1a:861:G:O4'	2.18	0.43
32:1a:1035:A:C4	32:1a:1036:G:N2	2.86	0.43
32:1a:1464:G:H2'	32:1a:1465:C:C6	2.53	0.43
33:1b:92:TYR:HE1	33:1b:94:ASN:HB2	1.84	0.43
35:1d:117:ALA:O	35:1d:121:VAL:HG23	2.17	0.43
43:1l:54:LYS:HD2	43:1l:54:LYS:N	2.33	0.43
44:1m:70:LEU:HD23	44:1m:70:LEU:HA	1.76	0.43
1:2A:83:G:OP1	20:2Y:95:LYS:NZ	2.36	0.43
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.53	0.43
1:2A:2258:C:O2'	1:2A:2427:C:OP2	2.32	0.43
1:2A:2298:A:N6	1:2A:2318:G:C8	2.86	0.43
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.19	0.43
10:2O:80:ASP:OD1	15:2T:64:ARG:NH2	2.51	0.43
16:2U:81:HIS:O	16:2U:84:LYS:HB3	2.18	0.43
24:22:35:LEU:HD12	24:22:50:ILE:HG13	2.00	0.43
24:22:58:ALA:O	24:22:62:THR:OG1	2.36	0.43
25:23:44:ARG:O	25:23:48:GLU:HG3	2.18	0.43
32:2a:134:A:H61	47:2p:25:ARG:HH12	1.66	0.43
32:2a:458:C:H2'	32:2a:460:G:C8	2.52	0.43
32:2a:620:C:H2'	32:2a:621:A:O4'	2.18	0.43
32:2a:1371:G:O3'	40:2i:69:GLY:HA3	2.19	0.43
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.53	0.43
40:2i:49:PRO:HG3	40:2i:101:PHE:HD1	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:22:ILE:HB	44:2m:25:ILE:HD12	2.00	0.43
45:2n:23:ARG:CZ	45:2n:30:ALA:HB2	2.48	0.43
1:1A:910:A:N1	1:1A:2277:G:H1'	2.34	0.43
1:1A:1051:G:H4'	1:1A:2752:C:H4'	1.99	0.43
1:1A:1054:A:N6	1:1A:1105:U:H3	2.14	0.43
1:1A:1951:U:O2'	1:1A:1953:A:N7	2.44	0.43
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.53	0.43
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.19	0.43
25:13:55:ARG:C	25:13:55:ARG:HE	2.27	0.43
32:1a:45:U:H2'	32:1a:46:G:C8	2.54	0.43
32:1a:262:A:C6	32:1a:263:A:C6	3.06	0.43
32:1a:741:G:H2'	32:1a:742:G:O4'	2.18	0.43
32:1a:976:G:OP1	45:1n:32:SER:N	2.49	0.43
32:1a:1429:C:H2'	32:1a:1430:C:H6	1.83	0.43
38:1g:22:LEU:HG	38:1g:62:PHE:HE2	1.84	0.43
54:1w:20:U:OP1	54:1w:20:U:H4'	2.18	0.43
54:1y:19:G:C4'	54:1y:57:G:H22	2.31	0.43
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.18	0.43
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.54	0.43
1:2A:2143:C:N4	1:2A:2148:G:H1	2.12	0.43
1:2A:2282:G:H4'	1:2A:2389:G:O2'	2.17	0.43
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.50	0.43
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.40	0.43
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	2.00	0.43
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.35	0.43
12:2Q:1:MET:HE2	12:2Q:1:MET:HB2	1.87	0.43
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	2.01	0.43
26:24:1:MET:HB3	26:24:6:HIS:CD2	2.54	0.43
32:2a:266:G:H2'	32:2a:266:G:N3	2.34	0.43
32:2a:1135:U:H2'	32:2a:1137:C:C4	2.54	0.43
33:2b:118:LEU:HD12	33:2b:118:LEU:HA	1.77	0.43
33:2b:153:ARG:C	33:2b:155:LEU:H	2.26	0.43
35:2d:33:MET:HB2	59:2d:302:SF4:S2	2.59	0.43
36:2e:31:LEU:HD23	36:2e:31:LEU:HA	1.81	0.43
38:2g:115:ARG:O	38:2g:119:ARG:HG3	2.18	0.43
54:2w:51:U:H2'	54:2w:52:G:C8	2.54	0.43
55:2x:23:C:H2'	55:2x:24:U:C6	2.53	0.43
1:1A:1510:G:H2'	1:1A:1511:C:C6	2.53	0.43
8:1I:47:LEU:HD22	8:1I:47:LEU:HA	1.77	0.43
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	2.01	0.43
21:1Z:155:LEU:HD12	21:1Z:156:LYS:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:381:C:H2'	32:1a:382:A:O4'	2.19	0.43
32:1a:735:C:H2'	32:1a:736:C:H6	1.83	0.43
32:1a:949:A:C6	32:1a:950:U:C4	3.07	0.43
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.53	0.43
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.53	0.43
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	2.01	0.43
36:1e:148:VAL:O	36:1e:152:ARG:HG3	2.19	0.43
47:1p:6:LEU:HB3	47:1p:17:TYR:CD1	2.54	0.43
48:1q:45:HIS:CE1	48:1q:47:PRO:HG3	2.54	0.43
54:1y:58:A:O2'	54:1y:60:U:OP2	2.32	0.43
1:2A:127:A:H5''	1:2A:128:C:C6	2.54	0.43
1:2A:687:C:H2'	1:2A:688:U:O4'	2.19	0.43
1:2A:1349:A:OP1	61:2A:3844:HOH:O	2.21	0.43
1:2A:2336:A:H61	22:20:43:THR:CG2	2.32	0.43
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.83	0.43
32:2a:953:G:H2'	32:2a:954:G:O4'	2.18	0.43
32:2a:1386:G:C2	32:2a:1387:G:C8	3.06	0.43
33:2b:10:LEU:HD12	33:2b:10:LEU:HA	1.84	0.43
33:2b:55:PHE:CE1	33:2b:218:ALA:HA	2.50	0.43
38:2g:26:PHE:CD2	38:2g:62:PHE:HE1	2.36	0.43
39:2h:103:VAL:HG21	39:2h:109:ILE:C	2.44	0.43
1:1A:71:A:H5''	1:1A:73:A:C8	2.53	0.43
1:1A:236:C:H2'	1:1A:237:C:C6	2.53	0.43
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.19	0.43
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.19	0.43
1:1A:2251:OMG:HM23	1:1A:2251:OMG:H1'	1.88	0.43
1:1A:2522:U:O2'	1:1A:2647:U:OP1	2.28	0.43
61:1A:4590:HOH:O	29:17:43:THR:HB	2.18	0.43
3:1D:96:HIS:NE2	3:1D:102:LYS:HE2	2.33	0.43
32:1a:501:C:H2'	32:1a:502:G:H8	1.84	0.43
32:1a:528:C:H41	43:11:49:ASN:CG	2.27	0.43
32:1a:690:G:C6	32:1a:691:G:C6	3.07	0.43
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.48	0.43
33:1b:219:VAL:O	33:1b:223:ILE:HG13	2.18	0.43
40:1i:49:PRO:HD3	40:1i:78:LYS:HG3	2.01	0.43
1:2A:579:G:H2'	1:2A:580:C:C6	2.53	0.43
1:2A:1263:U:C4	1:2A:1264:G:C6	3.07	0.43
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.19	0.43
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.54	0.43
7:2H:2:SER:O	7:2H:3:ARG:HG2	2.19	0.43
21:2Z:47:VAL:HG13	21:2Z:51:ALA:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:20:36:ILE:HD12	22:20:58:THR:HG21	1.99	0.43
32:2a:501:C:H2'	32:2a:502:G:C8	2.53	0.43
32:2a:523:A:N1	43:2l:92:0TD:H6	2.34	0.43
32:2a:629:G:H2'	32:2a:630:G:O4'	2.19	0.43
32:2a:1350:A:C2	32:2a:1351:U:C2	3.07	0.43
32:2a:1401:G:H2'	32:2a:1402:4OC:O4'	2.19	0.43
33:2b:27:LYS:HB2	33:2b:194:PRO:HD2	1.99	0.43
35:2d:17:VAL:HG12	35:2d:19:LEU:HD12	2.01	0.43
47:2p:58:TYR:O	47:2p:61:SER:OG	2.28	0.43
1:1A:444:C:H4'	5:1F:49:ALA:HB2	2.00	0.43
1:1A:566:U:H5''	11:1P:29:LYS:HE3	2.00	0.43
1:1A:1047:G:H2'	1:1A:1110:G:H1	1.83	0.43
1:1A:1453:U:OP1	13:1R:77:ARG:HD3	2.19	0.43
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.53	0.43
1:1A:2674:G:H5''	10:1O:26:LYS:HE3	2.01	0.43
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.49	0.43
5:1F:135:LYS:HB2	5:1F:138:GLU:CD	2.43	0.43
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.53	0.43
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.19	0.43
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.62	0.43
9:1N:104:LYS:HB2	9:1N:117:PHE:CE1	2.53	0.43
18:1W:23:LEU:HD21	27:15:25:LEU:HB2	2.00	0.43
26:14:16:CYS:HB2	26:14:36:CYS:HB3	2.01	0.43
32:1a:189(C):C:H2'	32:1a:189(D):C:O4'	2.19	0.43
32:1a:310:G:OP2	47:1p:27:LYS:HE2	2.18	0.43
32:1a:502:G:H2'	32:1a:503:C:O4'	2.19	0.43
32:1a:790:A:N1	32:1a:1497:G:H5''	2.34	0.43
32:1a:909:A:H2'	32:1a:910:C:O4'	2.18	0.43
50:1s:3:ARG:NH2	50:1s:7:LYS:HE2	2.34	0.43
1:2A:902:C:H2'	1:2A:903:C:C6	2.53	0.43
1:2A:1204:A:N6	1:2A:1240:U:H2'	2.34	0.43
1:2A:1902:C:H5'	3:2D:246:PRO:HD3	2.00	0.43
5:2F:137:LYS:HE2	5:2F:137:LYS:HB3	1.55	0.43
10:2O:20:MET:HE3	10:2O:44:LYS:HE3	2.00	0.43
12:2Q:82:ARG:H	22:20:7:LEU:HD21	1.84	0.43
32:2a:866:C:C4'	32:2a:919:A:H5'	2.49	0.43
32:2a:1130:A:H5''	40:2i:18:PHE:CE2	2.54	0.43
32:2a:1206:G:H2'	32:2a:1207:2MG:C8	2.54	0.43
32:2a:1411:C:H2'	32:2a:1412:C:H6	1.83	0.43
36:2e:78:HIS:HB3	39:2h:107:LEU:HD12	2.00	0.43
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:768:G:O2'	1:1A:1379:A:N1	2.48	0.43
1:1A:1176:G:N2	1:1A:1178:C:O5'	2.52	0.43
1:1A:1243:G:O3'	11:1P:7:ARG:NH2	2.51	0.43
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.34	0.43
2:1B:12:C:O2'	22:10:74:ARG:HB3	2.18	0.43
9:1N:138:LEU:HD23	9:1N:138:LEU:HA	1.81	0.43
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.34	0.43
21:1Z:150:LEU:H	21:1Z:150:LEU:HD23	1.84	0.43
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.54	0.43
32:1a:309:G:H1'	32:1a:608:A:C2	2.53	0.43
32:1a:966:M2G:HM13	32:1a:967:5MC:H1'	2.01	0.43
32:1a:1001(A):G:C2	32:1a:1002:G:H1'	2.54	0.43
1:2A:222:A:H3'	1:2A:421:U:H5'	2.01	0.43
1:2A:402:A:C2'	1:2A:403:U:H5'	2.49	0.43
1:2A:820:A:N3	1:2A:943:U:H4'	2.34	0.43
1:2A:1325:G:OP1	1:2A:1647:G:O2'	2.20	0.43
1:2A:1496:A:N3	1:2A:1577:C:O2'	2.42	0.43
1:2A:1592:C:H2'	1:2A:1593:G:C8	2.53	0.43
1:2A:2238:G:H5''	61:2A:4511:HOH:O	2.18	0.43
5:2F:196:LEU:HD23	5:2F:196:LEU:HA	1.78	0.43
6:2G:56:ALA:HA	6:2G:59:GLU:HG2	2.01	0.43
11:2P:98:GLU:O	11:2P:102:ARG:HD3	2.18	0.43
15:2T:102:ILE:HB	15:2T:110:ILE:HG12	2.01	0.43
21:2Z:35:ARG:HD3	21:2Z:35:ARG:HA	1.77	0.43
21:2Z:79:ARG:HB2	21:2Z:80:ARG:NH1	2.34	0.43
23:21:25:LYS:HE2	23:21:31:GLY:HA3	2.01	0.43
32:2a:109:A:H5'	32:2a:110:C:C5	2.53	0.43
32:2a:391:G:C6	32:2a:392:G:C5	3.07	0.43
32:2a:537:G:H5''	43:2l:113:ARG:NH1	2.34	0.43
32:2a:1096:C:C2'	32:2a:1097:C:H5'	2.48	0.43
32:2a:1122:U:C4	32:2a:1123:A:N7	2.87	0.43
53:2v:12:A:N3	53:2v:12:A:H2'	2.34	0.43
54:2w:4:C:H42	54:2w:69:G:H1	1.67	0.43
1:1A:882:G:H4'	54:1w:19:G:O6	2.17	0.43
1:1A:1053:C:N4	1:1A:1106:G:H1	2.15	0.43
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.54	0.43
2:1B:74:U:H2'	2:1B:75:G:O4'	2.19	0.43
11:1P:59:LEU:HD13	30:18:58:ILE:HD13	2.00	0.43
32:1a:1060:C:H5''	41:1j:51:ARG:HG2	2.01	0.43
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.18	0.43
34:1c:5:ILE:HG12	34:1c:6:HIS:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:95:ALA:O	36:1e:98:THR:HG23	2.19	0.43
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.99	0.43
1:2A:288:C:H2'	1:2A:289:A:H8	1.84	0.43
1:2A:764:A:H5''	3:2D:210:GLY:HA2	1.99	0.43
1:2A:892:G:C6	1:2A:893:C:H1'	2.54	0.43
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.82	0.43
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.54	0.43
20:2Y:16:ALA:HB2	20:2Y:73:ARG:HG3	2.00	0.43
21:2Z:55:HIS:HE1	21:2Z:135:GLU:HB2	1.84	0.43
32:2a:114:U:H2'	32:2a:115:G:C8	2.54	0.43
32:2a:625:G:H2'	32:2a:626:U:C6	2.53	0.43
32:2a:881:G:OP2	43:2l:12:ARG:NH2	2.52	0.43
32:2a:1277:C:HO2'	32:2a:1279:A:H8	1.58	0.43
36:2e:34:VAL:O	36:2e:42:GLY:N	2.47	0.43
36:2e:84:PHE:O	36:2e:86:ALA:N	2.50	0.43
39:2h:84:ARG:HH12	39:2h:86:ILE:HA	1.83	0.43
44:2m:60:VAL:HG13	44:2m:64:TRP:CE3	2.54	0.43
1:1A:620:G:H2'	1:1A:620:G:N3	2.33	0.42
1:1A:637:A:OP1	11:1P:133:SER:OG	2.24	0.42
1:1A:2515:C:O2'	1:1A:2516:G:H5'	2.19	0.42
3:1D:21:PHE:HB3	3:1D:24:ILE:HD12	2.01	0.42
4:1E:7:VAL:HG23	4:1E:51:PHE:CE2	2.52	0.42
10:1O:113:LYS:HE2	10:1O:117:LEU:HD11	2.01	0.42
11:1P:63:PRO:HG2	30:18:25:MET:HB2	2.01	0.42
18:1W:7:ALA:HB2	18:1W:50:VAL:HG22	2.01	0.42
28:16:47:THR:HG22	28:16:48:VAL:O	2.19	0.42
32:1a:1086:U:H3	32:1a:1099:G:N2	2.13	0.42
32:1a:1224:G:OP1	61:1a:1812:HOH:O	2.22	0.42
32:1a:1452:C:H3'	32:1a:1452:C:OP2	2.19	0.42
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.84	0.42
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.34	0.42
1:2A:852:G:H2'	1:2A:853:G:C8	2.50	0.42
1:2A:856:C:HO2'	1:2A:857:C:P	2.42	0.42
1:2A:2233:U:H2'	1:2A:2234:G:C8	2.54	0.42
1:2A:2853:C:H2'	1:2A:2854:G:H8	1.84	0.42
15:2T:56:GLY:O	15:2T:59:THR:HG22	2.18	0.42
28:26:12:GLU:OE1	28:26:19:ARG:NH1	2.52	0.42
32:2a:21:G:H2'	32:2a:22:G:C8	2.54	0.42
32:2a:37:U:H2'	32:2a:38:G:O4'	2.19	0.42
32:2a:671:G:H2'	32:2a:672:U:O4'	2.18	0.42
32:2a:922:G:N3	32:2a:1398:A:H2	2.17	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.19	0.42
40:2i:6:GLY:HA3	40:2i:80:GLY:O	2.19	0.42
55:2x:44:A:H2'	55:2x:45:G:C8	2.55	0.42
1:1A:603:A:O4'	1:1A:655:A:N6	2.52	0.42
1:1A:1448:G:H1'	1:1A:1528:A:N1	2.35	0.42
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.52	0.42
6:1G:167:GLU:OE1	6:1G:167:GLU:N	2.46	0.42
11:1P:119:GLU:OE2	25:23:3:ARG:NH1	2.52	0.42
20:1Y:5:MET:HE2	20:1Y:5:MET:HB2	1.84	0.42
21:1Z:48:PHE:CE1	21:1Z:71:VAL:HG11	2.54	0.42
32:1a:397:A:H3'	32:1a:397:A:N3	2.34	0.42
32:1a:542:G:H5'	35:1d:41:GLY:HA3	2.00	0.42
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.52	0.42
32:1a:1304:G:C6	32:1a:1305:G:N1	2.88	0.42
39:1h:77:GLU:HG3	39:1h:78:GLN:N	2.34	0.42
49:1r:59:SER:H	49:1r:62:GLU:HB2	1.82	0.42
51:1t:74:LYS:HE2	51:1t:74:LYS:HB3	1.91	0.42
1:2A:484:C:H2'	1:2A:485:C:C6	2.54	0.42
1:2A:1227:G:OP1	16:2U:13:LYS:HG2	2.18	0.42
1:2A:1800:C:OP1	3:2D:260:ARG:NH2	2.52	0.42
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.19	0.42
1:2A:2431:U:OP2	61:2A:3845:HOH:O	2.22	0.42
1:2A:2771:C:H2'	1:2A:2772:C:C6	2.54	0.42
1:2A:2773:C:H2'	1:2A:2774:C:H6	1.83	0.42
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.19	0.42
4:2E:183:LEU:HD21	15:2T:10:VAL:HG11	2.01	0.42
6:2G:76:SER:H	6:2G:84:LYS:HB2	1.84	0.42
15:2T:27:THR:C	15:2T:89:VAL:HG23	2.44	0.42
21:2Z:6:LYS:NZ	21:2Z:43:GLU:OE2	2.44	0.42
30:28:52:LYS:N	30:28:53:PRO:HD2	2.34	0.42
32:2a:157:G:H2'	32:2a:158:G:H8	1.84	0.42
32:2a:176:C:H2'	32:2a:177:C:C6	2.54	0.42
32:2a:868:C:H2'	32:2a:869:G:O4'	2.19	0.42
32:2a:1133:G:H2'	32:2a:1134:G:O4'	2.19	0.42
36:2e:19:MET:SD	36:2e:24:ARG:HG3	2.58	0.42
37:2f:76:ALA:O	37:2f:80:ARG:HG3	2.19	0.42
48:2q:54:GLY:O	48:2q:81:ARG:N	2.48	0.42
55:2x:66:C:H2'	55:2x:67:C:O4'	2.19	0.42
1:1A:218:A:C2	1:1A:235:U:H4'	2.54	0.42
1:1A:1968:G:OP1	61:1A:4137:HOH:O	2.22	0.42
1:1A:2203:U:O4'	3:1D:151:LYS:HE2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.52	0.42
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	2.01	0.42
19:1X:94:GLY:HA3	19:1X:95:LEU:HB2	2.01	0.42
32:1a:277:C:P	48:1q:68:ARG:HH12	2.42	0.42
32:1a:317:G:C6	32:1a:318:G:C5	3.07	0.42
32:1a:461:A:O2'	32:1a:470:C:H5'	2.19	0.42
32:1a:553:A:H5''	43:1l:24:VAL:HG21	2.00	0.42
32:1a:652:U:O4	32:1a:752:G:O2'	2.31	0.42
32:1a:1186:G:H4'	40:1i:110:GLU:OE2	2.19	0.42
32:1a:1273:G:H3'	32:1a:1274:G:C8	2.54	0.42
35:1d:101:LEU:HD21	35:1d:126:ILE:HG21	2.00	0.42
47:1p:60:LEU:HD12	47:1p:60:LEU:HA	1.89	0.42
1:2A:578:A:OP1	1:2A:1255:U:O2'	2.29	0.42
1:2A:581:C:H2'	1:2A:582:G:H8	1.83	0.42
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.33	0.42
1:2A:1743:C:H2'	1:2A:1744:C:O4'	2.19	0.42
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	2.01	0.42
16:2U:85:LYS:HE2	16:2U:85:LYS:HB3	1.83	0.42
32:2a:618:C:O2	32:2a:622:A:N6	2.52	0.42
32:2a:1004:A:N6	32:2a:1037:C:O2	2.30	0.42
33:2b:42:ILE:HG21	33:2b:202:PRO:O	2.19	0.42
1:1A:1006:C:C2	1:1A:1138:G:N2	2.88	0.42
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.65	0.42
4:1E:105:THR:OG1	4:1E:166:THR:OG1	2.27	0.42
10:1O:48:PRO:CB	32:1a:1422:G:H5''	2.50	0.42
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	2.01	0.42
32:1a:880:C:OP1	43:1l:8:ASN:ND2	2.39	0.42
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.54	0.42
32:1a:1144:G:N2	32:1a:1146:A:H62	2.17	0.42
54:1w:45:U:H5'	54:1w:46:G7M:OP2	2.18	0.42
1:2A:588:U:H2'	1:2A:589:C:C6	2.54	0.42
1:2A:731:C:H5''	61:2A:4271:HOH:O	2.19	0.42
1:2A:2303:G:O2'	6:2G:132:ASN:ND2	2.52	0.42
1:2A:2750:A:H1'	1:2A:2752:C:N4	2.35	0.42
6:2G:129:GLY:O	6:2G:161:THR:HB	2.18	0.42
10:2O:113:LYS:HD2	10:2O:113:LYS:HA	1.67	0.42
14:2S:11:LYS:O	14:2S:15:ARG:HB2	2.19	0.42
18:2W:57:ASN:HA	18:2W:61:ASN:HD22	1.85	0.42
24:22:7:ARG:HA	24:22:10:LEU:HD12	2.01	0.42
32:2a:649:G:H2'	32:2a:650:G:O4'	2.20	0.42
32:2a:901:A:O2'	32:2a:1513:A:OP1	2.26	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:204:ASN:O	33:2b:210:SER:HB3	2.20	0.42
35:2d:13:ARG:HB3	35:2d:38:TYR:O	2.19	0.42
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	2.00	0.42
40:2i:63:ILE:HD13	40:2i:77:ILE:HG23	2.00	0.42
40:2i:79:LEU:HG	40:2i:83:ARG:HD2	2.01	0.42
1:1A:1070:A:N3	1:1A:1070:A:H2'	2.35	0.42
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.19	0.42
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	2.02	0.42
1:1A:2101:G:H2'	1:1A:2102:U:C6	2.54	0.42
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.55	0.42
7:1H:3:ARG:HH22	7:1H:66:GLY:N	2.18	0.42
12:1Q:17:LEU:HD21	12:1Q:96:VAL:HG13	2.01	0.42
24:12:16:LEU:HB3	24:12:20:GLU:HB2	2.02	0.42
26:14:12:ALA:CB	26:14:26:SER:HB3	2.49	0.42
26:14:59:PHE:CD2	50:1s:64:GLU:HB3	2.55	0.42
32:1a:270:A:H2'	32:1a:271:C:C6	2.55	0.42
32:1a:735:C:H2'	32:1a:736:C:C6	2.54	0.42
32:1a:865:A:C2	32:1a:918:A:H4'	2.55	0.42
32:1a:1003:G:H2'	32:1a:1004:A:N3	2.35	0.42
32:1a:1367:C:H5'	41:1j:60:ARG:NH1	2.34	0.42
34:1c:53:ALA:HB2	34:1c:115:LEU:HD21	2.02	0.42
38:1g:113:GLU:HB2	38:1g:119:ARG:HG2	2.01	0.42
46:1o:29:VAL:HG13	46:1o:63:ARG:HG3	2.00	0.42
1:2A:271(R):G:OP1	23:21:76:ARG:NE	2.46	0.42
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.20	0.42
1:2A:1851:U:H2'	1:2A:1852:C:O4'	2.19	0.42
1:2A:2654:A:N1	1:2A:2665:A:H5''	2.34	0.42
6:2G:5:VAL:HG22	6:2G:8:LYS:HB2	2.01	0.42
6:2G:76:SER:N	6:2G:84:LYS:HB2	2.34	0.42
8:2I:82:ARG:NE	8:2I:82:ARG:H	2.18	0.42
10:2O:4:PRO:O	10:2O:5:GLN:HB2	2.19	0.42
32:2a:1233:G:H2'	32:2a:1234:C:C6	2.54	0.42
36:2e:78:HIS:CD2	36:2e:142:LEU:HD23	2.54	0.42
40:2i:82:ALA:O	40:2i:86:VAL:HG23	2.19	0.42
48:2q:29:HIS:CG	48:2q:30:PRO:HD2	2.54	0.42
51:2t:72:LEU:HD12	51:2t:72:LEU:HA	1.86	0.42
54:2w:22:G:H2'	54:2w:23:A:C8	2.54	0.42
1:1A:7:G:H2'	1:1A:8:A:O4'	2.20	0.42
1:1A:620:G:N3	1:1A:620:G:H5'	2.34	0.42
1:1A:762:U:H5''	61:1A:5146:HOH:O	2.19	0.42
1:1A:1364:G:C8	23:11:3:LYS:HD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.20	0.42
1:1A:1448:G:O2'	1:1A:1528(A):A:N1	2.48	0.42
1:1A:1800:C:OP2	3:1D:183:ARG:NH2	2.51	0.42
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.20	0.42
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	2.01	0.42
6:1G:66:GLN:HG3	26:14:1:MET:CE	2.50	0.42
32:1a:96:U:H2'	32:1a:97:G:C8	2.53	0.42
32:1a:266:G:H2'	32:1a:266:G:N3	2.34	0.42
32:1a:584:G:H5'	48:1q:91:ARG:NH2	2.34	0.42
33:1b:92:TYR:CE1	33:1b:94:ASN:HB2	2.55	0.42
39:1h:17:THR:HB	39:1h:78:GLN:OE1	2.20	0.42
39:1h:73:ASP:OD1	39:1h:75:ARG:NE	2.53	0.42
40:1i:8:GLY:O	40:1i:15:ALA:N	2.53	0.42
55:1x:23:C:H2'	55:1x:24:U:C6	2.55	0.42
1:2A:218:A:C2	1:2A:235:U:H4'	2.54	0.42
1:2A:900:A:H3'	1:2A:901:A:C8	2.53	0.42
1:2A:2335:A:C8	1:2A:2337:G:C5	3.08	0.42
1:2A:2663:G:H3'	1:2A:2664:G:C8	2.52	0.42
5:2F:158:THR:HB	5:2F:195:ASP:HB2	2.02	0.42
6:2G:16:ARG:NE	6:2G:31:VAL:HG11	2.34	0.42
15:2T:15:VAL:HG13	15:2T:79:HIS:CE1	2.53	0.42
21:2Z:70:LEU:HD12	21:2Z:71:VAL:N	2.35	0.42
32:2a:179:A:H2'	32:2a:180:U:C6	2.55	0.42
32:2a:432:A:H3'	32:2a:433:C:H6	1.85	0.42
32:2a:1261:A:H3'	32:2a:1262:C:H6	1.85	0.42
32:2a:1277:C:HO2'	32:2a:1279:A:H1'	1.84	0.42
32:2a:1466:C:H2'	32:2a:1467:G:O4'	2.20	0.42
33:2b:100:GLY:HA2	33:2b:103:THR:OG1	2.20	0.42
33:2b:102:LEU:HD13	33:2b:182:ILE:HD12	2.02	0.42
33:2b:150:SER:OG	33:2b:151:GLY:N	2.52	0.42
35:2d:11:LEU:O	35:2d:15:GLU:HG2	2.19	0.42
35:2d:153:ARG:HB3	35:2d:181:MET:HE3	2.01	0.42
38:2g:50:ILE:HD11	38:2g:58:PRO:HA	2.01	0.42
1:1A:616:G:H5'	5:1F:205:ARG:HD3	2.01	0.42
1:1A:652(D):C:H42	1:1A:652(U):G:H1	1.66	0.42
1:1A:898:C:H2'	1:1A:899:A:H5'	2.01	0.42
1:1A:1354:A:C5'	3:1D:38:LYS:HE3	2.47	0.42
1:1A:1815:A:H8	1:1A:1815:A:OP1	2.03	0.42
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.20	0.42
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	2.01	0.42
32:1a:663:A:H2'	32:1a:664:G:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1071:C:H2'	32:1a:1072:G:H8	1.85	0.42
42:1k:34:ASP:HB2	42:1k:35:PRO:HD2	2.02	0.42
48:1q:67:LYS:HA	48:1q:70:ARG:NH1	2.35	0.42
1:2A:94(A):G:H2'	1:2A:95:G:O4'	2.20	0.42
1:2A:747:U:O2	1:2A:2014:A:H1'	2.20	0.42
1:2A:829:A:N7	1:2A:2248:C:H5'	2.34	0.42
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	2.00	0.42
2:2B:40:U:C5	26:24:2:LYS:HG3	2.55	0.42
6:2G:3:LEU:H	6:2G:3:LEU:HG	1.67	0.42
7:2H:95:ARG:NH2	7:2H:97:ARG:HH11	2.17	0.42
15:2T:28:VAL:HG23	15:2T:88:ILE:HD13	2.01	0.42
19:2X:27:THR:HA	19:2X:79:ALA:O	2.20	0.42
20:2Y:20:TYR:CE2	20:2Y:43:ASN:HA	2.55	0.42
26:24:62:ARG:HB2	26:24:63:TYR:CE2	2.54	0.42
29:27:47:ARG:HE	29:27:47:ARG:HB3	1.39	0.42
32:2a:1118:C:H1'	32:2a:1179:A:C5	2.55	0.42
32:2a:1212:U:H5''	32:2a:1213:A:O5'	2.19	0.42
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.34	0.42
32:2a:1373:G:H5''	38:2g:36:LYS:HE2	2.02	0.42
33:2b:146:GLN:O	33:2b:150:SER:HB3	2.20	0.42
37:2f:82:ARG:HB2	37:2f:85:VAL:HG23	2.00	0.42
38:2g:131:LYS:HE2	38:2g:131:LYS:HB3	1.82	0.42
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	2.02	0.42
42:2k:34:ASP:OD2	42:2k:38:ASN:HB2	2.19	0.42
44:2m:89:GLY:O	44:2m:93:ARG:HG2	2.19	0.42
1:1A:272(F):C:H42	1:1A:363(D):G:H1	1.68	0.42
1:1A:831:G:O2'	11:1P:38:GLN:OE1	2.32	0.42
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.19	0.42
1:1A:2654:A:N1	1:1A:2665:A:H5''	2.34	0.42
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.19	0.42
32:1a:100:C:H2'	32:1a:101:A:C8	2.55	0.42
32:1a:445:G:H2'	32:1a:446:G:C8	2.54	0.42
32:1a:486:U:H2'	32:1a:487:A:C8	2.52	0.42
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.19	0.42
37:1f:44:GLY:HA2	37:1f:59:TYR:CD2	2.55	0.42
42:1k:67:ASP:OD1	42:1k:71:LYS:HE3	2.20	0.42
47:1p:47:ASP:OD1	47:1p:47:ASP:N	2.52	0.42
54:1w:1:G:H2'	54:1w:2:C:C6	2.55	0.42
1:2A:996:A:C2	1:2A:997:G:C8	3.08	0.42
1:2A:2029:G:H2'	1:2A:2031:A:OP1	2.20	0.42
1:2A:2484:G:C2	1:2A:2485:G:C8	3.08	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:23:PHE:HB2	6:2G:25:TYR:CZ	2.55	0.42
6:2G:148:MET:HE2	6:2G:148:MET:HB3	1.86	0.42
10:2O:1:MET:HE3	10:2O:32:TYR:CE1	2.54	0.42
22:20:27:GLU:HB2	22:20:69:PHE:HD1	1.85	0.42
32:2a:357:G:OP1	32:2a:367:U:H5''	2.20	0.42
32:2a:406:G:H5'	35:2d:5:ILE:HD11	2.00	0.42
32:2a:575:G:O2'	32:2a:821:G:H5'	2.20	0.42
32:2a:986:A:H1'	50:2s:54:GLY:O	2.20	0.42
32:2a:1120:G:O6	32:2a:1152:A:N6	2.53	0.42
32:2a:1128:C:HO2'	32:2a:1129:C:P	2.40	0.42
32:2a:1168:A:H2'	32:2a:1169:A:C8	2.54	0.42
32:2a:1289:A:OP1	52:2u:9:ARG:NH1	2.47	0.42
39:2h:85:ARG:NH1	39:2h:87:SER:O	2.53	0.42
1:1A:65:C:H5'	19:1X:71:GLY:HA3	2.02	0.42
1:1A:897:C:C2	1:1A:898:C:C4	3.07	0.42
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.20	0.42
1:1A:1417:C:H2'	1:1A:1418:G:O4'	2.20	0.42
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.54	0.42
1:1A:1594:G:H5''	61:1A:5725:HOH:O	2.20	0.42
1:1A:2064:C:H2'	1:1A:2065:C:C6	2.55	0.42
1:1A:2298:A:H2'	1:1A:2299:G:O4'	2.20	0.42
1:1A:2312:U:OP1	6:1G:73:ALA:HA	2.20	0.42
1:1A:2667:C:H1'	7:1H:109:PHE:CD1	2.54	0.42
3:1D:169:GLU:OE2	3:1D:184:LYS:NZ	2.47	0.42
6:1G:64:THR:HB	6:1G:94:LEU:HD11	2.02	0.42
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.84	0.42
32:1a:971:G:N2	32:1a:1363(A):A:OP2	2.50	0.42
32:1a:1164:G:H2'	32:1a:1165:C:C6	2.54	0.42
33:1b:80:ILE:O	33:1b:84:GLU:HG2	2.20	0.42
1:2A:994:C:O2'	1:2A:996:A:OP1	2.36	0.42
1:2A:2135:A:C8	1:2A:2136:C:H5	2.37	0.42
1:2A:2493:U:O2'	12:2Q:80:GLU:OE2	2.35	0.42
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.19	0.42
7:2H:16:SER:OG	7:2H:27:LYS:HB2	2.20	0.42
8:2I:117:GLU:H	8:2I:117:GLU:HG3	1.43	0.42
25:23:27:GLY:HA3	25:23:35:ARG:NE	2.35	0.42
32:2a:818:G:O2'	32:2a:819:A:H5'	2.20	0.42
32:2a:1091:U:H2'	32:2a:1093:A:OP2	2.20	0.42
35:2d:15:GLU:HB3	35:2d:63:LYS:HG2	2.02	0.42
38:2g:42:ILE:HG22	38:2g:120:ILE:HD12	2.02	0.42
38:2g:71:PRO:HG3	38:2g:103:TRP:CH2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2p:28:ARG:HG2	47:2p:28:ARG:HH11	1.85	0.42
48:2q:78:GLU:OE1	48:2q:81:ARG:NH1	2.53	0.42
1:1A:1174:A:H1'	1:1A:1175:U:H5''	2.01	0.42
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.85	0.42
15:1T:41:ARG:HH21	15:1T:43:GLN:NE2	2.18	0.42
21:1Z:43:GLU:O	21:1Z:46:LYS:HG3	2.19	0.42
21:1Z:72:ARG:HA	21:1Z:72:ARG:HD3	1.88	0.42
32:1a:353:A:H5'	32:1a:353:A:H8	1.85	0.42
40:1i:49:PRO:HG2	40:1i:81:ILE:HG23	2.02	0.42
1:2A:263:C:H2'	1:2A:264:C:O4'	2.20	0.42
1:2A:383:U:H2'	1:2A:385:C:H5	1.85	0.42
1:2A:1662:C:O2'	1:2A:2687:U:OP1	2.36	0.42
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.19	0.42
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.55	0.42
1:2A:2516:G:C6	1:2A:2517:C:N4	2.88	0.42
9:2N:103:VAL:O	9:2N:107:LEU:HG	2.20	0.42
32:2a:264:U:H2'	32:2a:265:G:O4'	2.20	0.42
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.35	0.42
32:2a:1055:A:C6	32:2a:1206:G:C5	3.08	0.42
32:2a:1256:A:H61	32:2a:1278:U:C2'	2.33	0.42
32:2a:1256:A:O3'	32:2a:1257:U:H4'	2.20	0.42
32:2a:1289:A:P	52:2u:9:ARG:HH22	2.43	0.42
33:2b:187:LEU:HD23	33:2b:201:ILE:O	2.19	0.42
55:2x:50:U:H3	55:2x:64:G:H1	1.66	0.42
54:2y:37:MIA:H2'	54:2y:38:A:O4'	2.19	0.42
1:1A:1042:G:H2'	1:1A:1043:C:O4'	2.20	0.41
1:1A:1441:G:H2'	1:1A:1442:G:H8	1.85	0.41
1:1A:1567:A:OP2	3:1D:84:TYR:OH	2.30	0.41
1:1A:1946:U:H2'	1:1A:1947:C:C6	2.55	0.41
1:1A:2168:G:N1	1:1A:2171:A:C8	2.88	0.41
1:1A:2854:G:H2'	1:1A:2855:C:C6	2.54	0.41
2:1B:13:A:N1	2:1B:69:G:O2'	2.48	0.41
8:1I:140:LEU:HD23	8:1I:140:LEU:HA	1.89	0.41
32:1a:376:G:P	47:1p:67:THR:HG21	2.60	0.41
32:1a:737:A:H2'	32:1a:738:C:C6	2.55	0.41
32:1a:1084:G:C5	32:1a:1085:U:C4	3.08	0.41
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.20	0.41
35:1d:116:GLN:HE22	35:1d:161:ASN:HD21	1.68	0.41
44:1m:87:TYR:CZ	44:1m:91:ARG:HD3	2.55	0.41
54:1w:43:C:H2'	54:1w:44:G:C8	2.55	0.41
1:2A:40:C:H2'	1:2A:41:C:C6	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:250:G:C6	1:2A:251:A:C6	3.08	0.41
1:2A:793:A:O2'	61:2A:3847:HOH:O	2.22	0.41
1:2A:1169:G:C2	1:2A:1170:G:N7	2.88	0.41
1:2A:1243:G:H2'	1:2A:1244:G:O4'	2.20	0.41
1:2A:1301:A:H2	1:2A:1626:G:N3	2.18	0.41
1:2A:1545:A:H2'	1:2A:1546:C:O4'	2.20	0.41
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.55	0.41
1:2A:2636:U:HO2'	4:2E:44:TYR:HH	1.61	0.41
3:2D:121:PRO:HB3	3:2D:135:PHE:CE2	2.55	0.41
6:2G:106:LEU:HG	6:2G:111:LEU:HD13	2.02	0.41
23:21:80:LEU:HD23	23:21:82:LEU:HD21	2.01	0.41
32:2a:540:G:H2'	32:2a:541:G:O4'	2.19	0.41
32:2a:961:U:H2'	32:2a:962:C:O4'	2.20	0.41
32:2a:974:A:C1'	45:2n:31:ARG:HE	2.33	0.41
32:2a:1265:G:C4	32:2a:1271:G:N2	2.87	0.41
35:2d:196:LEU:O	35:2d:198:VAL:N	2.45	0.41
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.29	0.41
48:2q:67:LYS:O	48:2q:68:ARG:HB2	2.20	0.41
1:1A:184:C:H2'	1:1A:185:U:H6	1.85	0.41
1:1A:459:U:H5''	29:17:40:TRP:CD2	2.55	0.41
1:1A:677:A:OP1	61:1A:4135:HOH:O	2.21	0.41
1:1A:2059:A:H2'	1:1A:2503:2MA:HM23	2.03	0.41
15:1T:127:ALA:O	15:1T:129:ARG:N	2.48	0.41
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.81	0.41
32:1a:437:U:H5'	35:1d:155:LEU:HD11	2.02	0.41
32:1a:985:C:H2'	32:1a:986:A:H8	1.85	0.41
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.20	0.41
32:1a:1123:A:O2'	41:1j:37:PRO:O	2.34	0.41
34:1c:121:ALA:O	34:1c:125:GLU:HG3	2.21	0.41
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	2.03	0.41
41:1j:49:VAL:HG13	45:1n:41:ARG:HB2	2.02	0.41
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.31	0.41
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.55	0.41
47:1p:50:LYS:HD2	47:1p:50:LYS:HA	1.91	0.41
49:1r:52:PRO:HG2	49:1r:54:ARG:HH11	1.85	0.41
1:2A:881:G:H3'	1:2A:882:G:H8	1.85	0.41
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.85	0.41
1:2A:1420:U:O5'	1:2A:1420:U:H6	2.03	0.41
1:2A:1999:C:H4'	1:2A:2723:C:O2	2.20	0.41
1:2A:2114:A:H2	1:2A:2171:A:H61	1.65	0.41
1:2A:2379:G:HO2'	14:2S:17:ARG:HH12	1.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2387:U:H1'	22:20:41:ARG:HE	1.85	0.41
1:2A:2689:U:OP2	1:2A:2719:G:N2	2.46	0.41
2:2B:118:G:OP2	61:2B:301:HOH:O	2.21	0.41
3:2D:71:ASP:CB	3:2D:103:ARG:HH12	2.32	0.41
3:2D:232:PRO:HB3	3:2D:244:ARG:CZ	2.50	0.41
4:2E:52:LEU:O	4:2E:76:ARG:N	2.45	0.41
6:2G:20:ILE:HA	6:2G:25:TYR:HD2	1.85	0.41
6:2G:63:ILE:HD13	6:2G:143:GLU:HB2	2.02	0.41
6:2G:120:LEU:HD11	6:2G:178:PHE:HD2	1.84	0.41
10:2O:35:VAL:HG23	10:2O:65:THR:HG23	2.01	0.41
12:2Q:3:MET:HB2	12:2Q:3:MET:HE3	1.84	0.41
12:2Q:130:LYS:HB3	12:2Q:130:LYS:HE2	1.86	0.41
15:2T:16:ARG:H	15:2T:16:ARG:HG3	1.74	0.41
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.38	0.41
15:2T:60:THR:HG22	15:2T:77:PRO:HA	2.02	0.41
16:2U:98:LEU:HD22	16:2U:105:VAL:HG11	2.02	0.41
20:2Y:90:LEU:HB3	20:2Y:92:ASN:H	1.85	0.41
21:2Z:27:VAL:HG12	21:2Z:85:HIS:HE1	1.86	0.41
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.55	0.41
32:2a:1287:A:H61	32:2a:1371:G:C1'	2.33	0.41
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.20	0.41
35:2d:57:ARG:HB3	35:2d:206:PHE:HB2	2.01	0.41
41:2j:61:GLU:OE2	45:2n:58:LYS:NZ	2.50	0.41
46:2o:37:ASN:O	46:2o:41:GLU:HG2	2.20	0.41
55:2x:10:G:N2	55:2x:26:G:H1'	2.35	0.41
55:2x:37:A:H2'	55:2x:38:A:O4'	2.21	0.41
1:1A:772:C:N4	61:1A:4176:HOH:O	2.53	0.41
1:1A:1919:A:O3'	32:1a:1517:G:H1'	2.20	0.41
3:1D:133:LEU:HD23	3:1D:133:LEU:HA	1.93	0.41
9:1N:120:LEU:HG	9:1N:122:VAL:HG23	2.02	0.41
13:1R:59:ASP:OD1	13:1R:59:ASP:N	2.48	0.41
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.20	0.41
32:1a:390:C:H2'	32:1a:391:G:C8	2.55	0.41
32:1a:864:A:H2'	32:1a:865:A:C8	2.55	0.41
32:1a:894:G:C6	32:1a:895:G:C5	3.08	0.41
34:1c:148:GLY:HA3	34:1c:172:ARG:H	1.86	0.41
39:1h:28:ALA:HA	39:1h:59:LEU:HG	2.02	0.41
1:2A:18:C:O2'	1:2A:554:U:OP1	2.34	0.41
1:2A:271(X):G:C2	1:2A:271(Y):U:O4	2.73	0.41
1:2A:724:U:H2'	1:2A:725:G:O4'	2.19	0.41
1:2A:819:A:OP2	1:2A:1187:G:N2	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.19	0.41
12:2Q:70:PRO:HA	12:2Q:95:ALA:HB2	2.03	0.41
13:2R:57:ARG:HE	13:2R:57:ARG:HB3	1.74	0.41
32:2a:1132:C:H2'	32:2a:1133:G:H8	1.84	0.41
32:2a:1206:G:H2'	32:2a:1207:2MG:H8	1.85	0.41
32:2a:1272:G:C2	32:2a:1273:G:C8	3.08	0.41
32:2a:1326:C:H5''	52:2u:18:TYR:O	2.21	0.41
33:2b:28:PHE:CD2	33:2b:190:THR:HA	2.54	0.41
33:2b:54:THR:O	33:2b:58:ILE:HG13	2.20	0.41
35:2d:162:LEU:HG	35:2d:181:MET:SD	2.60	0.41
37:2f:44:GLY:HA2	37:2f:59:TYR:CZ	2.55	0.41
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.55	0.41
44:2m:70:LEU:O	44:2m:74:VAL:HG23	2.20	0.41
45:2n:50:LYS:HE3	45:2n:50:LYS:HB2	1.71	0.41
1:1A:1055:G:H1	1:1A:1104:C:H42	1.69	0.41
1:1A:1057:A:H61	1:1A:1081:U:H3	1.68	0.41
1:1A:1139:G:H5''	9:1N:70:LYS:NZ	2.36	0.41
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.86	0.41
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.53	0.41
1:1A:2352:A:C4	1:1A:2366:A:C2	3.09	0.41
1:1A:2679:A:H5'	4:1E:165:VAL:HG21	2.03	0.41
2:1B:29:A:H2'	2:1B:30:C:O4'	2.21	0.41
3:1D:25:THR:HG21	3:1D:113:VAL:HG21	2.03	0.41
5:1F:164:ARG:O	5:1F:168:ARG:HB3	2.19	0.41
30:18:62:LEU:HB3	30:18:65:GLU:CG	2.51	0.41
32:1a:1005:A:H5''	32:1a:1006:C:C5	2.56	0.41
32:1a:1486:G:H2'	32:1a:1487:G:O4'	2.20	0.41
33:1b:185:ILE:HG22	33:1b:199:TYR:HD2	1.85	0.41
34:1c:173:VAL:HG12	34:1c:175:LEU:HD22	2.02	0.41
35:1d:8:VAL:O	35:1d:11:LEU:HB2	2.21	0.41
39:1h:100:ILE:HD13	39:1h:112:LEU:HD21	2.02	0.41
1:2A:1999:C:H5''	1:2A:2723:C:O2'	2.21	0.41
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.56	0.41
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.20	0.41
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.19	0.41
4:2E:73:GLU:H	4:2E:73:GLU:HG3	1.44	0.41
4:2E:103:ASP:OD2	4:2E:168:MET:HE2	2.20	0.41
18:2W:1:MET:HE3	18:2W:62:HIS:HB3	2.02	0.41
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.46	0.41
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.49	0.41
32:2a:201:C:H5'	32:2a:202:U:OP2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:271:C:H2'	32:2a:272:C:C6	2.55	0.41
32:2a:404:U:H2'	32:2a:405:U:H6	1.84	0.41
32:2a:512:U:H2'	32:2a:513:C:C6	2.55	0.41
32:2a:625:G:H4'	47:2p:16:HIS:CD2	2.55	0.41
32:2a:1092:A:H5''	38:2g:4:ARG:CZ	2.50	0.41
33:2b:21:ARG:HA	33:2b:39:ILE:HA	2.01	0.41
33:2b:100:GLY:O	33:2b:104:ASN:N	2.49	0.41
34:2c:159:GLY:HA2	34:2c:193:TYR:CE1	2.55	0.41
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.44	0.41
40:2i:18:PHE:HD2	40:2i:62:TYR:HD2	1.66	0.41
43:2l:77:LEU:HD21	43:2l:107:ALA:HB2	2.02	0.41
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.21	0.41
1:1A:81:G:HO2'	1:1A:295:G:HO2'	1.67	0.41
1:1A:271(X):G:C2	1:1A:271(Y):U:O4	2.74	0.41
1:1A:1062:G:P	1:1A:1070:A:H1'	2.60	0.41
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.20	0.41
1:1A:2056:G:C2	1:1A:2057:A:C8	3.08	0.41
1:1A:2183:C:HO2'	1:1A:2184:G:P	2.42	0.41
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	2.02	0.41
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.20	0.41
7:1H:3:ARG:NH2	7:1H:5:GLY:HA3	2.35	0.41
9:1N:16:ILE:HG21	9:1N:26:LEU:HD11	2.02	0.41
19:1X:60:ARG:NH1	29:17:47:ARG:HH22	2.18	0.41
24:12:24:LEU:HD13	24:12:60:LEU:HD11	2.02	0.41
32:1a:167:G:H2'	32:1a:168:G:C8	2.55	0.41
32:1a:407:G:H2'	32:1a:408:A:C8	2.56	0.41
32:1a:649:G:H2'	32:1a:650:G:H8	1.85	0.41
32:1a:1136:U:H5''	32:1a:1137:C:C4	2.55	0.41
33:1b:153:ARG:HE	33:1b:153:ARG:HB3	1.74	0.41
37:1f:39:LYS:HE3	37:1f:39:LYS:HB3	1.92	0.41
39:1h:81:HIS:HB2	39:1h:138:TRP:CD1	2.55	0.41
54:1w:48:C:C2	54:1w:59:U:H1'	2.54	0.41
1:2A:184:C:H2'	1:2A:185:U:H6	1.85	0.41
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.53	0.41
4:2E:50:GLY:HA2	4:2E:77:ILE:O	2.20	0.41
10:2O:91:LEU:HB3	10:2O:111:PHE:CE1	2.56	0.41
10:2O:120:GLU:OE2	10:2O:122:LEU:HD21	2.20	0.41
16:2U:16:LYS:HE2	16:2U:16:LYS:HB3	1.85	0.41
19:2X:55:ASN:O	19:2X:79:ALA:HA	2.20	0.41
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.42	0.41
32:2a:1260:C:P	32:2a:1284:C:H4'	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1490:C:H2'	32:2a:1491:G:O4'	2.20	0.41
1:1A:271(J):C:H4'	1:1A:271(K):U:OP1	2.19	0.41
1:1A:1173:G:H2'	1:1A:1173:G:OP2	2.21	0.41
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.46	0.41
1:1A:2110:G:C5	1:1A:2120:G:C8	3.09	0.41
8:1I:109:ILE:HD12	8:1I:130:TYR:CE2	2.56	0.41
11:1P:44:GLY:HA2	61:1P:316:HOH:O	2.20	0.41
32:1a:109:A:C6	32:1a:326:G:C6	3.08	0.41
32:1a:171:A:H2'	32:1a:172:A:C8	2.55	0.41
32:1a:761:G:H4'	48:1q:97:SER:OG	2.21	0.41
32:1a:894:G:H2'	32:1a:895:G:O4'	2.21	0.41
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.52	0.41
33:1b:44:LEU:HA	33:1b:47:THR:OG1	2.21	0.41
39:1h:98:LYS:HE2	39:1h:98:LYS:HB2	1.87	0.41
40:1i:33:PHE:HD2	40:1i:34:ASN:ND2	2.19	0.41
48:1q:5:VAL:HA	48:1q:59:ILE:O	2.21	0.41
50:1s:16:LEU:O	50:1s:19:VAL:HG12	2.21	0.41
54:1w:25:C:H2'	54:1w:26:A:H8	1.85	0.41
54:1y:35:A:H3'	54:1y:36:A:C8	2.56	0.41
1:2A:415:A:H2'	1:2A:416:C:O4'	2.20	0.41
1:2A:832:G:H5'	11:2P:45:LEU:HD11	2.03	0.41
1:2A:920:G:H2'	1:2A:921:G:H8	1.86	0.41
1:2A:2356:C:H2'	1:2A:2357:U:O4'	2.19	0.41
1:2A:2489:G:C2'	1:2A:2490:G:H5'	2.51	0.41
1:2A:2748:A:H5'	7:2H:4:ILE:CD1	2.50	0.41
2:2B:73:A:C4	2:2B:105:A:C2	3.08	0.41
2:2B:100:A:H3'	2:2B:101:G:H8	1.84	0.41
5:2F:53:THR:HG22	5:2F:56:GLU:HG3	2.02	0.41
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	2.01	0.41
11:2P:126:VAL:HA	11:2P:146:VAL:HB	2.02	0.41
14:2S:4:LEU:HD23	14:2S:4:LEU:HA	1.87	0.41
23:21:32:LYS:HB3	23:21:32:LYS:HE3	1.90	0.41
23:21:80:LEU:HD12	23:21:80:LEU:HA	1.91	0.41
32:2a:435:C:H2'	32:2a:436:C:C6	2.55	0.41
32:2a:1029:C:H1'	32:2a:1033:G:N2	2.36	0.41
33:2b:16:HIS:O	33:2b:18:GLY:N	2.54	0.41
38:2g:51:GLN:O	38:2g:55:GLY:HA2	2.20	0.41
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	2.03	0.41
44:2m:27:LYS:HD2	44:2m:27:LYS:HA	1.68	0.41
1:1A:286:C:H2'	1:1A:287:C:C6	2.56	0.41
1:1A:1025:G:O2'	61:1A:4117:HOH:O	2.11	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2142:C:N3	1:1A:2149:G:O6	2.53	0.41
3:1D:218:ARG:HB3	3:1D:219:PRO:HD2	2.03	0.41
11:1P:42:SER:O	61:1P:301:HOH:O	2.22	0.41
15:1T:41:ARG:HH21	15:1T:43:GLN:HE21	1.69	0.41
17:1V:29:PRO:HA	17:1V:61:VAL:HG22	2.02	0.41
21:1Z:30:ASN:HA	21:1Z:89:PHE:HE1	1.86	0.41
29:17:11:LYS:HE3	29:17:15:THR:OG1	2.20	0.41
30:18:52:LYS:N	30:18:53:PRO:HD2	2.36	0.41
32:1a:520:A:N1	32:1a:536:C:H1'	2.35	0.41
32:1a:708:C:H2'	32:1a:709:G:C8	2.55	0.41
32:1a:727:G:N2	32:1a:730:G:OP2	2.43	0.41
32:1a:1095:U:H2'	32:1a:1096:C:C6	2.56	0.41
32:1a:1142:G:H2'	32:1a:1143:G:O4'	2.21	0.41
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.21	0.41
32:1a:1364:U:C6	52:1u:14:TRP:HH2	2.38	0.41
32:1a:1376:U:OP1	38:1g:98:SER:OG	2.38	0.41
33:1b:54:THR:HG23	33:1b:199:TYR:HB3	2.01	0.41
47:1p:48:TRP:HH2	47:1p:76:GLN:NE2	2.19	0.41
55:1x:61:C:H2'	55:1x:62:C:H6	1.84	0.41
54:1y:35:A:H3'	54:1y:36:A:H8	1.85	0.41
54:1y:40:C:H2'	54:1y:41:C:C6	2.55	0.41
1:2A:402:A:H2'	1:2A:403:U:H5'	2.02	0.41
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	2.01	0.41
1:2A:2683:C:H4'	4:2E:13:ARG:CZ	2.51	0.41
1:2A:2705:A:H2'	1:2A:2706:G:O4'	2.21	0.41
8:2I:121:LYS:HE2	8:2I:121:LYS:HB3	1.87	0.41
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.85	0.41
26:24:34:GLU:HB2	44:2m:57:ARG:HE	1.86	0.41
32:2a:381:C:H2'	32:2a:382:A:O4'	2.20	0.41
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.54	0.41
32:2a:1223:C:P	50:2s:78:ARG:HH21	2.44	0.41
40:2i:18:PHE:CD2	40:2i:62:TYR:HD2	2.37	0.41
41:2j:16:LEU:HD23	41:2j:16:LEU:HA	1.88	0.41
41:2j:33:GLN:HG2	41:2j:34:VAL:H	1.84	0.41
45:2n:34:TYR:O	45:2n:38:GLY:N	2.53	0.41
47:2p:26:ARG:HG3	47:2p:27:LYS:O	2.21	0.41
54:2w:22:G:H2'	54:2w:23:A:H8	1.85	0.41
54:2w:52:G:H2'	54:2w:53:G:O4'	2.20	0.41
1:1A:1289:C:H2'	1:1A:1290:C:C6	2.56	0.41
6:1G:34:LEU:HD12	6:1G:100:TRP:CH2	2.56	0.41
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:108:ARG:NH2	15:1T:112:ARG:HD3	2.36	0.41
18:1W:62:HIS:O	18:1W:64:MET:HG3	2.21	0.41
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.54	0.41
32:1a:580:U:H2'	32:1a:581:G:O4'	2.21	0.41
32:1a:911:U:H2'	32:1a:912:C:C6	2.56	0.41
32:1a:1312:G:O6	50:1s:2:PRO:HD2	2.21	0.41
1:2A:251:A:C5	1:2A:252:G:H1'	2.55	0.41
1:2A:286:C:H2'	1:2A:287:C:C6	2.56	0.41
1:2A:479:A:N3	1:2A:481:G:H5''	2.36	0.41
1:2A:855:G:H2'	1:2A:856:C:C6	2.56	0.41
1:2A:1186:G:C2	1:2A:1187:G:H1'	2.55	0.41
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.36	0.41
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.56	0.41
1:2A:2322:A:H2'	1:2A:2323:G:O4'	2.20	0.41
2:2B:88:C:H2'	2:2B:89:G:O4'	2.20	0.41
3:2D:16:MET:HE3	3:2D:16:MET:HB2	1.74	0.41
3:2D:275:LYS:HB2	3:2D:276:LYS:H	1.63	0.41
6:2G:37:VAL:HG21	6:2G:103:LEU:HD11	2.03	0.41
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	2.02	0.41
8:2I:51:ILE:HD13	8:2I:51:ILE:HA	1.85	0.41
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	2.02	0.41
14:2S:99:LYS:NZ	14:2S:103:GLU:OE2	2.40	0.41
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.57	0.41
28:26:38:LYS:HE3	28:26:38:LYS:HB3	1.91	0.41
32:2a:19:C:H5''	36:2e:86:ALA:HB1	2.02	0.41
32:2a:107:G:C2	32:2a:108:G:H1'	2.56	0.41
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.56	0.41
32:2a:137:C:H2'	32:2a:138:G:H8	1.85	0.41
32:2a:865:A:H5'	32:2a:1078:U:H5	1.85	0.41
32:2a:1266:G:N2	32:2a:1268:A:H3'	2.36	0.41
32:2a:1324:A:H4'	32:2a:1362:C:O3'	2.21	0.41
32:2a:1441:G:H1'	32:2a:1461:G:N2	2.35	0.41
33:2b:111:ARG:HA	33:2b:111:ARG:HD3	1.79	0.41
34:2c:125:GLU:HB2	34:2c:190:ARG:HH21	1.86	0.41
38:2g:120:ILE:O	38:2g:124:LEU:HB2	2.20	0.41
39:2h:119:LEU:HB3	39:2h:123:GLU:HB3	2.02	0.41
1:1A:41:C:H2'	1:1A:42:G:O4'	2.21	0.41
1:1A:118:A:C8	1:1A:119:A:C8	3.08	0.41
1:1A:548:A:H3'	1:1A:548:A:OP2	2.21	0.41
1:1A:593:G:C4'	30:18:4:MET:HE2	2.51	0.41
1:1A:647:G:H2'	1:1A:648:G:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:847:U:OP2	61:1A:4136:HOH:O	2.21	0.41
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.54	0.41
1:1A:1095:A:C8	1:1A:1096:A:C8	3.09	0.41
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.21	0.41
1:1A:1338:G:O2'	1:1A:1393:A:N1	2.39	0.41
1:1A:1431:U:H2'	1:1A:1432:C:C6	2.56	0.41
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.20	0.41
1:1A:2306:C:N4	6:1G:42:GLY:O	2.36	0.41
1:1A:2477:C:N4	31:19:10:ILE:HG23	2.35	0.41
1:1A:2478:A:H5'	31:19:31:LYS:HE2	2.02	0.41
1:1A:2627:G:O2'	1:1A:2781:A:N1	2.44	0.41
5:1F:39:TRP:O	5:1F:43:LYS:HG2	2.20	0.41
5:1F:170:LEU:HD13	5:1F:172:TRP:CZ2	2.56	0.41
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.56	0.41
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.20	0.41
11:1P:125:VAL:CG1	11:1P:138:LEU:HD21	2.51	0.41
15:1T:91:ARG:HB2	15:1T:121:ILE:HG13	2.03	0.41
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	2.03	0.41
26:14:34:GLU:H	26:14:34:GLU:CD	2.29	0.41
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.72	0.41
32:1a:103:C:O2'	32:1a:172:A:N1	2.44	0.41
32:1a:708:C:H2'	32:1a:709:G:H8	1.86	0.41
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.43	0.41
33:1b:63:MET:HG2	33:1b:225:ALA:HB1	2.03	0.41
34:1c:77:ILE:H	34:1c:77:ILE:HG12	1.63	0.41
34:1c:137:ALA:O	34:1c:141:VAL:HG23	2.21	0.41
35:1d:65:ARG:HG3	35:1d:75:PHE:CD1	2.56	0.41
35:1d:172:PRO:C	35:1d:174:LEU:H	2.29	0.41
36:1e:90:VAL:O	36:1e:120:THR:HA	2.21	0.41
38:1g:50:ILE:CD1	38:1g:61:VAL:HG11	2.51	0.41
39:1h:17:THR:HG22	39:1h:63:LEU:HD13	2.03	0.41
42:1k:48:ILE:O	42:1k:48:ILE:HG12	2.20	0.41
43:1l:56:ALA:HB2	43:1l:70:ILE:HD11	2.03	0.41
52:1u:15:ARG:H	52:1u:15:ARG:HG2	1.47	0.41
54:1w:4:C:H2'	54:1w:5:G:H8	1.85	0.41
54:1y:20:U:O3'	54:1y:21:A:H4'	2.20	0.41
1:2A:56:A:H2'	1:2A:57:C:O4'	2.20	0.41
1:2A:265:A:H1'	1:2A:266:G:O4'	2.21	0.41
1:2A:272(B):G:H2'	1:2A:272(C):G:H8	1.84	0.41
1:2A:489:G:H2'	1:2A:491:G:O4'	2.21	0.41
1:2A:597:U:H2'	1:2A:598:G:H8	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:600:G:O3'	5:2F:108:LYS:HE3	2.21	0.41
1:2A:616:G:H5'	5:2F:205:ARG:HE	1.86	0.41
1:2A:661:C:H2'	1:2A:662:G:C8	2.55	0.41
1:2A:925:C:H2'	1:2A:926:A:C8	2.54	0.41
1:2A:1580:A:H8	1:2A:1580:A:OP2	2.04	0.41
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.51	0.41
1:2A:1830:C:H2'	1:2A:1831:G:H8	1.85	0.41
1:2A:1996:C:OP1	10:2O:31:LYS:HE3	2.21	0.41
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.21	0.41
1:2A:2406:U:H6	1:2A:2406:U:H2'	1.73	0.41
1:2A:2611:U:H3'	1:2A:2611:U:OP2	2.21	0.41
1:2A:2740:A:C6	1:2A:2741:A:C6	3.09	0.41
8:2I:29:TYR:CD2	8:2I:30:LEU:HD23	2.55	0.41
11:2P:89:ALA:O	11:2P:121:LYS:NZ	2.42	0.41
14:2S:56:LEU:C	14:2S:58:LEU:H	2.29	0.41
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.45	0.41
21:2Z:125:LEU:HD23	21:2Z:164:ALA:HB3	2.03	0.41
27:25:35:GLU:HG3	27:25:51:TYR:CG	2.56	0.41
32:2a:34:C:H2'	32:2a:35:G:C8	2.56	0.41
32:2a:203:U:H2'	32:2a:203:U:OP2	2.20	0.41
32:2a:841:U:C5	32:2a:848:C:H1'	2.55	0.41
32:2a:1172:C:H2'	32:2a:1173:G:C8	2.56	0.41
38:2g:97:GLN:O	38:2g:101:LEU:HG	2.21	0.41
38:2g:106:GLN:HE21	38:2g:106:GLN:HB3	1.70	0.41
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.21	0.41
40:2i:28:VAL:HG13	40:2i:63:ILE:HB	2.02	0.41
46:2o:26:GLU:HG3	46:2o:81:LEU:HD13	2.03	0.41
51:2t:79:ARG:O	51:2t:83:ARG:HG3	2.20	0.41
54:2y:52:G:H1	54:2y:62:C:H42	1.68	0.41
1:1A:1380:G:N2	1:1A:1570:A:N1	2.62	0.41
1:1A:1762:A:H2'	61:1A:5566:HOH:O	2.21	0.41
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.86	0.41
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.21	0.41
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.21	0.41
21:1Z:45:ASP:O	21:1Z:49:ARG:HB2	2.21	0.41
26:14:26:SER:OG	26:14:27:THR:N	2.54	0.41
32:1a:115:G:H4'	32:1a:116:A:O5'	2.20	0.41
32:1a:313:A:H2'	32:1a:314:C:C6	2.56	0.41
32:1a:591:U:H2'	32:1a:592:G:C8	2.55	0.41
32:1a:1030(A):G:O2'	32:1a:1031:G:N2	2.54	0.41
33:1b:76:GLN:O	33:1b:208:ILE:HG22	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:56:ASP:HB2	34:1c:67:THR:HB	2.02	0.41
51:1t:29:LYS:O	51:1t:33:ILE:HG13	2.20	0.41
54:1y:9:A:H4'	54:1y:46:G7M:OP2	2.22	0.41
1:2A:244:A:H4'	11:2P:74:GLU:HB2	2.03	0.41
1:2A:443:A:H5''	1:2A:444:C:OP1	2.21	0.41
1:2A:1779:U:H2'	61:2A:4408:HOH:O	2.21	0.41
1:2A:2162:G:O2'	1:2A:2172:U:H5'	2.21	0.41
1:2A:2516:G:C6	1:2A:2517:C:C4	3.09	0.41
3:2D:186:HIS:HE1	3:2D:188:GLU:HG2	1.84	0.41
5:2F:53:THR:HG22	5:2F:56:GLU:CG	2.51	0.41
8:2I:44:LEU:HD12	8:2I:44:LEU:HA	1.88	0.41
15:2T:91:ARG:HD2	15:2T:120:ARG:NH1	2.35	0.41
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	2.02	0.41
32:2a:302:G:N3	32:2a:556:C:H4'	2.36	0.41
32:2a:517:G:H5'	32:2a:519:C:C2	2.56	0.41
32:2a:581:G:OP1	46:2o:61:GLY:HA3	2.21	0.41
32:2a:986:A:H2'	32:2a:987:G:C8	2.56	0.41
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.55	0.41
32:2a:1074:G:O2'	32:2a:1101:A:N1	2.52	0.41
32:2a:1121:U:H2'	32:2a:1122:U:H6	1.86	0.41
34:2c:193:TYR:HE1	34:2c:196:LEU:HD11	1.86	0.41
36:2e:89:ILE:HG21	36:2e:135:THR:HA	2.03	0.41
47:2p:1:MET:HE2	47:2p:1:MET:HB3	1.86	0.41
47:2p:3:LYS:O	47:2p:21:VAL:HA	2.20	0.41
47:2p:41:PRO:O	47:2p:43:LYS:HE3	2.21	0.41
53:2v:14:A:C2	54:2y:34:G:C2	3.09	0.41
1:1A:272:G:N7	1:1A:421:U:H2'	2.36	0.40
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.36	0.40
2:1B:78:A:C2	2:1B:100:A:C4	3.08	0.40
8:1I:101:LEU:HD12	8:1I:107:VAL:HB	2.03	0.40
32:1a:1030(A):G:H1'	32:1a:1031:G:H22	1.86	0.40
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.56	0.40
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.33	0.40
33:1b:100:GLY:N	33:1b:176:GLU:OE2	2.33	0.40
36:1e:82:VAL:HG11	36:1e:137:GLU:HB3	2.03	0.40
41:1j:81:THR:C	41:1j:83:GLU:N	2.78	0.40
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.21	0.40
54:1y:54:5MU:C4	54:1y:55:PSU:C2	3.09	0.40
1:2A:480:A:OP2	20:2Y:47:LYS:HE3	2.21	0.40
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.37	0.40
1:2A:1372:U:H2'	1:2A:1373:A:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1777:U:O2'	1:2A:1778:U:H5'	2.20	0.40
1:2A:1799:G:O2'	3:2D:181:GLU:OE2	2.35	0.40
1:2A:2144:U:O3'	1:2A:2145:C:H6	2.04	0.40
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.56	0.40
1:2A:2262:U:OP2	22:20:16:SER:OG	2.34	0.40
3:2D:5:LYS:HE3	3:2D:5:LYS:HB3	1.90	0.40
4:2E:179:GLU:HB2	4:2E:181:LEU:HG	2.03	0.40
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.33	0.40
17:2V:29:PRO:HA	17:2V:61:VAL:HG22	2.03	0.40
21:2Z:151:HIS:HB3	21:2Z:152:ALA:H	1.80	0.40
32:2a:100:C:H2'	32:2a:101:A:C8	2.55	0.40
32:2a:390:C:H4'	47:2p:28:ARG:HH21	1.87	0.40
32:2a:975:A:N1	41:2j:48:THR:HB	2.36	0.40
32:2a:1122:U:C2	32:2a:1123:A:C8	3.08	0.40
32:2a:1189:C:OP1	34:2c:5:ILE:HD12	2.20	0.40
32:2a:1381:U:H1'	38:2g:79:ARG:HD2	2.02	0.40
34:2c:109:PRO:C	34:2c:111:LEU:H	2.29	0.40
44:2m:94:ARG:NH2	50:2s:81:ARG:HA	2.35	0.40
46:2o:15:PHE:CZ	46:2o:84:LYS:HD2	2.56	0.40
55:2x:14:A:C2	55:2x:15:G:H1'	2.55	0.40
1:1A:228:A:C8	1:1A:229:A:H5'	2.55	0.40
1:1A:285:C:H2'	1:1A:286:C:C6	2.56	0.40
1:1A:888:C:O5'	44:1m:93:ARG:HD3	2.21	0.40
1:1A:1142(A):A:C4	1:1A:1144:G:N7	2.89	0.40
1:1A:1812:A:O2'	3:1D:45:ASN:N	2.52	0.40
1:1A:2396:G:OP1	23:11:25:LYS:NZ	2.52	0.40
1:1A:2717:G:H1'	15:1T:96:ARG:HH21	1.85	0.40
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.56	0.40
11:1P:37:GLY:C	11:1P:38:GLN:O	2.63	0.40
14:1S:3:ARG:HA	14:1S:3:ARG:HD3	1.81	0.40
21:1Z:101:PRO:HA	21:1Z:123:ASP:HB3	2.03	0.40
32:1a:572:A:N3	32:1a:917:G:H1'	2.35	0.40
32:1a:685:G:C2	32:1a:686:U:C4	3.09	0.40
32:1a:971:G:N1	32:1a:1363(A):A:OP2	2.45	0.40
33:1b:85:ALA:HB1	33:1b:90:MET:O	2.21	0.40
33:1b:178:ARG:HH12	39:1h:68:ARG:HH22	1.69	0.40
33:1b:204:ASN:OD1	33:1b:206:ASP:N	2.35	0.40
34:1c:159:GLY:HA2	34:1c:193:TYR:CD1	2.57	0.40
34:1c:172:ARG:NH2	34:1c:206:GLU:OE2	2.54	0.40
44:1m:25:ILE:HD11	44:1m:60:VAL:HG13	2.04	0.40
47:1p:43:LYS:HA	47:1p:48:TRP:CG	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1v:23:A:H4'	53:1v:24:A:C5'	2.51	0.40
1:2A:68:G:H2'	1:2A:69:C:O4'	2.22	0.40
1:2A:861:A:C2	1:2A:917:A:C4	3.09	0.40
1:2A:1270:C:H5''	1:2A:1271:G:O5'	2.21	0.40
1:2A:1473:G:C6	1:2A:1474:C:C4	3.09	0.40
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.21	0.40
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	2.04	0.40
1:2A:2309:A:H2'	1:2A:2310:A:O4'	2.21	0.40
1:2A:2579:C:H2'	1:2A:2580:U:O4'	2.22	0.40
1:2A:2752:C:H2'	1:2A:2753:A:O4'	2.20	0.40
2:2B:12:C:O5'	2:2B:12:C:H6	2.04	0.40
4:2E:34:VAL:HG21	4:2E:78:LEU:HD11	2.04	0.40
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.85	0.40
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	2.02	0.40
9:2N:28:THR:HG22	9:2N:29:LYS:N	2.36	0.40
15:2T:61:PHE:CE2	15:2T:76:PHE:HB2	2.57	0.40
18:2W:15:ARG:NH1	61:2W:301:HOH:O	2.53	0.40
24:22:66:GLU:HA	24:22:69:ARG:HH12	1.85	0.40
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.57	0.40
32:2a:1080:A:H5''	32:2a:1081:G:OP2	2.21	0.40
32:2a:1263:C:H1'	32:2a:1273:G:N2	2.35	0.40
32:2a:1530:G:H2'	32:2a:1531:A:O4'	2.21	0.40
34:2c:63:ASN:HA	34:2c:98:ASN:H	1.87	0.40
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.21	0.40
50:2s:80:TYR:C	50:2s:82:GLY:H	2.29	0.40
55:2x:17:C:H2'	55:2x:17(A):U:C5	2.56	0.40
1:1A:893:C:H2'	1:1A:894:C:C6	2.56	0.40
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.56	0.40
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.51	0.40
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.56	0.40
32:1a:226:G:H2'	32:1a:227:G:O4'	2.22	0.40
32:1a:1313:U:P	50:1s:5:LEU:HG	2.61	0.40
32:1a:1346:A:H5''	40:1i:120:ARG:NH1	2.36	0.40
34:1c:130:VAL:HG11	34:1c:153:VAL:HG11	2.01	0.40
35:1d:74:GLN:O	35:1d:78:LEU:HD12	2.22	0.40
38:1g:28:ASN:HD22	38:1g:28:ASN:HA	1.63	0.40
41:1j:49:VAL:HG21	45:1n:44:LEU:HD22	2.04	0.40
1:2A:407:G:H2'	1:2A:408:G:C8	2.57	0.40
1:2A:992:C:OP1	16:2U:47:TYR:OH	2.33	0.40
1:2A:1300:U:H4'	1:2A:1301:A:H5'	2.03	0.40
1:2A:2365:G:O6	30:28:39:LYS:HE3	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	2.03	0.40
4:2E:105:THR:HG21	4:2E:164:ARG:CZ	2.52	0.40
5:2F:11:VAL:HG22	5:2F:125:LEU:HD13	2.02	0.40
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.53	0.40
6:2G:15:VAL:HG12	6:2G:19:LEU:HD12	2.03	0.40
6:2G:59:GLU:OE2	6:2G:153:ARG:NE	2.50	0.40
8:2I:84:GLY:O	8:2I:85:GLU:HB3	2.21	0.40
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.20	0.40
17:2V:76:LYS:HB2	17:2V:81:TYR:HD2	1.86	0.40
32:2a:202:U:H3'	32:2a:203:U:C5	2.56	0.40
32:2a:423:G:N3	32:2a:423:G:H3'	2.36	0.40
33:2b:114:ARG:HD2	33:2b:117:GLU:HB3	2.02	0.40
36:2e:62:ALA:C	36:2e:64:ARG:H	2.29	0.40
36:2e:148:VAL:HG21	39:2h:107:LEU:HD22	2.02	0.40
37:2f:24:GLU:O	37:2f:28:ARG:N	2.42	0.40
39:2h:17:THR:HA	39:2h:65:TYR:HE1	1.86	0.40
40:2i:46:ALA:HA	40:2i:78:LYS:HB2	2.02	0.40
46:2o:62:GLN:O	46:2o:66:LEU:HG	2.21	0.40
47:2p:19:ILE:N	47:2p:37:GLY:O	2.53	0.40
48:2q:32:TYR:O	48:2q:34:LYS:N	2.45	0.40
55:2x:15:G:H2'	55:2x:59:A:N1	2.35	0.40
1:1A:264:C:O2'	1:1A:265:A:H2'	2.22	0.40
1:1A:586:A:N1	1:1A:809:G:O2'	2.46	0.40
1:1A:1045:A:OP1	1:1A:1046:A:H3'	2.21	0.40
1:1A:2115:G:N2	1:1A:2171:A:H61	2.19	0.40
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.22	0.40
3:1D:181:GLU:OE2	3:1D:270:ILE:HD12	2.22	0.40
4:1E:35:GLN:OE1	4:1E:66:HIS:HE1	2.05	0.40
12:1Q:17:LEU:HD23	12:1Q:17:LEU:HA	1.71	0.40
12:1Q:84:GLY:O	12:1Q:85:LYS:HB2	2.21	0.40
20:1Y:75:ILE:HD13	20:1Y:82:PRO:HB3	2.04	0.40
32:1a:399:G:H2'	32:1a:400:C:C6	2.57	0.40
32:1a:1436:U:H2'	32:1a:1437:C:O4'	2.21	0.40
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.57	0.40
35:1d:102:ASP:OD1	35:1d:103:ASN:N	2.55	0.40
37:1f:91:VAL:HG11	49:1r:72:ARG:NH1	2.36	0.40
44:1m:16:ASP:N	44:1m:16:ASP:OD1	2.55	0.40
45:1n:14:PRO:HB2	45:1n:19:ARG:HB2	2.04	0.40
1:2A:1006:C:C2	1:2A:1138:G:N2	2.89	0.40
1:2A:2393:A:H5''	11:2P:63:PRO:HB3	2.03	0.40
1:2A:2743:C:OP1	31:29:33:LYS:NZ	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	2.03	0.40
13:2R:29:LEU:HD22	13:2R:79:LEU:HD13	2.02	0.40
15:2T:113:LYS:HD3	15:2T:113:LYS:HA	1.83	0.40
16:2U:65:ILE:CD1	16:2U:95:LEU:HB3	2.51	0.40
26:24:46:GLN:C	26:24:48:ARG:N	2.77	0.40
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.39	0.40
32:2a:436:C:H2'	32:2a:437:U:C6	2.55	0.40
32:2a:707:C:H2'	32:2a:708:C:C6	2.56	0.40
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.56	0.40
32:2a:1070:U:H2'	32:2a:1071:C:H6	1.86	0.40
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.48	0.40
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	2.03	0.40
40:2i:5:TYR:CD1	40:2i:18:PHE:HE1	2.40	0.40
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.85	0.40
49:2r:48:GLY:O	49:2r:74:ARG:NH2	2.52	0.40
51:2t:54:LYS:HE2	51:2t:54:LYS:HB3	1.87	0.40
54:2y:66:U:H2'	54:2y:67:C:O4'	2.20	0.40
1:1A:637:A:H2'	11:1P:117:GLU:OE1	2.22	0.40
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.57	0.40
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.56	0.40
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.20	0.40
5:1F:148:LEU:HD23	5:1F:191:ARG:NH1	2.36	0.40
7:1H:52:VAL:HG12	7:1H:65:HIS:CD2	2.56	0.40
22:10:46:LYS:HD2	22:10:78:TYR:CZ	2.56	0.40
26:14:58:ARG:HG2	50:1s:68:GLY:H	1.87	0.40
32:1a:300:A:O2'	32:1a:564:C:N3	2.50	0.40
32:1a:924:C:H2'	32:1a:925:G:C8	2.57	0.40
33:1b:13:ALA:HB2	33:1b:44:LEU:HD13	2.03	0.40
33:1b:73:THR:OG1	33:1b:170:GLU:OE1	2.31	0.40
41:1j:75:ILE:O	41:1j:77:PRO:HD3	2.21	0.40
42:1k:98:LEU:HD23	42:1k:98:LEU:HA	1.86	0.40
44:1m:108:ARG:HA	44:1m:108:ARG:HD3	1.91	0.40
45:1n:3:ARG:HG3	45:1n:4:LYS:N	2.36	0.40
1:2A:35:G:H1'	1:2A:454:A:C4	2.57	0.40
1:2A:38:A:H2'	1:2A:39:C:C6	2.56	0.40
1:2A:455:C:N3	1:2A:473:G:H5'	2.35	0.40
1:2A:577:G:C6	1:2A:578:A:C6	3.10	0.40
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.21	0.40
1:2A:1711:C:H2'	1:2A:1712:C:H6	1.86	0.40
1:2A:2331:G:O2'	22:20:43:THR:HG22	2.21	0.40
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:48:GLU:HG3	8:2I:52:ARG:NH1	2.36	0.40
15:2T:19:LEU:HD13	15:2T:86:ILE:HD12	2.03	0.40
17:2V:4:ILE:HD12	17:2V:39:LEU:HB3	2.04	0.40
19:2X:92:LEU:HD12	19:2X:92:LEU:HA	1.83	0.40
21:2Z:67:LEU:HD12	21:2Z:67:LEU:HA	1.88	0.40
25:23:59:VAL:HG12	25:23:60:GLU:H	1.85	0.40
32:2a:4:U:O4	39:2h:105:ARG:HD3	2.21	0.40
32:2a:130:A:N3	32:2a:263:A:O2'	2.45	0.40
32:2a:187:C:H2'	32:2a:188:C:C6	2.57	0.40
32:2a:684:A:C6	32:2a:685:G:C6	3.09	0.40
32:2a:828:A:H2'	32:2a:829:G:O4'	2.21	0.40
32:2a:1289:A:OP1	52:2u:10:ARG:NH2	2.55	0.40
32:2a:1413:A:H2'	32:2a:1414:U:O4'	2.22	0.40
33:2b:115:LEU:HD21	33:2b:146:GLN:HG3	2.04	0.40
35:2d:150:GLU:HA	35:2d:153:ARG:HG3	2.03	0.40
38:2g:99:LEU:HD23	38:2g:102:ARG:HH12	1.86	0.40
39:2h:121:ASP:OD1	39:2h:121:ASP:N	2.54	0.40
41:2j:33:GLN:O	41:2j:75:ILE:N	2.53	0.40
42:2k:38:ASN:HA	42:2k:39:PRO:HD3	1.95	0.40
47:2p:60:LEU:HD12	47:2p:60:LEU:HA	1.91	0.40
55:2x:53:G:H2'	55:2x:54:5MU:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	43
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1F	200/210 (95%)	194 (97%)	5 (2%)	1 (0%)	24	43
5	2F	200/210 (95%)	187 (94%)	10 (5%)	3 (2%)	8	16
6	1G	179/182 (98%)	163 (91%)	14 (8%)	2 (1%)	11	22
6	2G	179/182 (98%)	149 (83%)	24 (13%)	6 (3%)	3	4
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	38
7	2H	172/180 (96%)	155 (90%)	15 (9%)	2 (1%)	10	20
8	1I	144/148 (97%)	130 (90%)	14 (10%)	0	100	100
8	2I	144/148 (97%)	126 (88%)	15 (10%)	3 (2%)	5	9
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	4 (3%)	2 (1%)	9	17
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	31
11	1P	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	9	17
11	2P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	4	6
12	1Q	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
12	2Q	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	14	27
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	31
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	10
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	24
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	5	9
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	12	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	2Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
21	1Z	148/206 (72%)	136 (92%)	9 (6%)	3 (2%)	6	10
21	2Z	156/206 (76%)	128 (82%)	24 (15%)	4 (3%)	4	7
22	10	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
22	20	77/85 (91%)	71 (92%)	5 (6%)	1 (1%)	9	18
23	11	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	22
23	21	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	1 (2%)	1 (2%)	6	12
26	14	67/71 (94%)	54 (81%)	11 (16%)	2 (3%)	3	5
26	24	67/71 (94%)	54 (81%)	12 (18%)	1 (2%)	8	16
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	196 (86%)	26 (11%)	7 (3%)	3	5
33	2b	229/256 (90%)	178 (78%)	44 (19%)	7 (3%)	3	5
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	171 (84%)	28 (14%)	5 (2%)	4	7
35	1d	206/209 (99%)	194 (94%)	12 (6%)	0	100	100
35	2d	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
36	1e	146/162 (90%)	133 (91%)	12 (8%)	1 (1%)	18	34
36	2e	146/162 (90%)	129 (88%)	14 (10%)	3 (2%)	5	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	1f	98/101 (97%)	97 (99%)	0	1 (1%)	12	24
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	18	34
38	2g	153/156 (98%)	138 (90%)	11 (7%)	4 (3%)	4	7
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	122 (90%)	13 (10%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	16	31
40	2i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	16	31
41	1j	95/105 (90%)	80 (84%)	11 (12%)	4 (4%)	2	2
41	2j	94/105 (90%)	78 (83%)	13 (14%)	3 (3%)	3	4
42	1k	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	14	27
42	2k	112/129 (87%)	95 (85%)	15 (13%)	2 (2%)	6	12
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
44	1m	121/126 (96%)	104 (86%)	15 (12%)	2 (2%)	7	13
44	2m	120/126 (95%)	105 (88%)	14 (12%)	1 (1%)	16	31
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	47 (81%)	11 (19%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	20
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	18
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12	24
48	2q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	12	24
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	16
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	64 (79%)	15 (18%)	2 (2%)	4	7
51	1t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	3	4
51	2t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5	9
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11358/12128 (94%)	10454 (92%)	798 (7%)	106 (1%)	14	27

