



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 09:58 AM EDT

PDB ID : 9MTP / pdb_00009mtp
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with mRNA, A-site Q230-N5-methylated Release Factor 1, and P-site fM EAAAKC-peptidyl-tRNA_{cys} at 2.40Å resolution
Authors : Aleksandrova, E.V.; Syroegin, E.A.; Basu, R.S.; Vassilevski, A.A.; Gagnon, M.G.; Polikanov, Y.S.
Deposited on : 2025-01-12
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

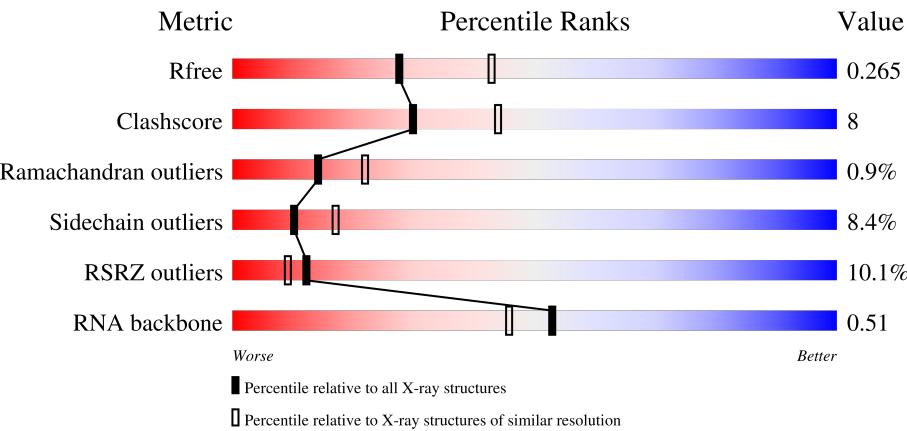
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.40 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.



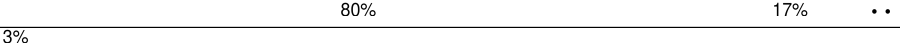
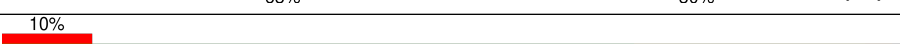
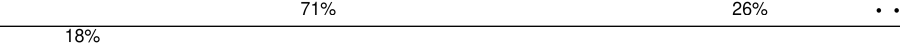
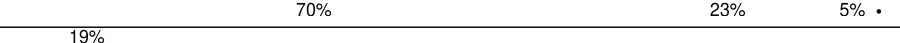
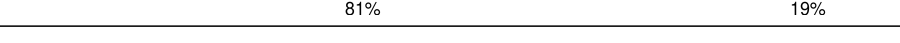
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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	
1	2A	2915	
2	1B	121	

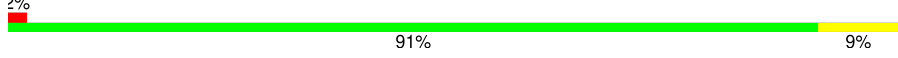
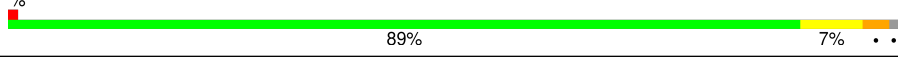
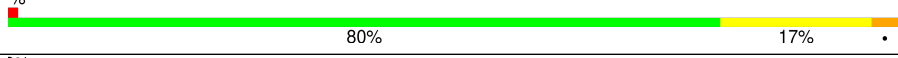
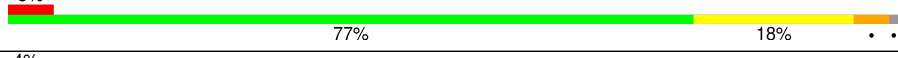
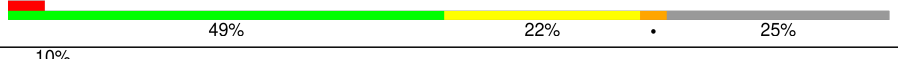
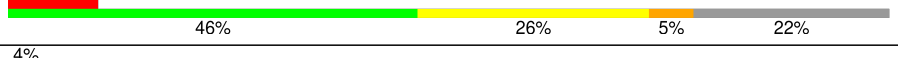
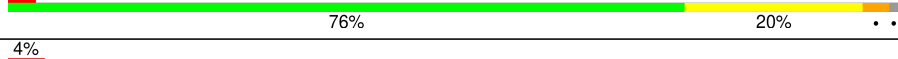
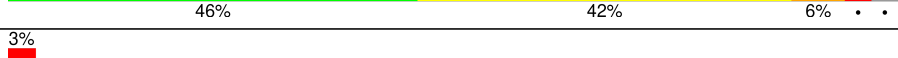
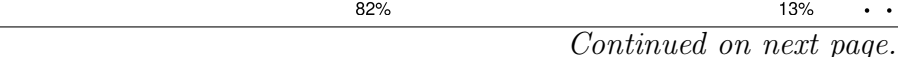
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	354	
54	2w	354	
55	1x	74	
55	2x	74	
56	1z	7	
56	2z	7	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1U	211	-	-	-	X
57	MG	1a	1640	-	-	-	X
57	MG	1a	1716	-	-	-	X
57	MG	2A	3263	-	-	-	X

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 297056 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	249	Total	C	N	O	S	0	0	0
			1939	1199	360	371	9			
54	2w	253	Total	C	N	O	S	0	0	0
			1957	1210	361	377	9			

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMEAAAKC-tRNA_{cys} RNA-part.

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

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMEAAAKC-tRNA_{cys} Peptide-part.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1101	Total	Mg	0	0
			1101	1101		
57	1B	38	Total	Mg	0	0
			38	38		
57	1D	14	Total	Mg	0	0
			14	14		
57	1E	13	Total	Mg	0	0
			13	13		
57	1F	16	Total	Mg	0	0
			16	16		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	4	Total 4	Mg 4	0	0
57	1O	4	Total 4	Mg 4	0	0
57	1P	7	Total 7	Mg 7	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	4	Total 4	Mg 4	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	3	Total 3	Mg 3	0	0
57	1U	11	Total 11	Mg 11	0	0
57	1V	7	Total 7	Mg 7	0	0
57	1W	5	Total 5	Mg 5	0	0
57	1X	5	Total 5	Mg 5	0	0
57	1Y	4	Total 4	Mg 4	0	0
57	1Z	2	Total 2	Mg 2	0	0
57	10	7	Total 7	Mg 7	0	0
57	11	4	Total 4	Mg 4	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	3	Total 3	Mg 3	0	0
57	15	9	Total 9	Mg 9	0	0
57	16	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	17	5	Total 5	Mg 5	0	0
57	18	4	Total 4	Mg 4	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	215	Total 215	Mg 215	0	0
57	1b	2	Total 2	Mg 2	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	3	Total 3	Mg 3	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1k	1	Total 1	Mg 1	0	0
57	1l	2	Total 2	Mg 2	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	2	Total 2	Mg 2	0	0
57	1r	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	4	Total 4	Mg 4	0	0
57	1w	1	Total 1	Mg 1	0	0
57	1x	12	Total 12	Mg 12	0	0
57	2A	852	Total 852	Mg 852	0	0
57	2B	19	Total 19	Mg 19	0	0
57	2D	7	Total 7	Mg 7	0	0
57	2E	8	Total 8	Mg 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2F	7	Total 7	Mg 7	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	2	Total 2	Mg 2	0	0
57	2P	2	Total 2	Mg 2	0	0
57	2Q	4	Total 4	Mg 4	0	0
57	2R	1	Total 1	Mg 1	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2U	2	Total 2	Mg 2	0	0
57	2V	2	Total 2	Mg 2	0	0
57	2W	2	Total 2	Mg 2	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	1	Total 1	Mg 1	0	0
57	21	2	Total 2	Mg 2	0	0
57	23	4	Total 4	Mg 4	0	0
57	25	7	Total 7	Mg 7	0	0
57	26	1	Total 1	Mg 1	0	0
57	28	3	Total 3	Mg 3	0	0
57	29	1	Total 1	Mg 1	0	0
57	2a	185	Total 185	Mg 185	0	0
57	2d	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2e	2	Total Mg 2 2	0	0
57	2f	1	Total Mg 1 1	0	0
57	2g	1	Total Mg 1 1	0	0
57	2i	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2l	2	Total Mg 2 2	0	0
57	2n	1	Total Mg 1 1	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	1	Total Mg 1 1	0	0
57	2x	5	Total Mg 5 5	0	0