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
11	1P	38	GLN
11	1P	45	LEU
17	1V	43	GLU
19	1X	93	GLU
21	1Z	53	ILE
23	11	3	LYS
33	1b	17	PHE
33	1b	22	LYS
40	1i	54	ASP
44	1m	67	GLU
5	2F	130	ALA
8	2I	10	GLU
11	2P	36	LYS
26	24	45	GLY
33	2b	17	PHE
33	2b	123	ALA
34	2c	156	ARG
38	2g	55	GLY
38	2g	80	VAL
6	1G	43	LEU
15	1T	37	GLY
17	1V	79	VAL
20	1Y	54	LYS
21	1Z	156	LYS
26	14	49	PHE
26	14	62	ARG
33	1b	126	GLU
38	1g	79	ARG
41	1j	79	ARG
51	1t	47	GLY
6	2G	42	GLY
6	2G	124	SER
7	2H	47	GLU
7	2H	126	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	2O	5	GLN
17	2V	79	VAL
21	2Z	144	LEU
34	2c	91	LEU
36	2e	85	GLY
40	2i	121	ARG
41	2j	75	ILE
44	2m	106	ASN
48	2q	68	ARG
19	1X	2	LYS
33	1b	8	LYS
48	1q	61	GLU
4	2E	52	LEU
5	2F	18	ARG
6	2G	84	LYS
11	2P	38	GLN
11	2P	44	GLY
33	2b	16	HIS
33	2b	20	GLU
33	2b	21	ARG
34	2c	95	THR
38	2g	4	ARG
38	2g	52	GLU
41	2j	79	ARG
49	2r	36	ASN
50	2s	81	ARG
51	2t	95	ALA
4	1E	52	LEU
6	1G	150	ASP
41	1j	55	LYS
41	1j	77	PRO
41	1j	78	ASN
44	1m	106	ASN
46	1o	88	ARG
6	2G	50	ALA
8	2I	41	GLU
9	2N	2	LYS
14	2S	84	GLN
34	2c	110	ASN
41	2j	78	ASN
47	2p	81	ARG
33	1b	125	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1e	85	GLY
51	1t	95	ALA
5	2F	21	ALA
8	2I	40	THR
11	2P	29	LYS
34	2c	53	ALA
36	2e	96	PRO
33	1b	16	HIS
37	1f	40	VAL
6	2G	43	LEU
6	2G	127	GLY
21	2Z	134	PRO
22	20	12	ASN
25	23	59	VAL
36	2e	69	VAL
42	2k	49	GLY
50	2s	9	VAL
33	1b	231	GLU
21	2Z	158	PRO
42	1k	49	GLY
51	1t	100	ILE
9	2N	129	PRO
21	2Z	146	ILE
51	2t	47	GLY
33	2b	125	PRO
33	2b	231	GLU
42	2k	105	VAL
21	1Z	157	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	202 (94%)	13 (6%)	17	36
3	2D	215/218 (99%)	203 (94%)	12 (6%)	19	39
4	1E	164/166 (99%)	155 (94%)	9 (6%)	19	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	2E	164/166 (99%)	150 (92%)	14 (8%)	10	22
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	15
5	2F	159/166 (96%)	146 (92%)	13 (8%)	10	23
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	19
6	2G	143/156 (92%)	121 (85%)	22 (15%)	2	5
7	1H	144/148 (97%)	130 (90%)	14 (10%)	8	17
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7	14
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	4
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2	4
9	1N	118/119 (99%)	111 (94%)	7 (6%)	18	37
9	2N	118/119 (99%)	105 (89%)	13 (11%)	6	13
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	44
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	36
11	1P	115/116 (99%)	106 (92%)	9 (8%)	11	24
11	2P	115/116 (99%)	103 (90%)	12 (10%)	7	14
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	16	34
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	34
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	20
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28	54
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	23
14	2S	85/88 (97%)	71 (84%)	14 (16%)	2	4
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	29
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	24
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26	51
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10	21
17	1V	80/82 (98%)	75 (94%)	5 (6%)	16	34
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4	9
18	1W	90/92 (98%)	86 (96%)	4 (4%)	25	50
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	31
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	68
19	2X	77/78 (99%)	76 (99%)	1 (1%)	61	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	14
20	2Y	85/91 (93%)	72 (85%)	13 (15%)	3	5
21	1Z	135/179 (75%)	121 (90%)	14 (10%)	7	14
21	2Z	137/179 (76%)	118 (86%)	19 (14%)	3	7
22	10	61/67 (91%)	56 (92%)	5 (8%)	10	23
22	20	62/67 (92%)	60 (97%)	2 (3%)	34	62
23	11	80/83 (96%)	76 (95%)	4 (5%)	22	44
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	26
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	48
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	19
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	24
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	24
26	14	59/63 (94%)	47 (80%)	12 (20%)	1	2
26	24	53/63 (84%)	43 (81%)	10 (19%)	1	3
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	36
27	25	50/52 (96%)	47 (94%)	3 (6%)	17	36
28	16	51/52 (98%)	48 (94%)	3 (6%)	18	37
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	10
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	27
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	10
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	39
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	27
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	30 (88%)	4 (12%)	5	11
33	1b	192/220 (87%)	161 (84%)	31 (16%)	2	4
33	2b	187/220 (85%)	154 (82%)	33 (18%)	2	3
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	14
34	2c	140/188 (74%)	120 (86%)	20 (14%)	3	6
35	1d	169/181 (93%)	140 (83%)	29 (17%)	2	4
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	19
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	2e	114/123 (93%)	98 (86%)	16 (14%)	3	7
37	1f	84/90 (93%)	74 (88%)	10 (12%)	5	11
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23	47
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	15
38	2g	120/127 (94%)	104 (87%)	16 (13%)	4	8
39	1h	114/119 (96%)	106 (93%)	8 (7%)	14	29
39	2h	114/119 (96%)	99 (87%)	15 (13%)	4	8
40	1i	90/99 (91%)	81 (90%)	9 (10%)	7	15
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	12
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5	10
41	2j	69/92 (75%)	57 (83%)	12 (17%)	2	3
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7	16
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10	22
43	1l	96/108 (89%)	92 (96%)	4 (4%)	26	52
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8	18
44	1m	93/101 (92%)	81 (87%)	12 (13%)	4	9
44	2m	92/101 (91%)	85 (92%)	7 (8%)	12	26
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17	35
45	2n	49/50 (98%)	46 (94%)	3 (6%)	17	35
46	1o	78/80 (98%)	70 (90%)	8 (10%)	7	14
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5	11
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	11
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	11
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	27
48	2q	94/97 (97%)	86 (92%)	8 (8%)	10	22
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21	43
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	22
50	1s	69/80 (86%)	62 (90%)	7 (10%)	7	15
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2	4
51	1t	70/82 (85%)	65 (93%)	5 (7%)	13	29
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6	12
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	12
All	All	9296/10064 (92%)	8402 (90%)	894 (10%)	8	17

All (894) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	14	ARG
3	1D	37	LEU
3	1D	38	LYS
3	1D	61	LEU
3	1D	99	ASP
3	1D	111	LEU
3	1D	142	VAL
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
4	1E	12	THR
4	1E	47	VAL
4	1E	49	LEU
4	1E	73	GLU
4	1E	78	LEU
4	1E	89	ASP
4	1E	116	VAL
4	1E	119	ARG
4	1E	184	VAL
5	1F	24	LEU
5	1F	28	ILE
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	137	LYS
5	1F	140	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	162	LEU
5	1F	168	ARG
5	1F	183	VAL
5	1F	192	LEU
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	9	ARG
6	1G	21	ARG
6	1G	22	ARG
6	1G	31	VAL
6	1G	43	LEU
6	1G	47	LYS
6	1G	49	ASP
6	1G	139	LEU
6	1G	140	ILE
6	1G	159	VAL
7	1H	13	LYS
7	1H	23	ARG
7	1H	24	VAL
7	1H	76	VAL
7	1H	77	LYS
7	1H	92	ILE
7	1H	98	LEU
7	1H	116	GLU
7	1H	122	THR
7	1H	124	GLU
7	1H	127	GLU
7	1H	129	THR
7	1H	130	ARG
7	1H	160	LYS
8	1I	5	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	38	LEU
8	1I	47	LEU
8	1I	61	ARG
8	1I	74	ASN
8	1I	77	LEU
8	1I	87	LYS
8	1I	92	VAL
8	1I	95	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1I	101	LEU
8	1I	109	ILE
8	1I	123	LEU
8	1I	127	VAL
8	1I	129	THR
8	1I	133	HIS
8	1I	142	VAL
8	1I	144	VAL
9	1N	8	GLN
9	1N	9	VAL
9	1N	10	GLU
9	1N	28	THR
9	1N	61	ARG
9	1N	62	VAL
9	1N	137	LYS
10	1O	35	VAL
10	1O	42	SER
10	1O	89	ASN
10	1O	108	GLU
10	1O	112	MET
11	1P	15	ARG
11	1P	75	ILE
11	1P	95	VAL
11	1P	98	GLU
11	1P	125	VAL
11	1P	126	VAL
11	1P	133	SER
11	1P	147	LEU
11	1P	148	LEU
12	1Q	1	MET
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	56	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	133	ARG
13	1R	6	SER
13	1R	15	SER
13	1R	24	GLN
13	1R	36	THR
13	1R	44	LEU
13	1R	100	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1R	102	GLU
13	1R	111	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	14	VAL
14	1S	25	ARG
14	1S	46	VAL
14	1S	69	VAL
14	1S	78	LEU
14	1S	110	LEU
15	1T	28	VAL
15	1T	30	VAL
15	1T	34	VAL
15	1T	36	GLU
15	1T	65	LYS
15	1T	96	ARG
15	1T	118	ARG
15	1T	128	GLU
16	1U	27	LEU
16	1U	31	SER
16	1U	74	LEU
16	1U	95	LEU
17	1V	10	LYS
17	1V	46	VAL
17	1V	56	SER
17	1V	61	VAL
17	1V	79	VAL
18	1W	4	LYS
18	1W	11	ARG
18	1W	17	VAL
18	1W	63	ASP
19	1X	57	LEU
19	1X	88	LYS
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	8	LYS
20	1Y	31	LEU
20	1Y	40	GLU
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	99	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	42	VAL
21	1Z	49	ARG
21	1Z	53	ILE
21	1Z	61	LEU
21	1Z	65	GLN
21	1Z	66	SER
21	1Z	129	SER
21	1Z	132	ASN
21	1Z	139	VAL
21	1Z	140	ASP
21	1Z	154	ASP
21	1Z	161	VAL
21	1Z	170	THR
21	1Z	171	ILE
22	10	10	THR
22	10	14	ARG
22	10	49	LYS
22	10	74	ARG
22	10	82	ARG
23	11	33	LYS
23	11	40	ARG
23	11	59	THR
23	11	83	GLU
24	12	24	LEU
24	12	38	GLN
24	12	55	ARG
25	13	23	LEU
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	5	ILE
26	14	30	GLU
26	14	32	TYR
26	14	46	GLN
26	14	49	PHE
26	14	50	VAL
26	14	53	GLU
26	14	60	GLN
26	14	61	ARG
26	14	63	TYR
26	14	67	TYR
26	14	69	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	15	6	VAL
27	15	40	LYS
27	15	59	GLU
28	16	5	VAL
28	16	6	ARG
28	16	19	ARG
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
31	19	19	ARG
33	1b	7	VAL
33	1b	8	LYS
33	1b	12	GLU
33	1b	15	VAL
33	1b	17	PHE
33	1b	20	GLU
33	1b	35	GLU
33	1b	37	ASN
33	1b	39	ILE
33	1b	44	LEU
33	1b	54	THR
33	1b	64	ARG
33	1b	73	THR
33	1b	80	ILE
33	1b	81	VAL
33	1b	82	ARG
33	1b	86	GLU
33	1b	112	VAL
33	1b	127	ILE
33	1b	137	ARG
33	1b	142	LEU
33	1b	160	ASP
33	1b	172	ILE
33	1b	185	ILE
33	1b	196	LEU
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	217	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	229	VAL
33	1b	236	TYR
34	1c	3	ASN
34	1c	5	ILE
34	1c	8	ILE
34	1c	15	THR
34	1c	64	VAL
34	1c	77	ILE
34	1c	89	GLU
34	1c	105	GLU
34	1c	165	THR
34	1c	175	LEU
34	1c	178	LEU
34	1c	195	VAL
34	1c	196	LEU
34	1c	198	VAL
34	1c	207	VAL
35	1d	3	ARG
35	1d	19	LEU
35	1d	31	CYS
35	1d	53	ASP
35	1d	59	ARG
35	1d	70	ILE
35	1d	76	ARG
35	1d	77	ASN
35	1d	85	LYS
35	1d	86	LYS
35	1d	88	VAL
35	1d	91	SER
35	1d	119	GLN
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	144	ASP
35	1d	155	LEU
35	1d	157	LEU
35	1d	158	ILE
35	1d	160	GLN
35	1d	177	ASP
35	1d	182	LYS
35	1d	187	ARG
35	1d	188	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	190	ASP
35	1d	193	ASP
35	1d	194	LEU
35	1d	200	GLU
36	1e	9	LYS
36	1e	12	LEU
36	1e	24	ARG
36	1e	31	LEU
36	1e	41	VAL
36	1e	51	VAL
36	1e	53	LEU
36	1e	56	GLN
36	1e	120	THR
36	1e	140	ARG
37	1f	10	LEU
37	1f	16	GLN
37	1f	19	LEU
37	1f	54	LYS
37	1f	55	ASP
37	1f	64	GLN
37	1f	72	VAL
37	1f	75	LEU
37	1f	81	ILE
37	1f	92	LYS
38	1g	10	ARG
38	1g	12	LEU
38	1g	24	THR
38	1g	27	ILE
38	1g	41	ARG
38	1g	50	ILE
38	1g	59	LEU
38	1g	61	VAL
38	1g	85	TYR
38	1g	104	LEU
38	1g	110	GLN
38	1g	114	ARG
39	1h	3	THR
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	77	GLU
39	1h	98	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	1h	112	LEU
39	1h	133	LEU
40	1i	23	ASN
40	1i	25	LYS
40	1i	50	LEU
40	1i	56	LEU
40	1i	64	THR
40	1i	88	TYR
40	1i	89	ASN
40	1i	96	LEU
40	1i	108	VAL
41	1j	38	ILE
41	1j	43	ARG
41	1j	66	ARG
41	1j	72	VAL
41	1j	81	THR
41	1j	92	THR
41	1j	94	VAL
41	1j	96	ILE
42	1k	31	THR
42	1k	40	ILE
42	1k	48	ILE
42	1k	77	MET
42	1k	87	THR
42	1k	91	ARG
42	1k	109	VAL
42	1k	114	VAL
43	1l	18	VAL
43	1l	22	SER
43	1l	83	VAL
43	1l	123	LYS
44	1m	3	ARG
44	1m	4	ILE
44	1m	11	ARG
44	1m	43	THR
44	1m	47	ASP
44	1m	49	THR
44	1m	70	LEU
44	1m	78	ILE
44	1m	98	VAL
44	1m	106	ASN
44	1m	109	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	1m	121	LYS
45	1n	3	ARG
45	1n	32	SER
45	1n	33	VAL
46	1o	3	ILE
46	1o	10	LYS
46	1o	39	LEU
46	1o	47	LYS
46	1o	76	GLU
46	1o	84	LYS
46	1o	87	ILE
46	1o	88	ARG
47	1p	16	HIS
47	1p	20	VAL
47	1p	21	VAL
47	1p	27	LYS
47	1p	43	LYS
47	1p	45	THR
47	1p	57	ARG
47	1p	62	VAL
48	1q	34	LYS
48	1q	53	LEU
48	1q	60	ILE
48	1q	85	VAL
48	1q	86	GLU
48	1q	89	LEU
48	1q	93	GLN
49	1r	35	ARG
49	1r	63	GLN
49	1r	76	LEU
50	1s	4	SER
50	1s	12	ASP
50	1s	28	LYS
50	1s	30	LEU
50	1s	41	VAL
50	1s	66	MET
50	1s	79	THR
51	1t	10	LEU
51	1t	13	LEU
51	1t	24	LEU
51	1t	84	LEU
51	1t	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	1u	15	ARG
52	1u	20	LYS
3	2D	20	ASP
3	2D	37	LEU
3	2D	38	LYS
3	2D	61	LEU
3	2D	99	ASP
3	2D	111	LEU
3	2D	142	VAL
3	2D	171	ASP
3	2D	173	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	1	MET
4	2E	12	THR
4	2E	14	ILE
4	2E	38	THR
4	2E	73	GLU
4	2E	77	ILE
4	2E	78	LEU
4	2E	90	THR
4	2E	94	GLU
4	2E	116	VAL
4	2E	119	ARG
4	2E	175	VAL
4	2E	184	VAL
4	2E	195	LEU
5	2F	20	LEU
5	2F	24	LEU
5	2F	28	ILE
5	2F	33	LEU
5	2F	41	LEU
5	2F	70	THR
5	2F	126	VAL
5	2F	137	LYS
5	2F	145	GLU
5	2F	154	VAL
5	2F	157	VAL
5	2F	183	VAL
5	2F	189	THR
6	2G	3	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	5	VAL
6	2G	7	LEU
6	2G	18	GLU
6	2G	26	GLN
6	2G	28	VAL
6	2G	31	VAL
6	2G	41	GLN
6	2G	43	LEU
6	2G	45	GLU
6	2G	49	ASP
6	2G	51	ARG
6	2G	53	LEU
6	2G	62	LEU
6	2G	91	ARG
6	2G	124	SER
6	2G	130	ASN
6	2G	133	LEU
6	2G	140	ILE
6	2G	159	VAL
6	2G	162	THR
6	2G	165	THR
7	2H	7	LEU
7	2H	13	LYS
7	2H	15	VAL
7	2H	17	VAL
7	2H	32	GLU
7	2H	76	VAL
7	2H	84	SER
7	2H	99	VAL
7	2H	122	THR
7	2H	129	THR
7	2H	130	ARG
7	2H	134	SER
7	2H	136	ILE
7	2H	141	VAL
7	2H	148	ILE
8	2I	15	VAL
8	2I	38	LEU
8	2I	44	LEU
8	2I	50	ARG
8	2I	51	ILE
8	2I	58	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2I	61	ARG
8	2I	68	LEU
8	2I	76	THR
8	2I	82	ARG
8	2I	86	THR
8	2I	87	LYS
8	2I	117	GLU
8	2I	123	LEU
8	2I	127	VAL
8	2I	142	VAL
8	2I	145	VAL
9	2N	1	MET
9	2N	9	VAL
9	2N	28	THR
9	2N	32	THR
9	2N	38	HIS
9	2N	48	MET
9	2N	55	VAL
9	2N	61	ARG
9	2N	62	VAL
9	2N	71	ILE
9	2N	73	THR
9	2N	83	LYS
9	2N	131	GLN
10	2O	52	VAL
10	2O	69	ILE
10	2O	71	ARG
10	2O	86	ILE
10	2O	91	LEU
10	2O	104	ARG
11	2P	3	LEU
11	2P	45	LEU
11	2P	65	ARG
11	2P	70	GLN
11	2P	95	VAL
11	2P	96	THR
11	2P	98	GLU
11	2P	101	VAL
11	2P	123	LEU
11	2P	125	VAL
11	2P	135	LEU
11	2P	147	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	2Q	1	MET
12	2Q	6	ARG
12	2Q	7	MET
12	2Q	10	ARG
12	2Q	22	LYS
12	2Q	38	GLU
12	2Q	110	THR
13	2R	36	THR
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	15	ARG
14	2S	35	ILE
14	2S	40	ILE
14	2S	43	GLU
14	2S	48	LEU
14	2S	63	THR
14	2S	64	GLU
14	2S	67	ARG
14	2S	75	GLU
14	2S	76	LYS
14	2S	78	LEU
14	2S	83	LYS
14	2S	84	GLN
14	2S	110	LEU
15	2T	16	ARG
15	2T	23	ARG
15	2T	28	VAL
15	2T	63	VAL
15	2T	72	VAL
15	2T	74	ARG
15	2T	89	VAL
15	2T	96	ARG
15	2T	115	ARG
16	2U	5	LYS
16	2U	8	VAL
16	2U	17	ILE
16	2U	27	LEU
16	2U	59	ARG
16	2U	74	LEU
16	2U	77	SER
16	2U	111	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	2V	7	THR
17	2V	46	VAL
17	2V	52	VAL
17	2V	53	GLU
17	2V	56	SER
17	2V	57	VAL
17	2V	61	VAL
17	2V	79	VAL
17	2V	82	ARG
17	2V	98	GLU
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	67	ASP
18	2W	92	ARG
18	2W	111	HIS
19	2X	81	VAL
20	2Y	1	MET
20	2Y	7	VAL
20	2Y	14	LEU
20	2Y	21	LYS
20	2Y	38	ILE
20	2Y	39	VAL
20	2Y	50	ARG
20	2Y	67	LEU
20	2Y	72	VAL
20	2Y	91	GLU
20	2Y	97	ARG
20	2Y	98	VAL
20	2Y	99	CYS
21	2Z	31	ARG
21	2Z	33	LEU
21	2Z	35	ARG
21	2Z	41	LEU
21	2Z	42	VAL
21	2Z	47	VAL
21	2Z	67	LEU
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	90	VAL
21	2Z	96	VAL
21	2Z	100	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	2Z	121	HIS
21	2Z	137	ILE
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	170	THR
21	2Z	171	ILE
22	20	10	THR
22	20	30	VAL
23	21	26	ARG
23	21	78	LYS
23	21	80	LEU
23	21	81	LYS
23	21	89	GLU
23	21	98	LEU
24	22	30	ARG
24	22	35	LEU
24	22	44	LEU
24	22	59	ARG
24	22	62	THR
24	22	70	GLN
25	23	3	ARG
25	23	31	LEU
25	23	54	VAL
25	23	59	VAL
26	24	5	ILE
26	24	10	VAL
26	24	26	SER
26	24	31	ILE
26	24	33	VAL
26	24	34	GLU
26	24	50	VAL
26	24	59	PHE
26	24	63	TYR
26	24	68	ARG
27	25	6	VAL
27	25	58	LEU
27	25	59	GLU
28	26	7	ILE
28	26	9	LEU
28	26	19	ARG
28	26	34	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	26	48	VAL
28	26	52	VAL
29	27	1	MET
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
29	27	47	ARG
30	28	14	VAL
30	28	15	LYS
30	28	29	LYS
30	28	37	SER
31	29	7	VAL
31	29	22	ARG
31	29	28	GLU
31	29	33	LYS
33	2b	8	LYS
33	2b	9	GLU
33	2b	10	LEU
33	2b	11	LEU
33	2b	16	HIS
33	2b	35	GLU
33	2b	47	THR
33	2b	48	MET
33	2b	49	GLU
33	2b	67	THR
33	2b	68	ILE
33	2b	71	VAL
33	2b	76	GLN
33	2b	82	ARG
33	2b	83	MET
33	2b	93	VAL
33	2b	110	GLN
33	2b	112	VAL
33	2b	117	GLU
33	2b	127	ILE
33	2b	138	LEU
33	2b	142	LEU
33	2b	157	ARG
33	2b	164	VAL
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	198	ASP
33	2b	200	ILE
33	2b	201	ILE
33	2b	224	GLN
33	2b	230	VAL
33	2b	236	TYR
34	2c	5	ILE
34	2c	15	THR
34	2c	16	ARG
34	2c	44	GLU
34	2c	54	ARG
34	2c	55	VAL
34	2c	57	ILE
34	2c	70	VAL
34	2c	77	ILE
34	2c	91	LEU
34	2c	101	LEU
34	2c	103	VAL
34	2c	105	GLU
34	2c	116	VAL
34	2c	132	ARG
34	2c	140	ARG
34	2c	153	VAL
34	2c	161	GLU
34	2c	190	ARG
34	2c	195	VAL
35	2d	8	VAL
35	2d	17	VAL
35	2d	31	CYS
35	2d	53	ASP
35	2d	58	LEU
35	2d	59	ARG
35	2d	83	SER
35	2d	86	LYS
35	2d	92	VAL
35	2d	112	VAL
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	156	GLU
35	2d	188	LEU
35	2d	196	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2e	13	ILE
36	2e	18	ARG
36	2e	20	GLN
36	2e	25	ARG
36	2e	31	LEU
36	2e	38	GLN
36	2e	41	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	64	ARG
36	2e	72	GLN
36	2e	73	ASN
36	2e	75	THR
36	2e	89	ILE
36	2e	91	LEU
36	2e	151	LEU
37	2f	21	LEU
37	2f	37	VAL
37	2f	63	TYR
37	2f	92	LYS
38	2g	6	ARG
38	2g	9	VAL
38	2g	13	GLN
38	2g	24	THR
38	2g	31	MET
38	2g	36	LYS
38	2g	45	ASP
38	2g	78	ARG
38	2g	79	ARG
38	2g	80	VAL
38	2g	94	ARG
38	2g	106	GLN
38	2g	114	ARG
38	2g	115	ARG
38	2g	131	LYS
38	2g	135	VAL
39	2h	24	THR
39	2h	25	ASP
39	2h	29	SER
39	2h	51	VAL
39	2h	52	ASP
39	2h	99	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	2h	103	VAL
39	2h	109	ILE
39	2h	112	LEU
39	2h	119	LEU
39	2h	127	LEU
39	2h	129	VAL
39	2h	133	LEU
39	2h	134	ILE
39	2h	137	VAL
40	2i	20	ARG
40	2i	27	THR
40	2i	38	GLN
40	2i	40	LEU
40	2i	47	LEU
40	2i	54	ASP
40	2i	65	VAL
40	2i	89	ASN
40	2i	102	LEU
40	2i	124	GLN
41	2j	8	LEU
41	2j	23	ILE
41	2j	34	VAL
41	2j	38	ILE
41	2j	43	ARG
41	2j	45	ARG
41	2j	49	VAL
41	2j	62	HIS
41	2j	67	THR
41	2j	97	GLU
41	2j	98	ILE
41	2j	100	THR
42	2k	14	VAL
42	2k	48	ILE
42	2k	81	ASP
42	2k	84	VAL
42	2k	105	VAL
42	2k	109	VAL
42	2k	114	VAL
43	2l	18	VAL
43	2l	42	THR
43	2l	43	VAL
43	2l	46	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	2l	47	LYS
43	2l	62	SER
43	2l	83	VAL
43	2l	116	SER
43	2l	117	ARG
44	2m	4	ILE
44	2m	32	GLU
44	2m	53	VAL
44	2m	90	LEU
44	2m	94	ARG
44	2m	103	THR
44	2m	106	ASN
45	2n	3	ARG
45	2n	22	THR
45	2n	33	VAL
46	2o	13	GLN
46	2o	26	GLU
46	2o	27	VAL
46	2o	39	LEU
46	2o	54	ARG
46	2o	60	VAL
46	2o	64	ARG
46	2o	83	GLU
46	2o	87	ILE
47	2p	2	VAL
47	2p	8	ARG
47	2p	20	VAL
47	2p	21	VAL
47	2p	42	ARG
47	2p	54	GLU
47	2p	60	LEU
47	2p	73	LEU
48	2q	5	VAL
48	2q	14	LYS
48	2q	19	VAL
48	2q	41	LYS
48	2q	63	ARG
48	2q	84	LEU
48	2q	97	SER
48	2q	100	LYS
49	2r	31	LEU
49	2r	35	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	2r	82	THR
49	2r	84	LYS
49	2r	86	VAL
50	2s	12	ASP
50	2s	23	ASN
50	2s	37	ARG
50	2s	43	GLU
50	2s	47	HIS
50	2s	48	THR
50	2s	49	ILE
50	2s	56	GLN
50	2s	57	HIS
50	2s	58	VAL
50	2s	83	HIS
51	2t	9	ASN
51	2t	24	LEU
51	2t	71	THR
51	2t	93	GLU
52	2u	7	ARG
52	2u	13	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	116	GLN
3	1D	164	GLN
4	1E	48	GLN
4	1E	143	ASN
5	1F	8	GLN
5	1F	203	GLN
6	1G	26	GLN
8	1I	104	GLN
9	1N	69	GLN
9	1N	94	HIS
9	1N	133	GLN
10	1O	89	ASN
12	1Q	12	GLN
13	1R	71	GLN
14	1S	95	HIS
15	1T	43	GLN
16	1U	81	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1U	94	ASN
18	1W	60	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	92	ASN
21	1Z	54	HIS
21	1Z	73	GLN
24	12	43	GLN
25	13	32	GLN
33	1b	40	HIS
34	1c	6	HIS
34	1c	102	ASN
34	1c	162	GLN
34	1c	170	GLN
34	1c	181	ASN
35	1d	74	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
36	1e	38	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	57	GLN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	86	GLN
39	1h	15	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
44	1m	77	ASN
46	1o	46	HIS
47	1p	13	HIS
47	1p	14	ASN
48	1q	93	GLN
49	1r	63	GLN
50	1s	23	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1s	47	HIS
50	1s	83	HIS
51	1t	90	GLN
3	2D	87	ASN
3	2D	112	GLN
3	2D	166	GLN
4	2E	48	GLN
4	2E	180	ASN
5	2F	40	GLN
5	2F	69	HIS
5	2F	75	HIS
5	2F	133	ASN
6	2G	132	ASN
7	2H	143	GLN
8	2I	54	GLN
8	2I	105	HIS
10	2O	5	GLN
11	2P	70	GLN
12	2Q	12	GLN
12	2Q	113	GLN
12	2Q	141	GLN
13	2R	31	HIS
13	2R	71	GLN
14	2S	38	GLN
15	2T	43	GLN
16	2U	72	HIS
16	2U	94	ASN
19	2X	31	HIS
21	2Z	55	HIS
21	2Z	73	GLN
24	22	38	GLN
24	22	70	GLN
25	23	32	GLN
33	2b	110	GLN
33	2b	135	GLN
34	2c	28	GLN
34	2c	98	ASN
34	2c	102	ASN
34	2c	123	GLN
34	2c	162	GLN
35	2d	77	ASN
35	2d	116	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	160	GLN
36	2e	38	GLN
36	2e	127	ASN
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	106	GLN
39	2h	78	GLN
40	2i	3	GLN
40	2i	23	ASN
40	2i	31	GLN
41	2j	21	GLN
41	2j	68	HIS
42	2k	22	HIS
42	2k	38	ASN
42	2k	62	GLN
42	2k	116	HIS
42	2k	117	ASN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
46	2o	62	GLN
47	2p	16	HIS
49	2r	63	GLN
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	422 (14%)	29 (1%)
1	2A	2791/2915 (95%)	446 (15%)	28 (1%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	26 (22%)	0
32	1a	1497/1521 (98%)	248 (16%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	2a	1501/1521 (98%)	309 (20%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	69/76 (90%)	21 (30%)	0
54	1y	72/76 (94%)	24 (33%)	0
54	2w	66/76 (86%)	22 (33%)	0
54	2y	70/76 (92%)	26 (37%)	0
55	1x	74/77 (96%)	12 (16%)	0
55	2x	74/77 (96%)	13 (17%)	0
All	All	9339/9620 (97%)	1581 (16%)	57 (0%)

All (1581) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A
1	1A	72	U
1	1A	74	A
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(A)	G
1	1A	154(A)	C
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	271(K)	U
1	1A	271(L)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	357	A
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	456	C
1	1A	457	A
1	1A	479	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	513	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	746	A
1	1A	747	U
1	1A	764	A
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	855	G
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	883	G
1	1A	884	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	892	G
1	1A	893	C
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
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	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1038	C
1	1A	1040	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1057	A
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1064	C
1	1A	1068	G
1	1A	1069	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1081	U
1	1A	1083	U
1	1A	1085	A
1	1A	1086	A
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1092	C
1	1A	1093	G
1	1A	1094	U
1	1A	1097	U
1	1A	1099	G
1	1A	1101	U
1	1A	1108	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1117	G
1	1A	1135	C
1	1A	1136	G
1	1A	1141	U
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	1253	A
1	1A	1256	G
1	1A	1271	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1513	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1745(A)	C
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1817	G
1	1A	1828	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1962	5MC
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2108	C
1	1A	2110	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2119	A
1	1A	2121	G
1	1A	2122	U
1	1A	2126	A
1	1A	2127	G
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2152	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2160	G
1	1A	2161	C
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2180	U
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2321	G
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2407	G
1	1A	2414	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2663	G
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2721	A
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2804	C
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2892	A
1	1A	2894	G
2	1B	35	U
2	1B	45	A
2	1B	56	G
2	1B	64	C
2	1B	67	G
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	73	G
32	1a	76	C
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	115	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	308	C
32	1a	309	G
32	1a	317	G
32	1a	328	C
32	1a	330	C
32	1a	332	G
32	1a	342	C
32	1a	345	C
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	392	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	451	A
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	475	G
32	1a	483	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	574	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	607	A
32	1a	616	G
32	1a	630	G
32	1a	639	G
32	1a	653	A
32	1a	660	G
32	1a	665	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	666	G
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	703	G
32	1a	717	C
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	874	G
32	1a	876	G
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	997	U
32	1a	999	C
32	1a	1000	U
32	1a	1001	A
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1043	C
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1124	G
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G
32	1a	1135	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1140	C
32	1a	1146	A
32	1a	1151	A
32	1a	1152	A
32	1a	1154	G
32	1a	1159	U
32	1a	1181	G
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	1204	A
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
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	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1331	G
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1364	U
32	1a	1365	G
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1492	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
53	1v	13	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	34	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	61	C
54	1w	62	C
54	1w	66	U
54	1w	68	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1w	73	A
55	1x	6	G
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	22	G
55	1x	42	G
55	1x	47	U
55	1x	61	C
55	1x	69	C
55	1x	70	G
54	1y	5	G
54	1y	6	G
54	1y	7	A
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	34	G
54	1y	35	A
54	1y	36	A
54	1y	44	G
54	1y	45	U
54	1y	46	G7M
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	53	G
54	1y	56	C
54	1y	57	G
54	1y	58	A
54	1y	59	U
54	1y	64	A
54	1y	65	G
54	1y	70	G
1	2A	8	A
1	2A	12	U
1	2A	15	G
1	2A	23	G
1	2A	34	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	266	G
1	2A	267	C
1	2A	271(A)	A
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	272(J)	C
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	391	G
1	2A	396	G
1	2A	403	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	586	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	793	A
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	852	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	874	G
1	2A	879	G
1	2A	880	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1043	C
1	2A	1117	G
1	2A	1118	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1144	G
1	2A	1171	G
1	2A	1181	C
1	2A	1188	U
1	2A	1195	G
1	2A	1196	C
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1236	G
1	2A	1244	G
1	2A	1247	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1435	G
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	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1582	C
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1699	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1896	G
1	2A	1900	A
1	2A	1906	G
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2142	C
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2183	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2294	C
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2376	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2491	U
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2757	A
1	2A	2761	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2879	C
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	23	G
2	2B	33	G
2	2B	34	U
2	2B	35	U
2	2B	40	U
2	2B	41	U
2	2B	42	C
2	2B	45	A
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	94	C
2	2B	108	U
2	2B	110	G
2	2B	113	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	70	G
32	2a	73	G
32	2a	76	C
32	2a	79	G
32	2a	89	C
32	2a	101	A
32	2a	105	G
32	2a	115	G
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	156	G
32	2a	163	C
32	2a	180	U
32	2a	182	U
32	2a	189(A)	C
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	217	C
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	281	G
32	2a	289	G
32	2a	301	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	339	C
32	2a	345	C
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	411	A
32	2a	412	A
32	2a	413	G
32	2a	415	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	470	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	553	A
32	2a	559	A
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	607	A
32	2a	619	U
32	2a	630	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	777	A
32	2a	787	A
32	2a	792	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	859	A
32	2a	870	U
32	2a	875	C
32	2a	880	C
32	2a	887	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	963	G
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	984	C
32	2a	989	C
32	2a	990	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	996	A
32	2a	997	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	999	C
32	2a	1000	U
32	2a	1001	A
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1050	G
32	2a	1053	G
32	2a	1062	U
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1078	U
32	2a	1079	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1087	G
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1104	G
32	2a	1108	G
32	2a	1109	C
32	2a	1115	C
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1133	G
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1143	G
32	2a	1146	A
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1182	G
32	2a	1184	G
32	2a	1191	A
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1214	C
32	2a	1227	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1232	U
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1253	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1264	C
32	2a	1265	G
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1319	A
32	2a	1320	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	1359	C
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1368	G
32	2a	1380	U
32	2a	1398	A
32	2a	1400	5MC
32	2a	1404	5MC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1416	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1497	G
32	2a	1499	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1519	MA6
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
54	2w	3	C
54	2w	5	G
54	2w	9	A
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	27	G
54	2w	34	G
54	2w	46	G7M
54	2w	48	C
54	2w	58	A
54	2w	62	C
54	2w	63	G
54	2w	65	G
54	2w	66	U
54	2w	68	C
54	2w	69	G
54	2w	70	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2w	71	G
54	2w	73	A
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	21	A
55	2x	22	G
55	2x	43	A
55	2x	46	G
55	2x	47	U
55	2x	48	C
55	2x	51	C
55	2x	52	G
55	2x	68	C
54	2y	5	G
54	2y	7	A
54	2y	15	G
54	2y	19	G
54	2y	23	A
54	2y	26	A
54	2y	27	G
54	2y	40	C
54	2y	41	C
54	2y	43	C
54	2y	45	U
54	2y	46	G7M
54	2y	48	C
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	54	5MU
54	2y	56	C
54	2y	58	A
54	2y	59	U
54	2y	60	U
54	2y	61	C
54	2y	62	C
54	2y	68	C
54	2y	69	G
54	2y	70	G

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(J)	C
1	1A	278	A
1	1A	548	A
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	827	U
1	1A	974	G
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1762	A
1	1A	1992	G
1	1A	2170	A
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	229	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	896	A
1	2A	900	A
1	2A	1026	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1497	U
1	2A	1530	C
1	2A	1653	G
1	2A	1698	A
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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	4SU	1w	8	54	18,21,22	1.79	4 (22%)	25,30,33	1.94	5 (20%)
54	5MU	2y	54	54	19,22,23	1.52	5 (26%)	27,32,35	1.79	8 (29%)
54	4SU	2y	8	54	18,21,22	1.76	4 (22%)	25,30,33	2.07	4 (16%)
1	5MU	2A	1939	56,1	19,22,23	1.39	5 (26%)	27,32,35	2.33	6 (22%)
55	4SU	1x	8	55	18,21,22	2.23	6 (33%)	25,30,33	1.64	6 (24%)
1	PSU	1A	2605	56,1	18,21,22	1.45	3 (16%)	21,30,33	2.18	5 (23%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
54	G7M	1w	46	54	23,26,27	1.55	4 (17%)	34,39,42	1.59	4 (11%)
1	PSU	1A	1911	1	18,21,22	1.41	2 (11%)	21,30,33	2.02	3 (14%)
32	PSU	1a	516	32	18,21,22	1.40	2 (11%)	21,30,33	1.96	4 (19%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.10	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MA	1A	2503	56,1	22,25,26	1.48	4 (18%)	32,37,40	2.21	9 (28%)
32	G7M	2a	527	32,56	23,26,27	1.48	4 (17%)	34,39,42	1.72	4 (11%)
32	5MC	1a	1407	32	19,22,23	1.55	2 (10%)	26,32,35	1.12	2 (7%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	27,32,35	2.07	8 (29%)
1	OMU	2A	2552	56,1	19,22,23	1.15	3 (15%)	25,31,34	1.87	6 (24%)
1	PSU	2A	2605	1	18,21,22	1.35	3 (16%)	21,30,33	2.07	4 (19%)
32	5MC	1a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.22	4 (15%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.89	3 (14%)
54	MIA	1w	37	54	28,31,32	2.42	7 (25%)	38,44,47	2.72	12 (31%)
43	0TD	1l	92	43	8,9,10	4.56	1 (12%)	6,11,13	6.66	2 (33%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	21,30,33	1.89	3 (14%)
55	5MC	1x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.15	3 (11%)
54	4SU	1y	8	54	18,21,22	1.81	6 (33%)	25,30,33	1.78	5 (20%)
54	PSU	1y	55	54	18,21,22	1.40	2 (11%)	21,30,33	2.06	3 (14%)
32	4OC	1a	1402	32	20,23,24	0.71	0	25,32,35	1.00	1 (4%)
32	2MG	1a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.26	9 (27%)
32	5MC	2a	1400	32	19,22,23	1.70	3 (15%)	26,32,35	1.20	3 (11%)
1	5MC	1A	1942	56,1	19,22,23	1.61	3 (15%)	26,32,35	1.22	2 (7%)
54	PSU	1w	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.07	4 (19%)
55	4SU	2x	8	55,56	18,21,22	2.03	6 (33%)	25,30,33	1.42	4 (16%)
32	5MC	1a	967	32	19,22,23	1.62	2 (10%)	26,32,35	1.07	2 (7%)
55	31H	1x	76	55,56	31,34,35	1.22	3 (9%)	35,47,50	1.78	8 (22%)
54	PSU	1y	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.91	3 (14%)
54	MIA	1y	37	54	21,24,32	1.60	4 (19%)	30,35,47	2.05	8 (26%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.01	4 (19%)
54	PSU	2y	55	54	18,21,22	1.39	2 (11%)	21,30,33	1.91	5 (23%)
1	2MA	2A	2503	56,1	22,25,26	1.44	4 (18%)	32,37,40	2.40	9 (28%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	0.99	1 (4%)
1	5MU	1A	1915	1	19,22,23	1.43	5 (26%)	27,32,35	2.12	6 (22%)
54	G7M	2w	46	54	23,26,27	1.42	4 (17%)	34,39,42	1.63	5 (14%)
54	4SU	2w	8	54	18,21,22	1.87	4 (22%)	25,30,33	2.10	5 (20%)
55	31H	2x	76	55,56	31,34,35	1.23	3 (9%)	35,47,50	2.57	13 (37%)
54	PSU	1w	32	54,56	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
32	5MC	2a	1404	32	19,22,23	1.61	3 (15%)	26,32,35	1.15	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1915	1	19,22,23	1.47	4 (21%)	27,32,35	2.08	6 (22%)
32	PSU	2a	516	32	18,21,22	1.33	2 (11%)	21,30,33	2.09	5 (23%)
54	PSU	2y	39	54	18,21,22	1.37	2 (11%)	21,30,33	1.84	3 (14%)
32	MA6	1a	1519	32	23,26,27	0.45	0	33,38,41	2.05	10 (30%)
54	G7M	1y	46	54	23,26,27	1.58	3 (13%)	34,39,42	1.72	4 (11%)
32	5MC	2a	967	32	19,22,23	1.80	3 (15%)	26,32,35	1.11	3 (11%)
54	PSU	2w	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.92	3 (14%)
54	5MU	2w	54	54	19,22,23	1.37	4 (21%)	27,32,35	1.73	6 (22%)
54	PSU	1y	39	54	18,21,22	1.42	3 (16%)	21,30,33	1.77	3 (14%)
32	5MC	2a	1407	32	19,22,23	1.63	3 (15%)	26,32,35	1.20	3 (11%)
55	PSU	1x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.01	4 (19%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	1.01	2 (8%)
1	OMG	2A	2251	55,56,1	23,26,27	1.21	3 (13%)	32,38,41	1.98	6 (18%)
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
55	5MU	1x	54	55	19,22,23	1.48	5 (26%)	27,32,35	1.78	5 (18%)
1	OMU	1A	2552	56,1	19,22,23	1.23	3 (15%)	25,31,34	1.91	5 (20%)
54	PSU	1w	39	54	18,21,22	1.31	2 (11%)	21,30,33	2.12	4 (19%)
55	5MC	2x	32	55	19,22,23	1.77	3 (15%)	26,32,35	1.21	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.68	3 (15%)	26,32,35	1.09	2 (7%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.02	9 (27%)
54	5MU	1w	54	54	19,22,23	1.36	4 (21%)	27,32,35	2.08	6 (22%)
1	OMC	2A	1920	1	19,22,23	0.77	0	25,31,34	0.97	1 (4%)
54	MIA	2w	37	54	24,27,32	1.98	5 (20%)	32,39,47	2.47	10 (31%)
32	2MG	2a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.24	9 (27%)
1	5MC	2A	1962	56,1	19,22,23	1.77	3 (15%)	26,32,35	1.14	3 (11%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	2.04	10 (30%)
32	G7M	1a	527	32,56	23,26,27	1.50	4 (17%)	34,39,42	1.62	4 (11%)
54	G7M	2y	46	54	23,26,27	1.63	3 (13%)	34,39,42	1.77	4 (11%)
1	OMG	1A	2251	55,56,1	23,26,27	1.18	3 (13%)	32,38,41	1.95	6 (18%)
54	5MU	1y	54	54	19,22,23	1.44	6 (31%)	27,32,35	1.92	6 (22%)
1	5MC	1A	1962	56,1	19,22,23	1.62	3 (15%)	26,32,35	1.17	4 (15%)
43	0TD	2l	92	43	8,9,10	4.58	2 (25%)	6,11,13	1.46	1 (16%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.16	3 (11%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.88	6 (18%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.90	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.76	4 (15%)
32	UR3	2a	1498	32,56	19,22,23	1.04	2 (10%)	26,32,35	1.77	4 (15%)
1	5MU	1A	1939	56,1	19,22,23	1.46	5 (26%)	27,32,35	2.27	7 (25%)
54	PSU	2y	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.89	3 (14%)
54	MIA	2y	37	54	21,24,32	1.62	3 (14%)	30,35,47	2.04	9 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	2MA	1A	2503	56,1	-	0/7/25/26	0/3/3/3
32	G7M	2a	527	32,56	-	2/7/25/26	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	3/15/33/34	0/3/3/3
43	0TD	1l	92	43	-	4/7/12/14	-
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1942	56,1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	31H	1x	76	55,56	-	7/22/40/41	0/3/3/3
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	1/7/25/26	0/2/2/2
1	2MA	2A	2503	56,1	-	1/7/25/26	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,56	-	6/22/40/41	0/3/3/3
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	1/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
54	G7M	1y	46	54	-	2/7/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	OMG	2A	2251	55,56,1	-	0/9/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
54	MIA	2w	37	54	-	4/11/29/34	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MC	2A	1962	56,1	-	2/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	G7M	1a	527	32,56	-	3/7/25/26	0/3/3/3
54	G7M	2y	46	54	-	1/7/25/26	0/3/3/3
1	OMG	1A	2251	55,56,1	-	0/9/27/28	0/3/3/3
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32,56	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3

All (251) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.47	1.69	1.82
43	1l	92	0TD	CB-SB	-12.32	1.69	1.82
54	1w	37	MIA	C2-S10	-7.77	1.69	1.75
54	1w	37	MIA	C13-C14	6.79	1.52	1.32
32	2a	967	5MC	C5-C4	6.69	1.49	1.44
1	2A	1962	5MC	C5-C4	6.60	1.49	1.44
55	2x	32	5MC	C5-C4	6.50	1.49	1.44
32	2a	1400	5MC	C5-C4	6.15	1.48	1.44
1	2A	1942	5MC	C5-C4	6.14	1.48	1.44
32	1a	1404	5MC	C5-C4	6.12	1.48	1.44
55	1x	32	5MC	C5-C4	5.92	1.48	1.44
1	1A	1962	5MC	C5-C4	5.85	1.48	1.44
32	1a	967	5MC	C5-C4	5.85	1.48	1.44
54	2w	37	MIA	C2-S10	-5.84	1.70	1.75
32	1a	1407	5MC	C5-C4	5.75	1.48	1.44
32	2a	1404	5MC	C5-C4	5.74	1.48	1.44
32	1a	1400	5MC	C5-C4	5.74	1.48	1.44
1	1A	1942	5MC	C5-C4	5.73	1.48	1.44
32	2a	1407	5MC	C5-C4	5.69	1.48	1.44
55	1x	8	4SU	C4-N3	-5.31	1.32	1.37
54	2y	46	G7M	C5-N7	-5.13	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	37	MIA	C5-C4	5.08	1.48	1.39
54	1y	37	MIA	C5-C4	5.02	1.48	1.39
54	2w	8	4SU	C4-S4	-5.00	1.59	1.68
54	2w	37	MIA	C5-C4	4.90	1.47	1.39
54	1w	37	MIA	C5-C4	4.86	1.47	1.39
55	1x	76	31H	C5-N7	-4.80	1.30	1.39
54	1w	8	4SU	C4-S4	-4.77	1.60	1.68
54	1w	46	G7M	C5-N7	-4.71	1.33	1.39
54	1y	46	G7M	C5-N7	-4.69	1.33	1.39
54	2y	8	4SU	C4-S4	-4.68	1.60	1.68
55	2x	8	4SU	C4-N3	-4.67	1.32	1.37
32	1a	527	G7M	C5-N7	-4.58	1.33	1.39
1	1A	2503	2MA	C5-C4	4.53	1.47	1.39
55	1x	8	4SU	C4-S4	-4.50	1.60	1.68
54	1y	8	4SU	C4-S4	-4.50	1.60	1.68
55	2x	8	4SU	C4-S4	-4.45	1.60	1.68
32	2a	527	G7M	C5-N7	-4.26	1.34	1.39
1	2A	2503	2MA	C5-C4	4.23	1.46	1.39
54	1y	55	PSU	C6-C5	4.07	1.39	1.35
54	1w	55	PSU	C6-C5	3.95	1.39	1.35
54	2y	39	PSU	C6-C5	3.94	1.39	1.35
54	2w	55	PSU	C6-C5	3.93	1.39	1.35
55	1x	8	4SU	C2-N3	-3.92	1.31	1.38
54	2w	46	G7M	C5-N7	-3.90	1.34	1.39
55	2x	76	31H	C5-C4	-3.87	1.32	1.39
54	1y	32	PSU	C6-C5	3.79	1.39	1.35
54	1y	39	PSU	C6-C5	3.78	1.39	1.35
54	2y	32	PSU	C6-C5	3.78	1.39	1.35
54	2w	39	PSU	C6-C5	3.78	1.39	1.35
54	2w	32	PSU	C6-C5	3.75	1.39	1.35
32	1a	516	PSU	C6-C5	3.71	1.39	1.35
54	1w	32	PSU	C6-C5	3.70	1.39	1.35
32	2a	516	PSU	C6-C5	3.67	1.39	1.35
1	2A	1911	PSU	C6-C5	3.67	1.39	1.35
55	2x	55	PSU	C6-C5	3.65	1.39	1.35
54	1y	8	4SU	C4-N3	-3.63	1.33	1.37
54	2w	8	4SU	C4-N3	-3.59	1.33	1.37
1	2A	1917	PSU	C6-C5	3.57	1.39	1.35
54	1y	46	G7M	C5-C4	3.56	1.47	1.38
1	1A	1917	PSU	C6-C5	3.52	1.39	1.35
1	2A	2605	PSU	C6-C5	3.49	1.39	1.35
54	2y	46	G7M	C5-C4	3.46	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2605	PSU	C4-N3	-3.45	1.32	1.38
55	1x	55	PSU	C6-C5	3.40	1.39	1.35
54	1w	46	G7M	C5-C4	3.39	1.46	1.38
54	2y	55	PSU	C6-C5	3.39	1.39	1.35
55	1x	8	4SU	C5-C4	-3.38	1.38	1.42
32	1a	527	G7M	C5-C4	3.33	1.46	1.38
1	1A	1911	PSU	C6-C5	3.33	1.39	1.35
54	1w	39	PSU	C6-C5	3.32	1.39	1.35
32	2a	1207	2MG	C5-C4	3.27	1.47	1.38
32	2a	527	G7M	C5-C4	3.25	1.46	1.38
54	2w	46	G7M	C5-C4	3.22	1.46	1.38
32	1a	966	M2G	C2-N2	3.21	1.41	1.35
32	2a	966	M2G	C5-C4	3.19	1.47	1.38
1	2A	2251	OMG	C5-C4	3.17	1.47	1.38
54	2y	8	4SU	C4-N3	-3.09	1.34	1.37
1	2A	1939	5MU	C6-C5	3.06	1.39	1.34
54	2y	54	5MU	C2-N1	3.04	1.43	1.38
1	1A	2251	OMG	C5-C4	3.03	1.47	1.38
54	1w	8	4SU	C4-N3	-3.03	1.34	1.37
55	2x	76	31H	C5-N7	-3.02	1.33	1.39
32	1a	966	M2G	C5-C4	3.01	1.47	1.38
54	2w	37	MIA	C5-C6	2.98	1.49	1.41
32	1a	1207	2MG	C5-C4	2.98	1.46	1.38
1	1A	1942	5MC	C6-C5	2.96	1.39	1.34
1	2A	1915	5MU	C6-C5	2.95	1.39	1.34
55	1x	32	5MC	C6-C5	2.95	1.39	1.34
55	2x	8	4SU	C2-N3	-2.94	1.32	1.38
55	2x	8	4SU	C5-C4	-2.93	1.39	1.42
32	2a	1407	5MC	C6-C5	2.93	1.39	1.34
32	2a	1404	5MC	C6-C5	2.90	1.39	1.34
32	2a	967	5MC	C6-C5	2.89	1.39	1.34
54	1y	37	MIA	C5-C6	2.89	1.49	1.41
32	1a	967	5MC	C6-C5	2.88	1.39	1.34
54	2y	54	5MU	C6-C5	2.88	1.39	1.34
54	2y	37	MIA	C5-C6	2.88	1.49	1.41
1	2A	1942	5MC	C6-C5	2.86	1.39	1.34
55	2x	32	5MC	C6-C5	2.86	1.39	1.34
55	1x	76	31H	C5-C4	-2.86	1.34	1.39
54	2w	54	5MU	C6-C5	2.86	1.39	1.34
32	2a	1400	5MC	C6-C5	2.85	1.39	1.34
32	1a	1404	5MC	C6-C5	2.84	1.39	1.34
1	1A	1939	5MU	C6-N1	-2.84	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C4-N3	-2.83	1.33	1.38
1	1A	2552	OMU	C4-N3	-2.83	1.33	1.38
54	1y	54	5MU	C6-C5	2.82	1.39	1.34
55	1x	54	5MU	C6-C5	2.82	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.81	1.33	1.38
32	1a	1400	5MC	C6-C5	2.81	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.79	1.33	1.38
54	1w	37	MIA	C5-C6	2.76	1.48	1.41
54	1y	39	PSU	C4-N3	-2.75	1.33	1.38
1	2A	1915	5MU	C4-C5	2.74	1.49	1.44
1	2A	1939	5MU	C4-N3	-2.73	1.33	1.38
32	2a	966	M2G	C2-N2	2.73	1.40	1.35
55	2x	54	5MU	C6-C5	2.73	1.39	1.34
1	2A	1915	5MU	C2-N1	2.71	1.42	1.38
54	1y	54	5MU	C4-N3	-2.69	1.33	1.38
1	1A	1915	5MU	C6-C5	2.69	1.39	1.34
1	1A	1915	5MU	C2-N1	2.69	1.42	1.38
54	1w	54	5MU	C6-C5	2.68	1.39	1.34
1	1A	2503	2MA	C5-C6	2.67	1.48	1.41
54	2w	8	4SU	C5-C4	-2.67	1.39	1.42
54	1w	8	4SU	C5-C4	-2.66	1.39	1.42
54	1w	32	PSU	C4-N3	-2.62	1.33	1.38
55	2x	76	31H	C5-C6	-2.59	1.33	1.41
1	1A	1939	5MU	C6-C5	2.59	1.38	1.34
54	2y	55	PSU	C4-N3	-2.58	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.58	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.58	1.33	1.38
55	2x	54	5MU	C4-C5	2.57	1.49	1.44
54	2y	54	5MU	C4-C5	2.57	1.49	1.44
55	1x	54	5MU	C2-N1	2.57	1.42	1.38
1	2A	1962	5MC	C6-N1	-2.56	1.33	1.38
54	2w	54	5MU	C4-N3	-2.55	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.55	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.55	1.33	1.37
1	2A	2251	OMG	C6-N1	-2.54	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.53	1.34	1.38
54	2y	54	5MU	C4-N3	-2.53	1.34	1.38
54	1w	54	5MU	C2-N1	2.53	1.42	1.38
1	1A	1915	5MU	C4-N3	-2.53	1.34	1.38
32	1a	1407	5MC	C6-C5	2.53	1.38	1.34
32	2a	527	G7M	C6-N1	-2.52	1.34	1.38
1	1A	2552	OMU	C2-N3	-2.52	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	55	PSU	C4-N3	-2.51	1.34	1.38
1	1A	2605	PSU	C6-C5	2.51	1.38	1.35
55	2x	55	PSU	C4-N3	-2.51	1.34	1.38
32	2a	1498	UR3	C2-N1	2.51	1.42	1.38
32	1a	516	PSU	C4-N3	-2.50	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.50	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.49	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.49	1.34	1.38
54	1y	8	4SU	C5-C4	-2.48	1.39	1.42
1	1A	2503	2MA	C8-N7	2.47	1.36	1.31
32	1a	1404	5MC	C6-N1	-2.47	1.33	1.38
54	1y	54	5MU	C4-C5	2.47	1.48	1.44
55	2x	54	5MU	C4-N3	-2.47	1.34	1.38
54	2y	39	PSU	C4-N3	-2.46	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.45	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.45	1.34	1.38
55	1x	54	5MU	C4-C5	2.44	1.48	1.44
54	2w	8	4SU	C2-N3	-2.43	1.33	1.38
1	1A	2251	OMG	C6-N1	-2.42	1.34	1.38
54	1w	39	PSU	C4-N3	-2.42	1.34	1.38
54	2y	8	4SU	C5-C4	-2.42	1.39	1.42
54	1w	37	MIA	C5-N7	-2.41	1.34	1.39
55	2x	54	5MU	C2-N1	2.40	1.42	1.38
54	1y	37	MIA	C8-N7	2.40	1.36	1.31
1	1A	1915	5MU	C4-C5	2.40	1.48	1.44
32	1a	1400	5MC	C6-N1	-2.40	1.33	1.38
54	2y	46	G7M	C6-N1	-2.39	1.34	1.38
54	1w	37	MIA	C8-N7	2.39	1.36	1.31
1	2A	2503	2MA	C5-N7	-2.38	1.34	1.39
54	1y	32	PSU	C4-N3	-2.38	1.34	1.38
1	2A	1962	5MC	C6-C5	2.37	1.38	1.34
54	1y	46	G7M	C6-N1	-2.36	1.34	1.38
55	1x	55	PSU	C4-N3	-2.36	1.34	1.38
32	1a	1498	UR3	C2-N1	2.36	1.41	1.38
55	1x	32	5MC	C6-N1	-2.36	1.34	1.38
1	2A	2503	2MA	C5-C6	2.35	1.47	1.41
54	2y	32	PSU	C4-N3	-2.34	1.34	1.38
1	1A	1962	5MC	C6-C5	2.33	1.38	1.34
54	2w	39	PSU	C4-N3	-2.33	1.34	1.38
54	2w	37	MIA	C8-N7	2.33	1.36	1.31
54	2y	8	4SU	C2-N1	2.33	1.42	1.38
54	2y	37	MIA	C8-N7	2.32	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	C6-N1	-2.32	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.32	1.34	1.38
54	1w	8	4SU	C2-N1	2.31	1.42	1.38
54	1w	54	5MU	C4-N3	-2.31	1.34	1.38
54	1w	55	PSU	C4-N3	-2.30	1.34	1.38
54	1y	55	PSU	C4-N3	-2.30	1.34	1.38
32	2a	966	M2G	C6-N1	-2.30	1.34	1.38
1	1A	1939	5MU	C4-C5	2.29	1.48	1.44
54	2w	32	PSU	C4-N3	-2.28	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.27	1.34	1.38
54	1y	54	5MU	C2-N1	2.27	1.42	1.38
54	2w	54	5MU	C4-C5	2.26	1.48	1.44
55	1x	76	31H	C5-C6	-2.25	1.34	1.41
32	1a	966	M2G	C6-N1	-2.25	1.34	1.38
32	2a	516	PSU	C4-N3	-2.25	1.34	1.38
54	1w	54	5MU	C4-C5	2.25	1.48	1.44
55	2x	8	4SU	O2-C2	2.22	1.27	1.23
55	2x	54	5MU	C6-N1	-2.20	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.20	1.34	1.38
54	1w	46	G7M	C4-N9	-2.20	1.32	1.38
32	2a	1400	5MC	C6-N1	-2.19	1.34	1.38
32	1a	527	G7M	C6-N1	-2.19	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.18	1.34	1.38
32	1a	527	G7M	C4-N9	-2.18	1.32	1.38
54	1y	8	4SU	C2-N1	2.18	1.41	1.38
55	1x	8	4SU	O2-C2	2.17	1.26	1.23
32	2a	1404	5MC	C6-N1	-2.16	1.34	1.38
54	2w	37	MIA	C5-N7	-2.16	1.35	1.39
54	1y	54	5MU	C2-N3	-2.16	1.34	1.38
1	2A	1939	5MU	C4-C5	2.16	1.48	1.44
32	2a	527	G7M	C5-C6	2.16	1.49	1.43
54	1y	54	5MU	C6-N1	-2.16	1.34	1.38
54	2y	54	5MU	O2-C2	2.15	1.26	1.23
1	1A	2251	OMG	C5-N7	-2.15	1.34	1.39
54	2w	46	G7M	C4-N9	-2.14	1.32	1.38
55	2x	32	5MC	C6-N1	-2.14	1.34	1.38
1	2A	2552	OMU	C2-N3	-2.14	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.14	1.34	1.39
1	2A	2503	2MA	C8-N7	2.13	1.35	1.31
32	2a	966	M2G	C5-N7	-2.13	1.34	1.39
54	1y	8	4SU	C2-N3	-2.12	1.34	1.38
54	1y	37	MIA	C5-N7	-2.11	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-CA	2.10	1.55	1.54
1	2A	2552	OMU	C6-C5	2.10	1.39	1.35
55	1x	54	5MU	C2-N3	-2.09	1.34	1.38
55	2x	8	4SU	C2-N1	2.09	1.41	1.38
54	1y	8	4SU	C6-C5	2.08	1.39	1.35
54	1w	37	MIA	C4-N9	-2.06	1.33	1.37
1	1A	1915	5MU	C6-N1	-2.06	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.04	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.04	1.35	1.39
54	2w	54	5MU	C2-N1	2.04	1.41	1.38
32	1a	966	M2G	C5-N7	-2.04	1.35	1.39
32	2a	1498	UR3	C6-C5	2.04	1.39	1.35
55	1x	8	4SU	C6-C5	2.03	1.39	1.35
1	1A	1942	5MC	C6-N1	-2.03	1.34	1.38
54	1y	39	PSU	C2-N3	-2.02	1.34	1.37
1	1A	2552	OMU	C6-C5	2.02	1.39	1.35
32	2a	967	5MC	C6-N1	-2.02	1.34	1.38
54	2w	46	G7M	C5-C6	2.02	1.48	1.43
32	2a	1207	2MG	C2-N3	2.02	1.35	1.32
1	2A	2605	PSU	C2-N3	-2.00	1.34	1.37

All (423) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-16.03	73.56	102.36
54	1w	37	MIA	C12-C13-C14	-9.26	110.38	127.01
54	2w	37	MIA	C5-C4-N3	-8.23	118.51	127.18
1	2A	2503	2MA	C5-C4-N3	-8.21	118.53	127.18
55	2x	76	31H	O4'-C1'-N9	7.97	123.39	108.09
1	1A	2503	2MA	C5-C4-N3	-7.56	119.22	127.18
54	1w	37	MIA	C5-C4-N3	-7.35	119.43	127.18
32	2a	1207	2MG	C2-N3-C4	7.11	120.89	112.00
32	1a	1207	2MG	C2-N3-C4	6.98	120.73	112.00
1	2A	2503	2MA	N3-C4-N9	6.86	135.69	126.99
32	2a	1498	UR3	C4-N3-C2	-6.85	119.06	124.58
1	1A	2605	PSU	N1-C2-N3	6.82	122.36	115.17
54	1y	55	PSU	N1-C2-N3	6.67	122.21	115.17
1	2A	1917	PSU	N1-C2-N3	6.55	122.07	115.17
54	2w	37	MIA	N3-C4-N9	6.53	135.27	126.99
54	1w	39	PSU	N1-C2-N3	6.47	121.99	115.17
1	1A	1917	PSU	N1-C2-N3	6.42	121.94	115.17
32	1a	1498	UR3	C4-N3-C2	-6.37	119.46	124.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	55	PSU	N1-C2-N3	6.36	121.88	115.17
32	2a	516	PSU	N1-C2-N3	6.33	121.85	115.17
55	2x	55	PSU	N1-C2-N3	6.32	121.83	115.17
1	1A	1911	PSU	N1-C2-N3	6.32	121.83	115.17
32	2a	966	M2G	C5-C4-N3	-6.29	118.38	128.39
1	2A	2605	PSU	N1-C2-N3	6.22	121.72	115.17
55	1x	55	PSU	N1-C2-N3	6.19	121.69	115.17
54	1w	32	PSU	N1-C2-N3	6.12	121.62	115.17
54	1w	55	PSU	N1-C2-N3	6.08	121.58	115.17
32	2a	1207	2MG	C5-C4-N3	-6.08	118.72	128.39
32	1a	966	M2G	C5-C4-N3	-6.07	118.73	128.39
32	1a	516	PSU	N1-C2-N3	6.05	121.55	115.17
54	2y	8	4SU	C4-N3-C2	-6.01	121.55	127.31
55	2x	76	31H	N1-C2-N3	-5.98	119.54	128.58
54	2w	8	4SU	C5-C4-N3	5.95	120.29	114.75
1	2A	2251	OMG	C5-C4-N3	-5.94	118.93	128.39
1	2A	1911	PSU	N1-C2-N3	5.94	121.43	115.17
1	1A	2251	OMG	C5-C4-N3	-5.93	118.96	128.39
54	2w	32	PSU	N1-C2-N3	5.92	121.42	115.17
54	1y	37	MIA	C5-C4-N3	-5.92	118.56	126.72
54	2w	8	4SU	C4-N3-C2	-5.92	121.64	127.31
54	2y	32	PSU	N1-C2-N3	5.90	121.39	115.17
54	2w	39	PSU	N1-C2-N3	5.87	121.36	115.17
55	2x	76	31H	C5-C4-N3	-5.83	118.68	126.72
54	1y	32	PSU	N1-C2-N3	5.83	121.32	115.17
1	2A	1939	5MU	C4-N3-C2	-5.81	119.72	127.34
54	1y	46	G7M	N9-C4-N3	5.75	137.45	125.95
54	2y	55	PSU	N1-C2-N3	5.75	121.23	115.17
54	2y	46	G7M	N9-C4-N3	5.75	137.45	125.95
32	1a	1207	2MG	C5-C4-N3	-5.70	119.32	128.39
54	2y	39	PSU	N1-C2-N3	5.70	121.18	115.17
1	1A	2503	2MA	N3-C4-N9	5.68	134.20	126.99
54	1w	37	MIA	N3-C4-N9	5.62	134.12	126.99
54	1y	39	PSU	N1-C2-N3	5.61	121.08	115.17
1	1A	1939	5MU	C4-N3-C2	-5.61	119.99	127.34
54	2y	37	MIA	C5-C4-N3	-5.56	119.06	126.72
1	2A	1939	5MU	N3-C2-N1	5.53	122.09	114.89
32	2a	527	G7M	C5-C4-N3	-5.48	117.79	128.15
32	2a	527	G7M	N9-C4-N3	5.48	136.90	125.95
54	2y	46	G7M	C5-C4-N3	-5.46	117.83	128.15
55	1x	76	31H	N1-C2-N3	-5.36	120.47	128.58
54	1w	8	4SU	C5-C4-N3	5.30	119.68	114.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	8	4SU	C4-N3-C2	-5.29	122.24	127.31
54	1y	46	G7M	C5-C4-N3	-5.27	118.19	128.15
54	2y	8	4SU	C5-C4-N3	5.24	119.62	114.75
1	2A	1939	5MU	C5-C4-N3	5.22	119.86	115.32
1	1A	1939	5MU	C5-C4-N3	5.15	119.80	115.32
1	1A	2251	OMG	C2-N3-C4	5.13	121.13	112.30
1	1A	1915	5MU	C4-N3-C2	-5.13	120.62	127.34
55	2x	54	5MU	N3-C2-N1	5.12	121.56	114.89
1	1A	2552	OMU	C4-N3-C2	-5.12	120.26	126.61
1	2A	1915	5MU	C4-N3-C2	-5.09	120.66	127.34
54	1w	46	G7M	N9-C4-N3	5.09	136.14	125.95
1	1A	1915	5MU	N3-C2-N1	5.07	121.49	114.89
32	1a	527	G7M	N9-C4-N3	5.04	136.03	125.95
54	1w	54	5MU	N3-C2-N1	5.00	121.40	114.89
54	1w	54	5MU	C4-N3-C2	-4.98	120.81	127.34
55	2x	54	5MU	C4-N3-C2	-4.97	120.83	127.34
54	1y	8	4SU	C4-N3-C2	-4.96	122.56	127.31
32	2a	1519	MA6	N1-C2-N3	-4.95	121.09	128.58
1	2A	1915	5MU	N3-C2-N1	4.95	121.33	114.89
32	1a	1519	MA6	N1-C2-N3	-4.94	121.11	128.58
1	1A	2552	OMU	N3-C2-N1	4.92	121.29	114.89
1	2A	2552	OMU	C4-N3-C2	-4.88	120.56	126.61
32	2a	1518	MA6	N1-C2-N3	-4.86	121.23	128.58
32	2a	527	G7M	C2-N3-C4	4.85	120.66	112.30
1	2A	2251	OMG	N9-C4-N3	4.85	135.64	125.95
1	1A	1939	5MU	N3-C2-N1	4.84	121.19	114.89
32	1a	1518	MA6	N1-C2-N3	-4.83	121.27	128.58
32	1a	527	G7M	C5-C4-N3	-4.76	119.16	128.15
1	2A	2251	OMG	C2-N3-C4	4.74	120.47	112.30
54	2y	37	MIA	N3-C4-N9	4.73	135.21	127.17
54	1y	54	5MU	N3-C2-N1	4.72	121.03	114.89
54	1y	37	MIA	N3-C4-N9	4.70	135.16	127.17
54	2y	46	G7M	C2-N3-C4	4.69	120.37	112.30
54	1y	46	G7M	C2-N3-C4	4.67	120.34	112.30
32	1a	966	M2G	C2-N3-C4	4.65	121.10	112.51
32	2a	1518	MA6	C5-C4-N3	-4.64	120.32	126.72
32	2a	966	M2G	N9-C4-N3	4.60	135.15	125.95
54	2w	46	G7M	C5-C4-N3	-4.58	119.50	128.15
54	1w	46	G7M	C5-C4-N3	-4.58	119.50	128.15
32	1a	966	M2G	N9-C4-N3	4.57	135.09	125.95
54	2w	46	G7M	N9-C4-N3	4.57	135.09	125.95
1	2A	1915	5MU	C5-C4-N3	4.53	119.26	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1915	5MU	C5-C4-N3	4.52	119.26	115.32
1	1A	2605	PSU	C4-N3-C2	-4.52	120.15	126.37
1	2A	1939	5MU	O4-C4-C5	-4.50	119.77	124.92
54	1w	54	5MU	O4-C4-C5	-4.49	119.78	124.92
1	2A	2605	PSU	C4-N3-C2	-4.47	120.21	126.37
32	2a	966	M2G	C2-N3-C4	4.45	120.74	112.51
54	1y	54	5MU	C4-N3-C2	-4.44	121.52	127.34
32	1a	1519	MA6	C5-C4-N3	-4.44	120.61	126.72
1	1A	1939	5MU	C5-C6-N1	-4.43	118.50	123.31
54	2w	46	G7M	C2-N3-C4	4.43	119.92	112.30
32	2a	1519	MA6	C5-C4-N3	-4.39	120.68	126.72
1	2A	1939	5MU	C5-C6-N1	-4.35	118.59	123.31
1	2A	2552	OMU	N3-C2-N1	4.34	120.54	114.89
54	1w	39	PSU	C4-N3-C2	-4.34	120.40	126.37
54	1w	54	5MU	C5-C4-N3	4.31	119.07	115.32
54	1y	8	4SU	C5-C4-N3	4.30	118.75	114.75
32	1a	527	G7M	C2-N3-C4	4.29	119.68	112.30
1	1A	2251	OMG	N9-C4-N3	4.28	134.51	125.95
55	1x	54	5MU	N3-C2-N1	4.28	120.46	114.89
1	1A	1917	PSU	C4-N3-C2	-4.26	120.51	126.37
32	2a	516	PSU	C4-N3-C2	-4.25	120.52	126.37
55	2x	55	PSU	C4-N3-C2	-4.21	120.57	126.37
54	1w	39	PSU	O2-C2-N1	-4.14	118.52	122.79
54	1w	37	MIA	C15-C14-C13	-4.14	110.23	122.66
1	1A	1939	5MU	O4-C4-C5	-4.08	120.25	124.92
32	1a	1519	MA6	C2-N1-C6	4.07	121.78	111.83
54	2y	54	5MU	C5-C4-N3	4.06	118.86	115.32
32	1a	1518	MA6	C2-N1-C6	4.04	121.70	111.83
32	2a	1519	MA6	C4-C5-N7	-4.03	105.98	110.58
32	2a	1519	MA6	C5-N7-C8	4.03	109.78	103.45
32	1a	1518	MA6	C5-C4-N3	-4.03	121.17	126.72
32	1a	1207	2MG	C6-C5-N7	4.02	137.61	130.29
32	2a	1207	2MG	N9-C4-N3	4.02	133.99	125.95
32	1a	516	PSU	C4-N3-C2	-4.01	120.84	126.37
55	2x	54	5MU	C5-C4-N3	4.01	118.81	115.32
54	2y	8	4SU	N3-C2-N1	4.00	120.10	114.89
54	1w	46	G7M	C2-N3-C4	4.00	119.19	112.30
55	1x	54	5MU	C4-N3-C2	-4.00	122.10	127.34
32	1a	1518	MA6	C5-N7-C8	3.99	109.72	103.45
32	2a	1518	MA6	C2-N1-C6	3.98	121.56	111.83
1	2A	1917	PSU	C4-N3-C2	-3.95	120.93	126.37
32	2a	1519	MA6	C2-N1-C6	3.95	121.47	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1915	5MU	O4-C4-C5	-3.92	120.43	124.92
54	1w	32	PSU	C4-N3-C2	-3.91	120.99	126.37
1	1A	1911	PSU	C4-N3-C2	-3.89	121.01	126.37
54	2w	32	PSU	C4-N3-C2	-3.88	121.02	126.37
54	1y	55	PSU	C4-N3-C2	-3.88	121.02	126.37
54	1y	8	4SU	N3-C2-N1	3.88	119.94	114.89
1	1A	1911	PSU	O2-C2-N1	-3.88	118.79	122.79
32	1a	1400	5MC	C5-C6-N1	-3.88	119.10	123.31
32	2a	1400	5MC	C5-C6-N1	-3.87	119.11	123.31
1	2A	1911	PSU	C4-N3-C2	-3.86	121.05	126.37
55	1x	55	PSU	C4-N3-C2	-3.85	121.07	126.37
32	1a	1519	MA6	C4-C5-N7	-3.84	106.19	110.58
54	2w	54	5MU	N3-C2-N1	3.83	119.88	114.89
54	2w	55	PSU	C4-N3-C2	-3.83	121.09	126.37
54	2w	54	5MU	C5-C4-N3	3.83	118.65	115.32
54	1w	37	MIA	C6-C5-N7	3.82	136.60	132.43
54	1y	54	5MU	C5-C4-N3	3.82	118.64	115.32
54	1y	32	PSU	C4-N3-C2	-3.81	121.12	126.37
54	1w	37	MIA	C16-C14-C13	-3.81	111.24	122.66
54	2w	55	PSU	O2-C2-N1	-3.80	118.87	122.79
32	1a	1207	2MG	N9-C4-N3	3.80	133.54	125.95
55	2x	76	31H	C6-C5-C4	3.78	122.34	117.18
55	1x	54	5MU	C5-C4-N3	3.77	118.60	115.32
54	2w	39	PSU	C4-N3-C2	-3.77	121.18	126.37
32	2a	516	PSU	O2-C2-N1	-3.76	118.91	122.79
54	1y	37	MIA	C2-N3-C4	3.76	121.02	111.83
1	1A	2552	OMU	C5-C4-N3	3.76	120.06	114.80
1	2A	1915	5MU	O4-C4-C5	-3.74	120.63	124.92
1	2A	1917	PSU	O2-C2-N1	-3.74	118.93	122.79
55	1x	8	4SU	O2-C2-N1	3.73	127.65	122.80
32	1a	1518	MA6	N9-C8-N7	-3.73	108.65	113.94
54	2w	54	5MU	C4-N3-C2	-3.72	122.47	127.34
54	2y	54	5MU	C4-N3-C2	-3.71	122.47	127.34
54	1w	55	PSU	O2-C2-N1	-3.71	118.96	122.79
54	2y	55	PSU	C4-N3-C2	-3.71	121.26	126.37
32	1a	1519	MA6	C5-N7-C8	3.70	109.27	103.45
1	2A	2552	OMU	C5-C4-N3	3.70	119.98	114.80
32	1a	1518	MA6	C4-C5-N7	-3.69	106.36	110.58
54	2y	32	PSU	C4-N3-C2	-3.68	121.31	126.37
54	1w	55	PSU	C4-N3-C2	-3.67	121.32	126.37
55	1x	55	PSU	O2-C2-N1	-3.66	119.01	122.79
54	1y	37	MIA	C4-C5-N7	-3.62	106.44	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	54	5MU	N3-C2-N1	3.62	119.61	114.89
54	2y	39	PSU	C4-N3-C2	-3.62	121.39	126.37
54	2y	37	MIA	N3-C2-N1	-3.62	123.11	128.58
54	2y	37	MIA	C2-N3-C4	3.61	120.65	111.83
32	2a	1207	2MG	C6-C5-N7	3.61	136.86	130.29
55	2x	76	31H	C5-C4-N9	3.61	109.74	105.81
55	1x	8	4SU	C6-C5-C4	-3.60	116.83	119.95
54	2w	54	5MU	O4-C4-C5	-3.60	120.80	124.92
1	1A	1917	PSU	O2-C2-N1	-3.58	119.10	122.79
54	2w	37	MIA	C2-N3-C4	3.58	121.67	112.29
55	2x	54	5MU	O4-C4-C5	-3.58	120.82	124.92
54	2w	37	MIA	C4-C5-N7	-3.57	106.50	110.58
54	1y	55	PSU	O2-C2-N1	-3.57	119.11	122.79
32	2a	1518	MA6	C5-N7-C8	3.57	109.06	103.45
55	2x	76	31H	C2-N3-C4	3.56	120.53	111.83
55	1x	76	31H	C5-C4-N3	-3.56	121.82	126.72
54	1y	37	MIA	N3-C2-N1	-3.54	123.22	128.58
32	2a	1519	MA6	N9-C8-N7	-3.54	108.91	113.94
32	2a	1518	MA6	C4-C5-N7	-3.54	106.54	110.58
1	2A	2552	OMU	O2-C2-N1	-3.53	118.20	122.80
54	2y	55	PSU	O2-C2-N1	-3.53	119.15	122.79
1	1A	2503	2MA	C4-C5-N7	-3.51	106.56	110.58
32	1a	1404	5MC	C5-C6-N1	-3.51	119.50	123.31
54	1w	8	4SU	C5-C4-S4	-3.51	120.30	124.31
1	1A	1942	5MC	C5-C6-N1	-3.51	119.50	123.31
54	2w	8	4SU	N3-C2-N1	3.50	119.45	114.89
1	2A	1915	5MU	C5-C6-N1	-3.49	119.52	123.31
32	2a	1519	MA6	C2-N3-C4	3.49	120.34	111.83
32	2a	1518	MA6	C2-N3-C4	3.47	120.31	111.83
55	1x	32	5MC	C5-C6-N1	-3.47	119.54	123.31
1	2A	1942	5MC	C5-C6-N1	-3.47	119.55	123.31
55	2x	8	4SU	C5-C4-N3	3.43	117.94	114.75
1	1A	1942	5MC	C5-C4-N3	-3.43	118.24	121.75
55	2x	8	4SU	C1'-N1-C2	3.43	123.75	117.59
32	1a	1519	MA6	C2-N3-C4	3.42	120.19	111.83
54	1w	37	MIA	C4-C5-N7	-3.42	106.67	110.58
54	2w	8	4SU	C5-C4-S4	-3.39	120.44	124.31
1	2A	2503	2MA	C4-N9-C8	3.37	109.28	105.74
54	2y	8	4SU	C5-C4-S4	-3.36	120.47	124.31
55	1x	76	31H	N9-C8-N7	-3.36	109.17	113.94
1	2A	2503	2MA	C4-C5-N7	-3.35	106.75	110.58
54	1y	54	5MU	O4-C4-C5	-3.34	121.09	124.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	32	PSU	O2-C2-N1	-3.34	119.35	122.79
1	2A	2503	2MA	N6-C6-N1	3.34	121.53	117.03
54	2y	37	MIA	C4-C5-N7	-3.33	106.77	110.58
54	2w	37	MIA	C6-C5-N7	3.32	136.05	132.43
54	2y	54	5MU	O4-C4-C5	-3.31	121.12	124.92
32	2a	967	5MC	C5-C6-N1	-3.31	119.72	123.31
32	2a	1404	5MC	C5-C6-N1	-3.31	119.72	123.31
54	1y	39	PSU	C4-N3-C2	-3.31	121.81	126.37
1	2A	1962	5MC	C5-C6-N1	-3.30	119.73	123.31
55	2x	32	5MC	C5-C6-N1	-3.30	119.73	123.31
1	1A	2503	2MA	N6-C6-N1	3.29	121.46	117.03
54	1w	8	4SU	N3-C2-N1	3.29	119.17	114.89
55	1x	54	5MU	O4-C4-C5	-3.29	121.16	124.92
32	2a	1407	5MC	C5-C6-N1	-3.28	119.75	123.31
54	2w	37	MIA	C12-N6-C6	-3.28	119.81	122.85
1	1A	2251	OMG	C6-C5-N7	3.27	136.24	130.29
54	1y	32	PSU	O2-C2-N1	-3.27	119.42	122.79
55	2x	76	31H	N9-C8-N7	-3.26	109.32	113.94
54	2y	32	PSU	O2-C2-N1	-3.24	119.44	122.79
32	1a	1518	MA6	C2-N3-C4	3.24	119.74	111.83
54	1w	37	MIA	C2-N3-C4	3.21	120.71	112.29
55	2x	76	31H	C4'-O4'-C1'	-3.19	102.43	109.47
32	1a	1407	5MC	C5-C6-N1	-3.17	119.87	123.31
32	2a	1498	UR3	C5-C4-N3	3.14	119.17	115.04
55	1x	76	31H	C5-N7-C8	3.13	108.36	103.45
54	1y	54	5MU	C5-C6-N1	-3.12	119.93	123.31
1	1A	1915	5MU	C5-C6-N1	-3.12	119.93	123.31
32	2a	1518	MA6	N9-C8-N7	-3.10	109.54	113.94
32	1a	1207	2MG	N1-C2-N2	3.09	119.72	116.56
1	1A	2605	PSU	O2-C2-N1	-3.08	119.61	122.79
32	1a	967	5MC	C5-C6-N1	-3.08	119.97	123.31
32	1a	1519	MA6	N9-C8-N7	-3.07	109.58	113.94
55	1x	54	5MU	C5-C6-N1	-3.07	119.98	123.31
1	2A	1939	5MU	O2-C2-N1	-3.07	118.80	122.80
32	1a	1498	UR3	C5-C4-N3	3.07	119.08	115.04
1	2A	2251	OMG	C6-C5-N7	3.07	135.87	130.29
32	1a	1207	2MG	C4-C5-N7	-3.06	105.82	110.67
54	2y	37	MIA	C4-N9-C8	3.06	108.95	105.74
32	2a	1407	5MC	C5-C4-N3	-3.06	118.62	121.75
32	2a	966	M2G	C6-C5-N7	3.04	135.82	130.29
55	2x	54	5MU	C5-C6-N1	-3.04	120.02	123.31
32	1a	966	M2G	C6-C5-N7	3.02	135.79	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	8	4SU	C5-C4-N3	3.02	117.56	114.75
1	1A	1962	5MC	C5-C6-N1	-3.01	120.04	123.31
1	1A	1939	5MU	O2-C2-N1	-3.01	118.88	122.80
55	1x	32	5MC	C5-C4-N3	-2.97	118.71	121.75
55	2x	55	PSU	O2-C2-N1	-2.95	119.75	122.79
32	2a	1207	2MG	C4-C5-N7	-2.93	106.02	110.67
32	1a	1404	5MC	C5-C4-N3	-2.93	118.75	121.75
54	2w	39	PSU	O2-C2-N1	-2.91	119.78	122.79
54	1w	32	PSU	O2-C2-N1	-2.90	119.80	122.79
55	1x	76	31H	C2-N3-C4	2.90	118.91	111.83
1	2A	2605	PSU	O2-C2-N1	-2.88	119.81	122.79
32	2a	1518	MA6	N3-C4-N9	2.84	132.00	127.17
1	2A	1942	5MC	C5-C4-N3	-2.83	118.85	121.75
1	1A	2552	OMU	O2-C2-N1	-2.83	119.11	122.80
55	2x	32	5MC	C5-C4-N3	-2.82	118.86	121.75
55	1x	8	4SU	S4-C4-N3	-2.81	117.26	120.20
54	1w	37	MIA	C2-N1-C6	2.81	122.87	117.54
1	2A	1911	PSU	O2-C2-N1	-2.80	119.90	122.79
32	2a	1207	2MG	N1-C2-N2	2.80	119.42	116.56
54	2y	54	5MU	C5-C6-N1	-2.79	120.28	123.31
55	1x	76	31H	C4'-O4'-C1'	-2.78	103.32	109.47
32	1a	1402	4OC	C6-C5-C4	2.78	120.35	117.00
1	2A	2503	2MA	C5-N7-C8	2.77	107.80	103.45
32	1a	516	PSU	O2-C2-N1	-2.76	119.94	122.79
55	1x	8	4SU	C1'-N1-C2	2.76	122.56	117.59
1	1A	2605	PSU	C5-C6-N1	-2.76	118.31	122.14
32	2a	967	5MC	C5-C4-N3	-2.74	118.95	121.75
1	1A	2503	2MA	C2-N1-C6	2.74	122.31	118.10
32	1a	1498	UR3	C1'-N1-C2	2.73	121.50	117.04
32	2a	966	M2G	C4-C5-N7	-2.71	106.38	110.67
54	2w	54	5MU	C5-C6-N1	-2.69	120.39	123.31
32	2a	1207	2MG	N2-C2-N3	-2.69	117.08	120.51
54	1y	37	MIA	C5-N7-C8	2.68	107.67	103.45
54	2w	37	MIA	C5-N7-C8	2.67	107.65	103.45
54	1w	54	5MU	C5-C6-N1	-2.67	120.42	123.31
32	2a	1404	5MC	C5-C4-N3	-2.64	119.05	121.75
55	1x	76	31H	CA-N-CN	-2.64	118.76	122.82
1	1A	2503	2MA	C4-N9-C8	2.64	108.51	105.74
32	1a	1207	2MG	N2-C2-N3	-2.64	117.15	120.51
54	2y	39	PSU	O2-C2-N1	-2.63	120.07	122.79
32	2a	1518	MA6	C4-C5-C6	2.63	118.63	115.91
54	2w	37	MIA	C4-N9-C8	2.61	108.48	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	37	MIA	N3-C2-N1	-2.61	122.23	127.00
1	2A	1962	5MC	C5-C4-N3	-2.61	119.08	121.75
54	2w	46	G7M	O6-C6-C5	-2.60	122.22	128.01
32	1a	1518	MA6	N3-C4-N9	2.60	131.58	127.17
32	1a	1400	5MC	C5-C4-N3	-2.59	119.10	121.75
54	2y	37	MIA	C5-N7-C8	2.59	107.51	103.45
55	2x	76	31H	N3-C4-N9	2.58	131.56	127.17
32	1a	1498	UR3	C6-N1-C2	-2.56	119.70	121.80
32	2a	1519	MA6	N3-C4-N9	2.56	131.52	127.17
55	2x	8	4SU	C6-C5-C4	-2.56	117.74	119.95
55	2x	76	31H	C5-N7-C8	2.54	107.45	103.45
1	1A	2552	OMU	O4-C4-C5	-2.52	120.81	125.16
32	1a	527	G7M	O6-C6-C5	-2.52	122.39	128.01
32	2a	1400	5MC	O2-C2-N3	-2.52	118.36	122.33
1	2A	2605	PSU	C5-C6-N1	-2.51	118.66	122.14
1	2A	2503	2MA	N9-C8-N7	-2.50	110.39	113.94
32	1a	967	5MC	C5-C4-N3	-2.50	119.20	121.75
55	1x	8	4SU	O2-C2-N3	-2.49	116.89	121.49
54	2y	54	5MU	C5M-C5-C4	2.49	121.44	118.78
32	1a	1519	MA6	N3-C4-N9	2.48	131.39	127.17
1	1A	2503	2MA	C5-N7-C8	2.47	107.34	103.45
32	1a	1407	5MC	C5-C4-N3	-2.47	119.22	121.75
32	1a	1519	MA6	C4-C5-C6	2.46	118.46	115.91
54	1w	37	MIA	N3-C2-N1	-2.46	122.50	127.00
1	2A	2552	OMU	O4-C4-C5	-2.46	120.92	125.16
55	2x	76	31H	C4-C5-N7	-2.45	107.78	110.58
32	1a	966	M2G	O6-C6-C5	-2.45	120.07	126.53
54	1w	37	MIA	C4-N9-C8	2.44	108.31	105.74
54	2w	37	MIA	C2-N1-C6	2.44	122.17	117.54
32	2a	1402	4OC	C6-C5-C4	2.44	119.94	117.00
54	1y	37	MIA	C4-N9-C8	2.43	108.29	105.74
55	2x	32	5MC	O2-C2-N3	-2.43	118.50	122.33
1	2A	1962	5MC	CM5-C5-C6	-2.41	119.58	122.85
55	2x	54	5MU	C5M-C5-C4	2.41	121.36	118.78
43	2l	92	0TD	CSB-SB-CB	2.41	106.69	102.36
32	1a	966	M2G	C4-C5-N7	-2.41	106.86	110.67
1	1A	2251	OMG	C4-C5-N7	-2.38	106.89	110.67
54	1w	37	MIA	C5-N7-C8	2.38	107.19	103.45
54	1w	46	G7M	O6-C6-C5	-2.37	122.71	128.01
1	2A	2251	OMG	C4-C5-N7	-2.36	106.92	110.67
32	1a	1404	5MC	O2-C2-N3	-2.36	118.61	122.33
1	1A	1962	5MC	C5-C4-N3	-2.35	119.34	121.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	8	4SU	C1'-N1-C2	2.33	121.78	117.59
1	1A	1962	5MC	CM5-C5-C6	-2.32	119.71	122.85
55	2x	54	5MU	O2-C2-N1	-2.31	119.78	122.80
55	1x	76	31H	OCN-CN-N	-2.31	119.35	125.32
54	1w	54	5MU	O2-C2-N1	-2.31	119.80	122.80
55	2x	8	4SU	O2-C2-N1	2.30	125.79	122.80
32	2a	1407	5MC	O2-C2-N3	-2.28	118.73	122.33
43	1l	92	0TD	OD2-CG-CB	2.28	118.07	113.15
54	1y	8	4SU	C5-C4-S4	-2.28	121.71	124.31
54	2y	46	G7M	O6-C6-C5	-2.27	122.94	128.01
54	2w	54	5MU	C5M-C5-C4	2.27	121.21	118.78
54	1w	8	4SU	C1'-N1-C2	2.27	121.67	117.59
1	1A	1962	5MC	C1'-N1-C6	-2.25	117.45	121.15
54	2y	54	5MU	C1'-N1-C2	2.24	121.62	117.59
1	1A	2251	OMG	O6-C6-C5	-2.23	120.64	126.53
32	2a	1498	UR3	C3U-N3-C4	2.23	120.97	117.87
55	2x	55	PSU	C5-C6-N1	-2.23	119.05	122.14
1	1A	2503	2MA	C6-C5-N7	2.22	136.38	132.09
1	2A	2503	2MA	C2-N1-C6	2.22	121.52	118.10
54	2y	54	5MU	C1'-N1-C6	-2.22	117.49	121.15
32	2a	1498	UR3	C6-N1-C2	-2.22	119.99	121.80
32	2a	527	G7M	C5-C6-N1	2.21	116.40	111.84
54	1y	8	4SU	C1'-N1-C2	2.21	121.56	117.59
55	1x	55	PSU	C5-C6-N1	-2.21	119.08	122.14
1	1A	1915	5MU	C5M-C5-C4	2.20	121.13	118.78
54	1w	39	PSU	C5-C6-N1	-2.19	119.09	122.14
54	1y	46	G7M	O6-C6-C5	-2.19	123.12	128.01
54	1y	39	PSU	O2-C2-N1	-2.19	120.53	122.79
54	2y	55	PSU	O4'-C1'-C2'	2.18	108.17	105.15
1	2A	2251	OMG	O6-C6-C5	-2.18	120.77	126.53
32	1a	1518	MA6	C4-N9-C8	2.17	108.02	105.74
32	1a	1207	2MG	CM2-N2-C2	-2.17	118.99	123.65
32	2a	516	PSU	O4'-C1'-C2'	2.17	108.15	105.15
1	1A	2605	PSU	O2-C2-N3	-2.16	118.03	121.86
1	1A	1939	5MU	C5M-C5-C4	2.15	121.08	118.78
54	1w	32	PSU	C6-C5-C4	-2.14	116.73	118.17
54	2y	55	PSU	C6-C5-C4	-2.14	116.73	118.17
32	2a	1402	4OC	CM4-N4-C4	-2.13	118.28	122.45
55	2x	76	31H	OCN-CN-N	-2.12	119.84	125.32
1	1A	1920	OMC	O2-C2-N3	-2.12	118.99	122.33
32	2a	1207	2MG	C2-N1-C6	-2.12	121.99	124.55
32	2a	1404	5MC	O2-C2-N3	-2.10	119.02	122.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1207	2MG	CM2-N2-C2	-2.10	119.14	123.65
54	1y	54	5MU	C5M-C5-C4	2.09	121.01	118.78
32	1a	1404	5MC	CM5-C5-C6	-2.08	120.04	122.85
1	2A	1917	PSU	C5-C6-N1	-2.08	119.26	122.14
32	1a	1207	2MG	C8-N7-C5	2.07	107.95	104.26
1	2A	2552	OMU	C5-C6-N1	-2.06	118.48	121.84
32	1a	1400	5MC	O2-C2-N3	-2.06	119.08	122.33
32	2a	1400	5MC	C5-C4-N3	-2.06	119.64	121.75
1	1A	2503	2MA	N9-C8-N7	-2.06	111.01	113.94
32	2a	516	PSU	C5-C6-N1	-2.06	119.28	122.14
54	1y	37	MIA	C6-C5-N7	2.06	136.05	132.09
55	1x	32	5MC	O2-C2-N3	-2.05	119.09	122.33
1	1A	1917	PSU	C5-C6-N1	-2.05	119.29	122.14
55	2x	54	5MU	C5M-C5-C6	-2.05	120.08	122.85
54	2y	37	MIA	N9-C8-N7	-2.05	111.03	113.94
32	1a	1518	MA6	C4-C5-C6	2.04	118.02	115.91
32	2a	1519	MA6	C4-C5-C6	2.03	118.01	115.91
32	2a	966	M2G	O6-C6-C5	-2.03	121.19	126.53
54	2y	37	MIA	C2-N1-C6	2.02	122.05	118.73
1	2A	1920	OMC	O2-C2-N3	-2.02	119.14	122.33
1	2A	2503	2MA	C6-C5-N7	2.02	135.98	132.09
32	1a	516	PSU	O4'-C1'-C2'	2.01	107.93	105.15
32	1a	1519	MA6	C5-C4-N9	2.01	108.00	105.81
54	2w	46	G7M	C5-C6-N1	2.00	115.98	111.84
1	2A	1915	5MU	C5M-C5-C4	2.00	120.92	118.78
32	2a	967	5MC	O2-C2-N3	-2.00	119.17	122.33
55	2x	76	31H	CA-N-CN	-2.00	119.74	122.82