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

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

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

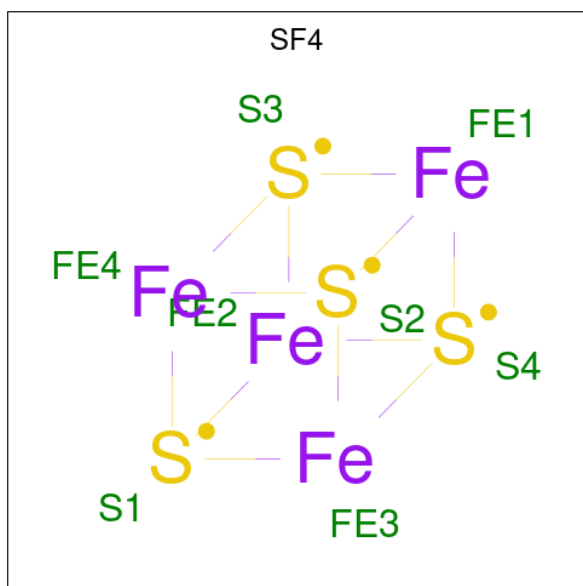
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2078	Total O 2078 2078	0	0
61	1B	64	Total O 64 64	0	0
61	1D	26	Total O 26 26	0	0
61	1E	25	Total O 25 25	0	0
61	1F	14	Total O 14 14	0	0
61	1G	3	Total O 3 3	0	0
61	1H	4	Total O 4 4	0	0
61	1I	1	Total O 1 1	0	0
61	1N	3	Total O 3 3	0	0
61	1O	8	Total O 8 8	0	0
61	1P	22	Total O 22 22	0	0
61	1Q	10	Total O 10 10	0	0
61	1R	14	Total O 14 14	0	0
61	1S	4	Total O 4 4	0	0
61	1T	5	Total O 5 5	0	0
61	1U	12	Total O 12 12	0	0
61	1V	9	Total O 9 9	0	0
61	1W	12	Total O 12 12	0	0
61	1X	2	Total O 2 2	0	0
61	1Y	3	Total O 3 3	0	0
61	1Z	1	Total O 1 1	0	0
61	10	10	Total O 10 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	11	10	Total 10	O 10	0	0
61	12	4	Total 4	O 4	0	0
61	13	5	Total 5	O 5	0	0
61	15	6	Total 6	O 6	0	0
61	16	2	Total 2	O 2	0	0
61	17	8	Total 8	O 8	0	0
61	18	13	Total 13	O 13	0	0
61	1a	287	Total 287	O 287	0	0
61	1d	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1f	2	Total 2	O 2	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	3	Total 3	O 3	0	0
61	1q	1	Total 1	O 1	0	0
61	1v	7	Total 7	O 7	0	0
61	1w	1	Total 1	O 1	0	0
61	1x	19	Total 19	O 19	0	0
61	2A	1124	Total 1124	O 1124	0	0
61	2B	19	Total 19	O 19	0	0
61	2D	23	Total 23	O 23	0	0
61	2E	17	Total 17	O 17	0	0

Continued on next page...

Continued from previous page...

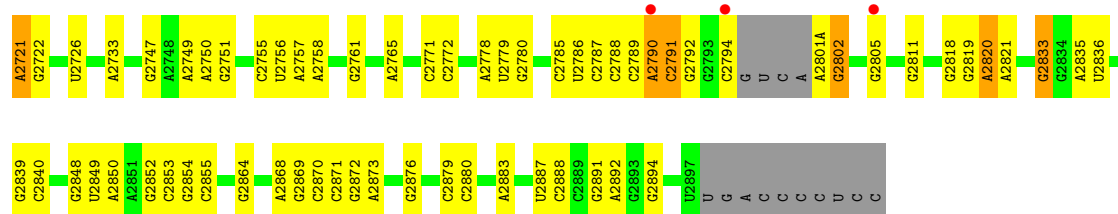
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2F	14	Total 14	O 14	0	0
61	2I	1	Total 1	O 1	0	0
61	2N	2	Total 2	O 2	0	0
61	2O	2	Total 2	O 2	0	0
61	2P	13	Total 13	O 13	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	4	Total 4	O 4	0	0
61	2T	3	Total 3	O 3	0	0
61	2U	2	Total 2	O 2	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	2	Total 2	O 2	0	0
61	2X	4	Total 4	O 4	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	5	Total 5	O 5	0	0
61	21	9	Total 9	O 9	0	0
61	22	1	Total 1	O 1	0	0
61	23	2	Total 2	O 2	0	0
61	25	1	Total 1	O 1	0	0
61	27	3	Total 3	O 3	0	0
61	28	4	Total 4	O 4	0	0

Continued on next page...

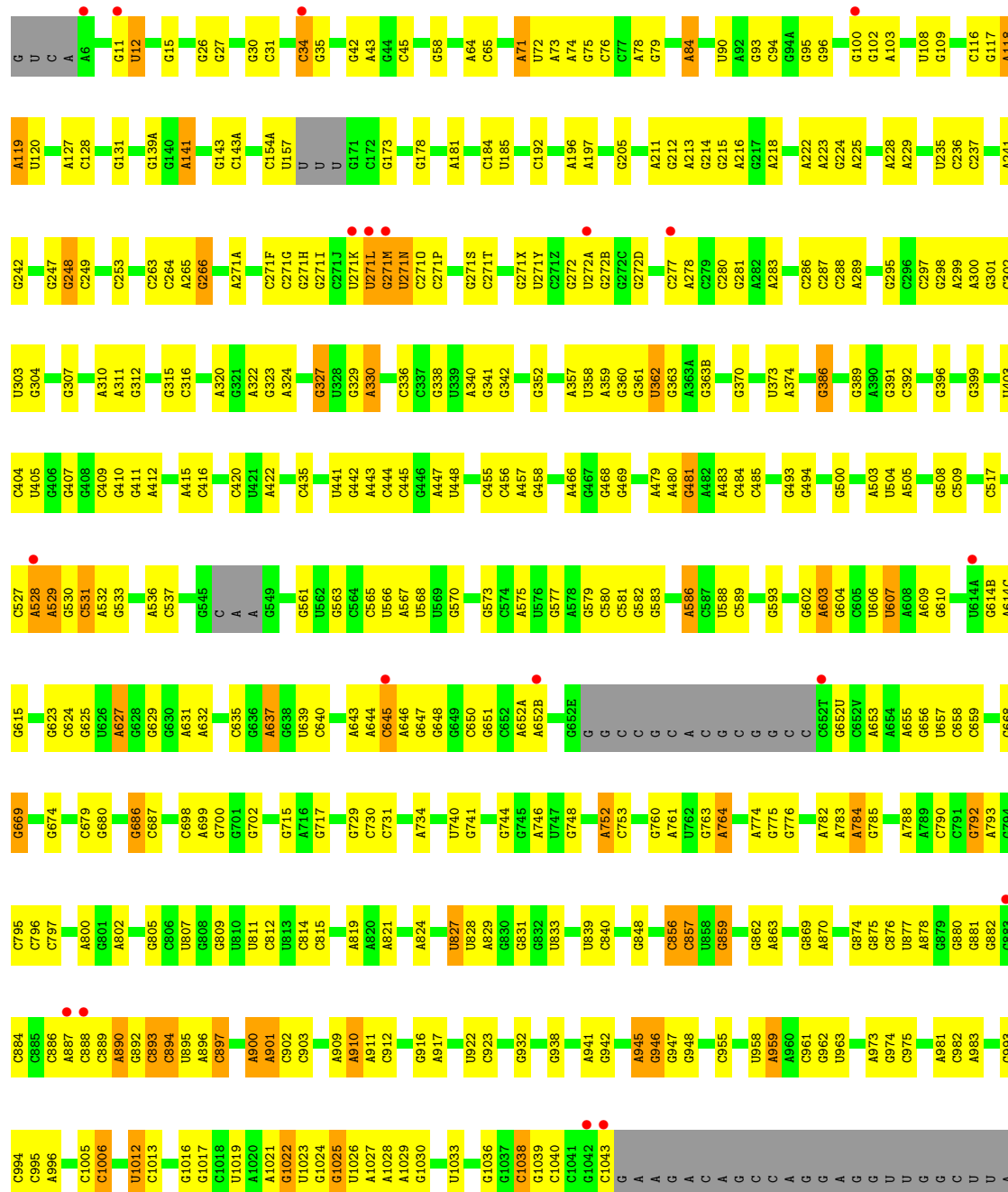
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	29	1	Total 1	O 1	0	0
61	2a	144	Total 144	O 144	0	0
61	2d	3	Total 3	O 3	0	0
61	2e	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	2	Total 2	O 2	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	4	Total 4	O 4	0	0
61	2q	2	Total 2	O 2	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	3	Total 3	O 3	0	0
61	2v	2	Total 2	O 2	0	0
61	2w	5	Total 5	O 5	0	0
61	2x	17	Total 17	O 17	0	0