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
54	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	37	MIA	C5-C6-N6-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	2w	37	MIA	N1-C6-N6-C12
54	2w	37	MIA	N1-C2-S10-C11
54	2w	37	MIA	N3-C2-S10-C11
54	2y	54	5MU	O4'-C4'-C5'-O5'
55	1x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	2y	54	5MU	C3'-C4'-C5'-O5'
55	1x	76	31H	N-CA-CB-CG
55	2x	76	31H	N-CA-CB-CG
55	1x	76	31H	CB-CG-SD-CE
55	2x	76	31H	CB-CG-SD-CE
1	2A	1962	5MC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
55	1x	76	31H	C-CA-CB-CG
55	1x	76	31H	C4'-C5'-O5'-P
55	2x	76	31H	C4'-C5'-O5'-P
54	2w	46	G7M	C4'-C5'-O5'-P
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	1962	5MC	C3'-C4'-C5'-O5'
55	1x	76	31H	CB-CA-N-CN
55	2x	76	31H	CB-CA-N-CN
43	2l	92	0TD	CG-CB-SB-CSB
54	2y	46	G7M	O4'-C1'-N9-C4
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
54	1y	55	PSU	O4'-C1'-C5-C4
54	1w	37	MIA	N6-C12-C13-C14
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	527	G7M	C4'-C5'-O5'-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	1y	46	G7M	C3'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
54	1y	55	PSU	O4'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6
1	1A	1920	OMC	C2'-C1'-N1-C2

There are no ring outliers.

33 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	1	0
55	1x	8	4SU	2	0
54	1w	46	G7M	2	0
32	2a	1519	MA6	2	0
1	1A	2503	2MA	2	0
55	2x	54	5MU	2	0
54	1y	8	4SU	2	0
54	1y	55	PSU	3	0
32	1a	1402	4OC	1	0
32	2a	1400	5MC	1	0
1	1A	1917	PSU	1	0
32	1a	967	5MC	1	0
54	1y	37	MIA	1	0
55	2x	55	PSU	1	0
54	2y	55	PSU	4	0
55	2x	76	31H	1	0
1	2A	1915	5MU	1	0
32	1a	1519	MA6	2	0
54	1y	46	G7M	1	0
32	2a	967	5MC	1	0
54	1y	39	PSU	1	0
32	2a	1402	4OC	2	0
1	2A	1917	PSU	1	0
1	1A	2552	OMU	1	0
32	2a	1518	MA6	2	0
32	2a	1207	2MG	2	0
32	1a	1518	MA6	2	0
54	2y	46	G7M	2	0
1	1A	2251	OMG	1	0
54	1y	54	5MU	1	0
43	2l	92	0TD	2	0
32	1a	966	M2G	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2y	37	MIA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2581 ligands modelled in this entry, 2577 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	SF4	2d	302	35	0,12,12	-	-	-		
57	A1A1L	2A	3783	-	34,39,39	3.52	10 (29%)	33,56,56	1.41	5 (15%)
59	SF4	1d	302	35	0,12,12	-	-	-		
57	A1A1L	1A	4060	-	34,39,39	3.35	12 (35%)	33,56,56	1.50	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	2d	302	35	-	-	0/6/5/5
57	A1A1L	2A	3783	-	-	6/30/74/74	0/3/4/4
59	SF4	1d	302	35	-	-	0/6/5/5
57	A1A1L	1A	4060	-	-	5/30/74/74	0/3/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3783	A1A1L	C23-C22	-11.84	1.35	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	4060	A1A1L	C23-C22	-10.87	1.37	1.53
57	2A	3783	A1A1L	O24-C23	9.74	1.52	1.42
57	1A	4060	A1A1L	C21-N20	9.40	1.54	1.34
57	2A	3783	A1A1L	C21-N20	9.23	1.53	1.34
57	1A	4060	A1A1L	O24-C23	8.79	1.51	1.42
57	2A	3783	A1A1L	C34-N35	-4.56	1.32	1.47
57	1A	4060	A1A1L	C34-N35	-4.41	1.32	1.47
57	2A	3783	A1A1L	C11-S10	3.96	1.85	1.82
57	1A	4060	A1A1L	C11-S10	3.65	1.85	1.82
57	2A	3783	A1A1L	O08-C09	2.86	1.47	1.42
57	1A	4060	A1A1L	O08-C09	2.80	1.46	1.42
57	2A	3783	A1A1L	C07-C19	2.78	1.56	1.53
57	1A	4060	A1A1L	O36-C21	-2.76	1.18	1.23
57	2A	3783	A1A1L	O36-C21	-2.64	1.18	1.23
57	1A	4060	A1A1L	O08-C07	2.57	1.48	1.44
57	2A	3783	A1A1L	O08-C07	2.45	1.47	1.44
57	1A	4060	A1A1L	C05-C03	-2.24	1.46	1.52
57	1A	4060	A1A1L	C28-C27	2.23	1.56	1.53
57	1A	4060	A1A1L	O24-C25	-2.22	1.40	1.43
57	2A	3783	A1A1L	O24-C25	-2.03	1.40	1.43
57	1A	4060	A1A1L	C07-C19	2.02	1.55	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3783	A1A1L	C09-O08-C07	-3.99	108.94	114.17
57	1A	4060	A1A1L	C12-C14-C15	-3.64	104.92	114.51
57	2A	3783	A1A1L	C11-S10-C09	3.61	106.82	100.12
57	1A	4060	A1A1L	C09-O08-C07	-3.28	109.87	114.17
57	1A	4060	A1A1L	O08-C07-C05	2.86	111.98	107.94
57	2A	3783	A1A1L	O08-C07-C05	2.75	111.83	107.94
57	2A	3783	A1A1L	C12-C14-C15	-2.61	107.65	114.51
57	1A	4060	A1A1L	C11-S10-C09	2.39	104.55	100.12
57	1A	4060	A1A1L	O36-C21-N20	-2.35	118.76	122.96
57	2A	3783	A1A1L	C32-C27-C26	-2.17	110.55	113.78
57	1A	4060	A1A1L	C32-C27-C26	-2.06	110.71	113.78

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1A	4060	A1A1L	C11-C12-C14-C15

Continued on next page...

Continued from previous page...

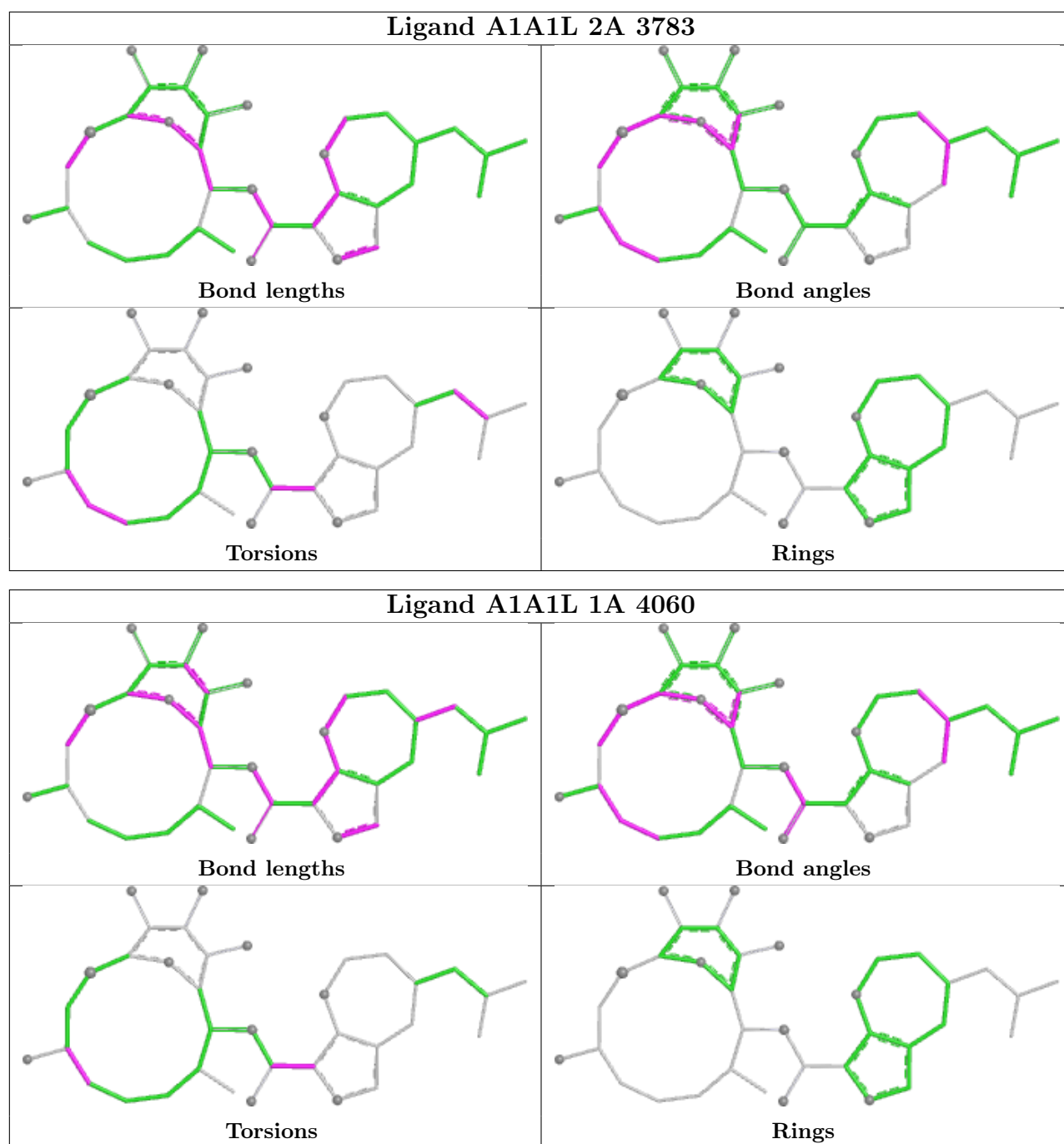
Mol	Chain	Res	Type	Atoms
57	1A	4060	A1A1L	F13-C12-C14-C15
57	2A	3783	A1A1L	C11-C12-C14-C15
57	2A	3783	A1A1L	F13-C12-C14-C15
57	1A	4060	A1A1L	O36-C21-C22-C23
57	2A	3783	A1A1L	O36-C21-C22-C23
57	1A	4060	A1A1L	N20-C21-C22-C23
57	2A	3783	A1A1L	N20-C21-C22-C23
57	1A	4060	A1A1L	O36-C21-C22-N35
57	2A	3783	A1A1L	C12-C14-C15-C16
57	2A	3783	A1A1L	C27-C28-C29-C31

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	2d	302	SF4	1	0
57	2A	3783	A1A1L	1	0
59	1d	302	SF4	1	0
57	1A	4060	A1A1L	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.47	128 (4%) 38 33	22, 38, 92, 107	0
1	2A	2789/2915 (95%)	0.10	110 (3%) 43 38	34, 59, 92, 104	0
2	1B	120/121 (99%)	-0.31	0 100 100	32, 52, 65, 90	0
2	2B	120/121 (99%)	0.97	3 (2%) 58 54	64, 81, 88, 92	0
3	1D	275/276 (99%)	-0.08	4 (1%) 72 68	23, 38, 52, 76	0
3	2D	275/276 (99%)	0.39	5 (1%) 67 64	32, 52, 63, 80	0
4	1E	204/206 (99%)	-0.06	2 (0%) 79 76	22, 40, 60, 73	0
4	2E	204/206 (99%)	0.58	3 (1%) 72 68	38, 60, 71, 78	0
5	1F	202/210 (96%)	0.09	2 (0%) 79 76	19, 43, 69, 84	0
5	2F	202/210 (96%)	0.77	10 (4%) 34 30	36, 68, 80, 86	0
6	1G	181/182 (99%)	0.75	13 (7%) 21 19	42, 62, 75, 88	0
6	2G	181/182 (99%)	1.75	61 (33%) 1 1	72, 81, 86, 91	0
7	1H	174/180 (96%)	0.32	3 (1%) 69 65	39, 54, 66, 72	0
7	2H	174/180 (96%)	1.65	55 (31%) 1 1	72, 82, 88, 92	0
8	1I	146/148 (98%)	1.05	13 (8%) 15 13	47, 74, 81, 84	0
8	2I	146/148 (98%)	1.30	20 (13%) 6 5	57, 73, 81, 85	0
9	1N	140/140 (100%)	-0.05	1 (0%) 84 81	28, 39, 61, 74	0
9	2N	140/140 (100%)	0.95	10 (7%) 22 19	49, 66, 78, 83	0
10	1O	122/122 (100%)	0.08	1 (0%) 82 80	30, 42, 59, 64	0
10	2O	122/122 (100%)	0.62	1 (0%) 82 80	48, 61, 71, 78	0
11	1P	149/150 (99%)	0.23	4 (2%) 56 51	23, 46, 67, 73	0
11	2P	149/150 (99%)	0.88	11 (7%) 20 18	39, 69, 81, 88	0
12	1Q	141/141 (100%)	0.12	2 (1%) 73 70	28, 43, 59, 75	0
12	2Q	141/141 (100%)	1.41	32 (22%) 2 2	50, 70, 78, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.17	0 100 100	26, 35, 50, 57	0
13	2R	118/118 (100%)	0.31	1 (0%) 82 80	42, 54, 64, 70	0
14	1S	110/112 (98%)	0.36	1 (0%) 81 78	40, 52, 64, 66	0
14	2S	110/112 (98%)	1.50	20 (18%) 3 2	68, 75, 82, 84	0
15	1T	131/146 (89%)	0.24	5 (3%) 44 39	32, 45, 67, 74	0
15	2T	131/146 (89%)	0.75	5 (3%) 44 39	53, 62, 73, 78	0
16	1U	116/118 (98%)	-0.31	0 100 100	23, 31, 46, 64	0
16	2U	116/118 (98%)	0.74	2 (1%) 69 65	48, 63, 76, 81	0
17	1V	101/101 (100%)	-0.20	1 (0%) 79 76	23, 41, 55, 67	0
17	2V	101/101 (100%)	0.91	3 (2%) 52 48	44, 72, 78, 81	0
18	1W	112/113 (99%)	-0.04	1 (0%) 81 78	25, 33, 53, 80	0
18	2W	112/113 (99%)	0.54	4 (3%) 46 41	41, 51, 65, 91	0
19	1X	95/96 (98%)	0.17	1 (1%) 78 75	28, 40, 62, 73	0
19	2X	95/96 (98%)	0.87	6 (6%) 26 23	48, 60, 74, 78	0
20	1Y	107/110 (97%)	0.42	2 (1%) 66 62	36, 51, 67, 78	0
20	2Y	107/110 (97%)	1.35	17 (15%) 5 4	59, 71, 81, 86	0
21	1Z	154/206 (74%)	1.01	20 (12%) 7 6	38, 65, 86, 88	0
21	2Z	160/206 (77%)	1.98	60 (37%) 1 1	71, 83, 91, 95	0
22	10	77/85 (90%)	0.11	2 (2%) 57 52	30, 39, 54, 62	0
22	20	79/85 (92%)	1.67	21 (26%) 1 1	51, 68, 75, 80	0
23	11	97/98 (98%)	0.37	1 (1%) 79 76	28, 45, 69, 77	0
23	21	97/98 (98%)	0.60	3 (3%) 51 47	42, 56, 74, 78	0
24	12	70/72 (97%)	0.22	0 100 100	36, 50, 60, 68	0
24	22	70/72 (97%)	0.92	0 100 100	60, 70, 78, 78	0
25	13	59/60 (98%)	-0.06	2 (3%) 48 43	28, 37, 62, 79	0
25	23	59/60 (98%)	0.91	3 (5%) 33 29	56, 68, 77, 85	0
26	14	69/71 (97%)	1.16	14 (20%) 3 2	57, 75, 87, 91	0
26	24	69/71 (97%)	2.14	36 (52%) 0 0	80, 87, 92, 96	0
27	15	59/60 (98%)	-0.23	1 (1%) 69 65	22, 32, 52, 63	0
27	25	59/60 (98%)	0.42	1 (1%) 69 65	40, 52, 66, 76	0
28	16	53/54 (98%)	0.03	0 100 100	35, 44, 58, 63	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%)	0.96	2 (3%) 44 39	55, 64, 71, 76	0
29	17	48/49 (97%)	-0.08	3 (6%) 26 23	22, 29, 55, 65	0
29	27	48/49 (97%)	0.33	4 (8%) 17 15	32, 43, 67, 71	0
30	18	64/65 (98%)	-0.15	0 100 100	27, 35, 42, 62	0
30	28	64/65 (98%)	0.79	2 (3%) 51 47	47, 58, 66, 67	0
31	19	37/37 (100%)	0.17	0 100 100	31, 41, 59, 60	0
31	29	37/37 (100%)	1.16	3 (8%) 18 15	64, 69, 76, 80	0
32	1a	1488/1521 (97%)	0.36	52 (3%) 47 42	37, 68, 92, 104	0
32	2a	1491/1521 (98%)	0.81	144 (9%) 13 11	50, 77, 95, 107	0
33	1b	231/256 (90%)	1.47	58 (25%) 1 1	66, 78, 87, 91	0
33	2b	231/256 (90%)	2.22	129 (55%) 0 0	73, 85, 89, 93	0
34	1c	206/239 (86%)	1.14	23 (11%) 10 8	62, 74, 83, 87	0
34	2c	206/239 (86%)	2.26	118 (57%) 0 0	74, 84, 88, 94	0
35	1d	208/209 (99%)	1.15	23 (11%) 10 8	57, 71, 80, 83	0
35	2d	208/209 (99%)	1.13	13 (6%) 26 23	61, 70, 78, 85	0
36	1e	148/162 (91%)	0.93	9 (6%) 27 23	53, 65, 75, 79	0
36	2e	148/162 (91%)	1.72	55 (37%) 1 1	63, 77, 84, 89	0
37	1f	100/101 (99%)	0.95	6 (6%) 27 24	58, 68, 77, 78	0
37	2f	100/101 (99%)	0.82	3 (3%) 52 48	59, 71, 78, 84	0
38	1g	155/156 (99%)	0.97	16 (10%) 12 10	59, 71, 83, 96	0
38	2g	155/156 (99%)	1.44	32 (20%) 2 2	69, 79, 86, 94	0
39	1h	137/138 (99%)	0.83	6 (4%) 39 34	57, 68, 73, 75	0
39	2h	137/138 (99%)	1.56	30 (21%) 2 2	68, 76, 82, 86	0
40	1i	127/128 (99%)	1.56	36 (28%) 1 1	57, 77, 84, 88	0
40	2i	127/128 (99%)	2.59	88 (69%) 0 0	73, 84, 88, 89	0
41	1j	97/105 (92%)	1.49	23 (23%) 2 1	62, 78, 85, 90	0
41	2j	96/105 (91%)	2.51	59 (61%) 0 0	77, 86, 91, 93	0
42	1k	114/129 (88%)	0.90	11 (9%) 13 11	46, 66, 76, 81	0
42	2k	114/129 (88%)	1.42	25 (21%) 2 2	57, 74, 81, 85	0
43	1l	121/132 (91%)	0.70	7 (5%) 29 25	46, 57, 68, 74	0
43	2l	121/132 (91%)	1.51	30 (24%) 2 1	57, 70, 77, 84	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.15	14 (11%) 10 8	56, 71, 79, 85	0
44	2m	122/126 (96%)	2.28	62 (50%) 0 0	75, 83, 87, 91	0
45	1n	60/61 (98%)	1.35	9 (15%) 5 4	62, 69, 75, 79	0
45	2n	60/61 (98%)	2.84	44 (73%) 0 0	79, 85, 89, 91	0
46	1o	88/89 (98%)	0.79	6 (6%) 23 20	49, 66, 74, 78	0
46	2o	88/89 (98%)	1.27	12 (13%) 7 5	62, 73, 81, 84	0
47	1p	82/88 (93%)	1.76	30 (36%) 1 1	58, 72, 77, 84	0
47	2p	82/88 (93%)	1.24	11 (13%) 7 5	60, 69, 77, 81	0
48	1q	99/105 (94%)	0.96	6 (6%) 27 23	54, 67, 77, 79	0
48	2q	99/105 (94%)	1.26	16 (16%) 4 3	63, 73, 80, 83	0
49	1r	68/88 (77%)	0.86	5 (7%) 20 18	58, 67, 76, 78	0
49	2r	68/88 (77%)	0.90	3 (4%) 39 34	64, 72, 81, 85	0
50	1s	83/93 (89%)	1.07	10 (12%) 9 7	64, 74, 81, 85	0
50	2s	83/93 (89%)	2.29	51 (61%) 0 0	81, 87, 91, 93	0
51	1t	96/106 (90%)	1.28	15 (15%) 5 4	63, 72, 80, 84	0
51	2t	96/106 (90%)	1.14	12 (12%) 8 6	58, 71, 80, 85	0
52	1u	23/27 (85%)	1.42	4 (17%) 4 3	64, 69, 72, 74	0
52	2u	23/27 (85%)	2.77	18 (78%) 0 0	74, 81, 85, 86	0
53	1v	13/24 (54%)	0.84	2 (15%) 5 4	51, 64, 86, 93	0
53	2v	13/24 (54%)	1.76	4 (30%) 1 1	72, 82, 93, 96	0
54	1w	64/76 (84%)	0.99	4 (6%) 26 23	63, 87, 96, 103	0
54	1y	67/76 (88%)	1.03	7 (10%) 11 10	38, 90, 98, 100	0
54	2w	62/76 (81%)	1.43	12 (19%) 3 2	82, 94, 100, 106	0
54	2y	66/76 (86%)	1.27	9 (13%) 7 5	56, 94, 99, 103	0
55	1x	71/77 (92%)	0.34	1 (1%) 73 70	29, 64, 85, 90	0
55	2x	71/77 (92%)	0.73	2 (2%) 55 50	48, 80, 90, 95	0
All	All	20855/21748 (95%)	0.58	2106 (10%) 12 10	19, 65, 89, 107	0