G2603	U2491	C2359	G2250	G2160	G2100	G1991	G1865	G1746	G1581	G1448	G1382	G1187	U1081
U2604	G2494	A2360	G2251	C2161	G2101	U1992	C1865	G1753	C1582	A1449	G1332	G1188	U1082
U2605	A2268	A2366	A2269	C2162	U2102	U1993	C1866	C1754	A1583	G1450	G1339	U1189	U1083
U2609	G2502	G2375	G2271	C2164	G2103	C1996	G1877	A1756	A1586	U1453	A1342	G1191	A1086
C2610	A2503	A2376	U2272	G2165	G2104	G1997	G1878	G1755	C1607	G1455	U1342	G1195	G1087
U2611	U2504	A2377	A2273	G2166	G2105	G1998	C1882	A1759	A1608	A1460	U1352	C1196	A1088
C2612	G2505	U2378	A2274	U2167	G2106	G1999	G1883	A1760	A1610	G1466	A1353	C1197	A1089
U2615	U2506	G2379	G2275	A2169	U2109	A2001	A1889	G1762	A1610	G1467	A1354	U1197	U1090
C2616	C2507	G2382	G2277	A2170	G2110	G2002	A1890	G1763	G1622	C1468	G1355	U1198	C1092
C2617	G2512	A2383	G2280	A2171	C2111	C2006	G1891	G1764	G1636	A1469	A1359	C1201	G1093
A2629	G2513	G2385	G2281	A2172	U2112	G2006	C1892	G1769	A1637	G1482	A1360	U1205	U1094
G2630	A2518	C2385	C2283	A2173	U2113	G2010	G1899	G1769	A1637	G1484	U1205	U1205	A1095
U2647	G2525	U2390	A2286	C2175	G2114	A2013	G1899	G1769	A1637	G1484	A1360	U1205	A1096
C2648	U2529	U2406	A2288	C2176	G2115	A2014	A1900	A1773	A1641	G1485	A1365	A1210	U1097
U2649	G2532	G2407	G2289	C2177	A2116	A2014	A1900	A1773	A1641	G1485	A1365	G1212	A1098
U2650	G2535	G2422	G2290	C2178	U2117	A2014	G1906	A1780	G1642	C1483	C1370	C1218	C1100
A2654	U2537	A2423	G2291	C2179	G2118	A2020	U1911	G1781	G1645	A1507	G1371	G1219	U1101
C2658	C2538	C2424	G2292	U2180	G2119	C2021	G1915	C1782	C1646	A1508	G1372	G1219	C1102
U2657	G2539	A2425	A2305	G2181	G2120	U2022	C1914	A1783	G1647	C1509	A1373	A1220	A1103
G2663	U2540	A2426	G2306	C2182	G2121	U2022	C1914	A1783	C1648	A1509A	A1379	G1239	U1105
G2673	C2551	G2428	G2307	U2189	G2122	G2023	U1915	A1786	G1663	A1509B	G1380	U1240	G1106
U2678	U2552	G2429	G2308	G2190	G2123	C2040	U1916	A1786	G1663	A1509B	G1380	U1240	G1106
A2679	G2553	A2430	G2309	C2191	U2130	U2041	U1917	A1791	A1654	U1518	A1384	A1241	G1110
U2687	U2554	U2431	U2312	G2198	U2131	A2042	C1920	U1796	U1659	G1519	G1385	G1242	A1111
G2683	U2555	A2435	G2313	A2199	G2132	C2043	G1929	U1797	U1659	G1519	G1385	G1242	A1111
G2685	G2557	G2436	A2134	C2200	G2133	G2043	G1930	U1797	U1659	G1519	G1385	G1242	A1111
G2686	U2558	A2439	G2321	C2200	G2134	G2043	G1931	U1797	U1659	G1519	G1385	G1242	A1111
U2688	U2563	C2440	G2325	C2206	G2135	G2043	A1932	U1797	U1659	G1519	G1385	G1242	A1111
U2689	A2565	C2441	C2326	G2207	G2136	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
C2690	A2566	G2447	A2327	A2208	G2137	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
G2691	G2567	A2448	G2329	U2218	G2138	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
C2692	G2568	A2451	G2331	G2224	G2139	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
A2693	C2573	G2461	G2334	A2225	G2140	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
G2694	U2574	U2462	A2335	C2226	G2141	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
U2702	A2577	U2463	A2336	U2233	G2142	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
G2703	G2578	C2464	A2337	G2234	G2143	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
G2706	G2581	G2468	U2347	G2235	G2144	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
A2711	U2585	A2469	U2348	C2236	G2145	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
A2712A	G2586	G2476	G2349	G2237	G2146	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
A2713	C2591	A2477	C2350	G2238	G2147	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
G2714	G2592	G2478	G2351	G2239	G2148	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
U2715	C2601	C2483	C2355	U2243	G2149	G2043	A1933	U1797	U1659	G1519	G1385	G1242	A1111
U2716	A2602			U2244	U2150	U2079	C1962	A1847	G1740	U1578	A1445A	G1319	C1179
				U2245	G2151	U2086	G1963	A1848	A1741	U1579	C1445A	G1319	C1179
					G2152	U2087	G1964	A1848	A1741	U1579	C1445A	G1319	C1179
					G2153	G2087	A1966	A1848	A1741	U1579	C1445A	G1319	C1179
					G2154	G2087	A1966	A1848	A1741	U1579	C1445A	G1319	C1179
					G2155	G2087	A1966	A1848	A1741	U1579	C1445A	G1319	C1179
					G2156	G2087	A1966	A1848	A1741	U1579	C1445A	G1319	C1179
					G2157	G2087	A1966	A1848	A1741	U1579	C1445A	G1319	C1179
					G2158	G2087	A1966	A1848	A1741	U1579	C1445A	G1319	C1179
					G2159	G2087	A1966	A1848	A1741	U1579	C1445A	G1319	C1179