All (2106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	7.8
40	2i	11	LYS	7.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	7.3
40	2i	102	LEU	7.2
44	1m	2	ALA	7.1
45	2n	2	ALA	7.0
33	2b	165	VAL	6.8
38	2g	82	GLY	6.5
33	2b	71	VAL	6.4
21	2Z	174	VAL	6.3
21	2Z	173	ALA	6.2
54	1w	73	A	6.2
44	1m	122	LYS	6.2
44	1m	123	ALA	6.1
22	20	7	LEU	6.1
41	2j	32	ALA	6.1
45	1n	2	ALA	6.0
23	11	2	SER	6.0
32	2a	1033	G	6.0
21	1Z	141	VAL	5.9
15	1T	131	ALA	5.8
38	1g	81	GLY	5.8
44	2m	123	ALA	5.8
44	2m	102	ARG	5.8
23	21	2	SER	5.7
1	2A	2155	G	5.7
45	2n	25	VAL	5.7
21	2Z	146	ILE	5.6
38	2g	16	LEU	5.6
45	2n	34	TYR	5.6
21	1Z	146	ILE	5.5
45	2n	39	LEU	5.5
44	2m	6	GLY	5.5
41	2j	47	PHE	5.4
26	24	51	ASP	5.3
34	2c	189	ALA	5.3
43	2l	64	TYR	5.2
33	2b	236	TYR	5.1
33	2b	237	ALA	5.1
38	2g	83	ALA	5.1
40	2i	14	VAL	5.1
33	2b	121	LEU	5.0
1	2A	1536	C	5.0
1	2A	2125	G	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	83	ALA	5.0
50	2s	84	GLY	5.0
41	2j	63	PHE	4.9
44	2m	104	ARG	4.8
41	2j	65	LEU	4.8
45	2n	6	LEU	4.8
33	2b	70	PHE	4.8
8	2I	146	ALA	4.8
20	2Y	90	LEU	4.8
38	2g	84	ASN	4.8
20	2Y	1	MET	4.7
42	1k	14	VAL	4.7
54	1w	71	G	4.7
34	2c	188	LEU	4.7
43	1l	18	VAL	4.7
38	2g	154	TYR	4.7
38	1g	80	VAL	4.6
38	2g	85	TYR	4.6
40	1i	15	ALA	4.6
44	2m	100	GLY	4.6
40	2i	5	TYR	4.6
33	2b	187	LEU	4.6
34	1c	207	VAL	4.6
40	2i	9	ARG	4.6
7	1H	2	SER	4.6
41	2j	76	ASN	4.6
40	2i	7	THR	4.6
32	2a	1149	C	4.5
26	24	49	PHE	4.5
38	2g	80	VAL	4.5
41	2j	36	GLY	4.5
50	2s	9	VAL	4.5
45	2n	38	GLY	4.5
52	2u	2	GLY	4.5
34	2c	195	VAL	4.5
1	1A	1057	A	4.5
38	1g	82	GLY	4.4
26	24	50	VAL	4.4
1	1A	1081	U	4.4
32	2a	1219	U	4.4
50	2s	80	TYR	4.4
41	2j	74	ILE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	237	ALA	4.4
53	2v	12	A	4.4
54	2w	73	A	4.4
41	2j	10	GLY	4.4
44	2m	72	ALA	4.4
22	20	8	GLY	4.4
33	1b	230	VAL	4.3
34	2c	149	ALA	4.3
52	2u	23	PRO	4.3
51	1t	103	GLY	4.3
34	1c	2	GLY	4.3
44	2m	65	LYS	4.3
34	2c	201	TYR	4.3
33	2b	201	ILE	4.3
41	2j	38	ILE	4.3
33	2b	7	VAL	4.3
34	2c	198	VAL	4.3
34	2c	129	ALA	4.3
40	2i	10	ARG	4.3
40	2i	126	SER	4.3
1	1A	1087	G	4.2
52	2u	14	TRP	4.2
45	2n	37	PHE	4.2
21	2Z	150	LEU	4.2
15	1T	130	ALA	4.2
40	2i	36	TYR	4.2
52	2u	24	ARG	4.2
40	2i	67	GLY	4.2
34	2c	182	ILE	4.2
34	2c	128	PHE	4.2
33	2b	185	ILE	4.2
1	2A	2154	G	4.2
21	2Z	144	LEU	4.2
45	2n	3	ARG	4.2
33	1b	33	TYR	4.2
12	2Q	15	GLY	4.2
33	2b	80	ILE	4.2
32	2a	1224	G	4.2
6	1G	48	GLU	4.1
1	1A	885	C	4.1
1	2A	896	A	4.1
6	2G	140	ILE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	229	VAL	4.1
33	2b	152	PHE	4.1
18	1W	112	GLY	4.1
34	2c	8	ILE	4.1
44	2m	7	VAL	4.1
44	2m	70	LEU	4.1
32	2a	1503	A	4.1
33	2b	122	PHE	4.1
21	2Z	149	SER	4.1
26	24	56	VAL	4.1
39	2h	2	LEU	4.1
44	1m	121	LYS	4.0
41	2j	41	PRO	4.0
41	2j	91	PRO	4.0
12	2Q	121	ALA	4.0
42	2k	117	ASN	4.0
32	2a	1532	U	4.0
44	2m	122	LYS	4.0
34	2c	87	LEU	4.0
32	1a	630	G	4.0
50	2s	2	PRO	4.0
29	27	45	ALA	4.0
32	2a	1030	C	4.0
18	2W	112	GLY	4.0
6	2G	20	ILE	4.0
50	2s	79	THR	4.0
40	2i	92	TYR	4.0
50	2s	45	VAL	4.0
3	2D	275	LYS	4.0
32	1a	1001(A)	G	4.0
1	2A	2138	C	4.0
1	2A	2146	C	4.0
21	2Z	121	HIS	4.0
41	2j	78	ASN	3.9
32	2a	1036	G	3.9
1	1A	1064	C	3.9
1	1A	1094	U	3.9
51	1t	13	LEU	3.9
34	2c	187	ALA	3.9
40	2i	13	ALA	3.9
1	2A	1026	U	3.9
26	24	32	TYR	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	94	ALA	3.9
33	2b	11	LEU	3.9
33	1b	133	LYS	3.9
39	1h	98	LYS	3.9
1	2A	2113	U	3.9
1	2A	2156	G	3.9
7	2H	52	VAL	3.9
33	2b	234	PRO	3.9
40	2i	17	VAL	3.9
40	2i	41	VAL	3.9
45	2n	33	VAL	3.9
34	2c	137	ALA	3.9
33	1b	11	LEU	3.9
40	1i	19	LEU	3.9
33	2b	97	TRP	3.8
1	1A	1058	G	3.8
32	2a	1030(A)	G	3.8
32	2a	1034	G	3.8
33	2b	120	ALA	3.8
41	1j	32	ALA	3.8
44	2m	5	ALA	3.8
51	2t	103	GLY	3.8
40	2i	104	ARG	3.8
41	2j	40	LEU	3.8
26	14	56	VAL	3.8
1	1A	1096	A	3.8
1	2A	2126	A	3.8
32	1a	1532	U	3.8
45	2n	61	TRP	3.8
32	1a	1027	C	3.8
44	2m	68	GLY	3.8
33	2b	211	ILE	3.8
52	2u	13	ILE	3.8
7	2H	39	PRO	3.8
33	1b	7	VAL	3.8
38	1g	85	TYR	3.8
21	2Z	171	ILE	3.8
32	2a	1002	G	3.8
54	2y	57	G	3.8
40	2i	27	THR	3.8
33	2b	123	ALA	3.8
34	2c	2	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	24	63	TYR	3.8
39	2h	15	ASN	3.8
43	1l	64	TYR	3.8
26	24	9	LEU	3.8
41	2j	75	ILE	3.8
40	2i	91	ASP	3.8
1	1A	2145	C	3.8
14	2S	46	VAL	3.7
34	2c	79	ARG	3.7
44	2m	75	ALA	3.7
7	2H	7	LEU	3.7
40	2i	96	LEU	3.7
50	2s	13	ASP	3.7
1	2A	2111	C	3.7
1	2A	2112	G	3.7
34	2c	124	ILE	3.7
34	2c	157	ILE	3.7
45	2n	18	VAL	3.7
1	2A	11	G	3.7
40	2i	101	PHE	3.7
1	1A	1078	U	3.7
47	1p	82	GLN	3.7
33	2b	48	MET	3.7
32	2a	1116	C	3.7
34	2c	194	GLY	3.7
33	2b	132	LYS	3.7
26	24	65	ASP	3.7
51	2t	98	PRO	3.7
7	2H	19	VAL	3.6
7	2H	45	VAL	3.6
7	2H	50	VAL	3.6
40	2i	103	THR	3.6
34	2c	133	ALA	3.6
19	1X	95	LEU	3.6
1	2A	883	G	3.6
1	2A	2802	G	3.6
32	1a	1021	G	3.6
32	2a	1220	G	3.6
35	1d	170	VAL	3.6
6	2G	163	ALA	3.6
35	1d	167	GLY	3.6
51	1t	69	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	17	PRO	3.6
50	2s	76	PRO	3.6
6	1G	146	TYR	3.6
42	2k	75	TYR	3.6
27	15	60	VAL	3.6
33	2b	197	VAL	3.6
40	1i	2	GLU	3.6
40	2i	28	VAL	3.6
32	1a	1035	A	3.6
53	2v	13	A	3.6
21	2Z	172	ALA	3.6
38	2g	81	GLY	3.6
40	2i	99	LEU	3.6
52	2u	11	GLY	3.6
33	2b	223	ILE	3.6
54	1w	72	C	3.6
42	1k	75	TYR	3.6
1	2A	2133	G	3.6
6	2G	15	VAL	3.6
32	2a	1001(A)	G	3.6
33	2b	136	VAL	3.6
33	2b	230	VAL	3.6
32	2a	1035	A	3.6
34	2c	78	GLY	3.6
34	2c	152	ILE	3.6
44	2m	4	ILE	3.6
45	2n	7	ILE	3.6
1	2A	2136	C	3.5
34	2c	6	HIS	3.5
20	2Y	54	LYS	3.5
51	2t	74	LYS	3.5
7	2H	15	VAL	3.5
14	2S	20	ARG	3.5
38	1g	4	ARG	3.5
44	2m	64	TRP	3.5
31	29	37	GLY	3.5
33	1b	10	LEU	3.5
34	2c	9	GLY	3.5
51	1t	10	LEU	3.5
1	2A	2170	A	3.5
22	20	69	PHE	3.5
33	1b	200	ILE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	163	PHE	3.5
12	2Q	22	LYS	3.5
50	1s	9	VAL	3.5
52	2u	15	ARG	3.5
26	24	25	TYR	3.5
33	2b	92	TYR	3.5
39	2h	58	TYR	3.5
3	2D	2	ALA	3.5
44	2m	66	LEU	3.5
34	2c	73	PRO	3.5
41	2j	77	PRO	3.5
33	1b	172	ILE	3.5
1	1A	899	A	3.5
12	2Q	104	PHE	3.5
32	2a	1117	G	3.5
1	1A	2111	C	3.5
1	2A	2137	C	3.5
33	2b	83	MET	3.5
34	2c	138	VAL	3.5
32	1a	1257	U	3.5
21	2Z	51	ALA	3.5
14	2S	29	PHE	3.5
9	2N	118	LYS	3.5
1	2A	2157	G	3.5
33	2b	21	ARG	3.5
40	2i	128	ARG	3.5
41	2j	44	VAL	3.5
44	2m	101	GLN	3.5
1	1A	1082	U	3.5
22	20	84	LEU	3.5
44	2m	96	LEU	3.5
48	1q	98	LEU	3.5
22	20	9	SER	3.5
45	2n	14	PRO	3.5
33	2b	200	ILE	3.5
1	2A	2166	G	3.4
32	2a	1032	G	3.4
33	2b	112	VAL	3.4
6	2G	3	LEU	3.4
33	2b	131	PRO	3.4
41	2j	37	PRO	3.4
29	17	45	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1030(B)	C	3.4
33	2b	31	TYR	3.4
33	2b	148	TYR	3.4
41	1j	4	ILE	3.4
1	1A	2159	G	3.4
7	2H	44	VAL	3.4
32	1a	1030(A)	G	3.4
5	2F	166	ALA	3.4
33	2b	188	ALA	3.4
34	2c	65	ALA	3.4
36	2e	109	ILE	3.4
1	2A	885	C	3.4
32	2a	1249	C	3.4
33	2b	140	HIS	3.4
45	2n	31	ARG	3.4
1	1A	2119	A	3.4
32	1a	1447	A	3.4
12	2Q	109	VAL	3.4
26	14	50	VAL	3.4
34	2c	207	VAL	3.4
44	2m	90	LEU	3.4
21	2Z	147	GLY	3.4
34	2c	158	GLY	3.4
8	1I	146	ALA	3.4
8	2I	82	ARG	3.4
34	2c	190	ARG	3.4
38	2g	5	ARG	3.4
1	2A	2145	C	3.4
47	2p	82	GLN	3.4
1	1A	896	A	3.4
21	2Z	76	LEU	3.4
25	13	2	PRO	3.4
33	1b	125	PRO	3.4
44	2m	105	THR	3.4
6	1G	50	ALA	3.4
21	2Z	164	ALA	3.4
45	2n	30	ALA	3.4
33	1b	134	GLU	3.4
41	2j	59	SER	3.4
1	1A	879	G	3.3
32	1a	1025	U	3.3
1	1A	886	C	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2138	C	3.3
7	2H	10	PRO	3.3
21	2Z	141	VAL	3.3
34	2c	151	VAL	3.3
43	2l	18	VAL	3.3
50	2s	63	THR	3.3
52	1u	23	PRO	3.3
45	2n	55	GLY	3.3
47	1p	78	GLY	3.3
40	2i	63	ILE	3.3
21	2Z	88	PHE	3.3
1	1A	1056	G	3.3
1	2A	2127	G	3.3
40	2i	105	ASP	3.3
20	2Y	106	LEU	3.3
25	23	2	PRO	3.3
33	2b	91	PRO	3.3
34	2c	196	LEU	3.3
38	1g	79	ARG	3.3
40	1i	66	ARG	3.3
40	2i	66	ARG	3.3
45	2n	13	THR	3.3
33	1b	129	GLU	3.3
40	2i	81	ILE	3.3
40	2i	62	TYR	3.3
50	1s	13	ASP	3.3
1	2A	2159	G	3.3
1	2A	2139	C	3.3
8	2I	38	LEU	3.3
36	2e	12	LEU	3.3
44	2m	60	VAL	3.3
34	2c	167	TRP	3.3
15	2T	130	ALA	3.3
33	2b	88	ALA	3.3
34	2c	77	ILE	3.3
35	1d	195	ALA	3.3
40	1i	106	ALA	3.3
41	2j	27	ALA	3.3
47	1p	4	ILE	3.3
1	1A	2117	A	3.3
33	2b	133	LYS	3.3
21	2Z	129	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	17	PHE	3.3
26	14	63	TYR	3.3
1	1A	1065	U	3.3
8	1I	38	LEU	3.3
21	2Z	95	PRO	3.3
40	2i	79	LEU	3.3
50	2s	15	LEU	3.3
50	2s	16	LEU	3.3
36	2e	51	VAL	3.3
34	2c	53	ALA	3.3
33	2b	17	PHE	3.2
6	2G	146	TYR	3.2
34	2c	184	TYR	3.2
38	1g	84	ASN	3.2
40	2i	114	TYR	3.2
1	1A	2118	U	3.2
32	2a	1150	U	3.2
33	2b	215	LEU	3.2
41	2j	49	VAL	3.2
47	1p	1	MET	3.2
43	2l	126	LYS	3.2
6	2G	52	ILE	3.2
14	2S	35	ILE	3.2
34	2c	202	ILE	3.2
41	2j	23	ILE	3.2
32	2a	999	C	3.2
33	2b	77	ALA	3.2
54	2w	3	C	3.2
54	2w	72	C	3.2
42	1k	13	GLN	3.2
1	1A	2135	A	3.2
1	2A	2134	A	3.2
42	2k	126	ARG	3.2
21	2Z	167	PRO	3.2
40	2i	125	TYR	3.2
46	1o	19	PRO	3.2
36	2e	34	VAL	3.2
26	14	54	GLY	3.2
41	2j	42	THR	3.2
34	2c	168	ALA	3.2
1	1A	880	G	3.2
32	1a	1034	G	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	142	PRO	3.2
21	2Z	157	LEU	3.2
33	2b	86	GLU	3.2
3	2D	38	LYS	3.2
33	1b	236	TYR	3.2
33	2b	101	MET	3.2
42	2k	25	TYR	3.2
6	2G	92	VAL	3.2
31	29	16	VAL	3.2
32	1a	204	U	3.2
33	1b	136	VAL	3.2
33	2b	93	VAL	3.2
41	2j	31	GLY	3.2
41	2j	72	VAL	3.2
6	2G	39	ILE	3.2
45	2n	10	ALA	3.2
33	1b	97	TRP	3.2
1	1A	1068	G	3.2
3	1D	276	LYS	3.2
33	2b	154	LEU	3.2
41	2j	71	LEU	3.2
1	2A	2169	A	3.2
34	2c	48	TYR	3.2
7	2H	49	VAL	3.2
45	2n	27	CYS	3.2
1	2A	888	C	3.1
32	1a	1028	C	3.1
39	2h	4	ASP	3.1
35	1d	194	LEU	3.1
46	1o	57	LEU	3.1
50	2s	14	HIS	3.1
32	1a	1023	G	3.1
32	1a	1024	G	3.1
7	2H	17	VAL	3.1
7	2H	43	VAL	3.1
21	2Z	106	GLY	3.1
26	24	54	GLY	3.1
43	1l	63	GLY	3.1
52	2u	8	THR	3.1
1	1A	2150	U	3.1
12	2Q	59	ARG	3.1
42	2k	13	GLN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	1D	275	LYS	3.1
5	2F	24	LEU	3.1
1	2A	2803	C	3.1
1	1A	2152	G	3.1
1	2A	2893	G	3.1
32	1a	1036	G	3.1
41	2j	34	VAL	3.1
34	1c	182	ILE	3.1
40	2i	4	TYR	3.1
54	2y	18	G	3.1
1	2A	899	A	3.1
32	1a	1286	A	3.1
33	2b	67	THR	3.1
34	2c	170	GLN	3.1
54	1y	20	U	3.1
20	2Y	94	LYS	3.1
40	2i	110	GLU	3.1
33	1b	234	PRO	3.1
6	1G	76	SER	3.1
6	2G	175	LEU	3.1
50	2s	5	LEU	3.1
50	2s	71	LEU	3.1
47	1p	48	TRP	3.1
1	1A	898	C	3.1
32	2a	1018	C	3.1
36	2e	29	GLY	3.1
52	2u	6	ARG	3.1
52	2u	16	GLY	3.1
8	2I	145	VAL	3.1
40	2i	65	VAL	3.1
7	2H	72	ILE	3.1
22	20	43	THR	3.1
45	2n	22	THR	3.1
48	2q	65	ILE	3.1
1	2A	2147	G	3.1
6	2G	139	LEU	3.1
21	2Z	136	PHE	3.1
40	2i	56	LEU	3.1
21	1Z	149	SER	3.1
41	2j	35	SER	3.1
43	2l	62	SER	3.1
43	2l	41	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	1u	24	ARG	3.1
50	2s	68	GLY	3.1
21	1Z	105	VAL	3.1
1	2A	884	C	3.1
33	2b	169	LYS	3.0
38	1g	2	ALA	3.0
45	2n	21	TYR	3.0
1	1A	2113	U	3.0
36	1e	10	MET	3.0
1	1A	2115	G	3.0
34	2c	52	LEU	3.0
29	27	48	LYS	3.0
34	2c	4	LYS	3.0
36	2e	74	GLY	3.0
33	1b	15	VAL	3.0
36	2e	100	VAL	3.0
46	2o	60	VAL	3.0
34	2c	67	THR	3.0
1	2A	2128	C	3.0
38	2g	2	ALA	3.0
33	2b	33	TYR	3.0
35	1d	181	MET	3.0
40	2i	117	HIS	3.0
40	2i	90	PRO	3.0
33	1b	187	LEU	3.0
33	2b	10	LEU	3.0
33	2b	44	LEU	3.0
34	2c	12	LEU	3.0
1	1A	1059	G	3.0
50	2s	78	ARG	3.0
54	1w	1	G	3.0
54	1y	18	G	3.0
33	2b	214	ILE	3.0
34	2c	55	VAL	3.0
34	2c	141	VAL	3.0
36	2e	55	VAL	3.0
7	2H	156	ALA	3.0
33	2b	161	ALA	3.0
40	2i	2	GLU	3.0
32	2a	1038	C	3.0
32	2a	1114	C	3.0
44	2m	23	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	131	PRO	3.0
43	2l	5	PRO	3.0
41	1j	90	LEU	3.0
45	2n	44	LEU	3.0
1	1A	1098	A	3.0
32	1a	1531	A	3.0
32	2a	1531	A	3.0
45	2n	29	ARG	3.0
21	2Z	104	PHE	3.0
32	1a	1003	G	3.0
32	2a	1094	G	3.0
7	2H	14	GLY	3.0
41	2j	93	GLY	3.0
46	2o	89	GLY	3.0
33	1b	127	ILE	3.0
33	2b	184	VAL	3.0
34	2c	66	VAL	3.0
40	1i	14	VAL	3.0
42	2k	48	ILE	3.0
26	14	52	THR	3.0
34	2c	15	THR	3.0
40	2i	49	PRO	3.0
12	2Q	10	ARG	3.0
1	2A	886	C	3.0
34	2c	204	LEU	3.0
3	2D	276	LYS	3.0
34	2c	62	ASP	3.0
42	2k	124	LYS	3.0
44	2m	121	LYS	3.0
21	1Z	136	PHE	3.0
21	2Z	48	PHE	3.0
50	2s	10	PHE	3.0
1	2A	2173	A	3.0
32	2a	1286	A	3.0
7	2H	2	SER	3.0
12	2Q	61	GLY	3.0
34	2c	171	GLY	3.0
38	2g	13	GLN	3.0
50	1s	84	GLY	3.0
29	27	46	VAL	2.9
43	2l	7	ILE	2.9
49	1r	86	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2156	G	2.9
44	2m	103	THR	2.9
41	2j	13	HIS	2.9
1	2A	889	C	2.9
2	2B	4	C	2.9
6	2G	102	PHE	2.9
1	2A	2167	U	2.9
1	1A	2114	A	2.9
1	2A	2158	A	2.9
21	1Z	1	MET	2.9
34	2c	5	ILE	2.9
40	1i	81	ILE	2.9
44	2m	58	GLU	2.9
45	1n	7	ILE	2.9
37	1f	88	VAL	2.9
36	2e	30	ALA	2.9
40	2i	42	ARG	2.9
40	2i	82	ALA	2.9
40	2i	106	ALA	2.9
1	1A	1063	G	2.9
1	1A	2151	G	2.9
1	2A	2153	G	2.9
41	2j	28	ARG	2.9
6	2G	74	LYS	2.9
21	2Z	156	LYS	2.9
41	2j	14	LYS	2.9
45	2n	4	LYS	2.9
33	1b	154	LEU	2.9
44	1m	87	TYR	2.9
44	2m	59	TYR	2.9
40	2i	37	PHE	2.9
1	1A	1076	C	2.9
1	2A	2140	C	2.9
12	2Q	12	GLN	2.9
32	2a	1148	U	2.9
32	2a	1257	U	2.9
34	2c	162	GLN	2.9
45	2n	32	SER	2.9
54	2y	56	C	2.9
20	1Y	1	MET	2.9
21	2Z	143	GLY	2.9
1	2A	2119	A	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	14	ILE	2.9
6	2G	28	VAL	2.9
26	24	10	VAL	2.9
34	2c	68	VAL	2.9
34	2c	7	PRO	2.9
6	2G	19	LEU	2.9
8	1I	72	LEU	2.9
21	2Z	125	LEU	2.9
1	1A	1176	G	2.9
1	2A	1533	G	2.9
1	2A	2131	G	2.9
32	2a	1021	G	2.9
7	2H	157	TYR	2.9
26	14	67	TYR	2.9
6	2G	80	PHE	2.9
38	2g	26	PHE	2.9
40	2i	18	PHE	2.9
47	1p	80	PHE	2.9
20	2Y	5	MET	2.9
33	1b	228	GLY	2.9
35	1d	87	GLY	2.9
1	1A	2136	C	2.9
1	2A	2896	C	2.9
32	1a	1008	C	2.9
36	2e	13	ILE	2.9
39	2h	86	ILE	2.9
44	2m	78	ILE	2.9
1	2A	2801(A)	A	2.9
6	2G	159	VAL	2.9
9	2N	61	ARG	2.9
21	1Z	139	VAL	2.9
40	2i	108	VAL	2.9
44	2m	92	HIS	2.9
32	1a	1503	A	2.9
32	2a	1250	A	2.9
26	24	52	THR	2.9
33	1b	120	ALA	2.9
33	1b	123	ALA	2.9
33	2b	125	PRO	2.9
50	2s	42	PRO	2.9
52	2u	17	THR	2.9
34	2c	163	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	118	ALA	2.9
11	1P	147	LEU	2.9
1	1A	2112	G	2.9
1	2A	2110	G	2.9
32	2a	1127	G	2.9
36	2e	10	MET	2.9
41	1j	86	MET	2.9
44	2m	21	TYR	2.9
34	2c	74	GLY	2.9
36	2e	22	GLY	2.9
43	2l	63	GLY	2.9
6	2G	21	ARG	2.8
26	14	58	ARG	2.8
33	2b	137	ARG	2.8
36	2e	118	ILE	2.8
38	2g	32	ARG	2.8
38	2g	37	ASN	2.8
33	1b	19	HIS	2.8
50	2s	81	ARG	2.8
33	2b	164	VAL	2.8
32	2a	1115	C	2.8
32	1a	1030(D)	A	2.8
32	2a	983	A	2.8
32	2a	1092	A	2.8
40	2i	98	PRO	2.8
33	1b	188	ALA	2.8
44	2m	42	ALA	2.8
33	2b	98	LEU	2.8
38	2g	12	LEU	2.8
45	2n	53	LEU	2.8
48	2q	98	LEU	2.8
6	1G	80	PHE	2.8
29	17	48	LYS	2.8
40	2i	68	GLY	2.8
1	1A	1089	G	2.8
33	1b	41	ILE	2.8
33	2b	127	ILE	2.8
1	1A	2132	U	2.8
9	2N	140	VAL	2.8
34	2c	116	VAL	2.8
39	2h	53	VAL	2.8
26	24	29	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	1e	21	ALA	2.8
41	2j	26	ALA	2.8
1	1A	229	A	2.8
1	1A	1069	A	2.8
6	2G	34	LEU	2.8
34	2c	178	LEU	2.8
49	1r	78	LEU	2.8
39	2h	9	MET	2.8
41	2j	83	GLU	2.8
38	2g	36	LYS	2.8
11	2P	35	HIS	2.8
14	2S	22	GLY	2.8
6	2G	157	ILE	2.8
34	1c	39	ILE	2.8
26	24	35	VAL	2.8
1	1A	2141	G	2.8
32	2a	1003	G	2.8
32	2a	1031	G	2.8
41	1j	77	PRO	2.8
1	2A	614(A)	U	2.8
36	2e	138	ALA	2.8
43	2l	68	ALA	2.8
50	1s	20	LEU	2.8
50	1s	71	LEU	2.8
1	1A	1075	C	2.8
1	1A	2161	C	2.8
45	2n	40	CYS	2.8
1	1A	1086	A	2.8
32	1a	1001	A	2.8
32	2a	1030(D)	A	2.8
32	2a	1225	A	2.8
33	1b	45	GLN	2.8
25	23	29	ARG	2.8
44	2m	88	ARG	2.8
48	2q	100	LYS	2.8
12	2Q	29	PHE	2.8
35	1d	110	PHE	2.8
40	1i	59	PHE	2.8
34	1c	18	TRP	2.8
36	2e	23	GLY	2.8
42	1k	90	GLY	2.8
47	2p	48	TRP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	9	ILE	2.8
36	2e	101	ILE	2.8
26	24	66	SER	2.8
7	2H	79	VAL	2.8
8	1I	136	VAL	2.8
40	2i	26	VAL	2.8
39	2h	3	THR	2.8
44	2m	37	THR	2.8
44	2m	76	ALA	2.8
50	2s	77	THR	2.8
1	1A	2160	G	2.8
1	2A	2308	G	2.8
54	2w	71	G	2.8
34	2c	142	MET	2.8
43	2l	13	LYS	2.8
33	2b	135	GLN	2.8
44	2m	69	GLU	2.8
32	2a	1001	A	2.8
32	2a	1447	A	2.8
54	2w	31	A	2.8
21	2Z	140	ASP	2.8
33	1b	227	GLY	2.7
33	2b	89	GLY	2.7
34	2c	185	GLY	2.7
45	2n	36	PHE	2.8
50	2s	46	GLY	2.7
48	2q	95	TYR	2.7
50	2s	52	TYR	2.7
21	1Z	52	SER	2.7
34	2c	76	VAL	2.7
41	1j	44	VAL	2.7
42	2k	114	VAL	2.7
50	2s	11	VAL	2.7
37	2f	21	LEU	2.7
51	2t	99	LEU	2.7
33	2b	29	ALA	2.7
1	1A	1060	U	2.7
7	1H	175	LYS	2.7
40	2i	95	LYS	2.7
29	17	47	ARG	2.7
29	27	47	ARG	2.7
51	2t	8	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2D	126	GLN	2.7
1	1A	2149	G	2.7
1	2A	882	G	2.7
1	2A	2116	G	2.7
32	1a	1002	G	2.7
1	1A	2134	A	2.7
1	1A	2137	C	2.7
1	1A	2158	A	2.7
1	1A	2794	C	2.7
1	2A	652(B)	A	2.7
1	2A	2310	A	2.7
32	2a	962	C	2.7
53	1v	13	A	2.7
36	2e	45	PHE	2.7
30	28	16	ILE	2.7
47	1p	66	PRO	2.7
6	2G	70	VAL	2.7
22	20	26	TYR	2.7
42	2k	14	VAL	2.7
44	2m	87	TYR	2.7
39	1h	2	LEU	2.7
41	1j	65	LEU	2.7
44	2m	19	LEU	2.7
34	2c	146	ALA	2.7
35	2d	164	ALA	2.7
40	1i	13	ALA	2.7
40	2i	43	ALA	2.7
41	2j	67	THR	2.7
44	2m	33	ALA	2.7
50	2s	33	THR	2.7
22	20	11	ARG	2.7
38	2g	76	ARG	2.7
51	1t	8	ARG	2.7
45	2n	49	HIS	2.7
1	2A	2751	G	2.7
14	2S	45	GLY	2.7
32	2a	1202	G	2.7
42	2k	49	GLY	2.7
51	2t	96	GLY	2.7
52	1u	2	GLY	2.7
54	2w	44	G	2.7
1	1A	888	C	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1095	A	2.7
32	2a	1037	C	2.7
32	2a	1357	A	2.7
33	2b	162	ILE	2.7
46	2o	75	PRO	2.7
3	1D	38	LYS	2.7
6	2G	76	SER	2.7
34	2c	130	VAL	2.7
39	2h	97	VAL	2.7
6	2G	7	LEU	2.7
6	2G	29	TRP	2.7
33	2b	213	LEU	2.7
34	1c	87	LEU	2.7
34	2c	33	LEU	2.7
44	2m	120	LYS	2.7
47	1p	43	LYS	2.7
7	2H	41	MET	2.7
50	2s	20	LEU	2.7
15	2T	112	ARG	2.7
27	25	29	THR	2.7
33	1b	130	ARG	2.7
33	2b	130	ARG	2.7
34	2c	24	ALA	2.7
34	2c	92	ALA	2.7
34	2c	200	ALA	2.7
42	1k	74	ALA	2.7
21	2Z	168	GLU	2.7
33	1b	9	GLU	2.7
36	2e	114	GLY	2.7
21	1Z	104	PHE	2.7
36	2e	84	PHE	2.7
21	1Z	159	PRO	2.7
1	2A	2115	G	2.7
32	2a	974	A	2.7
32	2a	977	A	2.7
32	2a	1222	G	2.7
32	2a	1253	G	2.7
32	2a	1223	C	2.7
41	1j	76	ASN	2.7
7	2H	67	LEU	2.7
7	2H	169	VAL	2.7
33	2b	229	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	47	LEU	2.7
36	2e	18	ARG	2.7
40	1i	17	VAL	2.7
40	1i	102	LEU	2.7
44	2m	98	VAL	2.7
20	2Y	55	TYR	2.7
40	2i	12	GLU	2.7
43	2l	26	ALA	2.7
1	1A	1066	U	2.7
33	2b	189	ASP	2.6
33	2b	38	GLY	2.6
40	2i	69	GLY	2.6
43	1l	29	GLY	2.6
52	2u	4	GLY	2.6
7	2H	8	PRO	2.6
14	2S	59	LYS	2.6
34	2c	147	LYS	2.6
36	2e	80	ILE	2.6
45	2n	58	LYS	2.6
34	2c	181	ASN	2.6
38	1g	5	ARG	2.6
1	1A	1046	A	2.6
6	2G	53	LEU	2.6
21	2Z	5	LEU	2.6
36	2e	115	VAL	2.6
40	1i	50	LEU	2.6
1	2A	2174	C	2.6
1	2A	2793	G	2.6
32	1a	1019	C	2.6
40	2i	86	VAL	2.6
22	20	68	GLU	2.6
32	2a	1190	G	2.6
54	2y	19	G	2.6
8	1I	65	ALA	2.6
22	20	10	THR	2.6
26	14	32	TYR	2.6
37	1f	16	GLN	2.6
40	1i	52	ALA	2.6
40	2i	119	ALA	2.6
41	2j	87	THR	2.6
49	1r	20	ALA	2.6
1	2A	2144	U	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	4	ASP	2.6
8	2I	16	GLY	2.6
22	20	6	GLY	2.6
35	1d	169	LYS	2.6
40	2i	112	LYS	2.6
44	2m	112	GLY	2.6
12	2Q	66	ILE	2.6
26	24	31	ILE	2.6
33	1b	232	PRO	2.6
35	1d	5	ILE	2.6
39	2h	67	PRO	2.6
41	2j	53	PRO	2.6
33	2b	175	ARG	2.6
41	1j	46	ARG	2.6
50	2s	29	ARG	2.6
21	1Z	150	LEU	2.6
35	1d	120	LEU	2.6
9	2N	5	VAL	2.6
20	2Y	45	VAL	2.6
26	24	57	GLU	2.6
33	2b	12	GLU	2.6
1	2A	887	A	2.6
32	2a	1016	A	2.6
32	2a	1248	A	2.6
1	1A	884	C	2.6
7	2H	20	ALA	2.6
8	2I	115	ALA	2.6
32	1a	1030	C	2.6
33	2b	13	ALA	2.6
34	2c	37	GLN	2.6
42	2k	89	ALA	2.6
50	2s	24	ALA	2.6
1	1A	1093	G	2.6
1	1A	2190	G	2.6
12	2Q	32	TYR	2.6
54	2y	15	G	2.6
50	2s	34	TRP	2.6
40	2i	70	LYS	2.6
19	2X	86	GLY	2.6
19	2X	94	GLY	2.6
34	2c	13	GLY	2.6
35	2d	2	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	1p	47	ASP	2.6
51	1t	47	GLY	2.6
12	2Q	6	ARG	2.6
15	1T	129	ARG	2.6
22	20	72	ARG	2.6
41	2j	39	PRO	2.6
34	2c	134	ILE	2.6
11	1P	149	GLU	2.6
33	2b	69	LEU	2.6
34	2c	91	LEU	2.6
34	2c	94	LEU	2.6
40	2i	40	LEU	2.6
41	2j	88	LEU	2.6
5	2F	6	VAL	2.6
16	2U	90	VAL	2.6
33	2b	15	VAL	2.6
36	2e	33	VAL	2.6
39	1h	93	VAL	2.6
50	2s	58	VAL	2.6
12	2Q	75	THR	2.6
33	2b	173	ALA	2.6
34	1c	60	ALA	2.6
40	2i	45	ALA	2.6
51	2t	94	ALA	2.6
32	1a	344	A	2.6
54	2w	4	C	2.6
9	2N	83	LYS	2.6
47	1p	3	LYS	2.6
1	1A	2162	G	2.6
1	2A	2165	G	2.6
32	2a	1310	G	2.6
47	1p	59	TRP	2.6
7	2H	170	ARG	2.6
33	2b	144	ARG	2.6
38	2g	34	GLY	2.6
40	2i	6	GLY	2.6
40	2i	20	ARG	2.6
41	2j	79	ARG	2.6
42	1k	36	ASP	2.6
45	1n	29	ARG	2.6
45	2n	54	PRO	2.6
50	2s	12	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	2Q	103	MET	2.6
12	2Q	64	ILE	2.6
34	2c	84	ILE	2.6
6	2G	23	PHE	2.6
41	2j	54	PHE	2.6
4	1E	73	GLU	2.6
6	2G	133	LEU	2.6
26	24	30	GLU	2.6
39	2h	63	LEU	2.6
6	2G	50	ALA	2.6
21	2Z	166	SER	2.6
36	2e	86	ALA	2.6
39	2h	115	SER	2.6
51	1t	11	SER	2.6
33	2b	168	THR	2.6
40	1i	64	THR	2.6
33	2b	27	LYS	2.6
34	2c	135	LYS	2.6
1	2A	878	A	2.6
1	2A	2135	A	2.6
32	2a	1183	A	2.6
53	1v	12	A	2.6
1	2A	2297	C	2.5
6	1G	51	ARG	2.5
32	2a	1054	C	2.5
32	2a	1226	C	2.5
33	1b	24	TRP	2.5
5	1F	14	PRO	2.5
7	2H	174	GLY	2.5
8	2I	1	MET	2.5
26	14	64	GLY	2.5
33	2b	90	MET	2.5
34	1c	22	TRP	2.5
40	2i	39	GLY	2.5
42	2k	36	ASP	2.5
46	2o	20	GLY	2.5
1	1A	2165	G	2.5
8	1I	71	ILE	2.5
32	2a	1221	G	2.5
21	2Z	2	GLU	2.5
26	14	59	PHE	2.5
33	2b	55	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	19	GLU	2.5
34	2c	161	GLU	2.5
1	2A	2130	U	2.5
7	2H	71	LEU	2.5
14	2S	54	LEU	2.5
32	2a	1020	U	2.5
34	2c	175	LEU	2.5
40	2i	85	LEU	2.5
14	2S	14	VAL	2.5
21	2Z	96	VAL	2.5
33	2b	81	VAL	2.5
35	1d	105	VAL	2.5
43	2l	8	ASN	2.5
48	2q	23	VAL	2.5
50	2s	41	VAL	2.5
6	1G	182	LYS	2.5
51	1t	74	LYS	2.5
6	2G	71	THR	2.5
15	2T	111	ARG	2.5
36	2e	25	ARG	2.5
39	2h	30	ARG	2.5
1	2A	528	A	2.5
32	2a	1110	A	2.5
34	2c	23	TYR	2.5
43	2l	69	TYR	2.5
36	2e	96	PRO	2.5
1	1A	2146	C	2.5
32	2a	866	C	2.5
32	2a	1354	C	2.5
40	1i	105	ASP	2.5
42	2k	102	GLY	2.5
7	2H	92	ILE	2.5
46	2o	3	ILE	2.5
12	2Q	65	PHE	2.5
33	1b	163	PHE	2.5
34	2c	43	LEU	2.5
39	1h	112	LEU	2.5
40	1i	56	LEU	2.5
40	2i	59	PHE	2.5
1	1A	2131	G	2.5
32	2a	973	G	2.5
51	1t	24	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	1y	19	G	2.5
32	2a	982	U	2.5
26	24	40	HIS	2.5
44	2m	117	VAL	2.5
45	2n	56	VAL	2.5
47	1p	20	VAL	2.5
50	2s	18	LYS	2.5
50	2s	32	LYS	2.5
33	2b	216	SER	2.5
38	2g	77	SER	2.5
50	1s	79	THR	2.5
45	2n	12	ARG	2.5
52	2u	22	ARG	2.5
33	1b	31	TYR	2.5
46	1o	69	TYR	2.5
46	2o	69	TYR	2.5
47	2p	38	TYR	2.5
1	1A	548	A	2.5
1	1A	1073	A	2.5
1	2A	2117	A	2.5
1	2A	2171	A	2.5
22	10	8	GLY	2.5
41	1j	10	GLY	2.5
6	2G	116	ASP	2.5
36	2e	149	GLU	2.5
1	1A	889	C	2.5
1	2A	894	C	2.5
32	1a	1029	C	2.5
32	2a	980	C	2.5
32	2a	1029	C	2.5
7	2H	64	LEU	2.5
26	14	49	PHE	2.5
33	2b	61	LEU	2.5
34	2c	47	LEU	2.5
42	2k	103	LEU	2.5
34	2c	45	LYS	2.5
20	2Y	42	VAL	2.5
40	1i	108	VAL	2.5
47	1p	2	VAL	2.5
54	2w	45	U	2.5
1	2A	652(U)	G	2.5
1	2A	1170	G	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	630	G	2.5
32	2a	1026	G	2.5
54	2w	15	G	2.5
36	1e	138	ALA	2.5
40	2i	52	ALA	2.5
41	2j	48	THR	2.5
43	2l	6	THR	2.5
47	2p	45	THR	2.5
50	2s	4	SER	2.5
50	2s	48	THR	2.5
9	2N	1	MET	2.5
5	2F	131	GLY	2.5
7	2H	22	GLY	2.5
12	2Q	30	GLY	2.5
34	2c	193	TYR	2.5
35	2d	34	GLU	2.5
39	2h	48	TYR	2.5
39	2h	94	TYR	2.5
44	2m	73	GLU	2.5
50	2s	61	TYR	2.5
33	1b	214	ILE	2.5
32	2a	1004	A	2.5
32	2a	1251	A	2.5
53	2v	24	A	2.5
6	2G	47	LYS	2.5
12	2Q	2	LEU	2.5
33	2b	149	LEU	2.5
34	2c	199	LYS	2.5
47	1p	74	LEU	2.5
11	2P	68	GLN	2.5
38	2g	156	TRP	2.5
40	2i	73	GLN	2.5
43	2l	32	PHE	2.5
32	1a	1030(B)	C	2.5
21	2Z	86	VAL	2.5
1	2A	2172	U	2.5
21	1Z	103	ARG	2.5
26	24	55	ARG	2.5
32	1a	65	U	2.5
40	2i	83	ARG	2.5
7	2H	102	ALA	2.5
21	2Z	21	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2133	G	2.5
40	2i	71	SER	2.5
6	2G	2	PRO	2.4
33	2b	26	PRO	2.4
33	2b	194	PRO	2.4
34	2c	197	GLY	2.4
48	2q	24	GLU	2.4
14	2S	36	TYR	2.4
33	2b	147	LYS	2.4
33	2b	199	TYR	2.4
39	2h	98	LYS	2.4
43	2l	28	LYS	2.4
52	2u	5	ASP	2.4
40	2i	19	LEU	2.4
1	1A	1103	A	2.4
54	1y	35	A	2.4
39	2h	18	ARG	2.4
41	2j	46	ARG	2.4
1	1A	897	C	2.4
1	2A	2175	C	2.4
7	2H	133	VAL	2.4
12	2Q	106	VAL	2.4
17	2V	14	VAL	2.4
21	2Z	139	VAL	2.4
28	26	48	VAL	2.4
32	2a	1109	C	2.4
33	1b	165	VAL	2.4
42	1k	117	ASN	2.4
34	2c	160	ALA	2.4
36	2e	17	ALA	2.4
41	1j	27	ALA	2.4
45	1n	10	ALA	2.4
51	2t	97	ALA	2.4
34	2c	191	THR	2.4
40	1i	103	THR	2.4
32	1a	1026	G	2.4
32	1a	1033	G	2.4
32	2a	1042	G	2.4
40	1i	127	LYS	2.4
47	1p	37	GLY	2.4
21	1Z	148	ASP	2.4
33	2b	39	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	1d	188	LEU	2.4
39	2h	10	LEU	2.4
52	2u	21	TYR	2.4
47	1p	16	HIS	2.4
44	2m	110	ARG	2.4
45	2n	16	PHE	2.4
1	1A	1070	A	2.4
32	2a	969	A	2.4
6	2G	31	VAL	2.4
6	2G	79	ASN	2.4
37	1f	90	VAL	2.4
39	2h	19	VAL	2.4
43	2l	55	VAL	2.4
50	2s	53	ASN	2.4
1	2A	645	C	2.4
5	2F	115	ALA	2.4
34	2c	60	ALA	2.4
34	2c	121	ALA	2.4
1	1A	1026	U	2.4
1	1A	1175	U	2.4
32	2a	1065	U	2.4
55	2x	47	U	2.4
44	2m	41	PRO	2.4
14	2S	19	LYS	2.4
36	2e	99	GLY	2.4
45	2n	51	GLY	2.4
34	1c	57	ILE	2.4
1	2A	2149	G	2.4
1	2A	2321	G	2.4
6	2G	41	GLN	2.4
14	2S	32	LEU	2.4
14	2S	58	LEU	2.4
32	2a	1024	G	2.4
32	2a	1311	G	2.4
37	1f	61	LEU	2.4
43	2l	60	LEU	2.4
48	2q	76	LEU	2.4
49	2r	66	LEU	2.4
34	2c	176	HIS	2.4
36	2e	107	ARG	2.4
40	2i	107	ARG	2.4
41	2j	62	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	2o	88	ARG	2.4
47	1p	81	ARG	2.4
6	2G	12	TYR	2.4
14	2S	92	TYR	2.4
34	1c	193	TYR	2.4
35	1d	138	TYR	2.4
33	2b	57	PHE	2.4
9	1N	9	VAL	2.4
9	2N	9	VAL	2.4
12	2Q	52	VAL	2.4
1	1A	1067	A	2.4
1	2A	2114	A	2.4
32	2a	949	A	2.4
32	2a	965	A	2.4
32	2a	1324	A	2.4
44	2m	106	ASN	2.4
35	2d	48	ALA	2.4
40	1i	55	ALA	2.4
8	2I	86	THR	2.4
21	2Z	170	THR	2.4
7	2H	21	PRO	2.4
21	1Z	95	PRO	2.4
21	2Z	15	PRO	2.4
25	13	60	GLU	2.4
26	24	38	LYS	2.4
33	2b	126	GLU	2.4
36	2e	81	GLU	2.4
40	2i	127	LYS	2.4
41	2j	92	THR	2.4
32	2a	961	U	2.4
32	2a	1039	C	2.4
48	1q	28	PRO	2.4
42	2k	101	SER	2.4
34	2c	205	GLY	2.4
33	1b	201	ILE	2.4
33	2b	58	ILE	2.4
47	2p	33	ILE	2.4
15	1T	111	ARG	2.4
26	24	47	GLN	2.4
33	2b	166	ASP	2.4
36	2e	27	ARG	2.4
40	1i	91	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	33	GLN	2.4
41	2j	90	LEU	2.4
42	2k	54	ARG	2.4
43	2l	84	LEU	2.4
48	1q	13	ASP	2.4
1	1A	1099	G	2.4
15	2T	22	PHE	2.4
32	1a	1030(C)	G	2.4
32	2a	1182	G	2.4
16	2U	8	VAL	2.4
34	2c	153	VAL	2.4
1	2A	1847	A	2.4
32	2a	1093	A	2.4
50	2s	75	ALA	2.4
36	2e	98	THR	2.3
41	2j	19	SER	2.3
1	1A	12	U	2.3
32	2a	204	U	2.3
1	1A	1100	C	2.3
1	1A	2140	C	2.3
1	2A	2143	C	2.3
1	2A	2789	C	2.3
11	1P	44	GLY	2.3
12	2Q	19	GLY	2.3
17	1V	101	GLY	2.3
19	2X	67	GLY	2.3
40	1i	8	GLY	2.3
41	1j	36	GLY	2.3
50	2s	8	GLY	2.3
6	1G	88	ILE	2.3
40	2i	111	ARG	2.3
45	2n	41	ARG	2.3
8	2I	20	ASP	2.3
21	2Z	33	LEU	2.3
33	1b	44	LEU	2.3
36	2e	5	ASP	2.3
36	2e	53	LEU	2.3
40	2i	47	LEU	2.3
40	2i	50	LEU	2.3
34	2c	186	PHE	2.3
40	1i	18	PHE	2.3
22	20	30	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	76	VAL	2.3
40	2i	118	LYS	2.3
47	1p	79	VAL	2.3
50	2s	51	VAL	2.3
1	1A	2116	G	2.3
1	2A	614(B)	G	2.3
1	2A	2151	G	2.3
1	2A	2162	G	2.3
32	1a	79	G	2.3
32	1a	1009	G	2.3
32	2a	867	G	2.3
32	2a	993	G	2.3
32	2a	1053	G	2.3
32	2a	1124	G	2.3
32	2a	1356	G	2.3
36	2e	54	ALA	2.3
38	1g	8	GLU	2.3
40	2i	61	ALA	2.3
45	2n	59	ALA	2.3
49	2r	24	ALA	2.3
51	1t	95	ALA	2.3
33	2b	232	PRO	2.3
1	1A	1077	A	2.3
42	1k	42	TRP	2.3
7	2H	38	SER	2.3
11	2P	79	ARG	2.3
37	2f	93	SER	2.3
44	2m	29	ARG	2.3
50	2s	38	SER	2.3
1	1A	614(A)	U	2.3
32	1a	1040	U	2.3
32	2a	1235	U	2.3
28	26	7	ILE	2.3
36	2e	131	ILE	2.3
39	2h	83	ILE	2.3
41	2j	68	HIS	2.3
1	2A	2142	C	2.3
1	2A	2163	C	2.3
6	2G	147	ASP	2.3
32	2a	948	C	2.3
32	2a	1007	C	2.3
32	2a	1027	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1119	C	2.3
22	20	49	LYS	2.3
22	20	60	PHE	2.3
26	24	59	PHE	2.3
41	2j	55	LYS	2.3
47	2p	80	PHE	2.3
7	2H	24	VAL	2.3
21	2Z	126	VAL	2.3
21	2Z	165	VAL	2.3
34	2c	29	TYR	2.3
40	2i	53	VAL	2.3
42	1k	25	TYR	2.3
47	2p	2	VAL	2.3
11	2P	149	GLU	2.3
35	1d	179	GLU	2.3
4	2E	28	ALA	2.3
4	2E	204	ALA	2.3
36	2e	94	ALA	2.3
36	2e	95	ALA	2.3
40	1i	49	PRO	2.3
44	1m	118	ALA	2.3
45	1n	5	ALA	2.3
45	2n	20	ALA	2.3
49	1r	73	ALA	2.3
1	2A	2148	G	2.3
32	1a	380	G	2.3
32	2a	1370	G	2.3
47	1p	22	THR	2.3
37	1f	46	ARG	2.3
54	2y	52	G	2.3
1	1A	529	A	2.3
1	1A	1084	A	2.3
8	2I	54	GLN	2.3
11	2P	24	GLY	2.3
26	24	45	GLY	2.3
32	2a	1280	A	2.3
33	1b	38	GLY	2.3
38	1g	130	GLY	2.3
38	1g	156	TRP	2.3
43	2l	88	GLY	2.3
45	2n	60	SER	2.3
53	2v	14	A	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	40	HIS	2.3
19	2X	92	LEU	2.3
21	1Z	120	ILE	2.3
33	2b	208	ILE	2.3
34	2c	57	ILE	2.3
35	2d	5	ILE	2.3
41	1j	98	ILE	2.3
44	1m	56	LEU	2.3
44	2m	22	ILE	2.3
1	2A	2150	U	2.3
32	2a	1159	U	2.3
39	2h	54	ASP	2.3
1	1A	1080	C	2.3
1	1A	1509	C	2.3
1	1A	2129	C	2.3
1	2A	897	C	2.3
6	2G	84	LYS	2.3
12	2Q	18	LYS	2.3
26	14	69	LYS	2.3
33	1b	28	PHE	2.3
48	1q	27	PHE	2.3
48	2q	71	PHE	2.3
8	1I	10	GLU	2.3
8	1I	107	VAL	2.3
11	2P	83	VAL	2.3
17	2V	61	VAL	2.3
40	2i	109	VAL	2.3
41	1j	34	VAL	2.3
47	1p	39	TYR	2.3
8	2I	53	ALA	2.3
40	2i	76	ALA	2.3
44	1m	106	ASN	2.3
47	1p	24	ALA	2.3
40	1i	9	ARG	2.3
40	2i	16	ARG	2.3
50	2s	3	ARG	2.3
6	2G	165	THR	2.3
21	2Z	32	HIS	2.3
44	2m	24	GLY	2.3
47	2p	76	GLN	2.3
1	2A	2318	G	2.3
1	2A	2805	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	14	66	SER	2.3
19	2X	95	LEU	2.3
21	2Z	155	LEU	2.3
32	2a	976	G	2.3
32	2a	998	G	2.3
33	2b	192	SER	2.3
48	2q	99	SER	2.3
1	1A	1088	A	2.3
1	1A	2790	A	2.3
1	2A	2298	A	2.3
6	2G	100	TRP	2.3
33	2b	138	LEU	2.3
36	2e	151	LEU	2.3
39	2h	112	LEU	2.3
44	2m	56	LEU	2.3
32	2a	1252	A	2.3
54	2y	58	A	2.3
33	2b	220	ASP	2.3
32	1a	1020	U	2.3
32	2a	997	U	2.3
1	2A	898	C	2.3
20	2Y	89	PHE	2.3
21	1Z	2	GLU	2.3
8	2I	15	VAL	2.3
42	2k	47	VAL	2.3
48	2q	77	VAL	2.3
6	2G	118	ARG	2.3
7	2H	29	PRO	2.3
36	1e	18	ARG	2.3
38	1g	154	TYR	2.3
38	2g	79	ARG	2.3
40	2i	120	ARG	2.3
41	2j	43	ARG	2.3
46	2o	2	PRO	2.3
47	1p	41	PRO	2.3
52	1u	9	ARG	2.3
12	2Q	49	ALA	2.2
42	1k	15	ALA	2.2
47	1p	56	ALA	2.2
49	2r	60	ALA	2.2
33	2b	73	THR	2.2
42	2k	31	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	66	GLY	2.2
43	1l	14	GLY	2.2
44	1m	24	GLY	2.2
48	2q	33	GLY	2.2
7	2H	175	LYS	2.2
8	2I	121	LYS	2.2
9	2N	116	LEU	2.2
21	2Z	41	LEU	2.2
22	20	62	LEU	2.2
23	21	85	LEU	2.2
33	1b	223	ILE	2.2
33	2b	233	SER	2.2
34	1c	72	LYS	2.2
36	2e	43	LEU	2.2
42	1k	51	LYS	2.2
44	1m	4	ILE	2.2
51	1t	43	LEU	2.2
51	1t	55	ILE	2.2
32	1a	143	A	2.2
32	2a	968	A	2.2
41	2j	58	ASP	2.2
1	1A	1173	G	2.2
1	1A	2157	G	2.2
32	2a	1009	G	2.2
32	2a	1030(C)	G	2.2
32	2a	1068	G	2.2
1	2A	2109	U	2.2
34	2c	203	PHE	2.2
6	2G	122	PRO	2.2
7	2H	55	PRO	2.2
14	1S	3	ARG	2.2
1	1A	1052	C	2.2
1	1A	1079	C	2.2
1	1A	1104	C	2.2
21	2Z	105	VAL	2.2
26	14	68	ARG	2.2
33	2b	202	PRO	2.2
34	1c	86	VAL	2.2
35	1d	153	ARG	2.2
39	2h	95	VAL	2.2
41	2j	70	ARG	2.2
47	1p	42	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	2q	92	ARG	2.2
32	2a	970	C	2.2
32	2a	1028	C	2.2
32	2a	1189	C	2.2
8	2I	65	ALA	2.2
33	1b	186	ALA	2.2
44	2m	30	ALA	2.2
42	2k	119	CYS	2.2
43	2l	98	TYR	2.2
34	1c	107	GLN	2.2
31	29	21	GLY	2.2
41	1j	31	GLY	2.2
43	2l	95	GLY	2.2
48	1q	14	LYS	2.2
22	10	84	LEU	2.2
33	2b	145	LEU	2.2
44	2m	34	LEU	2.2
6	2G	88	ILE	2.2
8	1I	109	ILE	2.2
10	2O	19	ILE	2.2
21	2Z	57	ILE	2.2
33	2b	108	ILE	2.2
34	1c	84	ILE	2.2
44	2m	39	ILE	2.2
35	1d	173	TRP	2.2
47	2p	59	TRP	2.2
1	1A	1174	A	2.2
32	2a	1285	A	2.2
33	2b	129	GLU	2.2
43	2l	16	GLU	2.2
1	2A	2132	U	2.2
1	2A	2897	U	2.2
32	2a	1040	U	2.2
1	1A	881	G	2.2
1	1A	2110	G	2.2
1	2A	880	G	2.2
1	2A	1171	G	2.2
7	2H	51	ARG	2.2
7	2H	60	ARG	2.2
26	24	68	ARG	2.2
32	1a	220	G	2.2
32	1a	1032	G	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	953	G	2.2
32	2a	1023	G	2.2
5	2F	14	PRO	2.2
7	2H	128	PRO	2.2
21	2Z	56	VAL	2.2
21	2Z	74	VAL	2.2
21	2Z	161	VAL	2.2
45	1n	33	VAL	2.2
1	2A	2164	C	2.2
32	2a	1362	C	2.2
32	2a	1369	C	2.2
40	2i	46	ALA	2.2
9	2N	69	GLN	2.2
11	2P	110	TYR	2.2
33	2b	22	LYS	2.2
33	2b	54	THR	2.2
34	2c	192	THR	2.2
35	2d	27	TYR	2.2
12	1Q	15	GLY	2.2
22	20	75	LEU	2.2
41	1j	93	GLY	2.2
7	2H	136	ILE	2.2
33	2b	68	ILE	2.2
14	2S	31	SER	2.2
40	1i	126	SER	2.2
34	1c	62	ASP	2.2
5	2F	127	GLU	2.2
20	1Y	91	GLU	2.2
6	1G	83	ARG	2.2
26	24	48	ARG	2.2
34	2c	88	ARG	2.2
34	2c	140	ARG	2.2
38	2g	4	ARG	2.2
1	1A	271(K)	U	2.2
1	1A	278	A	2.2
1	1A	1045	A	2.2
1	1A	1097	U	2.2
1	1A	2170	A	2.2
32	1a	149	A	2.2
26	24	7	PRO	2.2
32	1a	1000	U	2.2
32	2a	532	A	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	919	A	2.2
33	1b	122	PHE	2.2
34	2c	10	PHE	2.2
21	2Z	128	VAL	2.2
35	1d	140	VAL	2.2
1	1A	2153	G	2.2
1	1A	2166	G	2.2
1	1A	2207	G	2.2
1	2A	2141	G	2.2
1	2A	2168	G	2.2
6	1G	81	LYS	2.2
12	2Q	63	LYS	2.2
32	2a	485	G	2.2
33	1b	34	ALA	2.2
35	1d	111	ALA	2.2
35	1d	154	ASN	2.2
40	2i	84	ALA	2.2
41	2j	18	ALA	2.2
33	1b	83	MET	2.2
33	2b	224	GLN	2.2
1	2A	2129	C	2.2
20	2Y	80	GLY	2.2
22	20	59	LEU	2.2
32	1a	163	C	2.2
34	2c	95	THR	2.2
33	1b	18	GLY	2.2
34	1c	32	LEU	2.2
35	2d	21	LEU	2.2
35	2d	183	GLY	2.2
36	2e	142	LEU	2.2
40	2i	100	GLY	2.2
42	2k	90	GLY	2.2
43	2l	14	GLY	2.2
46	2o	81	LEU	2.2
50	1s	80	TYR	2.2
50	2s	82	GLY	2.2
54	1y	56	C	2.2
34	2c	39	ILE	2.2
38	2g	42	ILE	2.2
41	1j	75	ILE	2.2
41	2j	30	SER	2.2
7	1H	58	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	126	GLU	2.2
34	2c	90	GLU	2.2
50	1s	12	ASP	2.2
12	2Q	16	ARG	2.2
7	2H	173	PRO	2.2
20	2Y	53	PRO	2.2
30	28	34	TRP	2.2
1	1A	2189	U	2.2
1	1A	2897	U	2.2
1	2A	272(A)	U	2.2
2	2B	41	U	2.2
11	2P	76	LYS	2.2
26	24	42	PHE	2.2
40	1i	95	LYS	2.2
47	2p	9	PHE	2.2
5	1F	6	VAL	2.1
7	2H	113	VAL	2.1
32	2a	946	A	2.1
32	2a	1180	A	2.1
52	2u	3	LYS	2.2
44	2m	54	VAL	2.1
20	2Y	65	ALA	2.1
21	2Z	7	ALA	2.1
33	2b	78	GLN	2.1
45	2n	5	ALA	2.1
1	1A	614(B)	G	2.1
1	1A	1055	G	2.1
1	2A	1114	G	2.1
4	2E	195	LEU	2.1
5	2F	134	GLY	2.1
6	2G	162	THR	2.1
6	2G	173	LEU	2.1
7	2H	88	LEU	2.1
23	2I	46	LEU	2.1
32	1a	1224	G	2.1
33	2b	115	LEU	2.1
34	2c	145	GLY	2.1
36	1e	22	GLY	2.1
36	2e	35	GLY	2.1
39	2h	71	GLY	2.1
39	2h	127	LEU	2.1
41	1j	8	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	2o	31	LEU	2.1
49	1r	31	LEU	2.1
50	1s	26	GLY	2.1
50	2s	26	GLY	2.1
51	1t	53	LEU	2.1
51	1t	101	GLY	2.1
51	2t	24	LEU	2.1
36	2e	133	TYR	2.1
40	1i	4	TYR	2.1
46	1o	3	ILE	2.1
50	2s	62	ILE	2.1
1	1A	34	C	2.1
1	1A	2142	C	2.1
55	1x	69	C	2.1
6	2G	72	ARG	2.1
8	1I	67	ARG	2.1
20	2Y	91	GLU	2.1
26	24	61	ARG	2.1
34	2c	131	ARG	2.1
44	1m	102	ARG	2.1
45	2n	8	GLU	2.1
34	1c	56	ASP	2.1
7	2H	62	LYS	2.1
33	2b	156	LYS	2.1
34	2c	150	LYS	2.1
36	2e	106	PRO	2.1
39	2h	101	PRO	2.1
48	1q	100	LYS	2.1
18	2W	111	HIS	2.1
33	2b	219	VAL	2.1
34	1c	64	VAL	2.1
34	2c	86	VAL	2.1
38	2g	17	VAL	2.1
38	2g	21	VAL	2.1
1	1A	1054	A	2.1
1	1A	2173	A	2.1
3	1D	2	ALA	2.1
6	2G	57	ALA	2.1
8	2I	63	ALA	2.1
12	2Q	28	ALA	2.1
32	2a	975	A	2.1
41	1j	33	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2k	19	ALA	2.1
45	1n	59	ALA	2.1
51	2t	66	ALA	2.1
7	2H	48	GLY	2.1
8	1I	108	THR	2.1
8	2I	68	LEU	2.1
33	2b	118	LEU	2.1
33	2b	158	LEU	2.1
33	2b	227	GLY	2.1
35	1d	157	LEU	2.1
38	2g	24	THR	2.1
44	1m	100	GLY	2.1
44	2m	38	GLY	2.1
51	2t	47	GLY	2.1
6	2G	77	ILE	2.1
6	2G	144	ILE	2.1
36	1e	13	ILE	2.1
41	2j	6	ILE	2.1
6	2G	51	ARG	2.1
7	2H	59	ARG	2.1
15	1T	125	ARG	2.1
1	1A	1091	G	2.1
20	2Y	29	GLU	2.1
22	20	27	GLU	2.1
32	2a	1017	G	2.1
33	1b	12	GLU	2.1
36	1e	133	TYR	2.1
38	1g	6	ARG	2.1
38	2g	18	TYR	2.1
40	1i	10	ARG	2.1
44	2m	94	ARG	2.1
47	1p	5	ARG	2.1
50	2s	64	GLU	2.1
52	2u	7	ARG	2.1
54	1y	15	G	2.1
55	2x	70	G	2.1
1	1A	2128	C	2.1
1	1A	2143	C	2.1
1	1A	2164	C	2.1
21	1Z	153	SER	2.1
39	1h	4	ASP	2.1
54	2w	13	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	182	LYS	2.1
11	2P	78	PRO	2.1
21	1Z	158	PRO	2.1
21	2Z	159	PRO	2.1
41	1j	91	PRO	2.1
50	2s	59	PRO	2.1
21	2Z	151	HIS	2.1
35	2d	165	MET	2.1
41	2j	86	MET	2.1
8	2I	92	VAL	2.1
11	2P	38	GLN	2.1
12	2Q	113	GLN	2.1
36	2e	20	GLN	2.1
45	1n	25	VAL	2.1
1	1A	1101	U	2.1
1	1A	2130	U	2.1
8	2I	55	ALA	2.1
32	2a	5	U	2.1
32	2a	1196	U	2.1
33	1b	173	ALA	2.1
33	2b	186	ALA	2.1
34	2c	18	TRP	2.1
34	2c	180	ALA	2.1
39	2h	110	ALA	2.1
44	1m	18	ALA	2.1
45	1n	20	ALA	2.1
33	1b	37	ASN	2.1
1	2A	2176	A	2.1
6	2G	82	LEU	2.1
14	2S	80	LEU	2.1
19	2X	70	LEU	2.1
32	2a	1151	A	2.1
34	2c	148	GLY	2.1
35	2d	23	GLY	2.1
36	2e	123	LEU	2.1
46	2o	56	LEU	2.1
26	24	27	THR	2.1
26	24	44	THR	2.1
40	1i	27	THR	2.1
41	1j	87	THR	2.1
14	2S	3	ARG	2.1
34	1c	79	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	152	ARG	2.1
43	1l	19	ARG	2.1
48	2q	75	ARG	2.1
6	1G	77	ILE	2.1
6	2G	35	GLU	2.1
20	2Y	44	ILE	2.1
21	2Z	53	ILE	2.1
21	2Z	137	ILE	2.1
33	2b	170	GLU	2.1
36	2e	129	ILE	2.1
41	2j	82	ILE	2.1
44	2m	61	GLU	2.1
47	1p	36	ILE	2.1
36	2e	61	TYR	2.1
40	1i	88	TYR	2.1
52	2u	18	TYR	2.1
34	1c	26	LYS	2.1
35	1d	22	LYS	2.1
39	2h	64	LYS	2.1
40	1i	11	LYS	2.1
44	2m	31	LYS	2.1
47	1p	50	LYS	2.1
14	2S	50	SER	2.1
39	2h	29	SER	2.1
1	1A	545	G	2.1
1	1A	1062	G	2.1
1	2A	530	G	2.1
32	1a	1138	G	2.1
32	2a	1156	G	2.1
54	2w	19	G	2.1
6	2G	87	PRO	2.1
8	1I	132	PRO	2.1
32	2a	1019	C	2.1
33	2b	167	PRO	2.1
34	2c	109	PRO	2.1
40	2i	21	PRO	2.1
42	2k	115	PRO	2.1
33	2b	16	HIS	2.1
47	2p	16	HIS	2.1
38	1g	13	GLN	2.1
38	2g	11	GLN	2.1
7	2H	35	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	93	VAL	2.1
35	1d	88	VAL	2.1
41	2j	94	VAL	2.1
42	2k	125	PHE	2.1
50	2s	19	VAL	2.1
7	2H	96	ALA	2.1
1	1A	1105	U	2.1
1	1A	2167	U	2.1
7	2H	33	LEU	2.1
12	1Q	60	ARG	2.1
12	2Q	37	LEU	2.1
14	2S	30	ARG	2.1
18	2W	37	ARG	2.1
22	20	21	LEU	2.1
25	23	53	LEU	2.1
32	1a	182	U	2.1
32	2a	1126	U	2.1
32	2a	1205	U	2.1
33	2b	203	GLY	2.1
35	2d	167	GLY	2.1
37	2f	46	ARG	2.1
38	2g	115	ARG	2.1
39	2h	91	ARG	2.1
44	2m	3	ARG	2.1
46	1o	65	ARG	2.1
50	2s	36	ARG	2.1
40	2i	64	THR	2.1
47	1p	67	THR	2.1
48	2q	86	GLU	2.1
1	2A	901	A	2.1
26	24	5	ILE	2.1
32	2a	994	A	2.1
33	2b	41	ILE	2.1
39	1h	134	ILE	2.1
40	2i	74	ILE	2.1
50	2s	31	ILE	2.1
43	2l	111	LYS	2.1
6	2G	25	TYR	2.1
21	2Z	9	TYR	2.1
26	24	67	TYR	2.1
36	2e	60	TYR	2.1
41	2j	89	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	1p	38	TYR	2.1
5	2F	15	SER	2.1
4	1E	1	MET	2.1
6	2G	99	MET	2.1
21	2Z	1	MET	2.1
33	1b	140	HIS	2.1
1	2A	2206	G	2.0
32	1a	1010	G	2.0
32	2a	570	G	2.0
32	2a	963	G	2.0
32	2a	1006	C	2.1
32	2a	1010	G	2.0
32	2a	1048	G	2.0
32	2a	1058	G	2.0
32	2a	1113	C	2.1
34	2c	107	GLN	2.0
35	2d	201	GLN	2.0
36	1e	72	GLN	2.0
8	2I	107	VAL	2.0
12	2Q	97	VAL	2.0
14	2S	85	VAL	2.0
36	2e	82	VAL	2.0
37	1f	60	PHE	2.0
40	1i	37	PHE	2.0
9	2N	74	ARG	2.0
11	2P	15	ARG	2.0
33	1b	171	ALA	2.0
34	2c	126	ARG	2.0
34	2c	172	ARG	2.0
35	1d	164	ALA	2.0
42	2k	23	ALA	2.0
43	2l	56	ALA	2.0
47	1p	25	ARG	2.0
5	2F	12	LEU	2.0
6	1G	139	LEU	2.0
41	1j	78	ASN	2.0
44	2m	48	LEU	2.0
46	1o	66	LEU	2.0
6	2G	85	GLY	2.0
7	2H	82	GLY	2.0
8	2I	84	GLY	2.0
21	1Z	169	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	134	GLU	2.0
40	1i	39	GLY	2.0
40	1i	67	GLY	2.0
40	2i	72	GLY	2.0
1	1A	1963	U	2.0
32	1a	203	U	2.0
33	2b	107	THR	2.0
42	2k	123	LYS	2.0
43	1l	126	LYS	2.0
54	1y	45	U	2.0
43	2l	100	ILE	2.0
2	2B	120	A	2.0
32	1a	383	A	2.0
54	2y	36	A	2.0
12	2Q	26	TYR	2.0
21	2Z	148	ASP	2.0
33	2b	193	ASP	2.0
35	2d	51	PRO	2.0
38	2g	151	TYR	2.0
51	1t	98	PRO	2.0
36	2e	136	MET	2.0
50	2s	83	HIS	2.0
45	2n	24	CYS	2.0
7	2H	6	ARG	2.0
8	1I	27	ARG	2.0
11	1P	15	ARG	2.0
15	2T	108	ARG	2.0
20	2Y	85	VAL	2.0
22	20	79	VAL	2.0
26	24	58	ARG	2.0
32	1a	1007	C	2.0
32	2a	1112	C	2.0
33	2b	28	PHE	2.0
33	2b	174	VAL	2.0
41	1j	45	ARG	2.0
43	2l	39	VAL	2.0
45	2n	26	ARG	2.0
54	2w	25	C	2.0
1	1A	2147	G	2.0
1	2A	2120	G	2.0
1	2A	2123	G	2.0
32	2a	971	G	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1061	G	2.0
32	2a	1089	G	2.0
32	2a	1131	G	2.0
17	2V	94	LEU	2.0
6	1G	47	LYS	2.0
6	2G	48	GLU	2.0
10	1O	91	LEU	2.0
36	1e	94	ALA	2.0
33	2b	231	GLU	2.0
34	1c	175	LEU	2.0
34	2c	34	LEU	2.0
36	2e	119	LEU	2.0
38	2g	65	ALA	2.0
40	1i	46	ALA	2.0
12	2Q	33	GLY	2.0
18	2W	60	ASN	2.0
21	2Z	14	LYS	2.0
21	2Z	145	GLU	2.0
33	1b	50	GLU	2.0
34	2c	44	GLU	2.0
36	2e	8	GLU	2.0
43	2l	10	LEU	2.0
48	2q	43	LEU	2.0
50	1s	5	LEU	2.0
51	2t	93	GLU	2.0
26	24	64	GLY	2.0
43	2l	29	GLY	2.0
45	2n	28	GLY	2.0
21	1Z	69	THR	2.0
26	24	22	ILE	2.0
33	1b	42	ILE	2.0
33	2b	42	ILE	2.0
44	2m	63	THR	2.0
46	2o	4	THR	2.0
32	1a	723	U	2.0
54	2y	60	U	2.0
1	1A	1177	A	2.0
7	2H	12	PRO	2.0
7	2H	36	PRO	2.0
21	2Z	158	PRO	2.0
32	2a	1044	A	2.0
32	2a	1067	A	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1123	A	2.0
38	2g	33	ASP	2.0
48	2q	30	PRO	2.0
13	2R	6	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	G7M	2w	46	24/25	0.48	0.18	86,95,105,115	0
54	PSU	2y	55	20/21	0.56	0.17	92,100,112,113	0
54	G7M	1w	46	24/25	0.57	0.14	81,88,102,122	0
54	5MU	2y	54	21/22	0.59	0.18	90,96,105,123	0
54	G7M	1y	46	24/25	0.63	0.16	87,94,102,112	0
54	G7M	2y	46	24/25	0.63	0.15	91,94,99,119	0
54	MIA	2y	37	22/30	0.66	0.16	75,86,98,113	0
54	4SU	2w	8	20/21	0.69	0.14	93,96,104,114	0
54	PSU	1y	55	20/21	0.71	0.16	85,93,101,110	0
54	4SU	2y	8	20/21	0.71	0.13	89,94,101,109	0
54	5MU	1y	54	21/22	0.73	0.17	83,87,96,107	0
54	4SU	1y	8	20/21	0.77	0.12	88,90,99,100	0
54	PSU	2y	39	20/21	0.78	0.13	81,85,94,99	0
54	5MU	2w	54	21/22	0.79	0.13	74,84,90,94	0
54	PSU	2w	55	20/21	0.79	0.12	86,92,97,100	0
54	MIA	1y	37	22/30	0.80	0.13	72,79,86,96	0
32	2MG	2a	1207	24/25	0.82	0.14	81,88,93,96	0
54	PSU	2y	32	20/21	0.83	0.13	76,90,96,97	0
55	4SU	2x	8	20/21	0.83	0.13	79,85,89,89	0
55	5MU	2x	54	21/22	0.84	0.14	74,85,89,90	0
54	PSU	1w	55	20/21	0.84	0.12	63,83,88,89	0
54	PSU	1y	32	20/21	0.85	0.11	77,82,87,90	0
54	PSU	2w	32	20/21	0.85	0.16	85,89,97,102	0
55	PSU	2x	55	20/21	0.87	0.11	75,82,88,89	0
32	5MC	2a	967	21/22	0.87	0.16	68,74,83,87	0
54	PSU	1y	39	20/21	0.88	0.10	76,80,85,88	0
54	PSU	1w	32	20/21	0.88	0.13	63,71,83,85	0
54	4SU	1w	8	20/21	0.88	0.10	77,82,89,94	0
55	PSU	1x	55	20/21	0.89	0.12	62,67,77,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MU	2A	1915	21/22	0.89	0.14	67,74,76,86	0