• Molecule 1: 23S Ribosomal RNA

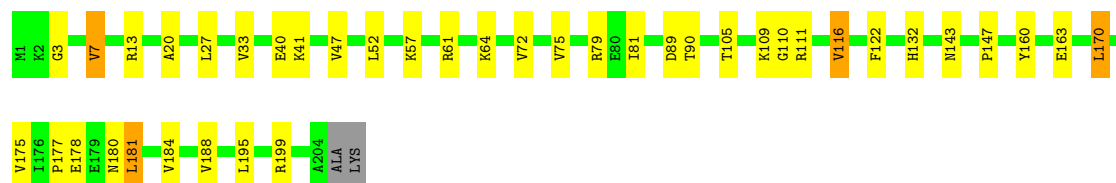


G2386	G2306	C2188	C2043	A1938	A1812	A1693	A1554	U1453	G1364	A1247	G1136	G
U2387	G2307	U2189	G2049	U1939	A1815	U1693	C1557	G1455	A1365	A1247	G1139	A
A2388	G2308	G2190	C2050	C1942	A1816	A1698	A1558	G1456	A1366	A1253	C1140	A
G2389	G2191	G2192	A2051	U1943	G1817	G1699	G1559	A1460	A1367	A1254	U1141	C
U2390	C2312	G2193	G2052	A1952	G1822	U1709	A1566	G1465	C1370	U1255	U1142	A
G2391	C2313	A2134	G2053	A1952	G1822	U1709	A1566	G1466	G1371	G1256	A1142A	C
G2396	C2314	A2135	A2054	U1955	C1827	U1710	A1569	C1467	U1372	C1261	A1143	C
C2404	G2316	C2136	G2055	U1956	G1828	G1721	A1570	G1470	A1262	U1263	G1144	C
G2405	G2317	C2137	G2056	U1957	A1829	A1722	A1571	G1471	C1376	G1149	G1149	A
U2406	G2318	C2138	C2057	C1958	U1833	U1739	A1572	A1472	G1264	C1150	C1150	U
G2410	A2320	C2139	A2060	C1958	U1833	U1739	A1572	A1472	A1268	G1154	G1154	C
G2410	G2321	C2140	G2061	C1958	U1834	G1740	U1578	G1473	A1269	G1155	G1155	U
A2422	A2322	G2141	A2062	C1962	U1834	G1740	U1578	G1473	A1269	G1155	G1155	U
U2423	C2226	C2142	A2062	U1963	G1835	A1741	A1579	A1477	A1270	A1155	A1155	U
U2424	A2227	C2143	C2064	U1963	G1836	G1742	A1580	A1477	C1270	A1155	A1155	U
C2424	G2325	U2144	C2065	C1967	C1837	C1743	A1583	G1478	G1271	G1169	G1169	A
A2425	G2326	C2145	C2066	C1968	C1838	G1746	A1584	G1482	A1272	G1170	G1170	A
A2426	G2327	C2146	C2066	A1969	C1839	G1746	A1586	A1490	U1273	G1171	G1171	A
G2427	A2328	G2147	G2069	A1970	G1839	G1756	A1587	A1490	A1274	G	G	A
G2428	G2329	C2148	G2070	A1971	A1847	G1762	A1593	U1405	A1275	U	U	A
G2429	G2239	U2150	A2071	G1973	A1848	G1763	G1594	U1406	A1276	U	U	A
A2430	A2335	G2151	G2080	A1981	G1858	A1762	G1593	U1407	A1284	A	A	C
U2431	A2336	G2152	G2080	A1981	A1859	G1764	G1594	C1407	G1297	C1178	C1178	C
A2434	C2343	G2153	U2086	G1984	C1866	C1765	G1604	C1408	C1297	C1179	C1179	G
A2435	U2344	G2154	G2087	G1984	A1876	U1766	G1604	C1409	C1297	C1180	C1180	U
G2443	G2345	G2155	U2096	U1991	A1877	C1767	A1608	G1410	U1300	G1184	G1184	A
G2445	G2346	G2156	U2097	U1991	A1877	C1767	A1609	C1411	A1301	G1184	G1184	A
A2439	A2346	G2157	U2098	G1992	A1878	U1769	A1610	A1412	A1302	G1187	G1187	U
C2441	C2347	A2158	U2098	U1993	G1878	G1769	A1611	G1413	G1303	U1188	U1188	A
C2442	C2348	G2159	U2099	G1983	A1883	A1773	G1630	G1414	G1303	U1188	U1188	A
G2442	C2349	G2160	G2100	G1983	G1883	A1773	G1630	G1414	G1303	U1188	U1188	A
G2443	G2251	G2161	G2101	A2001	A1889	U1778	G1631	C1509	G1310	A1189	A1189	C
G2445	G2255	G2162	U2102	G2002	A1890	U1779	G1631	C1509A	G1311	A1189	A1189	C
G2446	G2255	G2163	C2103	G2002	A1890	U1779	G1633	C1509B	G1311	A1189	A1189	C
G2447	G2273	C2164	C2104	G2010	G1999	G1781	G1636	G1510	C1314	G1191	G1191	C
A2448	A2274	G2165	C2105	G2011	A1900	C1782	G1636	G1510	C1314	G1191	G1191	C
U2449	G2275	G2166	G2106	U2011	A1901	C1782	G1637	U1514	U1316	C1200	C1200	C
A2450	G2276	U2167	C2107	G2012	G1902	A1783	C1638	G1426	A1317	C1201	C1201	C
U2457	G2277	G2168	C2108	A2013	G1903	A1785	U1639	G1427	C1318	C1202	C1202	C
U2457	G2280	A2169	U2109	A2014	G1906	A1786	G1647	A1427	C1319	C1203	C1203	C
U2462	G2283	A2170	G2110	A2015	G1907	A1786	G1648	G1428	A1204	U1205	U1205	C
C2465	C2287	A2171	G2111	A2015	C1908	U1790	G1648	G1429	C1320	A1210	A1210	A
G2468	U2291	C2174	G2112	A2019	U1911	A1791	G1651	C1532	G1324	U1211	U1211	A
A2469	C2292	A2175	A2114	A2020	U1911	A1791	G1651	U	G1339	G1212	G1212	A
A2476	U2296	C2176	G2115	C2021	C1914	U1794	A1652	A1434	A1342	A1220	A1220	A
C2477	G2299	A2176	G2116	G2023	U1915	C1796	A1654	G1435	A1342	C1221	C1221	A
U2480	G2300	C2177	A2117	G2023	A1916	C1797	G1667	G1436	G1346	C1221A	C1221A	A
C2483	C2301	C2178	U2118	G2027	U1917	U1798	G1667	G1437	G1346	C1222	C1222	A
G2484	G2302	C2179	A2119	A2030	C1920	U1799	G1667	U1362	U1362	G1223	G1223	A
G2485	G2303	U2180	G2120	A2030	C1920	U1799	G1667	A1445	A1353	A1226	A1226	A
G2486	G2304	G2181	G2121	A2031	G1801	A1542	C1543	A1448	A1354	A1226	A1226	A
G2486	G2305	G2182	U2122	G2032	A1802	C1543	C1546	G1449	A1355	G1229	G1229	A
G2486	G2306	G2183	G2123	A2033	A1803	C1546	C1547	G1450	G1356	G1239	G1239	A
G2486	G2307	G2184	G2124	A2033	U1931	C1547	C1548	C1450A	A1357	U1240	U1240	A
G2486	G2308	C2185	G2125	C2040	A1932	C1548	C1548	A1451	A1359	G1131	G1131	A
G2486	G2309	G2186	A2126	U2041	G1933	C1548	C1548	A1452	A1360	C1135	C1135	A
G2486	G2310	G2187	G2127	A2042	G1933	C1548	C1548	A1452	A1360	C1135	C1135	A



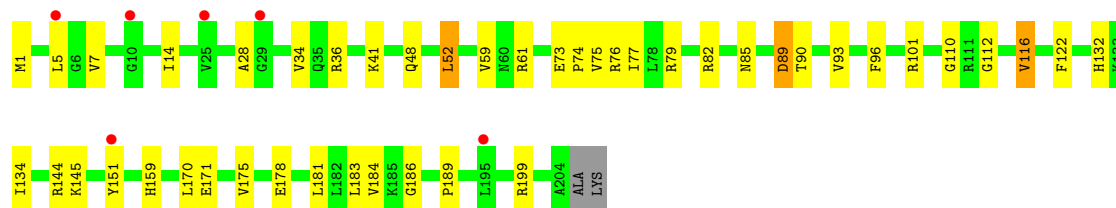
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 80% 17% ..



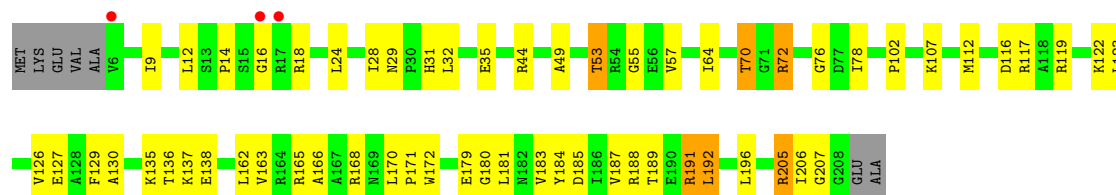
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 77% 20% ..



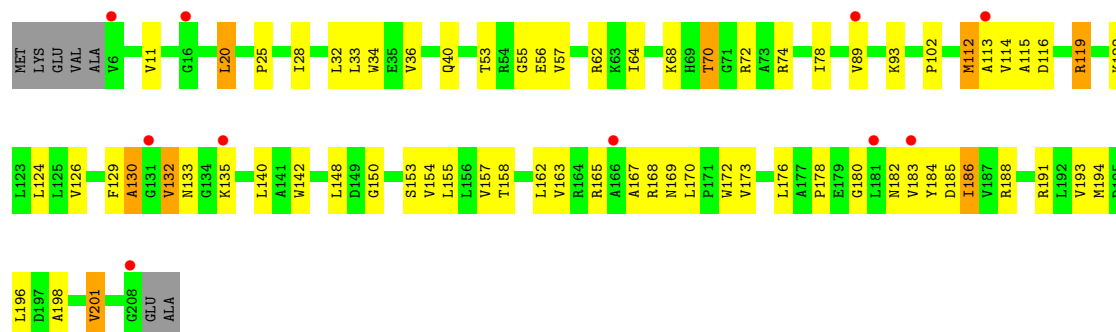
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 68% 26% ..

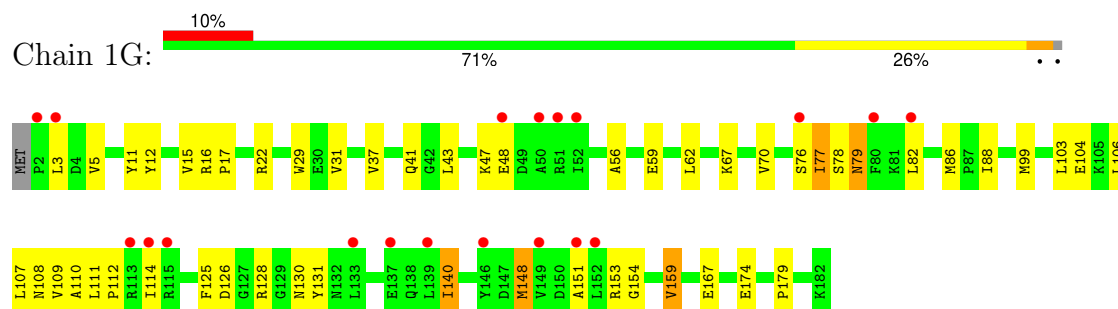


• Molecule 5: 50S ribosomal protein L4

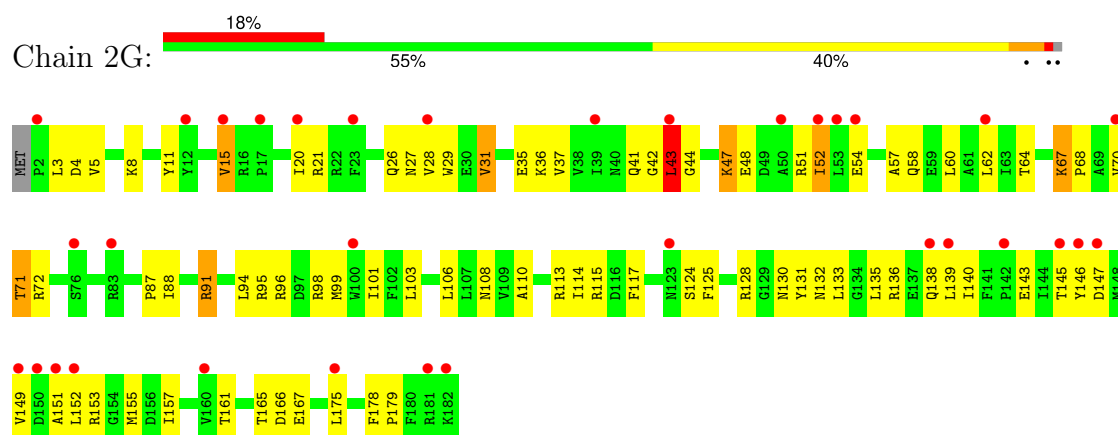
Chain 2F: 63% 30% ..



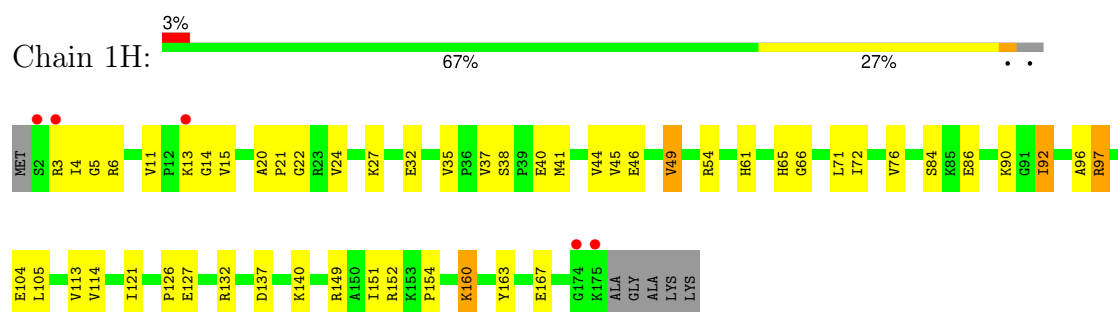
- Molecule 6: 50S ribosomal protein L5



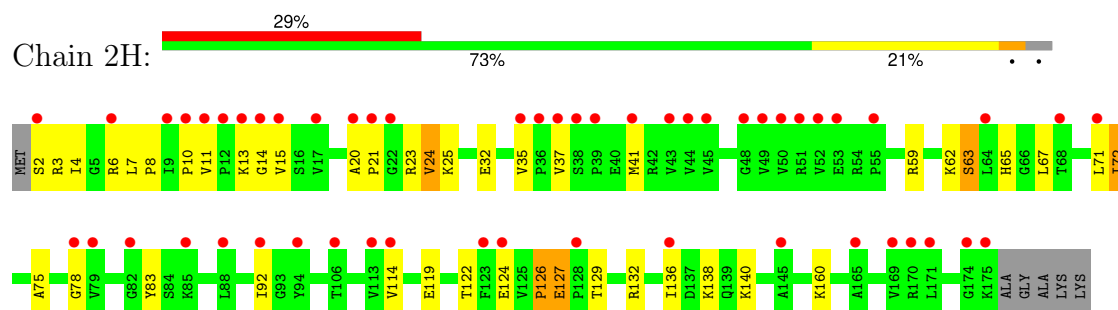
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6

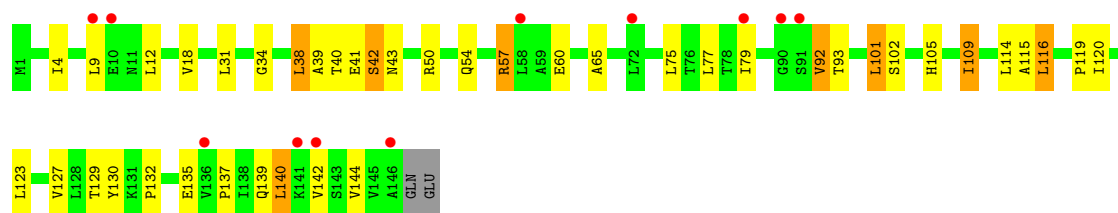


- Molecule 7: 50S ribosomal protein L6

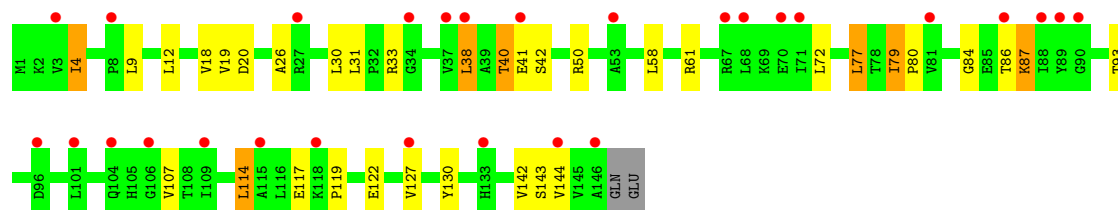
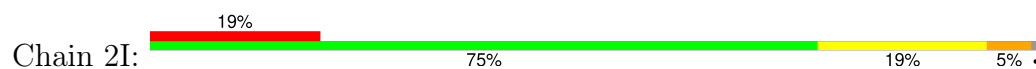


- Molecule 8: 50S ribosomal protein L9

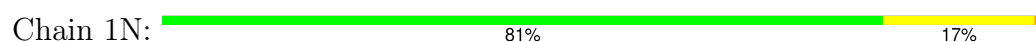




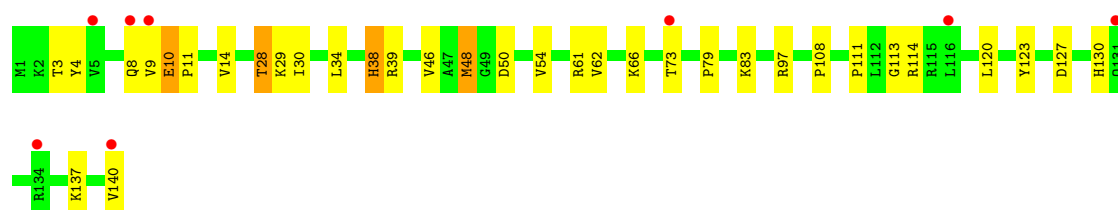
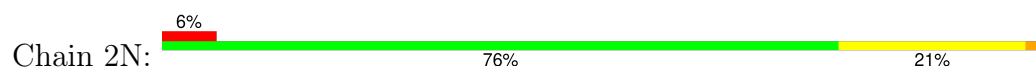
• Molecule 8: 50S ribosomal protein L9



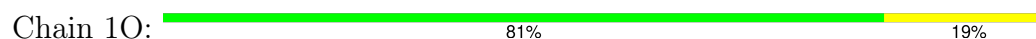
• Molecule 9: 50S ribosomal protein L13



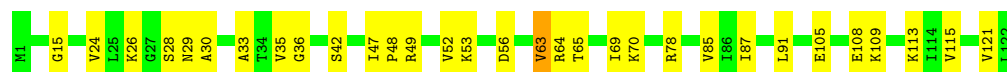
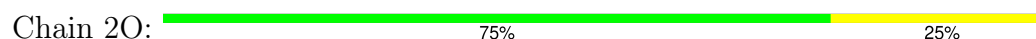
• Molecule 9: 50S ribosomal protein L13



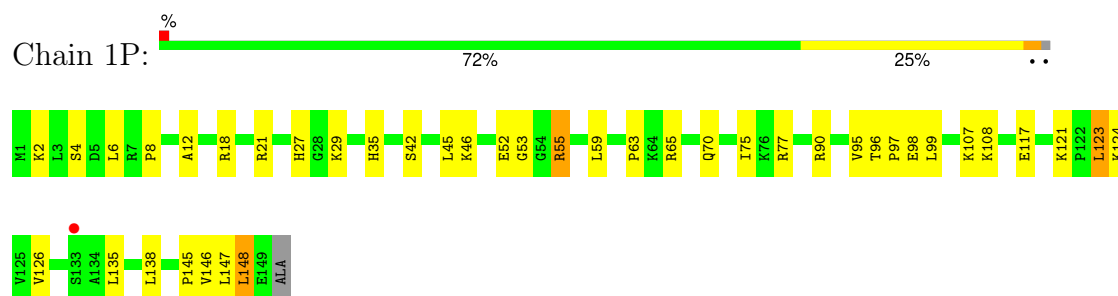
• Molecule 10: 50S ribosomal protein L14