32	5MC	2a	1404	21/22	0.89	0.13	51,59,66,66	0
32	PSU	2a	516	20/21	0.89	0.12	73,77,81,83	0
32	G7M	2a	527	24/25	0.89	0.15	65,70,75,79	0
32	M2G	2a	966	25/26	0.89	0.17	66,73,85,86	0
32	4OC	2a	1402	22/23	0.90	0.13	50,68,76,76	0
1	PSU	2A	1917	20/21	0.90	0.11	63,70,78,81	0
54	MIA	2w	37	25/30	0.90	0.14	74,79,87,90	0
43	0TD	2l	92	10/11	0.90	0.12	67,71,75,87	0
32	5MC	2a	1400	21/22	0.91	0.15	72,75,78,82	0
55	5MU	1x	54	21/22	0.91	0.11	60,69,74,86	0
1	PSU	2A	1911	20/21	0.91	0.10	61,67,70,70	0
43	0TD	1l	92	10/11	0.91	0.12	48,54,57,75	0
32	2MG	1a	1207	24/25	0.92	0.11	71,74,78,79	0
54	PSU	2w	39	20/21	0.92	0.11	77,82,90,92	0
55	5MC	2x	32	21/22	0.92	0.14	66,75,81,82	0
32	UR3	2a	1498	21/22	0.93	0.12	59,64,65,70	0
55	4SU	1x	8	20/21	0.93	0.09	61,70,77,77	0
54	MIA	1w	37	29/30	0.93	0.13	55,63,68,76	0
54	PSU	1w	39	20/21	0.93	0.10	59,70,78,79	0
32	5MC	2a	1407	21/22	0.93	0.11	55,60,64,67	0
32	PSU	1a	516	20/21	0.94	0.09	57,63,68,68	0
1	5MU	1A	1915	21/22	0.94	0.10	50,59,61,63	0
55	5MC	1x	32	21/22	0.94	0.13	55,59,66,72	0
32	MA6	2a	1518	24/25	0.94	0.12	54,69,74,75	0
32	MA6	2a	1519	24/25	0.94	0.12	57,68,74,77	0
1	OMC	2A	1920	21/22	0.94	0.11	52,64,68,72	0
1	5MC	2A	1962	21/22	0.94	0.10	35,50,56,63	0
54	5MU	1w	54	21/22	0.94	0.09	61,75,81,81	0
32	G7M	1a	527	24/25	0.95	0.11	48,53,56,57	0
32	M2G	1a	966	25/26	0.95	0.11	48,55,62,63	0
32	5MC	1a	967	21/22	0.95	0.11	50,57,61,63	0
1	5MC	2A	1942	21/22	0.95	0.09	48,57,64,67	0
1	5MU	2A	1939	21/22	0.96	0.08	32,41,47,50	0
55	31H	1x	76	32/33	0.96	0.09	23,32,38,68	10
32	4OC	1a	1402	22/23	0.96	0.10	40,47,51,53	0
1	OMG	2A	2251	24/25	0.96	0.09	37,46,49,51	0
1	OMU	2A	2552	21/22	0.96	0.10	43,48,53,61	0
32	MA6	1a	1519	24/25	0.96	0.11	39,44,49,53	0
32	5MC	1a	1404	21/22	0.97	0.09	37,43,46,47	0
32	5MC	1a	1407	21/22	0.97	0.09	37,42,46,47	0
1	2MA	2A	2503	23/24	0.97	0.09	34,42,43,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MA6	1a	1518	24/25	0.97	0.10	35,43,46,52	0
1	PSU	2A	2605	20/21	0.97	0.07	33,41,44,48	0
55	31H	2x	76	32/33	0.97	0.08	40,49,63,82	0
1	PSU	1A	1911	20/21	0.97	0.08	39,46,51,52	0
1	PSU	1A	1917	20/21	0.97	0.07	40,50,56,57	0
1	OMC	1A	1920	21/22	0.97	0.08	37,44,49,54	0
1	5MC	1A	1942	21/22	0.97	0.07	29,38,43,45	0
1	5MC	1A	1962	21/22	0.97	0.07	32,37,43,46	0
32	5MC	1a	1400	21/22	0.97	0.10	43,53,58,60	0
1	PSU	1A	2605	20/21	0.97	0.06	22,27,35,36	0
1	OMU	1A	2552	21/22	0.98	0.07	25,30,33,35	0
1	5MU	1A	1939	21/22	0.98	0.06	25,31,35,36	0
32	UR3	1a	1498	21/22	0.98	0.08	39,44,48,49	0
1	OMG	1A	2251	24/25	0.98	0.05	25,27,29,33	0
1	2MA	1A	2503	23/24	0.99	0.05	20,25,28,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
56	MG	1A	3939	1/1	0.43	0.20	83,83,83,83	0
56	MG	2G	201	1/1	0.48	0.25	84,84,84,84	0
56	MG	2a	1777	1/1	0.55	0.24	76,76,76,76	0
56	MG	2A	3615	1/1	0.57	0.21	86,86,86,86	0
56	MG	1A	3924	1/1	0.62	0.20	64,64,64,64	0
56	MG	2A	3752	1/1	0.62	0.27	67,67,67,67	0
56	MG	1A	3391	1/1	0.63	0.49	63,63,63,63	0
56	MG	1B	232	1/1	0.63	0.22	82,82,82,82	0
56	MG	1A	3990	1/1	0.64	0.16	50,50,50,50	0
56	MG	1A	3768	1/1	0.64	0.17	67,67,67,67	0
56	MG	1A	3989	1/1	0.65	0.30	65,65,65,65	0
56	MG	1A	3758	1/1	0.65	0.25	95,95,95,95	0
56	MG	2A	3659	1/1	0.65	0.18	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3979	1/1	0.66	0.13	78,78,78,78	0
56	MG	1A	3918	1/1	0.66	0.21	52,52,52,52	0
56	MG	2a	1613	1/1	0.66	0.17	75,75,75,75	0
56	MG	2A	3665	1/1	0.66	0.24	56,56,56,56	0
56	MG	1a	1657	1/1	0.67	0.14	62,62,62,62	0
56	MG	2A	3765	1/1	0.68	0.19	79,79,79,79	0
56	MG	2a	1614	1/1	0.68	0.25	78,78,78,78	0
56	MG	2A	3091	1/1	0.68	0.26	69,69,69,69	0
56	MG	2A	3700	1/1	0.69	0.26	72,72,72,72	0
56	MG	2A	3100	1/1	0.70	0.23	71,71,71,71	0
56	MG	2a	1619	1/1	0.70	0.18	80,80,80,80	0
56	MG	2a	1698	1/1	0.70	0.29	75,75,75,75	0
56	MG	2A	3166	1/1	0.70	0.25	76,76,76,76	0
56	MG	2a	1620	1/1	0.71	0.36	77,77,77,77	0
56	MG	2A	3657	1/1	0.71	0.30	74,74,74,74	0
56	MG	1A	3800	1/1	0.71	0.22	69,69,69,69	0
56	MG	1B	225	1/1	0.72	0.21	66,66,66,66	0
56	MG	1a	1741	1/1	0.72	0.21	76,76,76,76	0
56	MG	2A	3185	1/1	0.72	0.25	67,67,67,67	0
56	MG	2A	3499	1/1	0.72	0.23	60,60,60,60	0
56	MG	1a	1782	1/1	0.72	0.29	72,72,72,72	0
56	MG	2a	1764	1/1	0.72	0.21	87,87,87,87	0
56	MG	1P	206	1/1	0.72	0.25	58,58,58,58	0
56	MG	2a	1787	1/1	0.72	0.20	80,80,80,80	0
56	MG	1a	1781	1/1	0.73	0.22	80,80,80,80	0
56	MG	2a	1602	1/1	0.73	0.19	74,74,74,74	0
56	MG	1A	3315	1/1	0.73	0.27	52,52,52,52	0
56	MG	2A	3651	1/1	0.73	0.22	74,74,74,74	0
56	MG	18	104	1/1	0.73	0.20	69,69,69,69	0
56	MG	1A	3867	1/1	0.73	0.13	57,57,57,57	0
56	MG	2a	1634	1/1	0.73	0.37	72,72,72,72	0
56	MG	1O	206	1/1	0.73	0.21	66,66,66,66	0
56	MG	1a	1743	1/1	0.73	0.17	74,74,74,74	0
56	MG	2A	3330	1/1	0.73	0.26	80,80,80,80	0
56	MG	2A	3434	1/1	0.73	0.19	67,67,67,67	0
56	MG	2A	3630	1/1	0.74	0.18	57,57,57,57	0
56	MG	2A	3264	1/1	0.74	0.25	74,74,74,74	0
56	MG	1A	3677	1/1	0.74	0.16	43,43,43,43	0
56	MG	2A	3368	1/1	0.74	0.32	82,82,82,82	0
56	MG	1A	3369	1/1	0.74	0.18	69,69,69,69	0
56	MG	1A	3404	1/1	0.74	0.20	62,62,62,62	0
56	MG	2A	3582	1/1	0.74	0.22	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3595	1/1	0.74	0.19	66,66,66,66	0
56	MG	2a	1767	1/1	0.74	0.20	76,76,76,76	0
56	MG	2D	303	1/1	0.74	0.23	70,70,70,70	0
56	MG	2A	3048	1/1	0.74	0.25	69,69,69,69	0
56	MG	2a	1606	1/1	0.75	0.38	79,79,79,79	0
56	MG	1a	1656	1/1	0.75	0.26	79,79,79,79	0
56	MG	2A	3579	1/1	0.75	0.14	72,72,72,72	0
56	MG	2A	3255	1/1	0.75	0.37	77,77,77,77	0
56	MG	1B	233	1/1	0.75	0.13	79,79,79,79	0
56	MG	2A	3612	1/1	0.75	0.19	70,70,70,70	0
56	MG	2a	1643	1/1	0.75	0.28	68,68,68,68	0
56	MG	1A	3386	1/1	0.75	0.59	82,82,82,82	0
56	MG	2a	1702	1/1	0.75	0.34	73,73,73,73	0
56	MG	1A	3492	1/1	0.75	0.17	83,83,83,83	0
56	MG	2D	308	1/1	0.75	0.21	69,69,69,69	0
56	MG	2A	3647	1/1	0.75	0.20	76,76,76,76	0
56	MG	2a	1780	1/1	0.75	0.17	78,78,78,78	0
56	MG	1A	3805	1/1	0.75	0.20	62,62,62,62	0
56	MG	2A	3777	1/1	0.76	0.20	67,67,67,67	0
56	MG	2A	3603	1/1	0.76	0.27	62,62,62,62	0
56	MG	2A	3387	1/1	0.76	0.29	76,76,76,76	0
56	MG	2A	3722	1/1	0.76	0.22	65,65,65,65	0
56	MG	2A	3331	1/1	0.76	0.23	75,75,75,75	0
56	MG	1A	3952	1/1	0.76	0.13	37,37,37,37	0
56	MG	2a	1689	1/1	0.76	0.24	70,70,70,70	0
56	MG	2l	202	1/1	0.76	0.21	67,67,67,67	0
56	MG	2A	3441	1/1	0.77	0.28	58,58,58,58	0
56	MG	1A	3557	1/1	0.77	0.25	47,47,47,47	0
56	MG	2A	3201	1/1	0.77	0.25	53,53,53,53	0
56	MG	2A	3207	1/1	0.77	0.27	66,66,66,66	0
56	MG	2A	3591	1/1	0.77	0.23	73,73,73,73	0
56	MG	2A	3242	1/1	0.77	0.23	62,62,62,62	0
56	MG	1A	3966	1/1	0.77	0.14	67,67,67,67	0
56	MG	1x	111	1/1	0.77	0.35	75,75,75,75	0
56	MG	1D	311	1/1	0.77	0.28	49,49,49,49	0
56	MG	2A	3090	1/1	0.77	0.21	75,75,75,75	0
56	MG	2T	204	1/1	0.77	0.26	83,83,83,83	0
56	MG	1A	3993	1/1	0.77	0.21	63,63,63,63	0
56	MG	1A	3547	1/1	0.77	0.16	65,65,65,65	0
56	MG	2a	1798	1/1	0.77	0.30	74,74,74,74	0
56	MG	1a	1759	1/1	0.77	0.19	57,57,57,57	0
56	MG	1b	301	1/1	0.78	0.18	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3503	1/1	0.78	0.20	73,73,73,73	0
56	MG	1x	106	1/1	0.78	0.20	74,74,74,74	0
56	MG	1A	3959	1/1	0.78	0.16	31,31,31,31	0
56	MG	2a	1644	1/1	0.78	0.18	78,78,78,78	0
56	MG	1A	3850	1/1	0.78	0.20	35,35,35,35	0
56	MG	1E	313	1/1	0.78	0.16	60,60,60,60	0
56	MG	2A	3305	1/1	0.78	0.24	70,70,70,70	0
56	MG	2a	1729	1/1	0.78	0.25	75,75,75,75	0
56	MG	1F	312	1/1	0.78	0.20	66,66,66,66	0
56	MG	1A	4026	1/1	0.78	0.13	60,60,60,60	0
56	MG	2A	3343	1/1	0.78	0.18	59,59,59,59	0
56	MG	2A	3156	1/1	0.78	0.19	64,64,64,64	0
56	MG	1A	3475	1/1	0.78	0.18	64,64,64,64	0
56	MG	1A	3694	1/1	0.78	0.15	66,66,66,66	0
56	MG	2A	3195	1/1	0.78	0.30	52,52,52,52	0
56	MG	2A	3175	1/1	0.79	0.30	75,75,75,75	0
56	MG	1a	1666	1/1	0.79	0.23	78,78,78,78	0
56	MG	2a	1629	1/1	0.79	0.35	79,79,79,79	0
56	MG	1A	3965	1/1	0.79	0.17	81,81,81,81	0
56	MG	1A	3443	1/1	0.79	0.16	60,60,60,60	0
56	MG	2B	204	1/1	0.79	0.19	80,80,80,80	0
56	MG	2B	214	1/1	0.79	0.21	76,76,76,76	0
56	MG	2B	215	1/1	0.79	0.17	78,78,78,78	0
56	MG	1A	3238	1/1	0.79	0.30	75,75,75,75	0
56	MG	2a	1709	1/1	0.79	0.23	87,87,87,87	0
56	MG	1A	3163	1/1	0.79	0.14	48,48,48,48	0
56	MG	1A	3770	1/1	0.79	0.21	63,63,63,63	0
56	MG	2a	1766	1/1	0.79	0.26	75,75,75,75	0
56	MG	1A	3891	1/1	0.79	0.12	33,33,33,33	0
56	MG	2A	3286	1/1	0.79	0.19	78,78,78,78	0
56	MG	2A	3288	1/1	0.79	0.14	82,82,82,82	0
56	MG	2A	3580	1/1	0.79	0.18	75,75,75,75	0
56	MG	1x	105	1/1	0.79	0.23	79,79,79,79	0
56	MG	2a	1799	1/1	0.79	0.21	81,81,81,81	0
56	MG	2a	1617	1/1	0.79	0.24	79,79,79,79	0
56	MG	2A	3265	1/1	0.80	0.19	68,68,68,68	0
56	MG	1A	3983	1/1	0.80	0.10	65,65,65,65	0
56	MG	1W	206	1/1	0.80	0.26	50,50,50,50	0
56	MG	2A	3589	1/1	0.80	0.22	63,63,63,63	0
56	MG	2a	1662	1/1	0.80	0.23	69,69,69,69	0
56	MG	2A	3298	1/1	0.80	0.23	66,66,66,66	0
56	MG	1A	3801	1/1	0.80	0.18	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3312	1/1	0.80	0.29	69,69,69,69	0
56	MG	1a	1649	1/1	0.80	0.28	69,69,69,69	0
56	MG	1n	101	1/1	0.80	0.26	66,66,66,66	0
56	MG	2a	1752	1/1	0.80	0.24	73,73,73,73	0
56	MG	1A	3436	1/1	0.80	0.18	63,63,63,63	0
56	MG	2A	3643	1/1	0.80	0.20	75,75,75,75	0
56	MG	1A	3875	1/1	0.80	0.18	62,62,62,62	0
56	MG	2a	1776	1/1	0.80	0.18	78,78,78,78	0
56	MG	1A	3806	1/1	0.80	0.22	67,67,67,67	0
56	MG	1a	1679	1/1	0.80	0.17	57,57,57,57	0
56	MG	1A	4044	1/1	0.80	0.21	78,78,78,78	0
56	MG	2A	3258	1/1	0.80	0.34	69,69,69,69	0
56	MG	1B	216	1/1	0.80	0.19	73,73,73,73	0
56	MG	2A	3701	1/1	0.80	0.14	69,69,69,69	0
56	MG	2x	103	1/1	0.80	0.20	78,78,78,78	0
56	MG	2a	1607	1/1	0.81	0.27	75,75,75,75	0
56	MG	2A	3623	1/1	0.81	0.28	64,64,64,64	0
56	MG	2A	3250	1/1	0.81	0.14	62,62,62,62	0
56	MG	2A	3379	1/1	0.81	0.18	57,57,57,57	0
56	MG	1a	1726	1/1	0.81	0.29	81,81,81,81	0
56	MG	2A	3410	1/1	0.81	0.44	75,75,75,75	0
56	MG	2A	3423	1/1	0.81	0.23	68,68,68,68	0
56	MG	2A	3153	1/1	0.81	0.15	86,86,86,86	0
56	MG	2A	3261	1/1	0.81	0.31	59,59,59,59	0
56	MG	2A	3670	1/1	0.81	0.18	70,70,70,70	0
56	MG	1A	3388	1/1	0.81	0.29	70,70,70,70	0
56	MG	1A	3603	1/1	0.81	0.20	65,65,65,65	0
56	MG	2A	3703	1/1	0.81	0.18	67,67,67,67	0
56	MG	2a	1700	1/1	0.81	0.23	85,85,85,85	0
56	MG	2a	1701	1/1	0.81	0.32	67,67,67,67	0
56	MG	2A	3521	1/1	0.81	0.18	64,64,64,64	0
56	MG	2A	3748	1/1	0.81	0.13	56,56,56,56	0
56	MG	2A	3523	1/1	0.81	0.15	50,50,50,50	0
56	MG	2A	3525	1/1	0.81	0.18	71,71,71,71	0
56	MG	2A	3174	1/1	0.81	0.34	76,76,76,76	0
56	MG	1A	3821	1/1	0.81	0.15	67,67,67,67	0
56	MG	2A	3017	1/1	0.81	0.20	71,71,71,71	0
56	MG	2a	1774	1/1	0.81	0.18	74,74,74,74	0
56	MG	1A	3954	1/1	0.81	0.14	61,61,61,61	0
56	MG	2A	3054	1/1	0.81	0.20	81,81,81,81	0
56	MG	2A	3317	1/1	0.81	0.24	73,73,73,73	0
56	MG	2a	1784	1/1	0.81	0.10	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1785	1/1	0.81	0.18	71,71,71,71	0
56	MG	1A	3491	1/1	0.81	0.12	78,78,78,78	0
56	MG	2a	1789	1/1	0.81	0.20	79,79,79,79	0
56	MG	2A	3238	1/1	0.81	0.22	64,64,64,64	0
56	MG	25	105	1/1	0.81	0.16	67,67,67,67	0
56	MG	1a	1699	1/1	0.81	0.23	78,78,78,78	0
56	MG	2A	3622	1/1	0.81	0.28	63,63,63,63	0
56	MG	1F	314	1/1	0.82	0.28	55,55,55,55	0
56	MG	2A	3691	1/1	0.82	0.22	71,71,71,71	0
56	MG	2a	1621	1/1	0.82	0.39	78,78,78,78	0
56	MG	2a	1622	1/1	0.82	0.20	62,62,62,62	0
56	MG	2A	3697	1/1	0.82	0.17	59,59,59,59	0
56	MG	1A	3679	1/1	0.82	0.16	63,63,63,63	0
56	MG	1A	3403	1/1	0.82	0.17	75,75,75,75	0
56	MG	2A	3302	1/1	0.82	0.25	68,68,68,68	0
56	MG	2A	3707	1/1	0.82	0.22	64,64,64,64	0
56	MG	2A	3713	1/1	0.82	0.21	58,58,58,58	0
56	MG	2a	1697	1/1	0.82	0.18	79,79,79,79	0
56	MG	1A	4016	1/1	0.82	0.20	44,44,44,44	0
56	MG	1a	1740	1/1	0.82	0.16	72,72,72,72	0
56	MG	1A	3530	1/1	0.82	0.35	71,71,71,71	0
56	MG	2A	3587	1/1	0.82	0.18	78,78,78,78	0
56	MG	2A	3329	1/1	0.82	0.14	74,74,74,74	0
56	MG	2A	3219	1/1	0.82	0.25	77,77,77,77	0
56	MG	2a	1750	1/1	0.82	0.17	67,67,67,67	0
56	MG	2B	212	1/1	0.82	0.11	74,74,74,74	0
56	MG	2A	3229	1/1	0.82	0.15	75,75,75,75	0
56	MG	2a	1765	1/1	0.82	0.23	70,70,70,70	0
56	MG	2A	3234	1/1	0.82	0.23	73,73,73,73	0
56	MG	2A	3073	1/1	0.82	0.26	71,71,71,71	0
56	MG	2A	3080	1/1	0.82	0.22	70,70,70,70	0
56	MG	2E	307	1/1	0.82	0.17	65,65,65,65	0
56	MG	1a	1614	1/1	0.82	0.19	69,69,69,69	0
56	MG	1a	1623	1/1	0.82	0.20	76,76,76,76	0
56	MG	2Z	302	1/1	0.82	0.23	76,76,76,76	0
56	MG	1a	1629	1/1	0.82	0.28	73,73,73,73	0
56	MG	2A	3429	1/1	0.82	0.23	65,65,65,65	0
56	MG	1E	310	1/1	0.82	0.39	76,76,76,76	0
56	MG	1A	3619	1/1	0.82	0.11	65,65,65,65	0
56	MG	2A	3485	1/1	0.82	0.23	56,56,56,56	0
56	MG	2A	3496	1/1	0.82	0.16	76,76,76,76	0
56	MG	2q	202	1/1	0.82	0.20	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2w	103	1/1	0.82	0.30	83,83,83,83	0
56	MG	1A	3434	1/1	0.82	0.34	64,64,64,64	0
56	MG	2a	1639	1/1	0.83	0.32	75,75,75,75	0
56	MG	1G	203	1/1	0.83	0.13	71,71,71,71	0
56	MG	1A	3199	1/1	0.83	0.19	69,69,69,69	0
56	MG	2a	1646	1/1	0.83	0.26	71,71,71,71	0
56	MG	2a	1652	1/1	0.83	0.30	68,68,68,68	0
56	MG	1a	1692	1/1	0.83	0.35	70,70,70,70	0
56	MG	2A	3756	1/1	0.83	0.19	61,61,61,61	0
56	MG	2A	3760	1/1	0.83	0.14	72,72,72,72	0
56	MG	1A	3776	1/1	0.83	0.15	59,59,59,59	0
56	MG	2A	3365	1/1	0.83	0.37	70,70,70,70	0
56	MG	2A	3055	1/1	0.83	0.17	79,79,79,79	0
56	MG	2A	3611	1/1	0.83	0.15	58,58,58,58	0
56	MG	1a	1721	1/1	0.83	0.28	71,71,71,71	0
56	MG	2A	3385	1/1	0.83	0.20	75,75,75,75	0
56	MG	2A	3244	1/1	0.83	0.24	76,76,76,76	0
56	MG	1V	206	1/1	0.83	0.14	58,58,58,58	0
56	MG	1A	3571	1/1	0.83	0.14	43,43,43,43	0
56	MG	2A	3427	1/1	0.83	0.22	61,61,61,61	0
56	MG	2A	3645	1/1	0.83	0.18	69,69,69,69	0
56	MG	1A	3907	1/1	0.83	0.14	34,34,34,34	0
56	MG	1A	3483	1/1	0.83	0.15	66,66,66,66	0
56	MG	1A	3695	1/1	0.83	0.17	51,51,51,51	0
56	MG	1a	1780	1/1	0.83	0.35	82,82,82,82	0
56	MG	2A	3284	1/1	0.83	0.22	73,73,73,73	0
56	MG	1A	3708	1/1	0.83	0.13	56,56,56,56	0
56	MG	1a	1637	1/1	0.83	0.40	73,73,73,73	0
56	MG	2A	3518	1/1	0.83	0.18	73,73,73,73	0
56	MG	1A	3944	1/1	0.83	0.11	71,71,71,71	0
56	MG	1A	3609	1/1	0.83	0.17	55,55,55,55	0
56	MG	2A	3190	1/1	0.83	0.36	71,71,71,71	0
56	MG	1A	3027	1/1	0.83	0.17	82,82,82,82	0
56	MG	1a	1662	1/1	0.83	0.29	68,68,68,68	0
56	MG	2a	1632	1/1	0.83	0.16	79,79,79,79	0
56	MG	2A	3720	1/1	0.83	0.16	46,46,46,46	0
56	MG	1A	3747	1/1	0.84	0.14	45,45,45,45	0
56	MG	2A	3280	1/1	0.84	0.22	74,74,74,74	0
56	MG	2X	101	1/1	0.84	0.16	69,69,69,69	0
56	MG	2A	3086	1/1	0.84	0.17	75,75,75,75	0
56	MG	1A	3400	1/1	0.84	0.20	63,63,63,63	0
56	MG	1A	3318	1/1	0.84	0.16	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3913	1/1	0.84	0.11	74,74,74,74	0
56	MG	2A	3101	1/1	0.84	0.34	69,69,69,69	0
56	MG	2A	3124	1/1	0.84	0.13	63,63,63,63	0
56	MG	2A	3137	1/1	0.84	0.19	79,79,79,79	0
56	MG	2a	1615	1/1	0.84	0.26	66,66,66,66	0
56	MG	2A	3620	1/1	0.84	0.23	71,71,71,71	0
56	MG	1A	3999	1/1	0.84	0.17	50,50,50,50	0
56	MG	1A	3580	1/1	0.84	0.12	50,50,50,50	0
56	MG	1A	3188	1/1	0.84	0.24	61,61,61,61	0
56	MG	2A	3632	1/1	0.84	0.14	64,64,64,64	0
56	MG	2a	1623	1/1	0.84	0.17	63,63,63,63	0
56	MG	2A	3637	1/1	0.84	0.18	68,68,68,68	0
56	MG	2A	3167	1/1	0.84	0.27	77,77,77,77	0
56	MG	2A	3173	1/1	0.84	0.22	66,66,66,66	0
56	MG	2A	3344	1/1	0.84	0.19	63,63,63,63	0
56	MG	10	105	1/1	0.84	0.18	65,65,65,65	0
56	MG	2A	3654	1/1	0.84	0.14	75,75,75,75	0
56	MG	2a	1645	1/1	0.84	0.36	80,80,80,80	0
56	MG	1a	1750	1/1	0.84	0.16	62,62,62,62	0
56	MG	1A	4034	1/1	0.84	0.12	59,59,59,59	0
56	MG	1A	3795	1/1	0.84	0.15	50,50,50,50	0
56	MG	1A	4046	1/1	0.84	0.19	66,66,66,66	0
56	MG	2a	1695	1/1	0.84	0.23	80,80,80,80	0
56	MG	1A	3246	1/1	0.84	0.13	69,69,69,69	0
56	MG	2A	3204	1/1	0.84	0.16	61,61,61,61	0
56	MG	1a	1793	1/1	0.84	0.17	68,68,68,68	0
56	MG	1a	1797	1/1	0.84	0.16	68,68,68,68	0
56	MG	1a	1631	1/1	0.84	0.34	69,69,69,69	0
56	MG	1A	3493	1/1	0.84	0.23	77,77,77,77	0
56	MG	2A	3456	1/1	0.84	0.35	77,77,77,77	0
56	MG	2a	1731	1/1	0.84	0.15	79,79,79,79	0
56	MG	2a	1748	1/1	0.84	0.14	80,80,80,80	0
56	MG	2A	3467	1/1	0.84	0.11	44,44,44,44	0
56	MG	2A	3236	1/1	0.84	0.21	72,72,72,72	0
56	MG	2a	1759	1/1	0.84	0.29	74,74,74,74	0
56	MG	2a	1762	1/1	0.84	0.24	77,77,77,77	0
56	MG	2A	3739	1/1	0.84	0.13	63,63,63,63	0
56	MG	1A	3494	1/1	0.84	0.10	69,69,69,69	0
56	MG	1a	1655	1/1	0.84	0.23	60,60,60,60	0
56	MG	1A	3505	1/1	0.84	0.28	55,55,55,55	0
56	MG	2A	3759	1/1	0.84	0.13	64,64,64,64	0
56	MG	2A	3247	1/1	0.84	0.14	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3313	1/1	0.84	0.17	56,56,56,56	0
56	MG	1a	1661	1/1	0.84	0.19	63,63,63,63	0
56	MG	2B	203	1/1	0.84	0.28	77,77,77,77	0
56	MG	1A	3053	1/1	0.84	0.13	56,56,56,56	0
56	MG	2B	208	1/1	0.84	0.33	73,73,73,73	0
56	MG	2a	1788	1/1	0.84	0.14	80,80,80,80	0
56	MG	2A	3529	1/1	0.84	0.19	66,66,66,66	0
56	MG	2a	1790	1/1	0.84	0.33	75,75,75,75	0
56	MG	2A	3556	1/1	0.84	0.21	47,47,47,47	0
56	MG	2A	3565	1/1	0.84	0.17	57,57,57,57	0
56	MG	2B	218	1/1	0.84	0.34	76,76,76,76	0
56	MG	2l	205	1/1	0.84	0.15	71,71,71,71	0
56	MG	2A	3569	1/1	0.84	0.24	70,70,70,70	0
56	MG	1A	3555	1/1	0.84	0.16	50,50,50,50	0
56	MG	1a	1673	1/1	0.84	0.29	57,57,57,57	0
56	MG	14	101	1/1	0.85	0.24	77,77,77,77	0
56	MG	1A	3833	1/1	0.85	0.11	30,30,30,30	0
56	MG	1a	1613	1/1	0.85	0.15	69,69,69,69	0
56	MG	2A	3140	1/1	0.85	0.22	56,56,56,56	0
56	MG	1A	3261	1/1	0.85	0.30	68,68,68,68	0
56	MG	2a	1605	1/1	0.85	0.28	67,67,67,67	0
56	MG	2A	3309	1/1	0.85	0.21	76,76,76,76	0
56	MG	1A	3766	1/1	0.85	0.13	45,45,45,45	0
56	MG	2A	3164	1/1	0.85	0.24	72,72,72,72	0
56	MG	2A	3326	1/1	0.85	0.10	68,68,68,68	0
56	MG	1A	3399	1/1	0.85	0.13	52,52,52,52	0
56	MG	1A	3309	1/1	0.85	0.18	57,57,57,57	0
56	MG	1A	3159	1/1	0.85	0.30	66,66,66,66	0
56	MG	1a	1638	1/1	0.85	0.24	66,66,66,66	0
56	MG	1a	1790	1/1	0.85	0.23	65,65,65,65	0
56	MG	2A	3350	1/1	0.85	0.39	65,65,65,65	0
56	MG	2A	3356	1/1	0.85	0.35	70,70,70,70	0
56	MG	2A	3644	1/1	0.85	0.17	62,62,62,62	0
56	MG	1A	3682	1/1	0.85	0.20	67,67,67,67	0
56	MG	1a	1652	1/1	0.85	0.26	65,65,65,65	0
56	MG	1A	3024	1/1	0.85	0.23	57,57,57,57	0
56	MG	2A	3652	1/1	0.85	0.21	62,62,62,62	0
56	MG	2A	3200	1/1	0.85	0.13	57,57,57,57	0
56	MG	1A	3578	1/1	0.85	0.12	49,49,49,49	0
56	MG	2A	3406	1/1	0.85	0.27	82,82,82,82	0
56	MG	2A	3661	1/1	0.85	0.15	60,60,60,60	0
56	MG	2a	1658	1/1	0.85	0.17	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3408	1/1	0.85	0.20	59,59,59,59	0
56	MG	2a	1686	1/1	0.85	0.39	77,77,77,77	0
56	MG	2a	1688	1/1	0.85	0.28	66,66,66,66	0
56	MG	2A	3409	1/1	0.85	0.14	67,67,67,67	0
56	MG	2a	1692	1/1	0.85	0.35	71,71,71,71	0
56	MG	2A	3682	1/1	0.85	0.20	69,69,69,69	0
56	MG	1A	4011	1/1	0.85	0.21	72,72,72,72	0
56	MG	2A	3206	1/1	0.85	0.11	71,71,71,71	0
56	MG	1A	3702	1/1	0.85	0.17	65,65,65,65	0
56	MG	1A	4019	1/1	0.85	0.11	55,55,55,55	0
56	MG	2A	3002	1/1	0.85	0.31	71,71,71,71	0
56	MG	2A	3706	1/1	0.85	0.13	65,65,65,65	0
56	MG	2A	3014	1/1	0.85	0.20	67,67,67,67	0
56	MG	2A	3710	1/1	0.85	0.13	60,60,60,60	0
56	MG	1A	4023	1/1	0.85	0.13	50,50,50,50	0
56	MG	2A	3023	1/1	0.85	0.22	70,70,70,70	0
56	MG	2A	3721	1/1	0.85	0.15	50,50,50,50	0
56	MG	2A	3025	1/1	0.85	0.11	52,52,52,52	0
56	MG	1Q	205	1/1	0.85	0.14	57,57,57,57	0
56	MG	2A	3245	1/1	0.85	0.16	76,76,76,76	0
56	MG	2A	3502	1/1	0.85	0.18	50,50,50,50	0
56	MG	1a	1675	1/1	0.85	0.39	68,68,68,68	0
56	MG	1A	3513	1/1	0.85	0.11	69,69,69,69	0
56	MG	2A	3057	1/1	0.85	0.27	57,57,57,57	0
56	MG	1a	1689	1/1	0.85	0.14	67,67,67,67	0
56	MG	2A	3768	1/1	0.85	0.13	66,66,66,66	0
56	MG	1A	3528	1/1	0.85	0.29	54,54,54,54	0
56	MG	2A	3778	1/1	0.85	0.30	69,69,69,69	0
56	MG	1Z	302	1/1	0.85	0.11	58,58,58,58	0
56	MG	2A	3534	1/1	0.85	0.12	68,68,68,68	0
56	MG	2A	3536	1/1	0.85	0.11	38,38,38,38	0
56	MG	2B	209	1/1	0.85	0.25	71,71,71,71	0
56	MG	2A	3549	1/1	0.85	0.16	65,65,65,65	0
56	MG	1a	1701	1/1	0.85	0.46	70,70,70,70	0
56	MG	2A	3563	1/1	0.85	0.17	47,47,47,47	0
56	MG	2A	3269	1/1	0.85	0.20	71,71,71,71	0
56	MG	2A	3273	1/1	0.85	0.13	72,72,72,72	0
56	MG	2A	3574	1/1	0.85	0.18	75,75,75,75	0
56	MG	1A	3831	1/1	0.85	0.13	47,47,47,47	0
56	MG	1a	1723	1/1	0.85	0.17	67,67,67,67	0
56	MG	2A	3181	1/1	0.86	0.14	60,60,60,60	0
56	MG	1B	224	1/1	0.86	0.14	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1603	1/1	0.86	0.27	66,66,66,66	0
56	MG	2a	1604	1/1	0.86	0.20	72,72,72,72	0
56	MG	2A	3189	1/1	0.86	0.17	58,58,58,58	0
56	MG	1A	3350	1/1	0.86	0.21	64,64,64,64	0
56	MG	2A	3364	1/1	0.86	0.21	64,64,64,64	0
56	MG	2A	3192	1/1	0.86	0.15	65,65,65,65	0
56	MG	1A	3402	1/1	0.86	0.29	69,69,69,69	0
56	MG	2A	3374	1/1	0.86	0.18	64,64,64,64	0
56	MG	2a	1616	1/1	0.86	0.18	67,67,67,67	0
56	MG	1A	3815	1/1	0.86	0.13	65,65,65,65	0
56	MG	1A	3451	1/1	0.86	0.27	55,55,55,55	0
56	MG	1A	3717	1/1	0.86	0.12	48,48,48,48	0
56	MG	2A	3205	1/1	0.86	0.17	66,66,66,66	0
56	MG	1x	107	1/1	0.86	0.18	74,74,74,74	0
56	MG	1x	109	1/1	0.86	0.24	68,68,68,68	0
56	MG	1a	1660	1/1	0.86	0.23	69,69,69,69	0
56	MG	2A	3422	1/1	0.86	0.26	61,61,61,61	0
56	MG	1A	3729	1/1	0.86	0.11	23,23,23,23	0
56	MG	1A	3985	1/1	0.86	0.12	79,79,79,79	0
56	MG	2a	1641	1/1	0.86	0.12	56,56,56,56	0
56	MG	1A	3834	1/1	0.86	0.18	54,54,54,54	0
56	MG	1A	3458	1/1	0.86	0.15	47,47,47,47	0
56	MG	2A	3435	1/1	0.86	0.17	38,38,38,38	0
56	MG	1A	3466	1/1	0.86	0.19	61,61,61,61	0
56	MG	2a	1647	1/1	0.86	0.13	75,75,75,75	0
56	MG	1A	3765	1/1	0.86	0.11	26,26,26,26	0
56	MG	1a	1681	1/1	0.86	0.26	67,67,67,67	0
56	MG	1A	3352	1/1	0.86	0.21	59,59,59,59	0
56	MG	2a	1668	1/1	0.86	0.20	68,68,68,68	0
56	MG	2a	1673	1/1	0.86	0.22	72,72,72,72	0
56	MG	1A	4012	1/1	0.86	0.08	19,19,19,19	0
56	MG	1a	1695	1/1	0.86	0.18	68,68,68,68	0
56	MG	1A	3642	1/1	0.86	0.07	21,21,21,21	0
56	MG	2a	1691	1/1	0.86	0.35	66,66,66,66	0
56	MG	1A	3353	1/1	0.86	0.18	54,54,54,54	0
56	MG	2A	3089	1/1	0.86	0.35	76,76,76,76	0
56	MG	1A	4020	1/1	0.86	0.11	34,34,34,34	0
56	MG	1A	3409	1/1	0.86	0.22	51,51,51,51	0
56	MG	2a	1699	1/1	0.86	0.18	72,72,72,72	0
56	MG	2A	3738	1/1	0.86	0.11	68,68,68,68	0
56	MG	2A	3270	1/1	0.86	0.16	61,61,61,61	0
56	MG	2A	3745	1/1	0.86	0.17	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3099	1/1	0.86	0.17	57,57,57,57	0
56	MG	2a	1710	1/1	0.86	0.28	76,76,76,76	0
56	MG	2a	1718	1/1	0.86	0.36	82,82,82,82	0
56	MG	2A	3277	1/1	0.86	0.16	70,70,70,70	0
56	MG	15	108	1/1	0.86	0.16	60,60,60,60	0
56	MG	1a	1731	1/1	0.86	0.27	78,78,78,78	0
56	MG	2A	3285	1/1	0.86	0.29	80,80,80,80	0
56	MG	2A	3763	1/1	0.86	0.20	62,62,62,62	0
56	MG	2A	3562	1/1	0.86	0.24	75,75,75,75	0
56	MG	2A	3767	1/1	0.86	0.18	58,58,58,58	0
56	MG	16	103	1/1	0.86	0.30	53,53,53,53	0
56	MG	1A	3781	1/1	0.86	0.14	61,61,61,61	0
56	MG	1a	1604	1/1	0.86	0.18	66,66,66,66	0
56	MG	2A	3571	1/1	0.86	0.34	75,75,75,75	0
56	MG	2a	1771	1/1	0.86	0.17	67,67,67,67	0
56	MG	2A	3151	1/1	0.86	0.12	80,80,80,80	0
56	MG	1A	3925	1/1	0.86	0.10	31,31,31,31	0
56	MG	2A	3308	1/1	0.86	0.22	46,46,46,46	0
56	MG	1A	3316	1/1	0.86	0.24	58,58,58,58	0
56	MG	1A	3693	1/1	0.86	0.18	59,59,59,59	0
56	MG	1B	203	1/1	0.86	0.29	64,64,64,64	0
56	MG	1B	212	1/1	0.86	0.15	61,61,61,61	0
56	MG	2A	3593	1/1	0.86	0.13	61,61,61,61	0
56	MG	2D	307	1/1	0.86	0.18	67,67,67,67	0
56	MG	2A	3328	1/1	0.86	0.17	79,79,79,79	0
56	MG	2A	3596	1/1	0.86	0.24	66,66,66,66	0
56	MG	2F	306	1/1	0.86	0.18	67,67,67,67	0
56	MG	1a	1783	1/1	0.86	0.20	68,68,68,68	0
56	MG	2O	202	1/1	0.86	0.16	56,56,56,56	0
56	MG	1a	1788	1/1	0.86	0.28	74,74,74,74	0
56	MG	2w	101	1/1	0.86	0.33	71,71,71,71	0
56	MG	1A	3562	1/1	0.86	0.31	69,69,69,69	0
56	MG	2A	3613	1/1	0.86	0.12	66,66,66,66	0
56	MG	2E	305	1/1	0.87	0.17	68,68,68,68	0
56	MG	1A	4051	1/1	0.87	0.19	51,51,51,51	0
56	MG	2A	3152	1/1	0.87	0.11	68,68,68,68	0
56	MG	2A	3578	1/1	0.87	0.17	71,71,71,71	0
56	MG	1a	1758	1/1	0.87	0.14	62,62,62,62	0
56	MG	1a	1627	1/1	0.87	0.23	70,70,70,70	0
56	MG	1a	1765	1/1	0.87	0.12	69,69,69,69	0
56	MG	1A	3336	1/1	0.87	0.13	65,65,65,65	0
56	MG	1A	3153	1/1	0.87	0.14	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3169	1/1	0.87	0.32	74,74,74,74	0
56	MG	2A	3319	1/1	0.87	0.22	76,76,76,76	0
56	MG	2A	3170	1/1	0.87	0.15	74,74,74,74	0
56	MG	1a	1635	1/1	0.87	0.23	58,58,58,58	0
56	MG	2A	3597	1/1	0.87	0.13	66,66,66,66	0
56	MG	2A	3599	1/1	0.87	0.16	64,64,64,64	0
56	MG	1B	214	1/1	0.87	0.15	59,59,59,59	0
56	MG	2A	3604	1/1	0.87	0.12	52,52,52,52	0
56	MG	2A	3608	1/1	0.87	0.14	62,62,62,62	0
56	MG	1a	1784	1/1	0.87	0.14	69,69,69,69	0
56	MG	1A	3312	1/1	0.87	0.29	66,66,66,66	0
56	MG	2a	1618	1/1	0.87	0.16	76,76,76,76	0
56	MG	2A	3334	1/1	0.87	0.12	71,71,71,71	0
56	MG	2A	3339	1/1	0.87	0.23	47,47,47,47	0
56	MG	2A	3616	1/1	0.87	0.18	68,68,68,68	0
56	MG	2A	3340	1/1	0.87	0.20	59,59,59,59	0
56	MG	1B	218	1/1	0.87	0.10	55,55,55,55	0
56	MG	1a	1650	1/1	0.87	0.14	58,58,58,58	0
56	MG	1A	3579	1/1	0.87	0.12	34,34,34,34	0
56	MG	2a	1633	1/1	0.87	0.24	67,67,67,67	0
56	MG	2A	3351	1/1	0.87	0.31	67,67,67,67	0
56	MG	2a	1636	1/1	0.87	0.48	81,81,81,81	0
56	MG	1a	1798	1/1	0.87	0.18	67,67,67,67	0
56	MG	2A	3360	1/1	0.87	0.26	55,55,55,55	0
56	MG	2A	3362	1/1	0.87	0.17	58,58,58,58	0
56	MG	2A	3193	1/1	0.87	0.28	70,70,70,70	0
56	MG	1a	1653	1/1	0.87	0.16	65,65,65,65	0
56	MG	2A	3366	1/1	0.87	0.31	62,62,62,62	0
56	MG	2A	3198	1/1	0.87	0.11	56,56,56,56	0
56	MG	2a	1649	1/1	0.87	0.25	80,80,80,80	0
56	MG	2A	3369	1/1	0.87	0.29	62,62,62,62	0
56	MG	2a	1655	1/1	0.87	0.09	75,75,75,75	0
56	MG	1A	3968	1/1	0.87	0.09	27,27,27,27	0
56	MG	1u	101	1/1	0.87	0.23	70,70,70,70	0
56	MG	1A	3978	1/1	0.87	0.10	59,59,59,59	0
56	MG	1A	3251	1/1	0.87	0.16	56,56,56,56	0
56	MG	2a	1680	1/1	0.87	0.16	75,75,75,75	0
56	MG	2a	1685	1/1	0.87	0.19	72,72,72,72	0
56	MG	2A	3398	1/1	0.87	0.32	76,76,76,76	0
56	MG	1A	3595	1/1	0.87	0.20	59,59,59,59	0
56	MG	1A	3433	1/1	0.87	0.29	68,68,68,68	0
56	MG	2a	1690	1/1	0.87	0.12	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3213	1/1	0.87	0.17	70,70,70,70	0
56	MG	1A	3355	1/1	0.87	0.10	52,52,52,52	0
56	MG	2A	3224	1/1	0.87	0.24	65,65,65,65	0
56	MG	1A	3868	1/1	0.87	0.20	57,57,57,57	0
56	MG	2A	3704	1/1	0.87	0.15	68,68,68,68	0
56	MG	2A	3705	1/1	0.87	0.19	75,75,75,75	0
56	MG	1A	3097	1/1	0.87	0.13	68,68,68,68	0
56	MG	1a	1674	1/1	0.87	0.21	42,42,42,42	0
56	MG	2A	3708	1/1	0.87	0.19	88,88,88,88	0
56	MG	1A	3634	1/1	0.87	0.12	32,32,32,32	0
56	MG	2A	3239	1/1	0.87	0.26	74,74,74,74	0
56	MG	2a	1712	1/1	0.87	0.23	65,65,65,65	0
56	MG	2A	3437	1/1	0.87	0.22	81,81,81,81	0
56	MG	2a	1727	1/1	0.87	0.23	61,61,61,61	0
56	MG	1A	4010	1/1	0.87	0.11	66,66,66,66	0
56	MG	1A	3895	1/1	0.87	0.10	54,54,54,54	0
56	MG	2a	1736	1/1	0.87	0.12	68,68,68,68	0
56	MG	2A	3460	1/1	0.87	0.21	55,55,55,55	0
56	MG	1A	3265	1/1	0.87	0.11	53,53,53,53	0
56	MG	2a	1751	1/1	0.87	0.14	69,69,69,69	0
56	MG	2A	3472	1/1	0.87	0.14	50,50,50,50	0
56	MG	2A	3746	1/1	0.87	0.18	66,66,66,66	0
56	MG	2A	3479	1/1	0.87	0.13	69,69,69,69	0
56	MG	1a	1690	1/1	0.87	0.32	68,68,68,68	0
56	MG	1A	3674	1/1	0.87	0.14	30,30,30,30	0
56	MG	1A	3529	1/1	0.87	0.13	50,50,50,50	0
56	MG	1A	3317	1/1	0.87	0.14	54,54,54,54	0
56	MG	1A	3308	1/1	0.87	0.17	59,59,59,59	0
56	MG	2A	3506	1/1	0.87	0.12	63,63,63,63	0
56	MG	1a	1717	1/1	0.87	0.19	76,76,76,76	0
56	MG	1A	3938	1/1	0.87	0.14	80,80,80,80	0
56	MG	2a	1779	1/1	0.87	0.34	65,65,65,65	0
56	MG	1A	3319	1/1	0.87	0.24	66,66,66,66	0
56	MG	2a	1781	1/1	0.87	0.20	74,74,74,74	0
56	MG	1A	4043	1/1	0.87	0.14	54,54,54,54	0
56	MG	2A	3779	1/1	0.87	0.20	71,71,71,71	0
56	MG	2A	3780	1/1	0.87	0.16	61,61,61,61	0
56	MG	2A	3527	1/1	0.87	0.16	65,65,65,65	0
56	MG	1A	3804	1/1	0.87	0.11	56,56,56,56	0
56	MG	2A	3274	1/1	0.87	0.32	77,77,77,77	0
56	MG	2a	1792	1/1	0.87	0.22	64,64,64,64	0
56	MG	2A	3276	1/1	0.87	0.19	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1738	1/1	0.87	0.24	63,63,63,63	0
56	MG	2A	3279	1/1	0.87	0.21	70,70,70,70	0
56	MG	1A	4045	1/1	0.87	0.16	68,68,68,68	0
56	MG	2A	3134	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3333	1/1	0.87	0.12	57,57,57,57	0
56	MG	2A	3568	1/1	0.87	0.14	57,57,57,57	0
56	MG	1A	4050	1/1	0.87	0.16	62,62,62,62	0
56	MG	1A	3802	1/1	0.88	0.13	34,34,34,34	0
56	MG	1A	3803	1/1	0.88	0.11	40,40,40,40	0
56	MG	1A	3526	1/1	0.88	0.29	60,60,60,60	0
56	MG	2A	3291	1/1	0.88	0.15	67,67,67,67	0
56	MG	1A	3442	1/1	0.88	0.20	68,68,68,68	0
56	MG	2Q	202	1/1	0.88	0.26	65,65,65,65	0
56	MG	2R	201	1/1	0.88	0.13	64,64,64,64	0
56	MG	1O	205	1/1	0.88	0.13	67,67,67,67	0
56	MG	2V	202	1/1	0.88	0.17	71,71,71,71	0
56	MG	1A	3026	1/1	0.88	0.13	58,58,58,58	0
56	MG	2A	3108	1/1	0.88	0.26	77,77,77,77	0
56	MG	25	104	1/1	0.88	0.13	63,63,63,63	0
56	MG	2A	3109	1/1	0.88	0.16	57,57,57,57	0
56	MG	2A	3310	1/1	0.88	0.14	68,68,68,68	0
56	MG	1a	1706	1/1	0.88	0.21	68,68,68,68	0
56	MG	2A	3131	1/1	0.88	0.52	68,68,68,68	0
56	MG	1A	3259	1/1	0.88	0.17	62,62,62,62	0
56	MG	2A	3322	1/1	0.88	0.25	58,58,58,58	0
56	MG	1A	3820	1/1	0.88	0.16	46,46,46,46	0
56	MG	2a	1610	1/1	0.88	0.24	67,67,67,67	0
56	MG	1U	207	1/1	0.88	0.15	59,59,59,59	0
56	MG	1A	3684	1/1	0.88	0.14	59,59,59,59	0
56	MG	2A	3600	1/1	0.88	0.21	62,62,62,62	0
56	MG	1A	3996	1/1	0.88	0.15	58,58,58,58	0
56	MG	1a	1732	1/1	0.88	0.12	75,75,75,75	0
56	MG	1A	3827	1/1	0.88	0.15	58,58,58,58	0
56	MG	2A	3335	1/1	0.88	0.17	67,67,67,67	0
56	MG	2A	3336	1/1	0.88	0.34	59,59,59,59	0
56	MG	2A	3158	1/1	0.88	0.18	63,63,63,63	0
56	MG	1A	3100	1/1	0.88	0.10	38,38,38,38	0
56	MG	1A	3460	1/1	0.88	0.15	53,53,53,53	0
56	MG	2a	1626	1/1	0.88	0.28	66,66,66,66	0
56	MG	2A	3617	1/1	0.88	0.10	68,68,68,68	0
56	MG	15	107	1/1	0.88	0.16	61,61,61,61	0
56	MG	2A	3347	1/1	0.88	0.27	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3463	1/1	0.88	0.15	54,54,54,54	0
56	MG	2a	1635	1/1	0.88	0.28	63,63,63,63	0
56	MG	1a	1755	1/1	0.88	0.17	51,51,51,51	0
56	MG	2A	3171	1/1	0.88	0.22	70,70,70,70	0
56	MG	2A	3635	1/1	0.88	0.10	63,63,63,63	0
56	MG	1A	4013	1/1	0.88	0.16	63,63,63,63	0
56	MG	1A	3843	1/1	0.88	0.16	45,45,45,45	0
56	MG	1A	3241	1/1	0.88	0.09	61,61,61,61	0
56	MG	1a	1772	1/1	0.88	0.24	71,71,71,71	0
56	MG	1a	1776	1/1	0.88	0.14	62,62,62,62	0
56	MG	2A	3648	1/1	0.88	0.10	59,59,59,59	0
56	MG	1a	1607	1/1	0.88	0.27	65,65,65,65	0
56	MG	1A	3706	1/1	0.88	0.10	53,53,53,53	0
56	MG	2A	3370	1/1	0.88	0.30	61,61,61,61	0
56	MG	1A	3566	1/1	0.88	0.31	70,70,70,70	0
56	MG	1A	3286	1/1	0.88	0.23	70,70,70,70	0
56	MG	2A	3660	1/1	0.88	0.14	62,62,62,62	0
56	MG	2a	1676	1/1	0.88	0.15	68,68,68,68	0
56	MG	1a	1625	1/1	0.88	0.25	61,61,61,61	0
56	MG	2a	1681	1/1	0.88	0.18	62,62,62,62	0
56	MG	1a	1787	1/1	0.88	0.18	51,51,51,51	0
56	MG	2A	3667	1/1	0.88	0.28	65,65,65,65	0
56	MG	2A	3389	1/1	0.88	0.25	61,61,61,61	0
56	MG	1A	4033	1/1	0.88	0.12	53,53,53,53	0
56	MG	2A	3687	1/1	0.88	0.18	58,58,58,58	0
56	MG	1a	1789	1/1	0.88	0.20	64,64,64,64	0
56	MG	1A	3294	1/1	0.88	0.19	63,63,63,63	0
56	MG	2a	1694	1/1	0.88	0.24	76,76,76,76	0
56	MG	1A	4036	1/1	0.88	0.11	43,43,43,43	0
56	MG	2a	1696	1/1	0.88	0.17	67,67,67,67	0
56	MG	1a	1632	1/1	0.88	0.27	78,78,78,78	0
56	MG	1A	3296	1/1	0.88	0.27	58,58,58,58	0
56	MG	1A	3756	1/1	0.88	0.09	46,46,46,46	0
56	MG	2A	3218	1/1	0.88	0.26	67,67,67,67	0
56	MG	1l	202	1/1	0.88	0.15	60,60,60,60	0
56	MG	1A	3415	1/1	0.88	0.24	50,50,50,50	0
56	MG	2a	1703	1/1	0.88	0.22	68,68,68,68	0
56	MG	1a	1642	1/1	0.88	0.17	64,64,64,64	0
56	MG	1A	3764	1/1	0.88	0.11	28,28,28,28	0
56	MG	2A	3438	1/1	0.88	0.10	37,37,37,37	0
56	MG	2a	1714	1/1	0.88	0.24	69,69,69,69	0
56	MG	2A	3716	1/1	0.88	0.15	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1719	1/1	0.88	0.28	65,65,65,65	0
56	MG	1A	4049	1/1	0.88	0.29	52,52,52,52	0
56	MG	2A	3449	1/1	0.88	0.10	60,60,60,60	0
56	MG	1A	3431	1/1	0.88	0.23	47,47,47,47	0
56	MG	2A	3736	1/1	0.88	0.15	52,52,52,52	0
56	MG	2a	1742	1/1	0.88	0.16	74,74,74,74	0
56	MG	2A	3459	1/1	0.88	0.28	62,62,62,62	0
56	MG	1A	3076	1/1	0.88	0.10	29,29,29,29	0
56	MG	1a	1654	1/1	0.88	0.11	68,68,68,68	0
56	MG	1x	112	1/1	0.88	0.23	62,62,62,62	0
56	MG	1A	3495	1/1	0.88	0.14	76,76,76,76	0
56	MG	2A	3003	1/1	0.88	0.20	53,53,53,53	0
56	MG	2A	3754	1/1	0.88	0.11	61,61,61,61	0
56	MG	2A	3489	1/1	0.88	0.14	59,59,59,59	0
56	MG	1A	3613	1/1	0.88	0.13	67,67,67,67	0
56	MG	1A	3941	1/1	0.88	0.13	65,65,65,65	0
56	MG	2A	3257	1/1	0.88	0.16	63,63,63,63	0
56	MG	2a	1773	1/1	0.88	0.19	68,68,68,68	0
56	MG	1A	3387	1/1	0.88	0.20	63,63,63,63	0
56	MG	2a	1775	1/1	0.88	0.25	70,70,70,70	0
56	MG	2A	3504	1/1	0.88	0.19	78,78,78,78	0
56	MG	1A	3948	1/1	0.88	0.12	38,38,38,38	0
56	MG	2a	1778	1/1	0.88	0.19	68,68,68,68	0
56	MG	2A	3773	1/1	0.88	0.10	52,52,52,52	0
56	MG	2A	3776	1/1	0.88	0.18	72,72,72,72	0
56	MG	2A	3512	1/1	0.88	0.20	70,70,70,70	0
56	MG	2A	3515	1/1	0.88	0.18	67,67,67,67	0
56	MG	2A	3033	1/1	0.88	0.32	74,74,74,74	0
56	MG	2A	3036	1/1	0.88	0.16	63,63,63,63	0
56	MG	1A	3631	1/1	0.88	0.11	60,60,60,60	0
56	MG	1A	3329	1/1	0.88	0.18	53,53,53,53	0
56	MG	2B	205	1/1	0.88	0.19	65,65,65,65	0
56	MG	2A	3272	1/1	0.88	0.19	69,69,69,69	0
56	MG	1A	3955	1/1	0.88	0.11	54,54,54,54	0
56	MG	1A	3799	1/1	0.88	0.15	52,52,52,52	0
56	MG	2a	1800	1/1	0.88	0.28	60,60,60,60	0
56	MG	2a	1801	1/1	0.88	0.13	74,74,74,74	0
56	MG	2A	3058	1/1	0.88	0.30	69,69,69,69	0
56	MG	2A	3543	1/1	0.88	0.19	65,65,65,65	0
56	MG	2A	3070	1/1	0.88	0.18	55,55,55,55	0
56	MG	2r	101	1/1	0.88	0.14	79,79,79,79	0
56	MG	2v	101	1/1	0.88	0.31	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3514	1/1	0.88	0.14	72,72,72,72	0
56	MG	1D	312	1/1	0.88	0.18	39,39,39,39	0
56	MG	1A	3664	1/1	0.88	0.13	47,47,47,47	0
56	MG	2x	104	1/1	0.88	0.18	70,70,70,70	0
56	MG	1A	3928	1/1	0.89	0.10	45,45,45,45	0
56	MG	2P	202	1/1	0.89	0.20	55,55,55,55	0
56	MG	2A	3325	1/1	0.89	0.24	64,64,64,64	0
56	MG	1A	3501	1/1	0.89	0.08	67,67,67,67	0
56	MG	2R	202	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3327	1/1	0.89	0.16	69,69,69,69	0
56	MG	2V	201	1/1	0.89	0.36	48,48,48,48	0
56	MG	1A	3446	1/1	0.89	0.17	57,57,57,57	0
56	MG	2W	201	1/1	0.89	0.17	59,59,59,59	0
56	MG	2A	3159	1/1	0.89	0.20	57,57,57,57	0
56	MG	1A	3050	1/1	0.89	0.18	40,40,40,40	0
56	MG	20	101	1/1	0.89	0.16	72,72,72,72	0
56	MG	2A	3592	1/1	0.89	0.17	44,44,44,44	0
56	MG	1a	1626	1/1	0.89	0.14	62,62,62,62	0
56	MG	1A	3322	1/1	0.89	0.23	55,55,55,55	0
56	MG	1A	3704	1/1	0.89	0.11	54,54,54,54	0
56	MG	1B	201	1/1	0.89	0.09	49,49,49,49	0
56	MG	2A	3338	1/1	0.89	0.26	57,57,57,57	0
56	MG	1A	3357	1/1	0.89	0.11	50,50,50,50	0
56	MG	1a	1634	1/1	0.89	0.17	57,57,57,57	0
56	MG	2a	1609	1/1	0.89	0.45	76,76,76,76	0
56	MG	1a	1786	1/1	0.89	0.14	61,61,61,61	0
56	MG	2A	3606	1/1	0.89	0.15	57,57,57,57	0
56	MG	1A	3527	1/1	0.89	0.23	56,56,56,56	0
56	MG	2A	3178	1/1	0.89	0.14	64,64,64,64	0
56	MG	1A	3817	1/1	0.89	0.11	55,55,55,55	0
56	MG	1B	215	1/1	0.89	0.25	71,71,71,71	0
56	MG	2A	3614	1/1	0.89	0.15	76,76,76,76	0
56	MG	1A	3140	1/1	0.89	0.20	47,47,47,47	0
56	MG	1A	3961	1/1	0.89	0.20	28,28,28,28	0
56	MG	1A	3372	1/1	0.89	0.14	61,61,61,61	0
56	MG	2A	3619	1/1	0.89	0.10	35,35,35,35	0
56	MG	2A	3363	1/1	0.89	0.15	50,50,50,50	0
56	MG	1A	3735	1/1	0.89	0.11	38,38,38,38	0
56	MG	2A	3194	1/1	0.89	0.20	69,69,69,69	0
56	MG	2A	3628	1/1	0.89	0.15	60,60,60,60	0
56	MG	1B	226	1/1	0.89	0.18	64,64,64,64	0
56	MG	1A	3628	1/1	0.89	0.07	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1m	3002	1/1	0.89	0.19	61,61,61,61	0
56	MG	1A	3976	1/1	0.89	0.12	55,55,55,55	0
56	MG	2a	1638	1/1	0.89	0.16	63,63,63,63	0
56	MG	2A	3642	1/1	0.89	0.18	60,60,60,60	0
56	MG	1A	3630	1/1	0.89	0.07	21,21,21,21	0
56	MG	1w	101	1/1	0.89	0.09	73,73,73,73	0
56	MG	1x	104	1/1	0.89	0.18	66,66,66,66	0
56	MG	1A	3428	1/1	0.89	0.15	64,64,64,64	0
56	MG	1E	307	1/1	0.89	0.16	55,55,55,55	0
56	MG	2A	3394	1/1	0.89	0.15	66,66,66,66	0
56	MG	2A	3215	1/1	0.89	0.21	62,62,62,62	0
56	MG	2a	1651	1/1	0.89	0.09	66,66,66,66	0
56	MG	2A	3653	1/1	0.89	0.09	63,63,63,63	0
56	MG	2A	3399	1/1	0.89	0.29	63,63,63,63	0
56	MG	2A	3400	1/1	0.89	0.18	67,67,67,67	0
56	MG	1A	3180	1/1	0.89	0.10	50,50,50,50	0
56	MG	1A	3849	1/1	0.89	0.12	44,44,44,44	0
56	MG	2a	1672	1/1	0.89	0.21	68,68,68,68	0
56	MG	2A	3221	1/1	0.89	0.24	73,73,73,73	0
56	MG	2a	1674	1/1	0.89	0.23	71,71,71,71	0
56	MG	2A	3662	1/1	0.89	0.10	41,41,41,41	0
56	MG	1x	110	1/1	0.89	0.10	62,62,62,62	0
56	MG	2A	3414	1/1	0.89	0.22	71,71,71,71	0
56	MG	2a	1682	1/1	0.89	0.34	65,65,65,65	0
56	MG	2a	1683	1/1	0.89	0.24	65,65,65,65	0
56	MG	1a	1663	1/1	0.89	0.32	72,72,72,72	0
56	MG	2A	3672	1/1	0.89	0.13	58,58,58,58	0
56	MG	2a	1687	1/1	0.89	0.21	60,60,60,60	0
56	MG	2A	3676	1/1	0.89	0.16	42,42,42,42	0
56	MG	2A	3230	1/1	0.89	0.19	60,60,60,60	0
56	MG	1F	304	1/1	0.89	0.18	69,69,69,69	0
56	MG	1A	3298	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3694	1/1	0.89	0.20	76,76,76,76	0
56	MG	2A	3696	1/1	0.89	0.14	78,78,78,78	0
56	MG	1A	3862	1/1	0.89	0.17	74,74,74,74	0
56	MG	1A	3339	1/1	0.89	0.17	72,72,72,72	0
56	MG	1a	1678	1/1	0.89	0.28	67,67,67,67	0
56	MG	1A	3670	1/1	0.89	0.08	27,27,27,27	0
56	MG	1A	3873	1/1	0.89	0.09	50,50,50,50	0
56	MG	1a	1683	1/1	0.89	0.26	60,60,60,60	0
56	MG	2A	3451	1/1	0.89	0.20	67,67,67,67	0
56	MG	2A	3249	1/1	0.89	0.34	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3341	1/1	0.89	0.17	60,60,60,60	0
56	MG	2a	1707	1/1	0.89	0.29	62,62,62,62	0
56	MG	2A	3251	1/1	0.89	0.19	62,62,62,62	0
56	MG	2A	3462	1/1	0.89	0.22	61,61,61,61	0
56	MG	1A	3072	1/1	0.89	0.26	63,63,63,63	0
56	MG	1R	203	1/1	0.89	0.24	44,44,44,44	0
56	MG	2a	1716	1/1	0.89	0.34	77,77,77,77	0
56	MG	2a	1717	1/1	0.89	0.15	71,71,71,71	0
56	MG	1A	3777	1/1	0.89	0.12	45,45,45,45	0
56	MG	2A	3259	1/1	0.89	0.27	73,73,73,73	0
56	MG	2a	1725	1/1	0.89	0.28	65,65,65,65	0
56	MG	1A	3897	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	4015	1/1	0.89	0.15	53,53,53,53	0
56	MG	1a	1702	1/1	0.89	0.35	62,62,62,62	0
56	MG	1A	3570	1/1	0.89	0.10	57,57,57,57	0
56	MG	2a	1737	1/1	0.89	0.26	74,74,74,74	0
56	MG	2a	1738	1/1	0.89	0.15	68,68,68,68	0
56	MG	1a	1715	1/1	0.89	0.13	63,63,63,63	0
56	MG	2A	3083	1/1	0.89	0.15	51,51,51,51	0
56	MG	1A	3912	1/1	0.89	0.09	59,59,59,59	0
56	MG	2A	3507	1/1	0.89	0.25	63,63,63,63	0
56	MG	10	106	1/1	0.89	0.10	56,56,56,56	0
56	MG	2A	3514	1/1	0.89	0.09	66,66,66,66	0
56	MG	1a	1722	1/1	0.89	0.17	71,71,71,71	0
56	MG	2A	3761	1/1	0.89	0.13	66,66,66,66	0
56	MG	2A	3762	1/1	0.89	0.22	74,74,74,74	0
56	MG	10	107	1/1	0.89	0.09	71,71,71,71	0
56	MG	11	104	1/1	0.89	0.14	64,64,64,64	0
56	MG	2a	1770	1/1	0.89	0.17	68,68,68,68	0
56	MG	2A	3766	1/1	0.89	0.28	67,67,67,67	0
56	MG	1a	1730	1/1	0.89	0.09	61,61,61,61	0
56	MG	1A	3794	1/1	0.89	0.09	44,44,44,44	0
56	MG	2A	3769	1/1	0.89	0.19	59,59,59,59	0
56	MG	2A	3526	1/1	0.89	0.24	74,74,74,74	0
56	MG	1A	3914	1/1	0.89	0.13	64,64,64,64	0
56	MG	2A	3528	1/1	0.89	0.19	73,73,73,73	0
56	MG	1A	3284	1/1	0.89	0.09	39,39,39,39	0
56	MG	2A	3532	1/1	0.89	0.12	60,60,60,60	0
56	MG	2A	3110	1/1	0.89	0.10	53,53,53,53	0
56	MG	2A	3781	1/1	0.89	0.45	69,69,69,69	0
56	MG	2B	202	1/1	0.89	0.10	64,64,64,64	0
56	MG	2A	3535	1/1	0.89	0.09	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3111	1/1	0.89	0.12	74,74,74,74	0
56	MG	2A	3539	1/1	0.89	0.18	49,49,49,49	0
56	MG	2A	3293	1/1	0.89	0.12	67,67,67,67	0
56	MG	2A	3544	1/1	0.89	0.20	71,71,71,71	0
56	MG	2B	210	1/1	0.89	0.12	74,74,74,74	0
56	MG	1a	1739	1/1	0.89	0.12	67,67,67,67	0
56	MG	2A	3126	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3129	1/1	0.89	0.29	76,76,76,76	0
56	MG	2e	201	1/1	0.89	0.09	76,76,76,76	0
56	MG	2B	216	1/1	0.89	0.11	84,84,84,84	0
56	MG	2l	204	1/1	0.89	0.16	79,79,79,79	0
56	MG	1A	3919	1/1	0.89	0.11	58,58,58,58	0
56	MG	2A	3564	1/1	0.89	0.14	45,45,45,45	0
56	MG	1A	3922	1/1	0.89	0.08	50,50,50,50	0
56	MG	1a	1603	1/1	0.89	0.12	59,59,59,59	0
56	MG	1a	1746	1/1	0.89	0.16	63,63,63,63	0
56	MG	2A	3570	1/1	0.89	0.19	46,46,46,46	0
56	MG	1A	3574	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	3689	1/1	0.89	0.10	39,39,39,39	0
56	MG	2A	3321	1/1	0.90	0.19	63,63,63,63	0
56	MG	1Q	203	1/1	0.90	0.14	62,62,62,62	0
56	MG	1A	3832	1/1	0.90	0.13	59,59,59,59	0
56	MG	1A	3448	1/1	0.90	0.16	48,48,48,48	0
56	MG	1T	201	1/1	0.90	0.21	59,59,59,59	0
56	MG	1A	3006	1/1	0.90	0.15	55,55,55,55	0
56	MG	28	102	1/1	0.90	0.27	52,52,52,52	0
56	MG	2a	1601	1/1	0.90	0.17	68,68,68,68	0
56	MG	1A	3835	1/1	0.90	0.10	49,49,49,49	0
56	MG	1A	3838	1/1	0.90	0.06	37,37,37,37	0
56	MG	2A	3605	1/1	0.90	0.14	59,59,59,59	0
56	MG	1A	3381	1/1	0.90	0.28	61,61,61,61	0
56	MG	1A	3703	1/1	0.90	0.09	50,50,50,50	0
56	MG	1A	3568	1/1	0.90	0.14	44,44,44,44	0
56	MG	2A	3146	1/1	0.90	0.14	46,46,46,46	0
56	MG	2A	3147	1/1	0.90	0.33	70,70,70,70	0
56	MG	2a	1612	1/1	0.90	0.20	60,60,60,60	0
56	MG	2A	3150	1/1	0.90	0.13	59,59,59,59	0
56	MG	1a	1736	1/1	0.90	0.28	65,65,65,65	0
56	MG	2A	3341	1/1	0.90	0.28	58,58,58,58	0
56	MG	1A	3382	1/1	0.90	0.14	48,48,48,48	0
56	MG	1A	3461	1/1	0.90	0.21	56,56,56,56	0
56	MG	1A	3253	1/1	0.90	0.21	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3349	1/1	0.90	0.17	67,67,67,67	0
56	MG	1A	3870	1/1	0.90	0.13	39,39,39,39	0
56	MG	1A	3724	1/1	0.90	0.20	59,59,59,59	0
56	MG	2A	3163	1/1	0.90	0.23	62,62,62,62	0