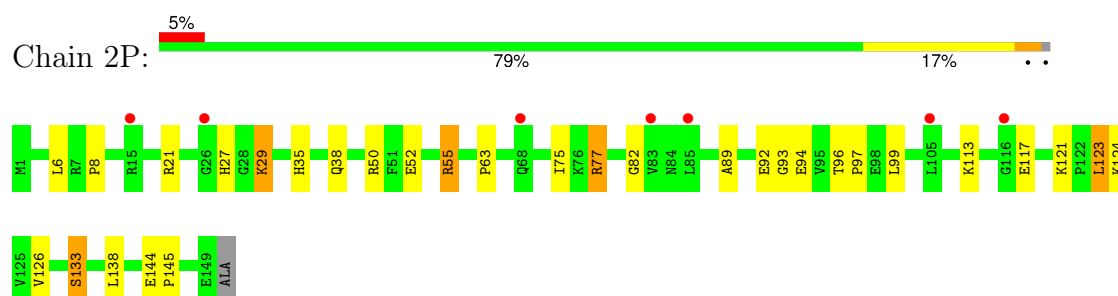
• Molecule 10: 50S ribosomal protein L14



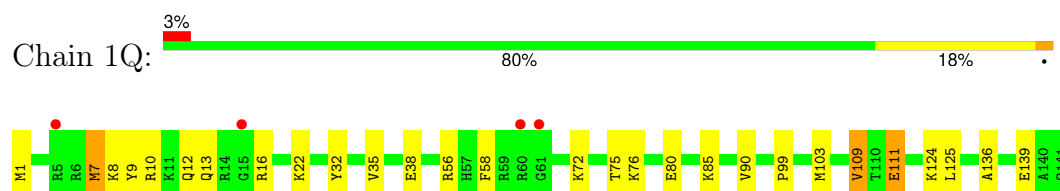
- Molecule 11: 50S ribosomal protein L15



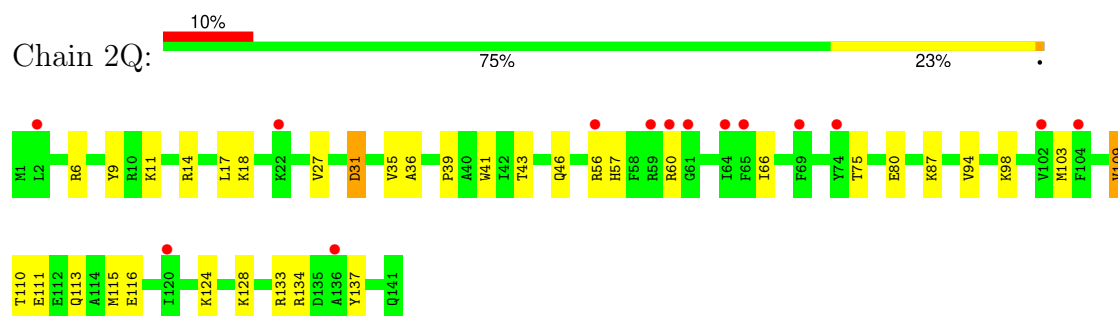
- Molecule 11: 50S ribosomal protein L15



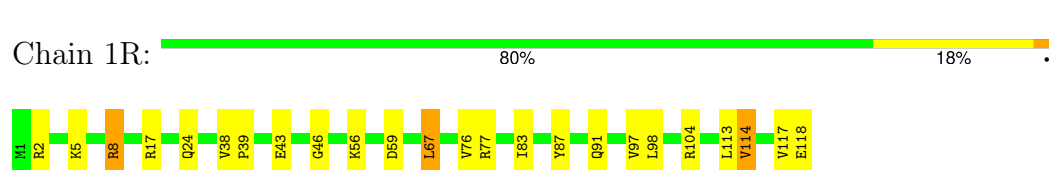
- Molecule 12: 50S ribosomal protein L16



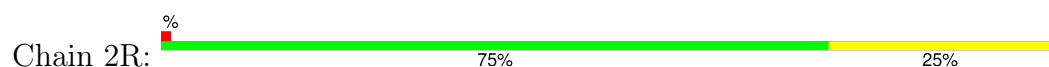
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

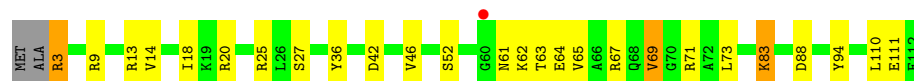
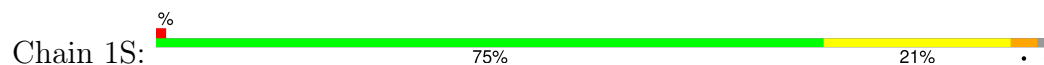


- Molecule 13: 50S ribosomal protein L17

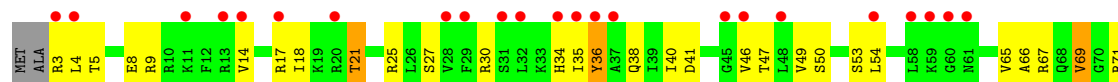




- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18



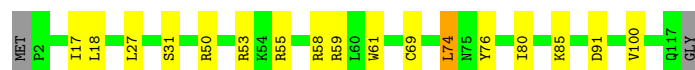
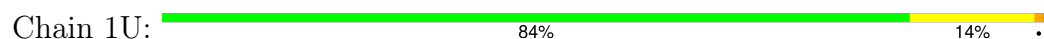
- Molecule 15: 50S ribosomal protein L19



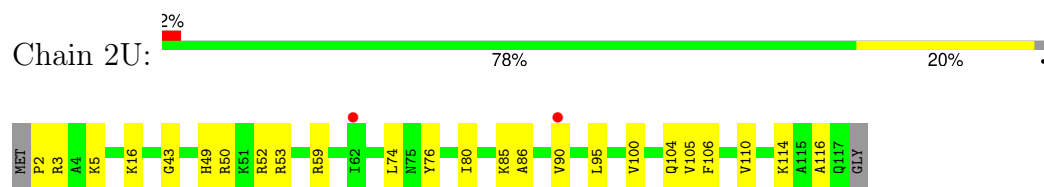
- Molecule 15: 50S ribosomal protein L19



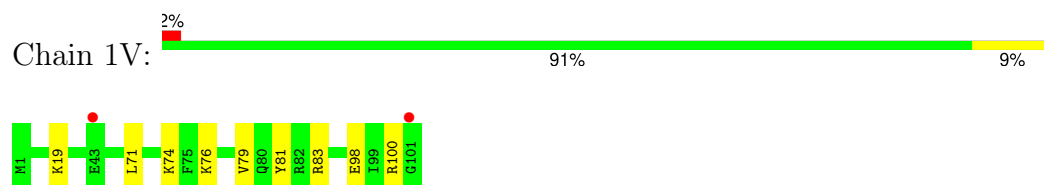
- Molecule 16: 50S ribosomal protein L20



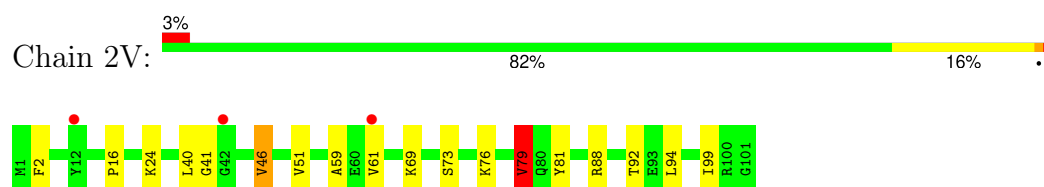
- Molecule 16: 50S ribosomal protein L20



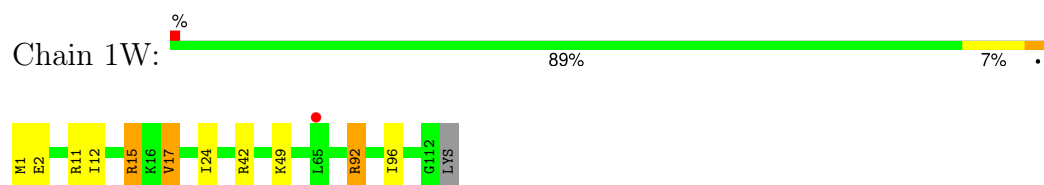
- Molecule 17: 50S ribosomal protein L21



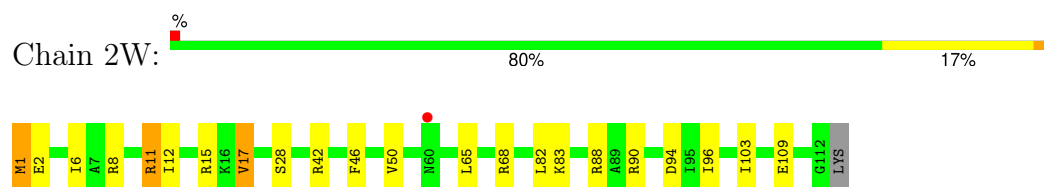
- Molecule 17: 50S ribosomal protein L21



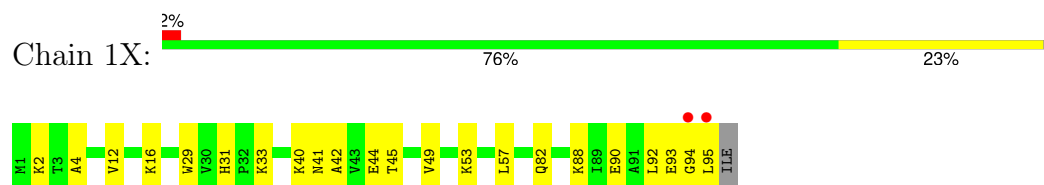
- Molecule 18: 50S ribosomal protein L22



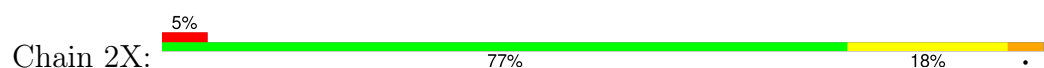
- Molecule 18: 50S ribosomal protein L22

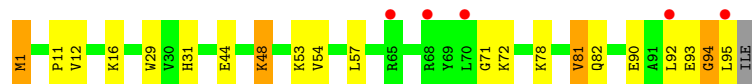


- Molecule 19: 50S ribosomal protein L23

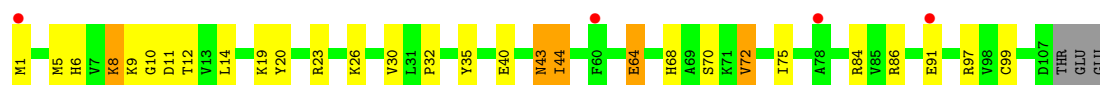


- Molecule 19: 50S ribosomal protein L23

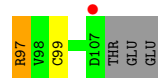
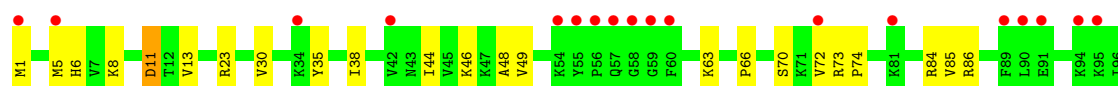
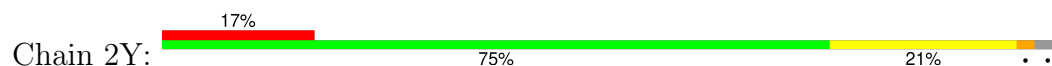




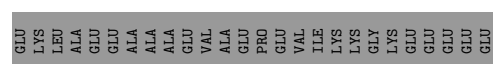
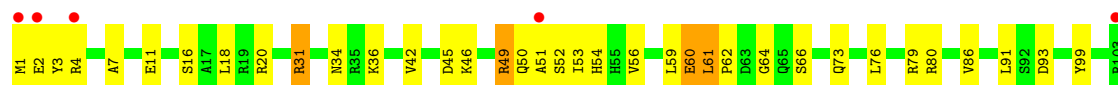
- Molecule 20: 50S ribosomal protein L24



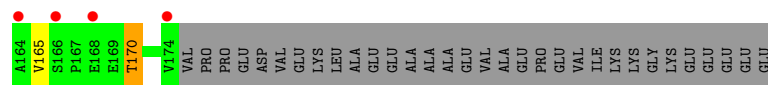
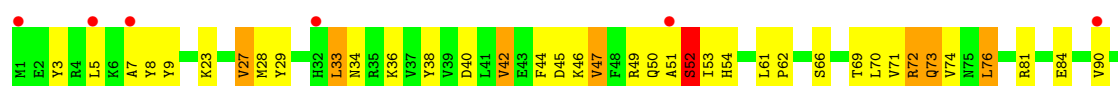
- Molecule 20: 50S ribosomal protein L24



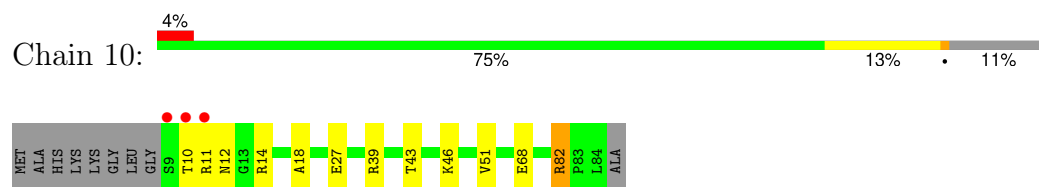
- Molecule 21: 50S ribosomal protein L25



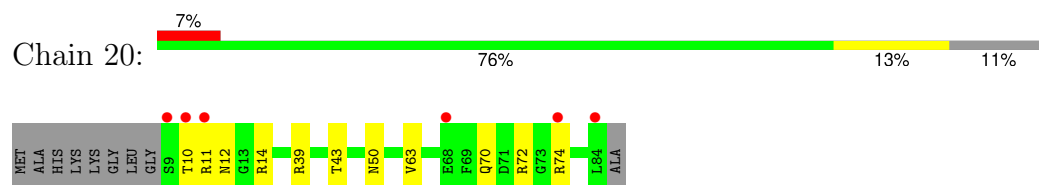
- Molecule 21: 50S ribosomal protein L25



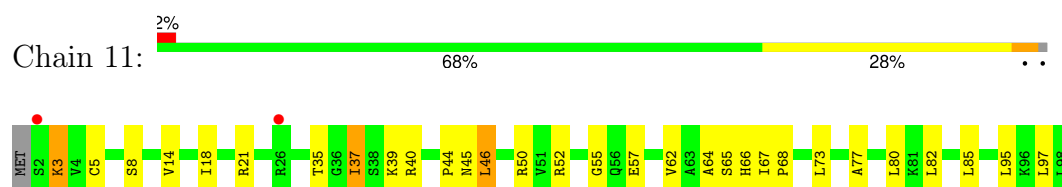
• Molecule 22: 50S ribosomal protein L27



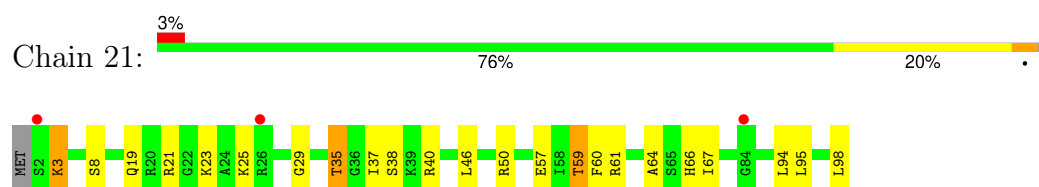
• Molecule 22: 50S ribosomal protein L27



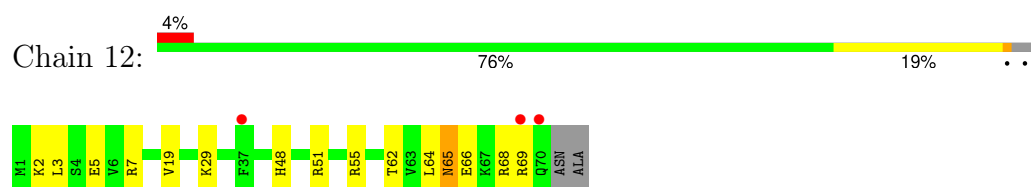
• Molecule 23: 50S ribosomal protein L28



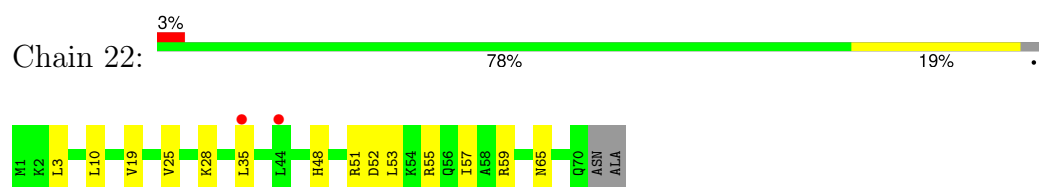
• Molecule 23: 50S ribosomal protein L28



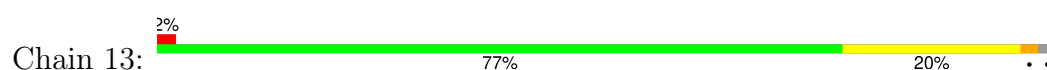
• Molecule 24: 50S ribosomal protein L29