56	MG	2A	3358	1/1	0.90	0.26	60,60,60,60	0
56	MG	2A	3634	1/1	0.90	0.16	50,50,50,50	0
56	MG	2a	1627	1/1	0.90	0.34	65,65,65,65	0
56	MG	2a	1628	1/1	0.90	0.11	88,88,88,88	0
56	MG	1A	3725	1/1	0.90	0.13	55,55,55,55	0
56	MG	1a	1748	1/1	0.90	0.11	64,64,64,64	0
56	MG	2A	3640	1/1	0.90	0.09	59,59,59,59	0
56	MG	1A	3881	1/1	0.90	0.11	25,25,25,25	0
56	MG	19	101	1/1	0.90	0.21	60,60,60,60	0
56	MG	1a	1601	1/1	0.90	0.25	62,62,62,62	0
56	MG	1A	4029	1/1	0.90	0.10	48,48,48,48	0
56	MG	1A	3577	1/1	0.90	0.09	27,27,27,27	0
56	MG	1a	1771	1/1	0.90	0.07	84,84,84,84	0
56	MG	1A	3099	1/1	0.90	0.11	68,68,68,68	0
56	MG	2A	3177	1/1	0.90	0.22	63,63,63,63	0
56	MG	1a	1609	1/1	0.90	0.25	57,57,57,57	0
56	MG	1a	1778	1/1	0.90	0.25	63,63,63,63	0
56	MG	1A	3471	1/1	0.90	0.13	45,45,45,45	0
56	MG	1A	3472	1/1	0.90	0.12	46,46,46,46	0
56	MG	1a	1621	1/1	0.90	0.13	64,64,64,64	0
56	MG	1A	3049	1/1	0.90	0.24	42,42,42,42	0
56	MG	2a	1653	1/1	0.90	0.19	80,80,80,80	0
56	MG	1a	1624	1/1	0.90	0.25	60,60,60,60	0
56	MG	2a	1656	1/1	0.90	0.24	67,67,67,67	0
56	MG	1A	3194	1/1	0.90	0.09	43,43,43,43	0
56	MG	1A	3606	1/1	0.90	0.12	65,65,65,65	0
56	MG	2a	1667	1/1	0.90	0.25	74,74,74,74	0
56	MG	1A	3608	1/1	0.90	0.11	40,40,40,40	0
56	MG	1A	3020	1/1	0.90	0.14	48,48,48,48	0
56	MG	2A	3673	1/1	0.90	0.16	62,62,62,62	0
56	MG	2A	3674	1/1	0.90	0.11	42,42,42,42	0
56	MG	1A	3204	1/1	0.90	0.08	47,47,47,47	0
56	MG	2A	3677	1/1	0.90	0.13	67,67,67,67	0
56	MG	2A	3678	1/1	0.90	0.27	70,70,70,70	0
56	MG	1A	3923	1/1	0.90	0.07	39,39,39,39	0
56	MG	1a	1633	1/1	0.90	0.12	51,51,51,51	0
56	MG	2a	1684	1/1	0.90	0.31	65,65,65,65	0
56	MG	2A	3689	1/1	0.90	0.09	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3287	1/1	0.90	0.17	65,65,65,65	0
56	MG	1B	208	1/1	0.90	0.18	66,66,66,66	0
56	MG	1e	202	1/1	0.90	0.10	74,74,74,74	0
56	MG	2A	3430	1/1	0.90	0.19	73,73,73,73	0
56	MG	2A	3432	1/1	0.90	0.12	77,77,77,77	0
56	MG	1a	1636	1/1	0.90	0.21	56,56,56,56	0
56	MG	1A	3288	1/1	0.90	0.14	55,55,55,55	0
56	MG	1A	3780	1/1	0.90	0.10	58,58,58,58	0
56	MG	2A	3220	1/1	0.90	0.09	69,69,69,69	0
56	MG	1t	201	1/1	0.90	0.16	61,61,61,61	0
56	MG	2A	3442	1/1	0.90	0.18	52,52,52,52	0
56	MG	1A	3930	1/1	0.90	0.14	43,43,43,43	0
56	MG	1a	1644	1/1	0.90	0.16	64,64,64,64	0
56	MG	2A	3452	1/1	0.90	0.09	40,40,40,40	0
56	MG	1w	103	1/1	0.90	0.15	67,67,67,67	0
56	MG	1a	1645	1/1	0.90	0.26	60,60,60,60	0
56	MG	1A	3937	1/1	0.90	0.09	64,64,64,64	0
56	MG	1B	217	1/1	0.90	0.11	62,62,62,62	0
56	MG	2A	3732	1/1	0.90	0.12	38,38,38,38	0
56	MG	1a	1651	1/1	0.90	0.20	57,57,57,57	0
56	MG	2a	1711	1/1	0.90	0.24	58,58,58,58	0
56	MG	1A	3234	1/1	0.90	0.33	46,46,46,46	0
56	MG	2A	3478	1/1	0.90	0.18	49,49,49,49	0
56	MG	1B	222	1/1	0.90	0.21	53,53,53,53	0
56	MG	1A	3237	1/1	0.90	0.19	67,67,67,67	0
56	MG	2A	3488	1/1	0.90	0.10	38,38,38,38	0
56	MG	1A	3342	1/1	0.90	0.12	59,59,59,59	0
56	MG	2a	1720	1/1	0.90	0.25	62,62,62,62	0
56	MG	1A	3427	1/1	0.90	0.15	64,64,64,64	0
56	MG	1A	3654	1/1	0.90	0.14	57,57,57,57	0
56	MG	2A	3004	1/1	0.90	0.10	51,51,51,51	0
56	MG	2a	1730	1/1	0.90	0.10	72,72,72,72	0
56	MG	2A	3011	1/1	0.90	0.22	77,77,77,77	0
56	MG	2a	1733	1/1	0.90	0.15	72,72,72,72	0
56	MG	1A	3659	1/1	0.90	0.11	26,26,26,26	0
56	MG	1B	235	1/1	0.90	0.09	55,55,55,55	0
56	MG	1B	237	1/1	0.90	0.11	65,65,65,65	0
56	MG	2a	1741	1/1	0.90	0.10	59,59,59,59	0
56	MG	2A	3260	1/1	0.90	0.21	53,53,53,53	0
56	MG	1A	3344	1/1	0.90	0.24	56,56,56,56	0
56	MG	2A	3262	1/1	0.90	0.17	66,66,66,66	0
56	MG	1A	3665	1/1	0.90	0.10	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1668	1/1	0.90	0.09	64,64,64,64	0
56	MG	2a	1758	1/1	0.90	0.16	54,54,54,54	0
56	MG	2A	3266	1/1	0.90	0.15	71,71,71,71	0
56	MG	2A	3267	1/1	0.90	0.22	68,68,68,68	0
56	MG	2A	3040	1/1	0.90	0.16	37,37,37,37	0
56	MG	2A	3041	1/1	0.90	0.25	70,70,70,70	0
56	MG	1a	1671	1/1	0.90	0.08	63,63,63,63	0
56	MG	2A	3053	1/1	0.90	0.10	53,53,53,53	0
56	MG	1E	301	1/1	0.90	0.14	38,38,38,38	0
56	MG	2B	201	1/1	0.90	0.20	77,77,77,77	0
56	MG	2A	3275	1/1	0.90	0.21	59,59,59,59	0
56	MG	1A	3525	1/1	0.90	0.14	39,39,39,39	0
56	MG	2A	3056	1/1	0.90	0.34	70,70,70,70	0
56	MG	2A	3278	1/1	0.90	0.10	55,55,55,55	0
56	MG	2B	206	1/1	0.90	0.21	74,74,74,74	0
56	MG	2A	3542	1/1	0.90	0.16	68,68,68,68	0
56	MG	1A	3085	1/1	0.90	0.16	38,38,38,38	0
56	MG	1a	1677	1/1	0.90	0.24	61,61,61,61	0
56	MG	2A	3547	1/1	0.90	0.19	62,62,62,62	0
56	MG	1E	311	1/1	0.90	0.12	26,26,26,26	0
56	MG	1A	3307	1/1	0.90	0.23	54,54,54,54	0
56	MG	1A	3091	1/1	0.90	0.15	60,60,60,60	0
56	MG	2A	3287	1/1	0.90	0.21	82,82,82,82	0
56	MG	1A	3681	1/1	0.90	0.08	61,61,61,61	0
56	MG	1a	1685	1/1	0.90	0.13	60,60,60,60	0
56	MG	2a	1791	1/1	0.90	0.22	63,63,63,63	0
56	MG	1A	3243	1/1	0.90	0.10	67,67,67,67	0
56	MG	2a	1796	1/1	0.90	0.18	58,58,58,58	0
56	MG	2A	3296	1/1	0.90	0.12	64,64,64,64	0
56	MG	1A	3162	1/1	0.90	0.10	40,40,40,40	0
56	MG	1N	206	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3304	1/1	0.90	0.29	72,72,72,72	0
56	MG	2N	201	1/1	0.90	0.07	57,57,57,57	0
56	MG	2A	3094	1/1	0.90	0.14	57,57,57,57	0
56	MG	2P	201	1/1	0.90	0.13	67,67,67,67	0
56	MG	1O	201	1/1	0.90	0.10	69,69,69,69	0
56	MG	1A	3825	1/1	0.90	0.11	61,61,61,61	0
56	MG	1A	3358	1/1	0.90	0.10	44,44,44,44	0
56	MG	2t	201	1/1	0.90	0.14	74,74,74,74	0
56	MG	2A	3311	1/1	0.90	0.25	63,63,63,63	0
56	MG	2T	203	1/1	0.90	0.30	65,65,65,65	0
56	MG	2A	3102	1/1	0.90	0.22	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3104	1/1	0.90	0.26	66,66,66,66	0
56	MG	1A	3247	1/1	0.90	0.12	76,76,76,76	0
56	MG	2A	3584	1/1	0.91	0.09	52,52,52,52	0
56	MG	1A	3496	1/1	0.91	0.07	53,53,53,53	0
56	MG	1A	3650	1/1	0.91	0.11	54,54,54,54	0
56	MG	1Y	201	1/1	0.91	0.16	67,67,67,67	0
56	MG	2A	3318	1/1	0.91	0.15	70,70,70,70	0
56	MG	1Y	202	1/1	0.91	0.11	71,71,71,71	0
56	MG	1A	3351	1/1	0.91	0.15	51,51,51,51	0
56	MG	1a	1737	1/1	0.91	0.10	66,66,66,66	0
56	MG	27	104	1/1	0.91	0.12	61,61,61,61	0
56	MG	2A	3323	1/1	0.91	0.12	70,70,70,70	0
56	MG	10	101	1/1	0.91	0.20	50,50,50,50	0
56	MG	2A	3143	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3602	1/1	0.91	0.17	74,74,74,74	0
56	MG	1A	3416	1/1	0.91	0.17	36,36,36,36	0
56	MG	1A	3661	1/1	0.91	0.12	75,75,75,75	0
56	MG	2A	3148	1/1	0.91	0.27	62,62,62,62	0
56	MG	2A	3149	1/1	0.91	0.17	51,51,51,51	0
56	MG	2A	3607	1/1	0.91	0.08	70,70,70,70	0
56	MG	1A	3997	1/1	0.91	0.09	49,49,49,49	0
56	MG	2A	3610	1/1	0.91	0.14	55,55,55,55	0
56	MG	1A	3998	1/1	0.91	0.06	33,33,33,33	0
56	MG	11	105	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	3507	1/1	0.91	0.29	59,59,59,59	0
56	MG	2A	3337	1/1	0.91	0.20	47,47,47,47	0
56	MG	1A	3508	1/1	0.91	0.26	54,54,54,54	0
56	MG	1a	1753	1/1	0.91	0.08	68,68,68,68	0
56	MG	1A	3666	1/1	0.91	0.12	37,37,37,37	0
56	MG	1A	3826	1/1	0.91	0.30	40,40,40,40	0
56	MG	17	104	1/1	0.91	0.16	55,55,55,55	0
56	MG	18	101	1/1	0.91	0.16	62,62,62,62	0
56	MG	1A	3016	1/1	0.91	0.27	54,54,54,54	0
56	MG	2A	3627	1/1	0.91	0.11	39,39,39,39	0
56	MG	1A	4014	1/1	0.91	0.15	47,47,47,47	0
56	MG	1A	3830	1/1	0.91	0.13	48,48,48,48	0
56	MG	2A	3631	1/1	0.91	0.15	62,62,62,62	0
56	MG	1a	1602	1/1	0.91	0.26	69,69,69,69	0
56	MG	1A	3120	1/1	0.91	0.21	54,54,54,54	0
56	MG	1A	3354	1/1	0.91	0.23	52,52,52,52	0
56	MG	1A	3256	1/1	0.91	0.11	53,53,53,53	0
56	MG	2A	3639	1/1	0.91	0.12	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3197	1/1	0.91	0.16	53,53,53,53	0
56	MG	1A	3198	1/1	0.91	0.09	37,37,37,37	0
56	MG	2A	3180	1/1	0.91	0.10	67,67,67,67	0
56	MG	1a	1785	1/1	0.91	0.30	67,67,67,67	0
56	MG	2A	3184	1/1	0.91	0.31	75,75,75,75	0
56	MG	1A	4027	1/1	0.91	0.11	24,24,24,24	0
56	MG	2A	3187	1/1	0.91	0.24	52,52,52,52	0
56	MG	2A	3649	1/1	0.91	0.13	60,60,60,60	0
56	MG	1A	3440	1/1	0.91	0.11	61,61,61,61	0
56	MG	2A	3371	1/1	0.91	0.11	49,49,49,49	0
56	MG	1a	1622	1/1	0.91	0.26	58,58,58,58	0
56	MG	1A	3367	1/1	0.91	0.32	31,31,31,31	0
56	MG	1A	3845	1/1	0.91	0.18	31,31,31,31	0
56	MG	1A	3846	1/1	0.91	0.13	65,65,65,65	0
56	MG	1A	3848	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3392	1/1	0.91	0.11	60,60,60,60	0
56	MG	2a	1664	1/1	0.91	0.20	55,55,55,55	0
56	MG	2A	3196	1/1	0.91	0.13	59,59,59,59	0
56	MG	2A	3395	1/1	0.91	0.27	69,69,69,69	0
56	MG	2a	1669	1/1	0.91	0.23	62,62,62,62	0
56	MG	1A	3126	1/1	0.91	0.14	68,68,68,68	0
56	MG	2A	3668	1/1	0.91	0.12	56,56,56,56	0
56	MG	2A	3669	1/1	0.91	0.15	67,67,67,67	0
56	MG	2a	1675	1/1	0.91	0.21	64,64,64,64	0
56	MG	1a	1628	1/1	0.91	0.36	66,66,66,66	0
56	MG	2a	1678	1/1	0.91	0.24	61,61,61,61	0
56	MG	1A	3134	1/1	0.91	0.12	42,42,42,42	0
56	MG	2A	3202	1/1	0.91	0.39	51,51,51,51	0
56	MG	1A	3380	1/1	0.91	0.10	41,41,41,41	0
56	MG	1A	4048	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3217	1/1	0.91	0.14	45,45,45,45	0
56	MG	2A	3413	1/1	0.91	0.21	61,61,61,61	0
56	MG	1A	3454	1/1	0.91	0.09	61,61,61,61	0
56	MG	2A	3418	1/1	0.91	0.11	70,70,70,70	0
56	MG	2A	3421	1/1	0.91	0.31	68,68,68,68	0
56	MG	1A	3456	1/1	0.91	0.11	54,54,54,54	0
56	MG	2A	3214	1/1	0.91	0.13	72,72,72,72	0
56	MG	1A	3324	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3216	1/1	0.91	0.31	74,74,74,74	0
56	MG	2A	3699	1/1	0.91	0.14	49,49,49,49	0
56	MG	1w	102	1/1	0.91	0.13	71,71,71,71	0
56	MG	1A	3227	1/1	0.91	0.12	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3433	1/1	0.91	0.12	59,59,59,59	0
56	MG	1x	101	1/1	0.91	0.29	72,72,72,72	0
56	MG	1x	102	1/1	0.91	0.10	73,73,73,73	0
56	MG	1A	3711	1/1	0.91	0.13	38,38,38,38	0
56	MG	2A	3225	1/1	0.91	0.12	56,56,56,56	0
56	MG	2A	3440	1/1	0.91	0.10	25,25,25,25	0
56	MG	2A	3709	1/1	0.91	0.12	61,61,61,61	0
56	MG	2a	1705	1/1	0.91	0.34	70,70,70,70	0
56	MG	2a	1706	1/1	0.91	0.21	60,60,60,60	0
56	MG	2A	3227	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3711	1/1	0.91	0.09	65,65,65,65	0
56	MG	2A	3228	1/1	0.91	0.21	67,67,67,67	0
56	MG	2A	3448	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3714	1/1	0.91	0.26	65,65,65,65	0
56	MG	1A	3716	1/1	0.91	0.12	44,44,44,44	0
56	MG	2a	1715	1/1	0.91	0.24	63,63,63,63	0
56	MG	1A	3086	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3726	1/1	0.91	0.11	68,68,68,68	0
56	MG	1x	108	1/1	0.91	0.14	37,37,37,37	0
56	MG	1A	3040	1/1	0.91	0.18	64,64,64,64	0
56	MG	1A	3465	1/1	0.91	0.18	48,48,48,48	0
56	MG	2a	1721	1/1	0.91	0.32	71,71,71,71	0
56	MG	1A	3727	1/1	0.91	0.17	59,59,59,59	0
56	MG	2A	3744	1/1	0.91	0.10	64,64,64,64	0
56	MG	1A	3390	1/1	0.91	0.17	73,73,73,73	0
56	MG	1A	3917	1/1	0.91	0.09	58,58,58,58	0
56	MG	2A	3246	1/1	0.91	0.18	68,68,68,68	0
56	MG	1A	3338	1/1	0.91	0.20	56,56,56,56	0
56	MG	2a	1734	1/1	0.91	0.15	74,74,74,74	0
56	MG	2A	3481	1/1	0.91	0.13	44,44,44,44	0
56	MG	2A	3482	1/1	0.91	0.17	43,43,43,43	0
56	MG	1A	3736	1/1	0.91	0.10	33,33,33,33	0
56	MG	1B	227	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3738	1/1	0.91	0.10	20,20,20,20	0
56	MG	2A	3252	1/1	0.91	0.37	73,73,73,73	0
56	MG	1A	3740	1/1	0.91	0.08	23,23,23,23	0
56	MG	1A	3586	1/1	0.91	0.11	18,18,18,18	0
56	MG	1A	3588	1/1	0.91	0.11	37,37,37,37	0
56	MG	1B	238	1/1	0.91	0.12	49,49,49,49	0
56	MG	1A	3594	1/1	0.91	0.12	49,49,49,49	0
56	MG	1A	3759	1/1	0.91	0.16	61,61,61,61	0
56	MG	1A	3394	1/1	0.91	0.21	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3042	1/1	0.91	0.10	54,54,54,54	0
56	MG	2A	3045	1/1	0.91	0.22	65,65,65,65	0
56	MG	1A	3474	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3049	1/1	0.91	0.25	63,63,63,63	0
56	MG	1A	3092	1/1	0.91	0.12	59,59,59,59	0
56	MG	1A	3478	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3769	1/1	0.91	0.08	47,47,47,47	0
56	MG	1F	302	1/1	0.91	0.28	38,38,38,38	0
56	MG	1A	3479	1/1	0.91	0.15	51,51,51,51	0
56	MG	1A	3610	1/1	0.91	0.08	25,25,25,25	0
56	MG	2A	3530	1/1	0.91	0.22	55,55,55,55	0
56	MG	2A	3065	1/1	0.91	0.14	72,72,72,72	0
56	MG	1a	1682	1/1	0.91	0.31	67,67,67,67	0
56	MG	1A	3611	1/1	0.91	0.08	20,20,20,20	0
56	MG	1A	3160	1/1	0.91	0.12	42,42,42,42	0
56	MG	1A	3956	1/1	0.91	0.17	43,43,43,43	0
56	MG	2B	213	1/1	0.91	0.19	60,60,60,60	0
56	MG	2A	3283	1/1	0.91	0.16	79,79,79,79	0
56	MG	2A	3085	1/1	0.91	0.15	64,64,64,64	0
56	MG	1A	3616	1/1	0.91	0.08	28,28,28,28	0
56	MG	1O	203	1/1	0.91	0.22	66,66,66,66	0
56	MG	1A	3783	1/1	0.91	0.11	33,33,33,33	0
56	MG	2a	1794	1/1	0.91	0.20	65,65,65,65	0
56	MG	2D	305	1/1	0.91	0.39	45,45,45,45	0
56	MG	2a	1797	1/1	0.91	0.23	70,70,70,70	0
56	MG	1A	3093	1/1	0.91	0.18	38,38,38,38	0
56	MG	1A	3624	1/1	0.91	0.12	47,47,47,47	0
56	MG	2E	302	1/1	0.91	0.12	67,67,67,67	0
56	MG	1A	3625	1/1	0.91	0.10	50,50,50,50	0
56	MG	2d	301	1/1	0.91	0.10	65,65,65,65	0
56	MG	1A	3052	1/1	0.91	0.12	56,56,56,56	0
56	MG	2A	3297	1/1	0.91	0.14	64,64,64,64	0
56	MG	1a	1708	1/1	0.91	0.11	66,66,66,66	0
56	MG	2A	3299	1/1	0.91	0.37	70,70,70,70	0
56	MG	1A	3349	1/1	0.91	0.17	47,47,47,47	0
56	MG	2A	3303	1/1	0.91	0.12	66,66,66,66	0
56	MG	2r	102	1/1	0.91	0.09	81,81,81,81	0
56	MG	1S	202	1/1	0.91	0.15	53,53,53,53	0
56	MG	2t	202	1/1	0.91	0.18	52,52,52,52	0
56	MG	1S	203	1/1	0.91	0.07	62,62,62,62	0
56	MG	1A	3408	1/1	0.91	0.24	58,58,58,58	0
56	MG	1A	3080	1/1	0.91	0.28	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2x	102	1/1	0.91	0.13	72,72,72,72	0
56	MG	2A	3581	1/1	0.91	0.15	68,68,68,68	0
56	MG	1a	1724	1/1	0.91	0.10	56,56,56,56	0
56	MG	2T	205	1/1	0.92	0.10	65,65,65,65	0
56	MG	2A	3320	1/1	0.92	0.16	66,66,66,66	0
56	MG	1A	3161	1/1	0.92	0.17	38,38,38,38	0
56	MG	1A	3058	1/1	0.92	0.08	50,50,50,50	0
56	MG	1A	3828	1/1	0.92	0.12	46,46,46,46	0
56	MG	2Z	301	1/1	0.92	0.24	67,67,67,67	0
56	MG	1A	3249	1/1	0.92	0.07	39,39,39,39	0
56	MG	1A	3297	1/1	0.92	0.13	44,44,44,44	0
56	MG	2I	101	1/1	0.92	0.23	56,56,56,56	0
56	MG	1A	3477	1/1	0.92	0.17	49,49,49,49	0
56	MG	1A	3707	1/1	0.92	0.10	49,49,49,49	0
56	MG	27	103	1/1	0.92	0.10	50,50,50,50	0
56	MG	1A	4000	1/1	0.92	0.08	57,57,57,57	0
56	MG	10	104	1/1	0.92	0.31	71,71,71,71	0
56	MG	1A	4003	1/1	0.92	0.09	36,36,36,36	0
56	MG	2A	3154	1/1	0.92	0.13	59,59,59,59	0
56	MG	2A	3155	1/1	0.92	0.28	61,61,61,61	0
56	MG	1A	4004	1/1	0.92	0.10	34,34,34,34	0
56	MG	1A	3401	1/1	0.92	0.13	52,52,52,52	0
56	MG	1a	1754	1/1	0.92	0.15	67,67,67,67	0
56	MG	1I	103	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3250	1/1	0.92	0.08	41,41,41,41	0
56	MG	1A	3343	1/1	0.92	0.12	56,56,56,56	0
56	MG	2A	3342	1/1	0.92	0.18	39,39,39,39	0
56	MG	1A	3300	1/1	0.92	0.09	56,56,56,56	0
56	MG	2A	3168	1/1	0.92	0.09	63,63,63,63	0
56	MG	2A	3346	1/1	0.92	0.41	71,71,71,71	0
56	MG	2A	3618	1/1	0.92	0.17	57,57,57,57	0
56	MG	1a	1766	1/1	0.92	0.12	49,49,49,49	0
56	MG	1A	3345	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	3346	1/1	0.92	0.23	55,55,55,55	0
56	MG	1A	3303	1/1	0.92	0.13	60,60,60,60	0
56	MG	2A	3354	1/1	0.92	0.19	55,55,55,55	0
56	MG	1a	1777	1/1	0.92	0.07	56,56,56,56	0
56	MG	1A	3726	1/1	0.92	0.09	24,24,24,24	0
56	MG	1A	3306	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	4021	1/1	0.92	0.15	63,63,63,63	0
56	MG	2A	3179	1/1	0.92	0.19	72,72,72,72	0
56	MG	1A	3852	1/1	0.92	0.13	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3853	1/1	0.92	0.13	31,31,31,31	0
56	MG	2A	3182	1/1	0.92	0.10	62,62,62,62	0
56	MG	2A	3367	1/1	0.92	0.27	64,64,64,64	0
56	MG	2A	3641	1/1	0.92	0.10	37,37,37,37	0
56	MG	2A	3183	1/1	0.92	0.17	68,68,68,68	0
56	MG	2a	1637	1/1	0.92	0.21	70,70,70,70	0
56	MG	1A	3859	1/1	0.92	0.13	27,27,27,27	0
56	MG	1A	4028	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3186	1/1	0.92	0.12	67,67,67,67	0
56	MG	1A	3861	1/1	0.92	0.09	26,26,26,26	0
56	MG	1A	4031	1/1	0.92	0.11	56,56,56,56	0
56	MG	1A	3612	1/1	0.92	0.12	50,50,50,50	0
56	MG	2A	3386	1/1	0.92	0.21	62,62,62,62	0
56	MG	1A	3863	1/1	0.92	0.08	43,43,43,43	0
56	MG	1A	4035	1/1	0.92	0.14	24,24,24,24	0
56	MG	2a	1650	1/1	0.92	0.25	65,65,65,65	0
56	MG	1a	1618	1/1	0.92	0.11	52,52,52,52	0
56	MG	2A	3655	1/1	0.92	0.07	57,57,57,57	0
56	MG	1A	3422	1/1	0.92	0.10	61,61,61,61	0
56	MG	1A	3425	1/1	0.92	0.16	58,58,58,58	0
56	MG	1A	3502	1/1	0.92	0.24	46,46,46,46	0
56	MG	1A	3131	1/1	0.92	0.14	46,46,46,46	0
56	MG	2a	1661	1/1	0.92	0.23	62,62,62,62	0
56	MG	1A	3224	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3663	1/1	0.92	0.11	55,55,55,55	0
56	MG	2a	1665	1/1	0.92	0.24	60,60,60,60	0
56	MG	1A	4047	1/1	0.92	0.09	61,61,61,61	0
56	MG	2A	3666	1/1	0.92	0.16	63,63,63,63	0
56	MG	1A	3878	1/1	0.92	0.18	43,43,43,43	0
56	MG	1A	3753	1/1	0.92	0.08	35,35,35,35	0
56	MG	1A	3882	1/1	0.92	0.12	40,40,40,40	0
56	MG	1A	3883	1/1	0.92	0.15	40,40,40,40	0
56	MG	2A	3211	1/1	0.92	0.17	58,58,58,58	0
56	MG	1A	3885	1/1	0.92	0.09	34,34,34,34	0
56	MG	1A	3255	1/1	0.92	0.08	47,47,47,47	0
56	MG	2a	1679	1/1	0.92	0.32	72,72,72,72	0
56	MG	1w	104	1/1	0.92	0.10	57,57,57,57	0
56	MG	1A	3893	1/1	0.92	0.14	54,54,54,54	0
56	MG	2A	3425	1/1	0.92	0.23	62,62,62,62	0
56	MG	1A	3432	1/1	0.92	0.09	53,53,53,53	0
56	MG	2A	3686	1/1	0.92	0.20	63,63,63,63	0
56	MG	1B	213	1/1	0.92	0.28	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3225	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3515	1/1	0.92	0.20	58,58,58,58	0
56	MG	1a	1639	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3034	1/1	0.92	0.27	41,41,41,41	0
56	MG	1A	3647	1/1	0.92	0.22	48,48,48,48	0
56	MG	2A	3436	1/1	0.92	0.23	65,65,65,65	0
56	MG	1A	3649	1/1	0.92	0.08	35,35,35,35	0
56	MG	1B	221	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3702	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	3314	1/1	0.92	0.31	63,63,63,63	0
56	MG	2A	3231	1/1	0.92	0.37	75,75,75,75	0
56	MG	2A	3233	1/1	0.92	0.24	74,74,74,74	0
56	MG	2A	3445	1/1	0.92	0.18	63,63,63,63	0
56	MG	1A	3652	1/1	0.92	0.11	41,41,41,41	0
56	MG	1A	3771	1/1	0.92	0.06	25,25,25,25	0
56	MG	1A	3182	1/1	0.92	0.13	34,34,34,34	0
56	MG	1A	3362	1/1	0.92	0.11	42,42,42,42	0
56	MG	2A	3453	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3454	1/1	0.92	0.08	44,44,44,44	0
56	MG	1B	229	1/1	0.92	0.12	55,55,55,55	0
56	MG	2a	1708	1/1	0.92	0.23	59,59,59,59	0
56	MG	1A	3263	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3018	1/1	0.92	0.24	70,70,70,70	0
56	MG	1A	3088	1/1	0.92	0.20	53,53,53,53	0
56	MG	2A	3723	1/1	0.92	0.10	57,57,57,57	0
56	MG	1a	1658	1/1	0.92	0.21	69,69,69,69	0
56	MG	2A	3248	1/1	0.92	0.36	69,69,69,69	0
56	MG	2A	3733	1/1	0.92	0.10	56,56,56,56	0
56	MG	2A	3735	1/1	0.92	0.09	65,65,65,65	0
56	MG	2A	3030	1/1	0.92	0.12	56,56,56,56	0
56	MG	1A	3267	1/1	0.92	0.09	49,49,49,49	0
56	MG	1B	236	1/1	0.92	0.10	68,68,68,68	0
56	MG	2A	3038	1/1	0.92	0.24	63,63,63,63	0
56	MG	2A	3253	1/1	0.92	0.17	64,64,64,64	0
56	MG	2A	3486	1/1	0.92	0.17	62,62,62,62	0
56	MG	2A	3747	1/1	0.92	0.08	44,44,44,44	0
56	MG	2A	3487	1/1	0.92	0.19	59,59,59,59	0
56	MG	2A	3751	1/1	0.92	0.09	61,61,61,61	0
56	MG	2A	3254	1/1	0.92	0.15	64,64,64,64	0
56	MG	2A	3753	1/1	0.92	0.14	50,50,50,50	0
56	MG	1A	3786	1/1	0.92	0.07	40,40,40,40	0
56	MG	2A	3256	1/1	0.92	0.12	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3757	1/1	0.92	0.14	65,65,65,65	0
56	MG	2A	3498	1/1	0.92	0.16	63,63,63,63	0
56	MG	1A	3788	1/1	0.92	0.07	27,27,27,27	0
56	MG	2a	1744	1/1	0.92	0.25	70,70,70,70	0
56	MG	2a	1745	1/1	0.92	0.10	52,52,52,52	0
56	MG	1a	1665	1/1	0.92	0.34	60,60,60,60	0
56	MG	2a	1749	1/1	0.92	0.20	70,70,70,70	0
56	MG	1D	301	1/1	0.92	0.15	55,55,55,55	0
56	MG	2A	3047	1/1	0.92	0.18	63,63,63,63	0
56	MG	1D	302	1/1	0.92	0.16	43,43,43,43	0
56	MG	1A	3554	1/1	0.92	0.22	46,46,46,46	0
56	MG	1A	3377	1/1	0.92	0.16	43,43,43,43	0
56	MG	2a	1760	1/1	0.92	0.21	77,77,77,77	0
56	MG	1A	3797	1/1	0.92	0.21	50,50,50,50	0
56	MG	1A	3672	1/1	0.92	0.13	55,55,55,55	0
56	MG	2A	3771	1/1	0.92	0.17	59,59,59,59	0
56	MG	1E	309	1/1	0.92	0.15	49,49,49,49	0
56	MG	2A	3520	1/1	0.92	0.12	55,55,55,55	0
56	MG	2a	1769	1/1	0.92	0.23	71,71,71,71	0
56	MG	1A	3945	1/1	0.92	0.11	60,60,60,60	0
56	MG	1A	3556	1/1	0.92	0.07	38,38,38,38	0
56	MG	2a	1772	1/1	0.92	0.16	60,60,60,60	0
56	MG	1A	3281	1/1	0.92	0.13	55,55,55,55	0
56	MG	1A	3953	1/1	0.92	0.09	49,49,49,49	0
56	MG	1A	3678	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3079	1/1	0.92	0.15	65,65,65,65	0
56	MG	1F	305	1/1	0.92	0.15	39,39,39,39	0
56	MG	2A	3082	1/1	0.92	0.28	53,53,53,53	0
56	MG	1a	1687	1/1	0.92	0.17	53,53,53,53	0
56	MG	1F	307	1/1	0.92	0.16	31,31,31,31	0
56	MG	1A	3320	1/1	0.92	0.18	60,60,60,60	0
56	MG	2A	3282	1/1	0.92	0.10	56,56,56,56	0
56	MG	2A	3537	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	3045	1/1	0.92	0.08	35,35,35,35	0
56	MG	2B	211	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3383	1/1	0.92	0.15	57,57,57,57	0
56	MG	1N	201	1/1	0.92	0.30	53,53,53,53	0
56	MG	1a	1700	1/1	0.92	0.27	66,66,66,66	0
56	MG	2A	3097	1/1	0.92	0.35	70,70,70,70	0
56	MG	1N	204	1/1	0.92	0.30	48,48,48,48	0
56	MG	1A	3285	1/1	0.92	0.23	51,51,51,51	0
56	MG	1A	3807	1/1	0.92	0.12	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3811	1/1	0.92	0.09	73,73,73,73	0
56	MG	2A	3103	1/1	0.92	0.15	55,55,55,55	0
56	MG	1a	1709	1/1	0.92	0.09	52,52,52,52	0
56	MG	2E	301	1/1	0.92	0.22	64,64,64,64	0
56	MG	1A	3814	1/1	0.92	0.09	49,49,49,49	0
56	MG	1a	1716	1/1	0.92	0.08	57,57,57,57	0
56	MG	1A	3970	1/1	0.92	0.13	40,40,40,40	0
56	MG	1A	3325	1/1	0.92	0.24	57,57,57,57	0
56	MG	2A	3113	1/1	0.92	0.12	61,61,61,61	0
56	MG	2A	3114	1/1	0.92	0.13	53,53,53,53	0
56	MG	1A	3691	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3692	1/1	0.92	0.15	50,50,50,50	0
56	MG	1Q	206	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3117	1/1	0.92	0.09	42,42,42,42	0
56	MG	1A	3054	1/1	0.92	0.12	50,50,50,50	0
56	MG	1A	3986	1/1	0.92	0.11	48,48,48,48	0
56	MG	2w	102	1/1	0.92	0.08	79,79,79,79	0
56	MG	2T	201	1/1	0.92	0.12	62,62,62,62	0
56	MG	2T	202	1/1	0.92	0.21	62,62,62,62	0
56	MG	2A	3138	1/1	0.92	0.14	67,67,67,67	0
56	MG	2A	3590	1/1	0.92	0.12	58,58,58,58	0
56	MG	2x	105	1/1	0.92	0.21	56,56,56,56	0
56	MG	2A	3294	1/1	0.93	0.35	75,75,75,75	0
56	MG	2A	3561	1/1	0.93	0.09	47,47,47,47	0
56	MG	2A	3295	1/1	0.93	0.15	62,62,62,62	0
56	MG	2A	3107	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3064	1/1	0.93	0.21	59,59,59,59	0
56	MG	1A	4001	1/1	0.93	0.10	48,48,48,48	0
56	MG	1U	204	1/1	0.93	0.25	38,38,38,38	0
56	MG	1a	1725	1/1	0.93	0.08	63,63,63,63	0
56	MG	1A	3509	1/1	0.93	0.09	55,55,55,55	0
56	MG	1a	1729	1/1	0.93	0.18	66,66,66,66	0
56	MG	2A	3573	1/1	0.93	0.09	67,67,67,67	0
56	MG	2A	3121	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3577	1/1	0.93	0.14	65,65,65,65	0
56	MG	2A	3306	1/1	0.93	0.11	63,63,63,63	0
56	MG	1A	3851	1/1	0.93	0.08	28,28,28,28	0
56	MG	1W	205	1/1	0.93	0.11	31,31,31,31	0
56	MG	1A	4007	1/1	0.93	0.11	57,57,57,57	0
56	MG	2A	3130	1/1	0.93	0.16	65,65,65,65	0
56	MG	1a	1735	1/1	0.93	0.13	60,60,60,60	0
56	MG	2A	3314	1/1	0.93	0.21	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3315	1/1	0.93	0.09	59,59,59,59	0
56	MG	2A	3316	1/1	0.93	0.11	61,61,61,61	0
56	MG	1A	3622	1/1	0.93	0.12	49,49,49,49	0
56	MG	2A	3135	1/1	0.93	0.21	54,54,54,54	0
56	MG	2A	3136	1/1	0.93	0.23	56,56,56,56	0
56	MG	2A	3594	1/1	0.93	0.12	72,72,72,72	0
56	MG	1A	3139	1/1	0.93	0.12	46,46,46,46	0
56	MG	1Z	301	1/1	0.93	0.15	69,69,69,69	0
56	MG	2A	3139	1/1	0.93	0.16	59,59,59,59	0
56	MG	1A	3019	1/1	0.93	0.15	44,44,44,44	0
56	MG	2a	1608	1/1	0.93	0.22	63,63,63,63	0
56	MG	2A	3324	1/1	0.93	0.10	63,63,63,63	0
56	MG	2A	3601	1/1	0.93	0.22	66,66,66,66	0
56	MG	2a	1611	1/1	0.93	0.23	68,68,68,68	0
56	MG	1A	3732	1/1	0.93	0.08	35,35,35,35	0
56	MG	2A	3144	1/1	0.93	0.08	60,60,60,60	0
56	MG	1A	3389	1/1	0.93	0.14	44,44,44,44	0
56	MG	1A	3629	1/1	0.93	0.07	24,24,24,24	0
56	MG	1a	1744	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3521	1/1	0.93	0.15	42,42,42,42	0
56	MG	1a	1747	1/1	0.93	0.07	72,72,72,72	0
56	MG	2A	3332	1/1	0.93	0.15	67,67,67,67	0
56	MG	2A	3333	1/1	0.93	0.14	59,59,59,59	0
56	MG	1A	3522	1/1	0.93	0.27	48,48,48,48	0
56	MG	1a	1749	1/1	0.93	0.15	72,72,72,72	0
56	MG	1A	3632	1/1	0.93	0.08	44,44,44,44	0
56	MG	2a	1625	1/1	0.93	0.11	66,66,66,66	0
56	MG	1A	3750	1/1	0.93	0.10	25,25,25,25	0
56	MG	1A	3144	1/1	0.93	0.29	42,42,42,42	0
56	MG	1A	3877	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3638	1/1	0.93	0.08	44,44,44,44	0
56	MG	1A	3242	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3643	1/1	0.93	0.12	26,26,26,26	0
56	MG	1A	3002	1/1	0.93	0.10	53,53,53,53	0
56	MG	17	105	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3624	1/1	0.93	0.12	58,58,58,58	0
56	MG	1A	3455	1/1	0.93	0.13	65,65,65,65	0
56	MG	1a	1774	1/1	0.93	0.18	58,58,58,58	0
56	MG	1A	3889	1/1	0.93	0.07	57,57,57,57	0
56	MG	2a	1640	1/1	0.93	0.14	68,68,68,68	0
56	MG	1A	3244	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3892	1/1	0.93	0.07	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3352	1/1	0.93	0.36	66,66,66,66	0
56	MG	2A	3353	1/1	0.93	0.28	61,61,61,61	0
56	MG	1A	4041	1/1	0.93	0.17	60,60,60,60	0
56	MG	1A	3118	1/1	0.93	0.35	51,51,51,51	0
56	MG	1A	3077	1/1	0.93	0.12	54,54,54,54	0
56	MG	2A	3359	1/1	0.93	0.14	71,71,71,71	0
56	MG	1A	3657	1/1	0.93	0.11	40,40,40,40	0
56	MG	2A	3361	1/1	0.93	0.13	44,44,44,44	0
56	MG	1A	3902	1/1	0.93	0.09	37,37,37,37	0
56	MG	1A	3658	1/1	0.93	0.16	30,30,30,30	0
56	MG	1A	3908	1/1	0.93	0.09	62,62,62,62	0
56	MG	2a	1657	1/1	0.93	0.18	53,53,53,53	0
56	MG	1A	3910	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3550	1/1	0.93	0.11	44,44,44,44	0
56	MG	1A	3321	1/1	0.93	0.10	39,39,39,39	0
56	MG	1A	4054	1/1	0.93	0.09	59,59,59,59	0
56	MG	1a	1792	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	4058	1/1	0.93	0.32	59,59,59,59	0
56	MG	1a	1794	1/1	0.93	0.12	55,55,55,55	0
56	MG	2A	3188	1/1	0.93	0.19	51,51,51,51	0
56	MG	2a	1670	1/1	0.93	0.12	71,71,71,71	0
56	MG	2A	3377	1/1	0.93	0.15	44,44,44,44	0
56	MG	1a	1795	1/1	0.93	0.07	59,59,59,59	0
56	MG	1A	3295	1/1	0.93	0.09	59,59,59,59	0
56	MG	1A	3915	1/1	0.93	0.14	55,55,55,55	0
56	MG	1A	3122	1/1	0.93	0.26	37,37,37,37	0
56	MG	2A	3664	1/1	0.93	0.25	44,44,44,44	0
56	MG	1B	209	1/1	0.93	0.18	67,67,67,67	0
56	MG	2A	3390	1/1	0.93	0.17	53,53,53,53	0
56	MG	2A	3391	1/1	0.93	0.16	64,64,64,64	0
56	MG	1B	211	1/1	0.93	0.14	51,51,51,51	0
56	MG	2A	3393	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3782	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3671	1/1	0.93	0.13	63,63,63,63	0
56	MG	2A	3197	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	3405	1/1	0.93	0.09	51,51,51,51	0
56	MG	1n	102	1/1	0.93	0.15	58,58,58,58	0
56	MG	1A	3920	1/1	0.93	0.09	49,49,49,49	0
56	MG	1A	3667	1/1	0.93	0.06	22,22,22,22	0
56	MG	1A	3668	1/1	0.93	0.23	64,64,64,64	0
56	MG	2A	3681	1/1	0.93	0.09	50,50,50,50	0
56	MG	2a	1693	1/1	0.93	0.07	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3669	1/1	0.93	0.09	32,32,32,32	0
56	MG	1A	3467	1/1	0.93	0.13	68,68,68,68	0
56	MG	2A	3412	1/1	0.93	0.34	69,69,69,69	0
56	MG	1A	3206	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3210	1/1	0.93	0.09	53,53,53,53	0
56	MG	2A	3417	1/1	0.93	0.24	57,57,57,57	0
56	MG	2A	3695	1/1	0.93	0.19	54,54,54,54	0
56	MG	1A	3929	1/1	0.93	0.10	22,22,22,22	0
56	MG	1A	3326	1/1	0.93	0.18	53,53,53,53	0
56	MG	1a	1643	1/1	0.93	0.16	57,57,57,57	0
56	MG	1A	3932	1/1	0.93	0.16	52,52,52,52	0
56	MG	1A	3933	1/1	0.93	0.12	58,58,58,58	0
56	MG	2A	3217	1/1	0.93	0.29	74,74,74,74	0
56	MG	1A	3934	1/1	0.93	0.15	62,62,62,62	0
56	MG	1A	3936	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3473	1/1	0.93	0.08	61,61,61,61	0
56	MG	1A	3410	1/1	0.93	0.12	63,63,63,63	0
56	MG	2A	3222	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3223	1/1	0.93	0.09	61,61,61,61	0
56	MG	1A	3364	1/1	0.93	0.12	58,58,58,58	0
56	MG	1A	3680	1/1	0.93	0.13	49,49,49,49	0
56	MG	2A	3226	1/1	0.93	0.17	65,65,65,65	0
56	MG	2A	3712	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3327	1/1	0.93	0.19	33,33,33,33	0
56	MG	1A	3420	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3421	1/1	0.93	0.12	45,45,45,45	0
56	MG	1A	3686	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3446	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3808	1/1	0.93	0.06	36,36,36,36	0
56	MG	1A	3481	1/1	0.93	0.17	56,56,56,56	0
56	MG	2A	3728	1/1	0.93	0.09	63,63,63,63	0
56	MG	2a	1732	1/1	0.93	0.08	76,76,76,76	0
56	MG	2A	3731	1/1	0.93	0.22	69,69,69,69	0
56	MG	2A	3450	1/1	0.93	0.14	35,35,35,35	0
56	MG	1A	3581	1/1	0.93	0.15	42,42,42,42	0
56	MG	1A	3209	1/1	0.93	0.07	46,46,46,46	0
56	MG	2A	3237	1/1	0.93	0.11	63,63,63,63	0
56	MG	2a	1739	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3958	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3026	1/1	0.93	0.14	52,52,52,52	0
56	MG	2A	3741	1/1	0.93	0.12	66,66,66,66	0
56	MG	2A	3458	1/1	0.93	0.13	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1747	1/1	0.93	0.16	74,74,74,74	0
56	MG	2A	3027	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3028	1/1	0.93	0.09	52,52,52,52	0
56	MG	2A	3461	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3029	1/1	0.93	0.11	41,41,41,41	0
56	MG	2A	3463	1/1	0.93	0.12	56,56,56,56	0
56	MG	2a	1753	1/1	0.93	0.20	61,61,61,61	0
56	MG	2a	1755	1/1	0.93	0.13	58,58,58,58	0
56	MG	2A	3465	1/1	0.93	0.12	61,61,61,61	0
56	MG	1A	3489	1/1	0.93	0.18	60,60,60,60	0
56	MG	2A	3469	1/1	0.93	0.11	47,47,47,47	0
56	MG	2A	3471	1/1	0.93	0.09	46,46,46,46	0
56	MG	1A	3370	1/1	0.93	0.59	48,48,48,48	0
56	MG	2A	3758	1/1	0.93	0.11	66,66,66,66	0
56	MG	2A	3035	1/1	0.93	0.17	73,73,73,73	0
56	MG	1A	3216	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3698	1/1	0.93	0.09	49,49,49,49	0
56	MG	1A	3599	1/1	0.93	0.07	34,34,34,34	0
56	MG	1A	3373	1/1	0.93	0.08	53,53,53,53	0
56	MG	1a	1676	1/1	0.93	0.33	58,58,58,58	0
56	MG	1A	3974	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3429	1/1	0.93	0.21	50,50,50,50	0
56	MG	1A	3607	1/1	0.93	0.11	56,56,56,56	0
56	MG	2A	3492	1/1	0.93	0.10	37,37,37,37	0
56	MG	2A	3494	1/1	0.93	0.08	44,44,44,44	0
56	MG	1a	1680	1/1	0.93	0.38	75,75,75,75	0
56	MG	2A	3497	1/1	0.93	0.08	49,49,49,49	0
56	MG	1A	3056	1/1	0.93	0.10	43,43,43,43	0
56	MG	1I	201	1/1	0.93	0.09	64,64,64,64	0
56	MG	2a	1783	1/1	0.93	0.30	70,70,70,70	0
56	MG	1A	3980	1/1	0.93	0.10	51,51,51,51	0
56	MG	1N	202	1/1	0.93	0.08	50,50,50,50	0
56	MG	2a	1786	1/1	0.93	0.12	71,71,71,71	0
56	MG	1a	1686	1/1	0.93	0.12	67,67,67,67	0
56	MG	2A	3263	1/1	0.93	0.09	58,58,58,58	0
56	MG	1A	3022	1/1	0.93	0.09	42,42,42,42	0
56	MG	2A	3063	1/1	0.93	0.08	55,55,55,55	0
56	MG	1a	1688	1/1	0.93	0.23	63,63,63,63	0
56	MG	1A	3984	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3710	1/1	0.93	0.10	24,24,24,24	0
56	MG	2A	3075	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3165	1/1	0.93	0.09	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1O	204	1/1	0.93	0.09	49,49,49,49	0
56	MG	1a	1697	1/1	0.93	0.20	49,49,49,49	0
56	MG	1A	3987	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3713	1/1	0.93	0.06	20,20,20,20	0
56	MG	1P	205	1/1	0.93	0.08	46,46,46,46	0
56	MG	1A	3166	1/1	0.93	0.29	42,42,42,42	0
56	MG	1a	1703	1/1	0.93	0.15	61,61,61,61	0
56	MG	1A	3841	1/1	0.93	0.28	34,34,34,34	0
56	MG	2A	3093	1/1	0.93	0.16	62,62,62,62	0
56	MG	1A	3435	1/1	0.93	0.13	34,34,34,34	0
56	MG	1A	3230	1/1	0.93	0.12	51,51,51,51	0
56	MG	1a	1713	1/1	0.93	0.13	55,55,55,55	0
56	MG	2A	3538	1/1	0.93	0.09	52,52,52,52	0
56	MG	1R	202	1/1	0.93	0.25	51,51,51,51	0
56	MG	2E	303	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3720	1/1	0.93	0.11	36,36,36,36	0
56	MG	1S	201	1/1	0.93	0.29	51,51,51,51	0
56	MG	2F	303	1/1	0.93	0.12	64,64,64,64	0
56	MG	1a	1718	1/1	0.93	0.15	59,59,59,59	0
56	MG	2A	3292	1/1	0.93	0.21	63,63,63,63	0
56	MG	1A	3722	1/1	0.93	0.08	42,42,42,42	0
56	MG	2A	3550	1/1	0.93	0.13	46,46,46,46	0
56	MG	2x	106	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3778	1/1	0.94	0.06	33,33,33,33	0
56	MG	2A	3290	1/1	0.94	0.10	64,64,64,64	0
56	MG	2E	308	1/1	0.94	0.11	43,43,43,43	0
56	MG	2F	302	1/1	0.94	0.07	43,43,43,43	0
56	MG	1D	305	1/1	0.94	0.07	37,37,37,37	0
56	MG	1a	1684	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3260	1/1	0.94	0.29	53,53,53,53	0
56	MG	2A	3087	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3552	1/1	0.94	0.10	38,38,38,38	0
56	MG	2A	3088	1/1	0.94	0.11	63,63,63,63	0
56	MG	2A	3558	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3218	1/1	0.94	0.09	56,56,56,56	0
56	MG	1A	3223	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3174	1/1	0.94	0.14	33,33,33,33	0
56	MG	1A	3175	1/1	0.94	0.13	63,63,63,63	0
56	MG	1A	3940	1/1	0.94	0.09	49,49,49,49	0
56	MG	2A	3567	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3095	1/1	0.94	0.16	58,58,58,58	0
56	MG	2A	3096	1/1	0.94	0.16	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2U	201	1/1	0.94	0.12	60,60,60,60	0
56	MG	1A	3272	1/1	0.94	0.14	35,35,35,35	0
56	MG	2A	3098	1/1	0.94	0.19	48,48,48,48	0
56	MG	2A	3572	1/1	0.94	0.27	56,56,56,56	0
56	MG	2A	3307	1/1	0.94	0.19	57,57,57,57	0
56	MG	2Y	201	1/1	0.94	0.30	62,62,62,62	0
56	MG	1a	1693	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3576	1/1	0.94	0.12	59,59,59,59	0
56	MG	1a	1694	1/1	0.94	0.23	51,51,51,51	0
56	MG	1E	312	1/1	0.94	0.12	27,27,27,27	0
56	MG	25	103	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3789	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	3790	1/1	0.94	0.08	33,33,33,33	0
56	MG	1A	3947	1/1	0.94	0.09	23,23,23,23	0
56	MG	1A	3275	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	3950	1/1	0.94	0.12	28,28,28,28	0
56	MG	2A	3585	1/1	0.94	0.08	57,57,57,57	0
56	MG	2A	3586	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3441	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	3796	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3660	1/1	0.94	0.07	26,26,26,26	0
56	MG	1G	204	1/1	0.94	0.15	62,62,62,62	0
56	MG	1A	3378	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3116	1/1	0.94	0.08	60,60,60,60	0
56	MG	2A	3117	1/1	0.94	0.17	74,74,74,74	0
56	MG	1a	1714	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	3663	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3379	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3445	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3960	1/1	0.94	0.09	19,19,19,19	0
56	MG	1A	3534	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3132	1/1	0.94	0.23	39,39,39,39	0
56	MG	1O	202	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3964	1/1	0.94	0.13	70,70,70,70	0
56	MG	1A	3539	1/1	0.94	0.26	38,38,38,38	0
56	MG	1A	3542	1/1	0.94	0.61	42,42,42,42	0
56	MG	1A	3543	1/1	0.94	0.09	44,44,44,44	0
56	MG	1a	1728	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3278	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	3972	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3447	1/1	0.94	0.23	63,63,63,63	0
56	MG	1Q	204	1/1	0.94	0.11	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3673	1/1	0.94	0.08	32,32,32,32	0
56	MG	1A	3813	1/1	0.94	0.17	58,58,58,58	0
56	MG	2a	1630	1/1	0.94	0.23	55,55,55,55	0
56	MG	2a	1631	1/1	0.94	0.27	56,56,56,56	0
56	MG	1A	3553	1/1	0.94	0.19	54,54,54,54	0
56	MG	1A	3676	1/1	0.94	0.09	38,38,38,38	0
56	MG	2A	3345	1/1	0.94	0.15	56,56,56,56	0
56	MG	1A	3816	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3323	1/1	0.94	0.18	48,48,48,48	0
56	MG	2A	3621	1/1	0.94	0.15	63,63,63,63	0
56	MG	2A	3348	1/1	0.94	0.27	61,61,61,61	0
56	MG	1A	3279	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3176	1/1	0.94	0.10	70,70,70,70	0
56	MG	1A	3385	1/1	0.94	0.32	64,64,64,64	0
56	MG	1A	3559	1/1	0.94	0.34	61,61,61,61	0
56	MG	1A	3561	1/1	0.94	0.28	59,59,59,59	0
56	MG	1A	3177	1/1	0.94	0.07	42,42,42,42	0
56	MG	2A	3160	1/1	0.94	0.13	52,52,52,52	0
56	MG	2A	3357	1/1	0.94	0.28	58,58,58,58	0
56	MG	2a	1648	1/1	0.94	0.10	68,68,68,68	0
56	MG	2A	3162	1/1	0.94	0.30	64,64,64,64	0
56	MG	2A	3636	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3994	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	3995	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3829	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3116	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3688	1/1	0.94	0.10	59,59,59,59	0
56	MG	1a	1756	1/1	0.94	0.09	62,62,62,62	0
56	MG	1Z	303	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3181	1/1	0.94	0.19	41,41,41,41	0
56	MG	1a	1762	1/1	0.94	0.11	54,54,54,54	0
56	MG	2a	1663	1/1	0.94	0.20	65,65,65,65	0
56	MG	10	103	1/1	0.94	0.24	47,47,47,47	0
56	MG	1A	3332	1/1	0.94	0.25	64,64,64,64	0
56	MG	2A	3650	1/1	0.94	0.18	57,57,57,57	0
56	MG	2A	3176	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3142	1/1	0.94	0.26	35,35,35,35	0
56	MG	1A	3573	1/1	0.94	0.09	34,34,34,34	0
56	MG	2a	1671	1/1	0.94	0.10	65,65,65,65	0
56	MG	2A	3375	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3837	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	4006	1/1	0.94	0.13	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3658	1/1	0.94	0.16	59,59,59,59	0
56	MG	2A	3384	1/1	0.94	0.13	69,69,69,69	0
56	MG	2a	1677	1/1	0.94	0.17	70,70,70,70	0
56	MG	1A	3335	1/1	0.94	0.17	38,38,38,38	0
56	MG	1A	4008	1/1	0.94	0.07	47,47,47,47	0
56	MG	1A	3393	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3239	1/1	0.94	0.25	53,53,53,53	0
56	MG	1A	3844	1/1	0.94	0.19	37,37,37,37	0
56	MG	16	102	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	3396	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3291	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3184	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3705	1/1	0.94	0.06	54,54,54,54	0
56	MG	2A	3397	1/1	0.94	0.07	57,57,57,57	0
56	MG	2A	3191	1/1	0.94	0.27	62,62,62,62	0
56	MG	18	103	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3584	1/1	0.94	0.08	25,25,25,25	0
56	MG	2A	3404	1/1	0.94	0.19	42,42,42,42	0
56	MG	1A	3585	1/1	0.94	0.06	35,35,35,35	0
56	MG	1A	3001	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	3148	1/1	0.94	0.18	44,44,44,44	0
56	MG	2A	3679	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3593	1/1	0.94	0.08	42,42,42,42	0
56	MG	2A	3411	1/1	0.94	0.12	50,50,50,50	0
56	MG	2A	3683	1/1	0.94	0.12	76,76,76,76	0
56	MG	1A	3476	1/1	0.94	0.11	62,62,62,62	0
56	MG	2A	3199	1/1	0.94	0.09	47,47,47,47	0
56	MG	1a	1605	1/1	0.94	0.08	63,63,63,63	0
56	MG	2A	3416	1/1	0.94	0.12	63,63,63,63	0
56	MG	2A	3692	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3693	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3004	1/1	0.94	0.07	29,29,29,29	0
56	MG	1A	3096	1/1	0.94	0.11	48,48,48,48	0
56	MG	1d	301	1/1	0.94	0.32	64,64,64,64	0
56	MG	1a	1612	1/1	0.94	0.08	72,72,72,72	0
56	MG	1f	3102	1/1	0.94	0.22	68,68,68,68	0
56	MG	1A	3865	1/1	0.94	0.09	55,55,55,55	0
56	MG	2a	1713	1/1	0.94	0.10	70,70,70,70	0
56	MG	2A	3209	1/1	0.94	0.21	53,53,53,53	0
56	MG	1A	3600	1/1	0.94	0.06	22,22,22,22	0
56	MG	1a	1615	1/1	0.94	0.14	61,61,61,61	0
56	MG	2A	3212	1/1	0.94	0.29	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3718	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3602	1/1	0.94	0.08	25,25,25,25	0
56	MG	1A	3299	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	4038	1/1	0.94	0.13	49,49,49,49	0
56	MG	2a	1724	1/1	0.94	0.31	58,58,58,58	0
56	MG	1A	4039	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3406	1/1	0.94	0.16	50,50,50,50	0
56	MG	2A	3439	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3482	1/1	0.94	0.17	52,52,52,52	0
56	MG	1A	3087	1/1	0.94	0.14	47,47,47,47	0
56	MG	2A	3714	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3485	1/1	0.94	0.18	39,39,39,39	0
56	MG	2A	3719	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3301	1/1	0.94	0.20	41,41,41,41	0
56	MG	1A	3730	1/1	0.94	0.06	37,37,37,37	0
56	MG	1A	3884	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3731	1/1	0.94	0.06	27,27,27,27	0
56	MG	2A	3724	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3490	1/1	0.94	0.13	42,42,42,42	0
56	MG	2a	1743	1/1	0.94	0.09	69,69,69,69	0
56	MG	1A	3890	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3730	1/1	0.94	0.07	75,75,75,75	0
56	MG	1A	3733	1/1	0.94	0.09	27,27,27,27	0
56	MG	1A	4055	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	4057	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	3124	1/1	0.94	0.20	55,55,55,55	0
56	MG	2A	3457	1/1	0.94	0.06	33,33,33,33	0
56	MG	2A	3232	1/1	0.94	0.16	53,53,53,53	0
56	MG	1a	1640	1/1	0.94	0.17	64,64,64,64	0
56	MG	1a	1641	1/1	0.94	0.10	57,57,57,57	0
56	MG	2a	1757	1/1	0.94	0.14	60,60,60,60	0
56	MG	2A	3743	1/1	0.94	0.08	71,71,71,71	0
56	MG	2A	3007	1/1	0.94	0.15	61,61,61,61	0
56	MG	1A	3413	1/1	0.94	0.22	43,43,43,43	0
56	MG	1B	202	1/1	0.94	0.22	54,54,54,54	0
56	MG	1A	3737	1/1	0.94	0.06	34,34,34,34	0
56	MG	2A	3240	1/1	0.94	0.15	58,58,58,58	0
56	MG	1B	205	1/1	0.94	0.19	55,55,55,55	0
56	MG	2A	3019	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3020	1/1	0.94	0.13	53,53,53,53	0
56	MG	2A	3475	1/1	0.94	0.12	49,49,49,49	0
56	MG	1a	1647	1/1	0.94	0.15	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3205	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3029	1/1	0.94	0.10	35,35,35,35	0
56	MG	1B	210	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3906	1/1	0.94	0.09	27,27,27,27	0
56	MG	1A	3743	1/1	0.94	0.12	66,66,66,66	0
56	MG	1A	3048	1/1	0.94	0.06	19,19,19,19	0
56	MG	1A	3909	1/1	0.94	0.12	64,64,64,64	0
56	MG	2A	3034	1/1	0.94	0.28	64,64,64,64	0
56	MG	1A	3749	1/1	0.94	0.14	63,63,63,63	0
56	MG	1A	3254	1/1	0.94	0.37	69,69,69,69	0
56	MG	2a	1782	1/1	0.94	0.28	58,58,58,58	0
56	MG	1A	3499	1/1	0.94	0.27	37,37,37,37	0
56	MG	1a	1659	1/1	0.94	0.13	62,62,62,62	0
56	MG	1A	3627	1/1	0.94	0.06	31,31,31,31	0
56	MG	1A	3310	1/1	0.94	0.10	45,45,45,45	0
56	MG	2A	3774	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3044	1/1	0.94	0.17	66,66,66,66	0
56	MG	1A	3424	1/1	0.94	0.18	63,63,63,63	0
56	MG	1A	3760	1/1	0.94	0.09	49,49,49,49	0
56	MG	1A	3504	1/1	0.94	0.16	42,42,42,42	0
56	MG	1A	3215	1/1	0.94	0.13	47,47,47,47	0
56	MG	2A	3509	1/1	0.94	0.15	59,59,59,59	0
56	MG	2a	1795	1/1	0.94	0.11	58,58,58,58	0
56	MG	2A	3510	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3050	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	3101	1/1	0.94	0.20	40,40,40,40	0
56	MG	1a	1669	1/1	0.94	0.25	57,57,57,57	0
56	MG	1a	1670	1/1	0.94	0.19	65,65,65,65	0
56	MG	2A	3271	1/1	0.94	0.07	49,49,49,49	0
56	MG	2a	1802	1/1	0.94	0.26	66,66,66,66	0
56	MG	2B	207	1/1	0.94	0.13	63,63,63,63	0
56	MG	1B	228	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3361	1/1	0.94	0.27	40,40,40,40	0
56	MG	2A	3524	1/1	0.94	0.25	64,64,64,64	0
56	MG	1A	3635	1/1	0.94	0.06	35,35,35,35	0
56	MG	2A	3059	1/1	0.94	0.20	55,55,55,55	0
56	MG	2A	3062	1/1	0.94	0.16	55,55,55,55	0
56	MG	1A	3637	1/1	0.94	0.08	31,31,31,31	0
56	MG	1B	234	1/1	0.94	0.11	67,67,67,67	0
56	MG	1A	3105	1/1	0.94	0.34	39,39,39,39	0
56	MG	2A	3071	1/1	0.94	0.26	60,60,60,60	0
56	MG	2A	3533	1/1	0.94	0.15	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3072	1/1	0.94	0.10	60,60,60,60	0
56	MG	2D	306	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3772	1/1	0.94	0.07	26,26,26,26	0
56	MG	1A	3510	1/1	0.94	0.24	60,60,60,60	0
56	MG	2A	3078	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3931	1/1	0.94	0.09	34,34,34,34	0
56	MG	1A	3512	1/1	0.94	0.10	62,62,62,62	0
56	MG	2x	107	1/1	0.94	0.07	59,59,59,59	0
60	K	2x	101	1/1	0.94	0.14	79,79,79,79	0
56	MG	1A	3283	1/1	0.95	0.19	34,34,34,34	0
56	MG	1A	3337	1/1	0.95	0.11	61,61,61,61	0
56	MG	27	102	1/1	0.95	0.21	59,59,59,59	0
56	MG	2A	3001	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3942	1/1	0.95	0.08	66,66,66,66	0
56	MG	2A	3380	1/1	0.95	0.19	66,66,66,66	0
56	MG	2A	3382	1/1	0.95	0.16	47,47,47,47	0
56	MG	1A	3582	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3017	1/1	0.95	0.13	70,70,70,70	0
56	MG	1A	3809	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	3226	1/1	0.95	0.27	45,45,45,45	0
56	MG	2A	3388	1/1	0.95	0.14	53,53,53,53	0
56	MG	1A	3949	1/1	0.95	0.14	37,37,37,37	0
56	MG	2A	3626	1/1	0.95	0.15	35,35,35,35	0
56	MG	2A	3016	1/1	0.95	0.14	50,50,50,50	0
56	MG	2A	3208	1/1	0.95	0.14	57,57,57,57	0
56	MG	2A	3629	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	3812	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3055	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3228	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3591	1/1	0.95	0.08	29,29,29,29	0
56	MG	2A	3022	1/1	0.95	0.21	50,50,50,50	0
56	MG	1a	1664	1/1	0.95	0.19	58,58,58,58	0
56	MG	1E	303	1/1	0.95	0.18	50,50,50,50	0
56	MG	1A	3486	1/1	0.95	0.31	36,36,36,36	0
56	MG	2A	3402	1/1	0.95	0.13	44,44,44,44	0
56	MG	2A	3403	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3701	1/1	0.95	0.10	64,64,64,64	0
56	MG	2A	3405	1/1	0.95	0.35	59,59,59,59	0
56	MG	2a	1624	1/1	0.95	0.12	69,69,69,69	0
56	MG	1A	3818	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3819	1/1	0.95	0.07	21,21,21,21	0
56	MG	2A	3646	1/1	0.95	0.12	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3487	1/1	0.95	0.31	44,44,44,44	0
56	MG	1A	3123	1/1	0.95	0.18	32,32,32,32	0
56	MG	1E	315	1/1	0.95	0.12	59,59,59,59	0
56	MG	1A	3962	1/1	0.95	0.09	24,24,24,24	0
56	MG	1A	3822	1/1	0.95	0.14	23,23,23,23	0
56	MG	1A	3824	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3041	1/1	0.95	0.11	37,37,37,37	0
56	MG	1F	309	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3018	1/1	0.95	0.10	39,39,39,39	0
56	MG	2A	3419	1/1	0.95	0.33	66,66,66,66	0
56	MG	2A	3043	1/1	0.95	0.18	67,67,67,67	0
56	MG	1A	3128	1/1	0.95	0.09	46,46,46,46	0
56	MG	1G	202	1/1	0.95	0.18	59,59,59,59	0
56	MG	2A	3424	1/1	0.95	0.13	54,54,54,54	0
56	MG	2a	1642	1/1	0.95	0.07	81,81,81,81	0
56	MG	1A	3414	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3605	1/1	0.95	0.09	29,29,29,29	0
56	MG	1A	3348	1/1	0.95	0.12	53,53,53,53	0
56	MG	2A	3235	1/1	0.95	0.10	64,64,64,64	0
56	MG	2A	3431	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	3059	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3051	1/1	0.95	0.13	57,57,57,57	0
56	MG	1A	3417	1/1	0.95	0.21	44,44,44,44	0
56	MG	1A	3240	1/1	0.95	0.16	43,43,43,43	0
56	MG	1N	205	1/1	0.95	0.16	56,56,56,56	0
56	MG	1A	3981	1/1	0.95	0.08	44,44,44,44	0
56	MG	2a	1654	1/1	0.95	0.26	64,64,64,64	0
56	MG	1A	3062	1/1	0.95	0.40	60,60,60,60	0
56	MG	1A	3135	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3836	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3503	1/1	0.95	0.18	48,48,48,48	0
56	MG	2a	1660	1/1	0.95	0.40	72,72,72,72	0
56	MG	1A	3187	1/1	0.95	0.23	39,39,39,39	0
56	MG	2A	3444	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3064	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3839	1/1	0.95	0.16	34,34,34,34	0
56	MG	2A	3067	1/1	0.95	0.15	50,50,50,50	0
56	MG	2A	3684	1/1	0.95	0.06	55,55,55,55	0
56	MG	1A	3614	1/1	0.95	0.11	24,24,24,24	0
56	MG	1A	3992	1/1	0.95	0.06	52,52,52,52	0
56	MG	2A	3688	1/1	0.95	0.07	71,71,71,71	0
56	MG	1A	3842	1/1	0.95	0.20	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3690	1/1	0.95	0.10	70,70,70,70	0
56	MG	1A	3615	1/1	0.95	0.08	32,32,32,32	0
56	MG	2A	3074	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3046	1/1	0.95	0.07	37,37,37,37	0
56	MG	2A	3077	1/1	0.95	0.10	57,57,57,57	0
56	MG	1A	3302	1/1	0.95	0.19	32,32,32,32	0
56	MG	1Q	207	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3620	1/1	0.95	0.11	57,57,57,57	0
56	MG	1A	3847	1/1	0.95	0.05	35,35,35,35	0
56	MG	1A	3621	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3084	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3245	1/1	0.95	0.07	33,33,33,33	0
56	MG	1A	3305	1/1	0.95	0.16	54,54,54,54	0
56	MG	1A	3189	1/1	0.95	0.07	44,44,44,44	0
56	MG	1T	202	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3190	1/1	0.95	0.27	40,40,40,40	0
56	MG	1U	205	1/1	0.95	0.19	34,34,34,34	0
56	MG	1A	3191	1/1	0.95	0.18	45,45,45,45	0
56	MG	1V	202	1/1	0.95	0.36	35,35,35,35	0
56	MG	1A	3365	1/1	0.95	0.14	43,43,43,43	0
56	MG	1W	201	1/1	0.95	0.24	49,49,49,49	0
56	MG	1A	3860	1/1	0.95	0.06	28,28,28,28	0
56	MG	2A	3484	1/1	0.95	0.08	36,36,36,36	0
56	MG	1A	3067	1/1	0.95	0.17	55,55,55,55	0
56	MG	1A	3520	1/1	0.95	0.15	37,37,37,37	0
56	MG	2A	3718	1/1	0.95	0.09	41,41,41,41	0
56	MG	1A	3368	1/1	0.95	0.16	30,30,30,30	0
56	MG	1A	3864	1/1	0.95	0.12	38,38,38,38	0
56	MG	2A	3281	1/1	0.95	0.12	61,61,61,61	0
56	MG	1A	3741	1/1	0.95	0.07	27,27,27,27	0
56	MG	1A	3866	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3439	1/1	0.95	0.08	50,50,50,50	0
56	MG	1A	3744	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3106	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3069	1/1	0.95	0.10	31,31,31,31	0
56	MG	1A	3872	1/1	0.95	0.17	57,57,57,57	0
56	MG	2A	3289	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	4022	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	3748	1/1	0.95	0.07	52,52,52,52	0
56	MG	1a	1745	1/1	0.95	0.11	59,59,59,59	0
56	MG	2A	3508	1/1	0.95	0.13	64,64,64,64	0
56	MG	11	102	1/1	0.95	0.10	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3740	1/1	0.95	0.11	70,70,70,70	0
56	MG	1A	4024	1/1	0.95	0.09	18,18,18,18	0
56	MG	2A	3115	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3636	1/1	0.95	0.05	24,24,24,24	0
56	MG	1A	3311	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3118	1/1	0.95	0.09	45,45,45,45	0
56	MG	2A	3119	1/1	0.95	0.21	49,49,49,49	0
56	MG	2a	1722	1/1	0.95	0.28	66,66,66,66	0
56	MG	2a	1723	1/1	0.95	0.32	60,60,60,60	0
56	MG	2A	3300	1/1	0.95	0.17	68,68,68,68	0
56	MG	2A	3750	1/1	0.95	0.19	54,54,54,54	0
56	MG	2A	3522	1/1	0.95	0.13	55,55,55,55	0
56	MG	2a	1728	1/1	0.95	0.11	61,61,61,61	0
56	MG	2A	3301	1/1	0.95	0.25	66,66,66,66	0
56	MG	2A	3120	1/1	0.95	0.06	51,51,51,51	0
56	MG	12	101	1/1	0.95	0.10	55,55,55,55	0
56	MG	13	102	1/1	0.95	0.15	45,45,45,45	0
56	MG	1A	3751	1/1	0.95	0.06	74,74,74,74	0
56	MG	2A	3127	1/1	0.95	0.12	42,42,42,42	0
56	MG	15	102	1/1	0.95	0.18	39,39,39,39	0
56	MG	1A	3371	1/1	0.95	0.25	36,36,36,36	0
56	MG	1A	3015	1/1	0.95	0.18	39,39,39,39	0
56	MG	1A	3444	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3645	1/1	0.95	0.05	24,24,24,24	0
56	MG	17	101	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3032	1/1	0.95	0.20	24,24,24,24	0
56	MG	1a	1767	1/1	0.95	0.14	69,69,69,69	0
56	MG	1A	3761	1/1	0.95	0.07	52,52,52,52	0
56	MG	1A	3762	1/1	0.95	0.05	23,23,23,23	0
56	MG	2A	3540	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3541	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3200	1/1	0.95	0.06	54,54,54,54	0
56	MG	2A	3775	1/1	0.95	0.11	73,73,73,73	0
56	MG	2A	3141	1/1	0.95	0.18	43,43,43,43	0
56	MG	1a	1775	1/1	0.95	0.07	57,57,57,57	0
56	MG	2A	3545	1/1	0.95	0.09	41,41,41,41	0
56	MG	2A	3546	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3149	1/1	0.95	0.06	39,39,39,39	0
56	MG	2A	3145	1/1	0.95	0.13	60,60,60,60	0
56	MG	2A	3782	1/1	0.95	0.32	64,64,64,64	0
56	MG	2a	1761	1/1	0.95	0.08	58,58,58,58	0
56	MG	1A	4042	1/1	0.95	0.11	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1763	1/1	0.95	0.19	49,49,49,49	0
56	MG	2A	3551	1/1	0.95	0.10	62,62,62,62	0
56	MG	1A	3540	1/1	0.95	0.20	43,43,43,43	0
56	MG	2A	3554	1/1	0.95	0.14	68,68,68,68	0
56	MG	1a	1779	1/1	0.95	0.27	66,66,66,66	0
56	MG	2A	3557	1/1	0.95	0.18	57,57,57,57	0
56	MG	1A	3767	1/1	0.95	0.08	48,48,48,48	0
56	MG	1A	3257	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3899	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3900	1/1	0.95	0.07	36,36,36,36	0
56	MG	1A	3655	1/1	0.95	0.07	24,24,24,24	0
56	MG	1A	3450	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3566	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3025	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3548	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	4052	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3154	1/1	0.95	0.08	51,51,51,51	0
56	MG	2D	302	1/1	0.95	0.33	59,59,59,59	0
56	MG	1a	1617	1/1	0.95	0.09	60,60,60,60	0
56	MG	1a	1791	1/1	0.95	0.08	40,40,40,40	0
56	MG	1A	3109	1/1	0.95	0.23	34,34,34,34	0
56	MG	1A	3262	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3210	1/1	0.95	0.15	34,34,34,34	0
56	MG	1A	3112	1/1	0.95	0.16	45,45,45,45	0
56	MG	1A	3114	1/1	0.95	0.18	34,34,34,34	0
56	MG	1A	3271	1/1	0.95	0.44	47,47,47,47	0
56	MG	1B	204	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	3785	1/1	0.95	0.23	29,29,29,29	0
56	MG	2A	3172	1/1	0.95	0.28	60,60,60,60	0
56	MG	2a	1793	1/1	0.95	0.27	69,69,69,69	0
56	MG	2E	309	1/1	0.95	0.10	70,70,70,70	0
56	MG	1e	201	1/1	0.95	0.33	67,67,67,67	0
56	MG	1B	206	1/1	0.95	0.11	45,45,45,45	0
56	MG	2F	304	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	3035	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3787	1/1	0.95	0.07	45,45,45,45	0
56	MG	1m	3001	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3921	1/1	0.95	0.13	50,50,50,50	0
56	MG	1A	3274	1/1	0.95	0.26	31,31,31,31	0
56	MG	1A	3563	1/1	0.95	0.13	54,54,54,54	0
56	MG	2A	3355	1/1	0.95	0.20	60,60,60,60	0
56	MG	2k	201	1/1	0.95	0.17	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3084	1/1	0.95	0.28	34,34,34,34	0
56	MG	2l	203	1/1	0.95	0.11	67,67,67,67	0
56	MG	1A	3793	1/1	0.95	0.06	33,33,33,33	0
56	MG	1A	3926	1/1	0.95	0.11	69,69,69,69	0
56	MG	2q	201	1/1	0.95	0.07	73,73,73,73	0
56	MG	1A	3468	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3598	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3328	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3276	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3395	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3798	1/1	0.95	0.16	56,56,56,56	0
56	MG	1x	103	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	3220	1/1	0.95	0.18	28,28,28,28	0
56	MG	1A	3575	1/1	0.95	0.10	30,30,30,30	0
56	MG	1A	3935	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3576	1/1	0.95	0.08	40,40,40,40	0
56	MG	1A	3398	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3164	1/1	0.95	0.23	59,59,59,59	0
56	MG	1A	3036	1/1	0.95	0.12	40,40,40,40	0
56	MG	25	101	1/1	0.95	0.27	59,59,59,59	0
58	ZN	24	501	1/1	0.95	0.17	126,126,126,126	0
56	MG	2A	3373	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	3590	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3051	1/1	0.96	0.13	31,31,31,31	0
56	MG	1A	3592	1/1	0.96	0.10	25,25,25,25	0
56	MG	1l	101	1/1	0.96	0.38	40,40,40,40	0
56	MG	1A	3155	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3426	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3498	1/1	0.96	0.17	44,44,44,44	0
56	MG	1A	3927	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3268	1/1	0.96	0.34	71,71,71,71	0
56	MG	2A	3455	1/1	0.96	0.14	66,66,66,66	0
56	MG	1A	3208	1/1	0.96	0.33	42,42,42,42	0
56	MG	12	102	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	4056	1/1	0.96	0.11	39,39,39,39	0
56	MG	1A	3258	1/1	0.96	0.16	46,46,46,46	0
56	MG	15	101	1/1	0.96	0.26	29,29,29,29	0
56	MG	1A	3042	1/1	0.96	0.15	32,32,32,32	0
56	MG	2A	3675	1/1	0.96	0.11	40,40,40,40	0
56	MG	15	103	1/1	0.96	0.19	35,35,35,35	0
56	MG	1A	4059	1/1	0.96	0.15	57,57,57,57	0
56	MG	1A	3090	1/1	0.96	0.12	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	16	101	1/1	0.96	0.13	51,51,51,51	0
56	MG	2A	3680	1/1	0.96	0.13	70,70,70,70	0
56	MG	2A	3468	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3211	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3043	1/1	0.96	0.29	35,35,35,35	0
56	MG	2A	3105	1/1	0.96	0.10	44,44,44,44	0
56	MG	2A	3473	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3506	1/1	0.96	0.08	25,25,25,25	0
56	MG	1A	3119	1/1	0.96	0.20	40,40,40,40	0
56	MG	1a	1757	1/1	0.96	0.05	71,71,71,71	0
56	MG	1A	3712	1/1	0.96	0.06	47,47,47,47	0
56	MG	1B	207	1/1	0.96	0.12	50,50,50,50	0
56	MG	1a	1760	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3112	1/1	0.96	0.24	61,61,61,61	0
56	MG	18	102	1/1	0.96	0.08	43,43,43,43	0
56	MG	1a	1763	1/1	0.96	0.10	58,58,58,58	0
56	MG	1a	1764	1/1	0.96	0.12	58,58,58,58	0
56	MG	1A	3008	1/1	0.96	0.11	26,26,26,26	0
56	MG	2A	3698	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3374	1/1	0.96	0.16	34,34,34,34	0
56	MG	2A	3493	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3438	1/1	0.96	0.12	42,42,42,42	0
56	MG	2A	3495	1/1	0.96	0.24	58,58,58,58	0
56	MG	1a	1768	1/1	0.96	0.08	77,77,77,77	0
56	MG	1A	3511	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3266	1/1	0.96	0.15	51,51,51,51	0
56	MG	2A	3123	1/1	0.96	0.17	44,44,44,44	0
56	MG	2A	3500	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3501	1/1	0.96	0.15	42,42,42,42	0
56	MG	1a	1773	1/1	0.96	0.07	67,67,67,67	0
56	MG	2A	3125	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3823	1/1	0.96	0.14	26,26,26,26	0
56	MG	1A	3075	1/1	0.96	0.15	36,36,36,36	0
56	MG	2A	3128	1/1	0.96	0.22	55,55,55,55	0
56	MG	1A	3269	1/1	0.96	0.07	23,23,23,23	0
56	MG	1a	1606	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3946	1/1	0.96	0.11	50,50,50,50	0
56	MG	1A	3723	1/1	0.96	0.10	61,61,61,61	0
56	MG	1a	1611	1/1	0.96	0.08	58,58,58,58	0
56	MG	1A	3270	1/1	0.96	0.20	36,36,36,36	0
56	MG	1A	3517	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3519	1/1	0.96	0.15	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3518	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3094	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3222	1/1	0.96	0.11	54,54,54,54	0
56	MG	1A	3623	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3028	1/1	0.96	0.27	38,38,38,38	0
56	MG	2A	3142	1/1	0.96	0.08	55,55,55,55	0
56	MG	1A	3523	1/1	0.96	0.16	38,38,38,38	0
56	MG	1A	3384	1/1	0.96	0.10	40,40,40,40	0
56	MG	1B	231	1/1	0.96	0.05	35,35,35,35	0
56	MG	1A	3734	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3167	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3172	1/1	0.96	0.06	18,18,18,18	0
56	MG	1A	3125	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3047	1/1	0.96	0.18	34,34,34,34	0
56	MG	1a	1796	1/1	0.96	0.29	64,64,64,64	0
56	MG	1a	1630	1/1	0.96	0.16	26,26,26,26	0
56	MG	1A	3739	1/1	0.96	0.07	59,59,59,59	0
56	MG	1A	3452	1/1	0.96	0.20	38,38,38,38	0
56	MG	1A	3280	1/1	0.96	0.20	54,54,54,54	0
56	MG	1A	3969	1/1	0.96	0.04	29,29,29,29	0
56	MG	1D	303	1/1	0.96	0.09	33,33,33,33	0
56	MG	2a	1704	1/1	0.96	0.18	63,63,63,63	0
56	MG	1f	3101	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3535	1/1	0.96	0.22	51,51,51,51	0
56	MG	2A	3161	1/1	0.96	0.09	46,46,46,46	0
56	MG	1D	306	1/1	0.96	0.10	33,33,33,33	0
56	MG	1D	307	1/1	0.96	0.11	43,43,43,43	0
56	MG	1D	308	1/1	0.96	0.09	52,52,52,52	0
56	MG	2A	3548	1/1	0.96	0.06	45,45,45,45	0
56	MG	1D	309	1/1	0.96	0.12	45,45,45,45	0
56	MG	1A	3127	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3745	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3334	1/1	0.96	0.13	68,68,68,68	0
56	MG	1A	3282	1/1	0.96	0.07	50,50,50,50	0
56	MG	1E	306	1/1	0.96	0.14	27,27,27,27	0
56	MG	1A	3459	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3544	1/1	0.96	0.09	36,36,36,36	0
56	MG	2A	3559	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3770	1/1	0.96	0.22	53,53,53,53	0
56	MG	2A	3560	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	3098	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3982	1/1	0.96	0.08	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3232	1/1	0.96	0.06	31,31,31,31	0
56	MG	2a	1726	1/1	0.96	0.20	64,64,64,64	0
56	MG	1A	3856	1/1	0.96	0.07	37,37,37,37	0
56	MG	1E	314	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3857	1/1	0.96	0.07	26,26,26,26	0
56	MG	1E	316	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3754	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3755	1/1	0.96	0.04	35,35,35,35	0
56	MG	1A	3011	1/1	0.96	0.06	37,37,37,37	0
56	MG	1F	306	1/1	0.96	0.06	41,41,41,41	0
56	MG	2a	1735	1/1	0.96	0.06	65,65,65,65	0
56	MG	1A	3552	1/1	0.96	0.06	46,46,46,46	0
56	MG	1A	3464	1/1	0.96	0.11	50,50,50,50	0
56	MG	1A	3235	1/1	0.96	0.14	49,49,49,49	0
56	MG	2A	3575	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3340	1/1	0.96	0.09	54,54,54,54	0
56	MG	1G	201	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3006	1/1	0.96	0.17	61,61,61,61	0
56	MG	1A	3132	1/1	0.96	0.17	33,33,33,33	0
56	MG	2A	3008	1/1	0.96	0.05	44,44,44,44	0
56	MG	1a	1667	1/1	0.96	0.13	66,66,66,66	0
56	MG	2A	3012	1/1	0.96	0.15	44,44,44,44	0
56	MG	2A	3013	1/1	0.96	0.05	35,35,35,35	0
56	MG	1A	3081	1/1	0.96	0.14	40,40,40,40	0
56	MG	1A	3470	1/1	0.96	0.14	36,36,36,36	0
56	MG	1A	3869	1/1	0.96	0.07	39,39,39,39	0
56	MG	2B	217	1/1	0.96	0.18	75,75,75,75	0
56	MG	2A	3588	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3372	1/1	0.96	0.08	64,64,64,64	0
56	MG	1A	3560	1/1	0.96	0.26	47,47,47,47	0
56	MG	2D	304	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3871	1/1	0.96	0.19	24,24,24,24	0
56	MG	1A	3083	1/1	0.96	0.21	30,30,30,30	0
56	MG	2A	3021	1/1	0.96	0.05	43,43,43,43	0
56	MG	2A	3203	1/1	0.96	0.25	51,51,51,51	0
56	MG	1A	3136	1/1	0.96	0.11	33,33,33,33	0
56	MG	2A	3381	1/1	0.96	0.24	48,48,48,48	0
56	MG	1A	3102	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3024	1/1	0.96	0.19	49,49,49,49	0
56	MG	2a	1768	1/1	0.96	0.09	70,70,70,70	0
56	MG	2E	306	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	4005	1/1	0.96	0.05	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3876	1/1	0.96	0.12	45,45,45,45	0
56	MG	1A	3564	1/1	0.96	0.24	57,57,57,57	0
56	MG	2F	301	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3030	1/1	0.96	0.21	32,32,32,32	0
56	MG	1A	3567	1/1	0.96	0.21	48,48,48,48	0
56	MG	1A	3775	1/1	0.96	0.33	29,29,29,29	0
56	MG	2A	3032	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3107	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3407	1/1	0.96	0.15	41,41,41,41	0
56	MG	1A	3143	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3886	1/1	0.96	0.07	68,68,68,68	0
56	MG	1A	3779	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	4018	1/1	0.96	0.05	22,22,22,22	0
56	MG	1A	3192	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3193	1/1	0.96	0.07	29,29,29,29	0
56	MG	2A	3401	1/1	0.96	0.09	71,71,71,71	0
56	MG	1A	3480	1/1	0.96	0.18	36,36,36,36	0
56	MG	1A	3675	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	3784	1/1	0.96	0.05	47,47,47,47	0
56	MG	1A	3411	1/1	0.96	0.07	56,56,56,56	0
56	MG	1a	1696	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3061	1/1	0.96	0.33	59,59,59,59	0
56	MG	1A	3248	1/1	0.96	0.20	31,31,31,31	0
56	MG	1U	201	1/1	0.96	0.16	30,30,30,30	0
56	MG	1A	3901	1/1	0.96	0.16	58,58,58,58	0
56	MG	1A	3146	1/1	0.96	0.23	37,37,37,37	0
56	MG	1A	3110	1/1	0.96	0.11	30,30,30,30	0
56	MG	1a	1704	1/1	0.96	0.20	66,66,66,66	0
56	MG	2A	3415	1/1	0.96	0.11	34,34,34,34	0
56	MG	1a	1705	1/1	0.96	0.15	58,58,58,58	0
56	MG	1A	3356	1/1	0.96	0.15	42,42,42,42	0
56	MG	1V	205	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3791	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3420	1/1	0.96	0.20	47,47,47,47	0
56	MG	2f	201	1/1	0.96	0.05	46,46,46,46	0
56	MG	2j	201	1/1	0.96	0.17	69,69,69,69	0
56	MG	1a	1711	1/1	0.96	0.15	44,44,44,44	0
56	MG	2l	201	1/1	0.96	0.10	73,73,73,73	0
56	MG	1a	1712	1/1	0.96	0.12	40,40,40,40	0
56	MG	2A	3638	1/1	0.96	0.07	39,39,39,39	0
56	MG	28	101	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3792	1/1	0.96	0.06	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3241	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3419	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3068	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3069	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	3583	1/1	0.96	0.09	57,57,57,57	0
56	MG	1X	101	1/1	0.96	0.35	43,43,43,43	0
56	MG	1X	106	1/1	0.96	0.08	33,33,33,33	0
56	MG	1A	3685	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	4040	1/1	0.96	0.14	50,50,50,50	0
56	MG	1Y	203	1/1	0.96	0.21	43,43,43,43	0
56	MG	2A	3076	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3007	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3687	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3151	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	3113	1/1	0.96	0.14	43,43,43,43	0
56	MG	2A	3081	1/1	0.96	0.11	39,39,39,39	0
57	A1A1L	2A	3783	36/36	0.96	0.09	33,42,49,58	0
58	ZN	14	102	1/1	0.96	0.12	118,118,118,118	0
56	MG	1A	3587	1/1	0.96	0.06	34,34,34,34	0
58	ZN	2n	501	1/1	0.96	0.07	89,89,89,89	0
56	MG	1A	3423	1/1	0.96	0.13	43,43,43,43	0
56	MG	2A	3376	1/1	0.97	0.40	53,53,53,53	0
56	MG	1A	3277	1/1	0.97	0.14	49,49,49,49	0
56	MG	2A	3378	1/1	0.97	0.09	21,21,21,21	0
56	MG	1A	3911	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3359	1/1	0.97	0.04	42,42,42,42	0
56	MG	1a	1616	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3553	1/1	0.97	0.08	49,49,49,49	0
56	MG	1A	3202	1/1	0.97	0.18	38,38,38,38	0
56	MG	2A	3555	1/1	0.97	0.08	37,37,37,37	0
56	MG	2A	3383	1/1	0.97	0.09	54,54,54,54	0
56	MG	2A	3734	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3104	1/1	0.97	0.16	37,37,37,37	0
56	MG	1a	1619	1/1	0.97	0.06	50,50,50,50	0
56	MG	1a	1620	1/1	0.97	0.32	63,63,63,63	0
56	MG	1A	3141	1/1	0.97	0.14	25,25,25,25	0
56	MG	1F	301	1/1	0.97	0.15	38,38,38,38	0
56	MG	2a	1666	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	4017	1/1	0.97	0.04	42,42,42,42	0
56	MG	2A	3742	1/1	0.97	0.09	27,27,27,27	0
56	MG	1A	3916	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3071	1/1	0.97	0.08	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3366	1/1	0.97	0.41	30,30,30,30	0
56	MG	1A	3412	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3662	1/1	0.97	0.08	29,29,29,29	0
56	MG	1F	310	1/1	0.97	0.06	47,47,47,47	0
56	MG	2A	3396	1/1	0.97	0.07	52,52,52,52	0
56	MG	1F	311	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3173	1/1	0.97	0.06	33,33,33,33	0
56	MG	1F	313	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3746	1/1	0.97	0.06	24,24,24,24	0
56	MG	1A	4025	1/1	0.97	0.12	36,36,36,36	0
56	MG	1A	3033	1/1	0.97	0.25	31,31,31,31	0
56	MG	1A	3108	1/1	0.97	0.17	33,33,33,33	0
56	MG	1A	3145	1/1	0.97	0.17	28,28,28,28	0
56	MG	1A	3212	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3469	1/1	0.97	0.10	38,38,38,38	0
56	MG	1A	4032	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3213	1/1	0.97	0.10	50,50,50,50	0
56	MG	2A	3764	1/1	0.97	0.15	43,43,43,43	0
56	MG	1A	3524	1/1	0.97	0.15	44,44,44,44	0
56	MG	2A	3583	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3073	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3330	1/1	0.97	0.18	29,29,29,29	0
56	MG	1A	3757	1/1	0.97	0.08	20,20,20,20	0
56	MG	1a	1646	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3376	1/1	0.97	0.18	35,35,35,35	0
56	MG	1A	3331	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3840	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3596	1/1	0.97	0.06	21,21,21,21	0
56	MG	1P	202	1/1	0.97	0.19	34,34,34,34	0
56	MG	1P	203	1/1	0.97	0.20	30,30,30,30	0
56	MG	1A	3598	1/1	0.97	0.06	31,31,31,31	0
56	MG	2A	3122	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3290	1/1	0.97	0.14	37,37,37,37	0
56	MG	1Q	202	1/1	0.97	0.04	46,46,46,46	0
56	MG	1A	3763	1/1	0.97	0.05	25,25,25,25	0
56	MG	2A	3426	1/1	0.97	0.06	72,72,72,72	0
56	MG	1A	3252	1/1	0.97	0.07	50,50,50,50	0
56	MG	2A	3428	1/1	0.97	0.07	68,68,68,68	0
56	MG	1A	3531	1/1	0.97	0.15	35,35,35,35	0
56	MG	1l	201	1/1	0.97	0.04	74,74,74,74	0
56	MG	1A	3532	1/1	0.97	0.06	25,25,25,25	0
56	MG	1A	3604	1/1	0.97	0.11	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1R	201	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	3683	1/1	0.97	0.04	15,15,15,15	0
56	MG	2A	3133	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3533	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3147	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3074	1/1	0.97	0.31	48,48,48,48	0
56	MG	1A	3536	1/1	0.97	0.27	41,41,41,41	0
56	MG	1A	3854	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3855	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3538	1/1	0.97	0.20	40,40,40,40	0
56	MG	2A	3443	1/1	0.97	0.10	43,43,43,43	0
56	MG	2D	301	1/1	0.97	0.11	42,42,42,42	0
56	MG	1U	202	1/1	0.97	0.25	38,38,38,38	0
56	MG	1a	1672	1/1	0.97	0.16	48,48,48,48	0
56	MG	1U	203	1/1	0.97	0.10	32,32,32,32	0
56	MG	2A	3447	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3111	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3858	1/1	0.97	0.05	29,29,29,29	0
56	MG	1A	3150	1/1	0.97	0.07	34,34,34,34	0
56	MG	1V	201	1/1	0.97	0.24	28,28,28,28	0
56	MG	1A	3957	1/1	0.97	0.05	40,40,40,40	0
56	MG	1V	204	1/1	0.97	0.17	53,53,53,53	0
56	MG	2E	304	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3430	1/1	0.97	0.21	56,56,56,56	0
56	MG	1A	3185	1/1	0.97	0.26	36,36,36,36	0
56	MG	1A	3066	1/1	0.97	0.07	32,32,32,32	0
56	MG	1W	202	1/1	0.97	0.18	48,48,48,48	0
56	MG	2a	1740	1/1	0.97	0.24	55,55,55,55	0
56	MG	1W	203	1/1	0.97	0.22	38,38,38,38	0
56	MG	1A	3546	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3697	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3005	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3129	1/1	0.97	0.05	45,45,45,45	0
56	MG	2F	305	1/1	0.97	0.16	48,48,48,48	0
56	MG	1X	102	1/1	0.97	0.07	39,39,39,39	0
56	MG	2A	3464	1/1	0.97	0.06	47,47,47,47	0
56	MG	1X	103	1/1	0.97	0.11	50,50,50,50	0
56	MG	2A	3466	1/1	0.97	0.07	56,56,56,56	0
56	MG	1X	104	1/1	0.97	0.12	38,38,38,38	0
56	MG	1A	3618	1/1	0.97	0.04	26,26,26,26	0
56	MG	2Q	201	1/1	0.97	0.12	64,64,64,64	0
56	MG	2a	1756	1/1	0.97	0.20	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3130	1/1	0.97	0.06	37,37,37,37	0
56	MG	2A	3470	1/1	0.97	0.06	48,48,48,48	0
56	MG	2A	3165	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3021	1/1	0.97	0.09	25,25,25,25	0
56	MG	1A	3488	1/1	0.97	0.09	33,33,33,33	0
56	MG	2A	3474	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3157	1/1	0.97	0.12	28,28,28,28	0
56	MG	2A	3476	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3063	1/1	0.97	0.10	34,34,34,34	0
56	MG	1a	1698	1/1	0.97	0.17	42,42,42,42	0
56	MG	2A	3480	1/1	0.97	0.09	48,48,48,48	0
56	MG	2A	3656	1/1	0.97	0.26	48,48,48,48	0
56	MG	1A	3973	1/1	0.97	0.05	35,35,35,35	0
56	MG	2X	102	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3089	1/1	0.97	0.15	56,56,56,56	0
56	MG	2A	3483	1/1	0.97	0.10	52,52,52,52	0
56	MG	10	102	1/1	0.97	0.05	48,48,48,48	0
56	MG	1A	3392	1/1	0.97	0.25	56,56,56,56	0
56	MG	1B	219	1/1	0.97	0.05	55,55,55,55	0
56	MG	23	101	1/1	0.97	0.06	54,54,54,54	0
56	MG	1B	220	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3977	1/1	0.97	0.07	62,62,62,62	0
56	MG	1A	3709	1/1	0.97	0.08	49,49,49,49	0
56	MG	2A	3490	1/1	0.97	0.07	41,41,41,41	0
56	MG	2A	3491	1/1	0.97	0.10	39,39,39,39	0
56	MG	1B	223	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3626	1/1	0.97	0.10	36,36,36,36	0
56	MG	1a	1710	1/1	0.97	0.05	39,39,39,39	0
56	MG	2A	3031	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3231	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3079	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3268	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3195	1/1	0.97	0.11	25,25,25,25	0
56	MG	1A	3715	1/1	0.97	0.07	52,52,52,52	0
56	MG	2A	3037	1/1	0.97	0.08	56,56,56,56	0
56	MG	1A	3497	1/1	0.97	0.08	54,54,54,54	0
56	MG	1A	3196	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3236	1/1	0.97	0.07	45,45,45,45	0
56	MG	1a	1720	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3887	1/1	0.97	0.12	36,36,36,36	0
56	MG	1A	3888	1/1	0.97	0.05	38,38,38,38	0
56	MG	15	105	1/1	0.97	0.26	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3685	1/1	0.97	0.05	50,50,50,50	0
56	MG	15	106	1/1	0.97	0.08	34,34,34,34	0
56	MG	1A	3719	1/1	0.97	0.04	43,43,43,43	0
56	MG	1A	3565	1/1	0.97	0.23	37,37,37,37	0
56	MG	1a	1727	1/1	0.97	0.20	44,44,44,44	0
56	MG	1A	3500	1/1	0.97	0.29	39,39,39,39	0
56	MG	2A	3052	1/1	0.97	0.05	53,53,53,53	0
56	MG	1B	239	1/1	0.97	0.06	37,37,37,37	0
56	MG	1A	3070	1/1	0.97	0.26	33,33,33,33	0
56	MG	1A	3273	1/1	0.97	0.24	31,31,31,31	0
56	MG	1A	3640	1/1	0.97	0.05	20,20,20,20	0
56	MG	1a	1734	1/1	0.97	0.05	56,56,56,56	0
56	MG	1A	3569	1/1	0.97	0.19	30,30,30,30	0
56	MG	1A	3137	1/1	0.97	0.05	18,18,18,18	0
56	MG	2A	3061	1/1	0.97	0.16	61,61,61,61	0
56	MG	1A	3810	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3138	1/1	0.97	0.08	49,49,49,49	0
56	MG	1A	4002	1/1	0.97	0.10	26,26,26,26	0
56	MG	2A	3531	1/1	0.97	0.08	45,45,45,45	0
56	MG	1D	310	1/1	0.97	0.14	26,26,26,26	0
56	MG	2A	3066	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3646	1/1	0.97	0.04	32,32,32,32	0
56	MG	1A	3903	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3904	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3572	1/1	0.97	0.05	25,25,25,25	0
56	MG	1E	305	1/1	0.97	0.16	28,28,28,28	0
56	MG	1A	3648	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3103	1/1	0.97	0.07	30,30,30,30	0
56	MG	1a	1608	1/1	0.97	0.06	55,55,55,55	0
56	MG	1E	308	1/1	0.97	0.12	35,35,35,35	0
57	A1A1L	1A	4060	36/36	0.97	0.08	19,28,35,44	0
56	MG	2A	3715	1/1	0.97	0.04	39,39,39,39	0
56	MG	1a	1751	1/1	0.97	0.08	62,62,62,62	0
56	MG	1a	1610	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	4009	1/1	0.97	0.06	27,27,27,27	0
56	MG	1A	3453	1/1	0.97	0.12	47,47,47,47	0
56	MG	1A	3003	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3178	1/1	0.98	0.09	40,40,40,40	0
56	MG	1A	3541	1/1	0.98	0.14	35,35,35,35	0
56	MG	1A	3203	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3690	1/1	0.98	0.07	26,26,26,26	0
56	MG	2A	3313	1/1	0.98	0.07	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3046	1/1	0.98	0.07	58,58,58,58	0
56	MG	1A	3179	1/1	0.98	0.06	40,40,40,40	0
56	MG	2A	3407	1/1	0.98	0.14	50,50,50,50	0
56	MG	1A	3589	1/1	0.98	0.08	54,54,54,54	0
56	MG	1A	3233	1/1	0.98	0.26	35,35,35,35	0
56	MG	1a	1707	1/1	0.98	0.11	57,57,57,57	0
56	MG	1A	3752	1/1	0.98	0.08	51,51,51,51	0
56	MG	2A	3505	1/1	0.98	0.05	32,32,32,32	0
56	MG	1X	105	1/1	0.98	0.05	47,47,47,47	0
56	MG	2a	1746	1/1	0.98	0.11	80,80,80,80	0
56	MG	1A	3639	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3545	1/1	0.98	0.18	32,32,32,32	0
56	MG	1A	3696	1/1	0.98	0.09	47,47,47,47	0
56	MG	1A	3289	1/1	0.98	0.07	33,33,33,33	0
56	MG	1A	3158	1/1	0.98	0.15	50,50,50,50	0
56	MG	1A	3700	1/1	0.98	0.03	26,26,26,26	0
56	MG	1A	3106	1/1	0.98	0.23	30,30,30,30	0
56	MG	2a	1754	1/1	0.98	0.08	59,59,59,59	0
56	MG	2A	3060	1/1	0.98	0.11	34,34,34,34	0
56	MG	1A	3292	1/1	0.98	0.11	41,41,41,41	0
56	MG	1A	3207	1/1	0.98	0.23	39,39,39,39	0
56	MG	1a	1719	1/1	0.98	0.05	45,45,45,45	0
56	MG	1A	3597	1/1	0.98	0.06	52,52,52,52	0
56	MG	1A	3264	1/1	0.98	0.14	28,28,28,28	0
56	MG	2A	3243	1/1	0.98	0.18	51,51,51,51	0
56	MG	1A	3013	1/1	0.98	0.16	29,29,29,29	0
56	MG	2a	1659	1/1	0.98	0.06	60,60,60,60	0
56	MG	2A	3717	1/1	0.98	0.10	45,45,45,45	0
56	MG	1A	3651	1/1	0.98	0.07	24,24,24,24	0
56	MG	1A	3943	1/1	0.98	0.09	53,53,53,53	0
56	MG	2A	3157	1/1	0.98	0.12	38,38,38,38	0
56	MG	1A	3360	1/1	0.98	0.16	29,29,29,29	0
56	MG	1A	3601	1/1	0.98	0.04	26,26,26,26	0
56	MG	1a	1648	1/1	0.98	0.09	47,47,47,47	0
56	MG	2O	201	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	3183	1/1	0.98	0.16	39,39,39,39	0
56	MG	2A	3725	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3656	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3397	1/1	0.98	0.16	39,39,39,39	0
56	MG	2A	3729	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3558	1/1	0.98	0.15	33,33,33,33	0
56	MG	1N	203	1/1	0.98	0.04	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3031	1/1	0.98	0.14	34,34,34,34	0
56	MG	1A	3951	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3363	1/1	0.98	0.10	49,49,49,49	0
56	MG	1A	3133	1/1	0.98	0.28	35,35,35,35	0
56	MG	1A	3516	1/1	0.98	0.28	34,34,34,34	0
56	MG	15	104	1/1	0.98	0.19	27,27,27,27	0
56	MG	1A	3121	1/1	0.98	0.16	34,34,34,34	0
56	MG	1A	3894	1/1	0.98	0.05	44,44,44,44	0
56	MG	1a	1742	1/1	0.98	0.07	55,55,55,55	0
56	MG	1A	3010	1/1	0.98	0.10	31,31,31,31	0
56	MG	1A	3214	1/1	0.98	0.16	42,42,42,42	0
56	MG	1P	201	1/1	0.98	0.28	33,33,33,33	0
56	MG	1A	3068	1/1	0.98	0.10	19,19,19,19	0
56	MG	1B	230	1/1	0.98	0.06	41,41,41,41	0
56	MG	1P	204	1/1	0.98	0.25	33,33,33,33	0
56	MG	2A	3092	1/1	0.98	0.05	28,28,28,28	0
56	MG	17	102	1/1	0.98	0.08	31,31,31,31	0
56	MG	17	103	1/1	0.98	0.10	35,35,35,35	0
56	MG	25	102	1/1	0.98	0.20	47,47,47,47	0
56	MG	1A	3304	1/1	0.98	0.08	37,37,37,37	0
56	MG	1A	3044	1/1	0.98	0.08	36,36,36,36	0
56	MG	2A	3009	1/1	0.98	0.07	46,46,46,46	0
56	MG	27	101	1/1	0.98	0.10	39,39,39,39	0
56	MG	2A	3755	1/1	0.98	0.04	54,54,54,54	0
56	MG	2A	3010	1/1	0.98	0.06	43,43,43,43	0
56	MG	1Q	201	1/1	0.98	0.07	31,31,31,31	0
56	MG	1A	3484	1/1	0.98	0.15	27,27,27,27	0
56	MG	1A	3060	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3671	1/1	0.98	0.03	16,16,16,16	0
56	MG	2A	3015	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	4030	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3617	1/1	0.98	0.03	27,27,27,27	0
56	MG	1A	3967	1/1	0.98	0.07	32,32,32,32	0
56	MG	1a	1761	1/1	0.98	0.06	68,68,68,68	0
56	MG	1A	3168	1/1	0.98	0.14	42,42,42,42	0
56	MG	1A	3219	1/1	0.98	0.14	32,32,32,32	0
56	MG	1A	3169	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3971	1/1	0.98	0.06	23,23,23,23	0
56	MG	1D	304	1/1	0.98	0.09	22,22,22,22	0
56	MG	1A	4037	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3375	1/1	0.98	0.07	30,30,30,30	0
56	MG	2A	3477	1/1	0.98	0.11	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3170	1/1	0.98	0.06	31,31,31,31	0
56	MG	1A	3152	1/1	0.98	0.21	30,30,30,30	0
56	MG	1A	3037	1/1	0.98	0.11	26,26,26,26	0
56	MG	1A	3082	1/1	0.98	0.12	31,31,31,31	0
56	MG	1A	3038	1/1	0.98	0.17	36,36,36,36	0
56	MG	1a	1691	1/1	0.98	0.15	47,47,47,47	0
56	MG	1A	3156	1/1	0.98	0.16	35,35,35,35	0
56	MG	1A	3457	1/1	0.98	0.15	40,40,40,40	0
56	MG	1E	302	1/1	0.98	0.22	35,35,35,35	0
56	MG	1A	3537	1/1	0.98	0.12	41,41,41,41	0
56	MG	1E	304	1/1	0.98	0.09	33,33,33,33	0
58	ZN	2Y	202	1/1	0.98	0.04	91,91,91,91	0
56	MG	1A	3742	1/1	0.98	0.03	44,44,44,44	0
58	ZN	29	501	1/1	0.98	0.05	74,74,74,74	0
56	MG	2A	3039	1/1	0.98	0.12	50,50,50,50	0
56	MG	1A	3347	1/1	0.98	0.09	42,42,42,42	0
56	MG	2A	3517	1/1	0.99	0.03	41,41,41,41	0
56	MG	2A	3625	1/1	0.99	0.05	34,34,34,34	0
56	MG	1A	3551	1/1	0.99	0.05	36,36,36,36	0
56	MG	1A	3012	1/1	0.99	0.03	30,30,30,30	0
56	MG	1F	303	1/1	0.99	0.16	33,33,33,33	0
56	MG	1A	3115	1/1	0.99	0.07	36,36,36,36	0
56	MG	1A	3653	1/1	0.99	0.06	30,30,30,30	0
56	MG	1A	3171	1/1	0.99	0.10	29,29,29,29	0
56	MG	1A	3773	1/1	0.99	0.03	46,46,46,46	0
56	MG	2A	3633	1/1	0.99	0.05	60,60,60,60	0
56	MG	1F	308	1/1	0.99	0.17	30,30,30,30	0
56	MG	2A	3749	1/1	0.99	0.05	44,44,44,44	0
56	MG	1A	4053	1/1	0.99	0.03	37,37,37,37	0
56	MG	1A	3975	1/1	0.99	0.06	34,34,34,34	0
56	MG	13	101	1/1	0.99	0.07	33,33,33,33	0
56	MG	1A	3095	1/1	0.99	0.11	24,24,24,24	0
56	MG	1A	3905	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	3005	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3186	1/1	0.99	0.24	26,26,26,26	0
56	MG	1A	3449	1/1	0.99	0.07	36,36,36,36	0
56	MG	1a	1770	1/1	0.99	0.04	52,52,52,52	0
56	MG	1U	206	1/1	0.99	0.28	35,35,35,35	0
56	MG	1A	3293	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3229	1/1	0.99	0.17	32,32,32,32	0
56	MG	1A	3633	1/1	0.99	0.04	37,37,37,37	0
56	MG	1V	203	1/1	0.99	0.15	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3078	1/1	0.99	0.09	38,38,38,38	0
56	MG	1A	3201	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3721	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3879	1/1	0.99	0.03	24,24,24,24	0
56	MG	1A	3988	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3880	1/1	0.99	0.03	27,27,27,27	0
56	MG	1W	204	1/1	0.99	0.09	40,40,40,40	0
56	MG	1a	1733	1/1	0.99	0.09	59,59,59,59	0
56	MG	2A	3772	1/1	0.99	0.06	57,57,57,57	0
56	MG	1A	3014	1/1	0.99	0.07	32,32,32,32	0
56	MG	1A	3991	1/1	0.99	0.03	22,22,22,22	0
56	MG	1A	3023	1/1	0.99	0.08	19,19,19,19	0
56	MG	1A	3519	1/1	0.99	0.09	27,27,27,27	0
56	MG	1A	3418	1/1	0.99	0.20	39,39,39,39	0
56	MG	1A	3437	1/1	0.99	0.23	37,37,37,37	0
56	MG	1A	3641	1/1	0.99	0.06	24,24,24,24	0
56	MG	1A	3057	1/1	0.99	0.07	25,25,25,25	0
56	MG	2A	3609	1/1	0.99	0.04	65,65,65,65	0
56	MG	1A	3699	1/1	0.99	0.08	31,31,31,31	0
56	MG	1A	3065	1/1	0.99	0.12	30,30,30,30	0
56	MG	1A	3644	1/1	0.99	0.04	24,24,24,24	0
56	MG	1A	3039	1/1	0.99	0.27	35,35,35,35	0
56	MG	1A	3963	1/1	0.99	0.03	35,35,35,35	0
56	MG	2A	3727	1/1	0.99	0.04	54,54,54,54	0
56	MG	1A	3221	1/1	0.99	0.14	33,33,33,33	0
56	MG	1A	3462	1/1	0.99	0.08	37,37,37,37	0
56	MG	1A	3549	1/1	0.99	0.10	39,39,39,39	0
56	MG	2A	3511	1/1	0.99	0.08	43,43,43,43	0
58	ZN	1Y	204	1/1	0.99	0.03	65,65,65,65	0
56	MG	1A	3009	1/1	0.99	0.03	23,23,23,23	0
58	ZN	15	109	1/1	0.99	0.08	49,49,49,49	0
58	ZN	1n	103	1/1	0.99	0.03	66,66,66,66	0
56	MG	2A	3513	1/1	0.99	0.07	66,66,66,66	0
56	MG	1A	3896	1/1	0.99	0.02	14,14,14,14	0
58	ZN	25	106	1/1	0.99	0.04	54,54,54,54	0
58	ZN	26	501	1/1	0.99	0.05	66,66,66,66	0
56	MG	1a	1752	1/1	0.99	0.09	56,56,56,56	0
56	MG	2A	3516	1/1	0.99	0.07	41,41,41,41	0
59	SF4	1d	302	8/8	0.99	0.05	62,68,71,74	0
59	SF4	2d	302	8/8	0.99	0.05	62,71,81,82	0
56	MG	2A	3737	1/1	0.99	0.03	36,36,36,36	0
56	MG	1A	3728	1/1	1.00	0.08	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3898	1/1	1.00	0.07	34,34,34,34	0
58	ZN	16	104	1/1	1.00	0.04	46,46,46,46	0
58	ZN	19	102	1/1	1.00	0.06	47,47,47,47	0
56	MG	1A	3874	1/1	1.00	0.07	39,39,39,39	0
56	MG	1a	1769	1/1	1.00	0.04	49,49,49,49	0
56	MG	1A	3774	1/1	1.00	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.