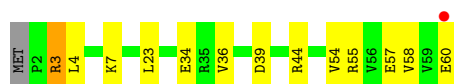


• Molecule 24: 50S ribosomal protein L29

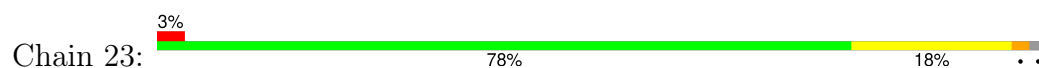


• Molecule 25: 50S ribosomal protein L30

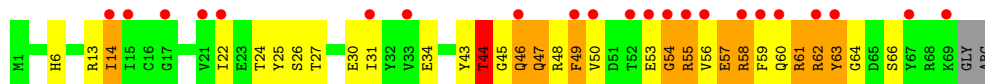




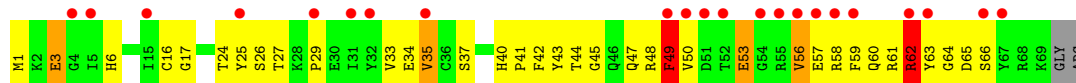
- Molecule 25: 50S ribosomal protein L30



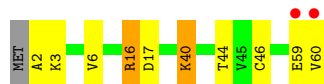
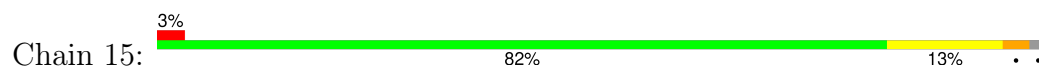
- Molecule 26: 50S ribosomal protein L31



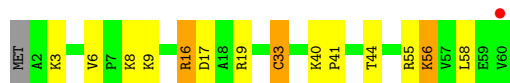
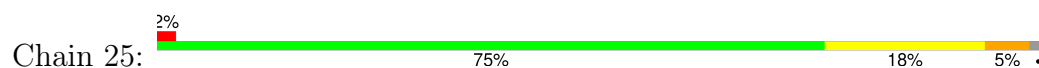
- Molecule 26: 50S ribosomal protein L31



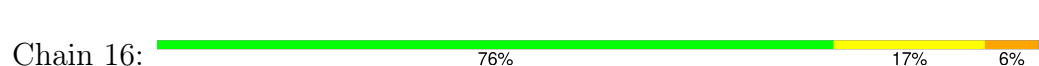
- Molecule 27: 50S ribosomal protein L32



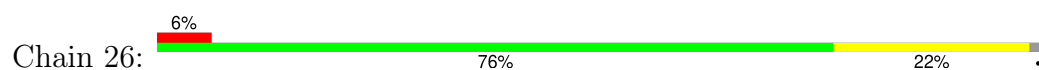
- Molecule 27: 50S ribosomal protein L32



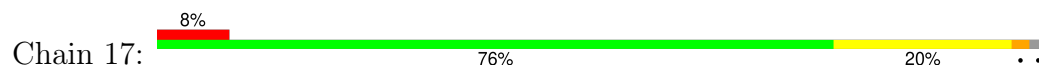
- Molecule 28: 50S ribosomal protein L33



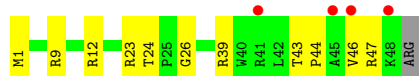
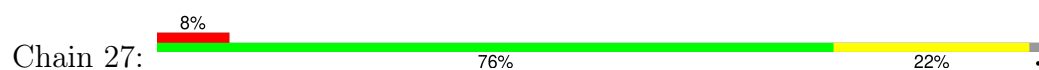
- Molecule 28: 50S ribosomal protein L33



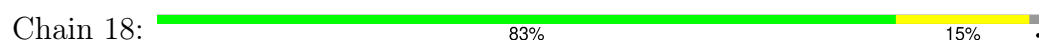
- Molecule 29: 50S ribosomal protein L34



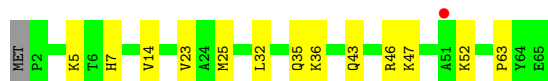
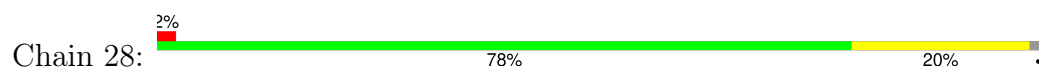
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



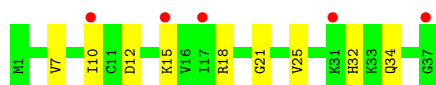
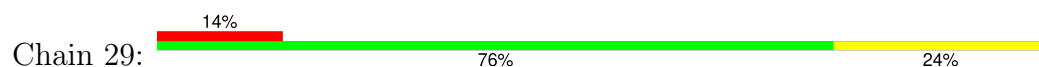
- Molecule 30: 50S ribosomal protein L35



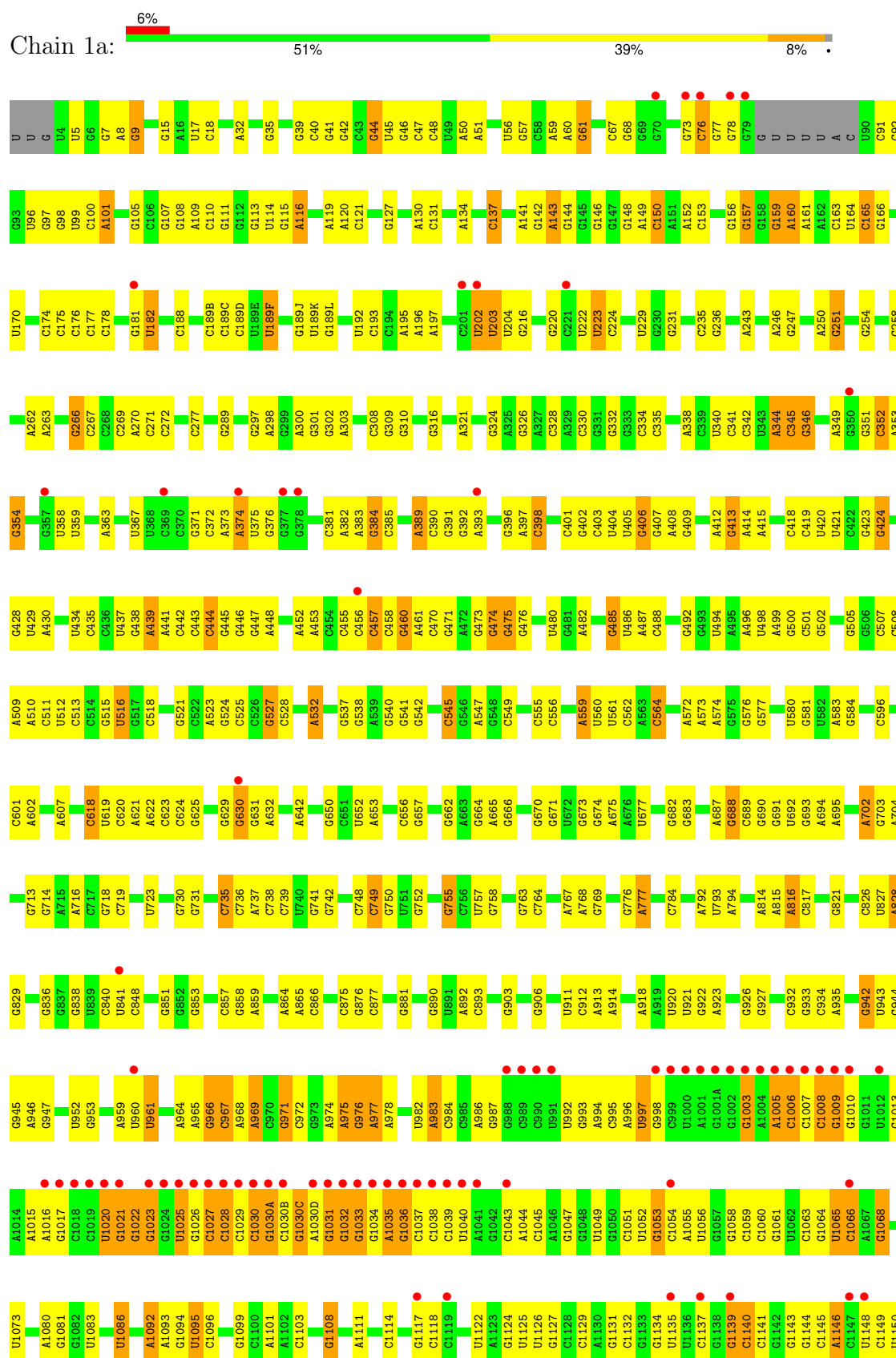
- Molecule 31: 50S ribosomal protein L36

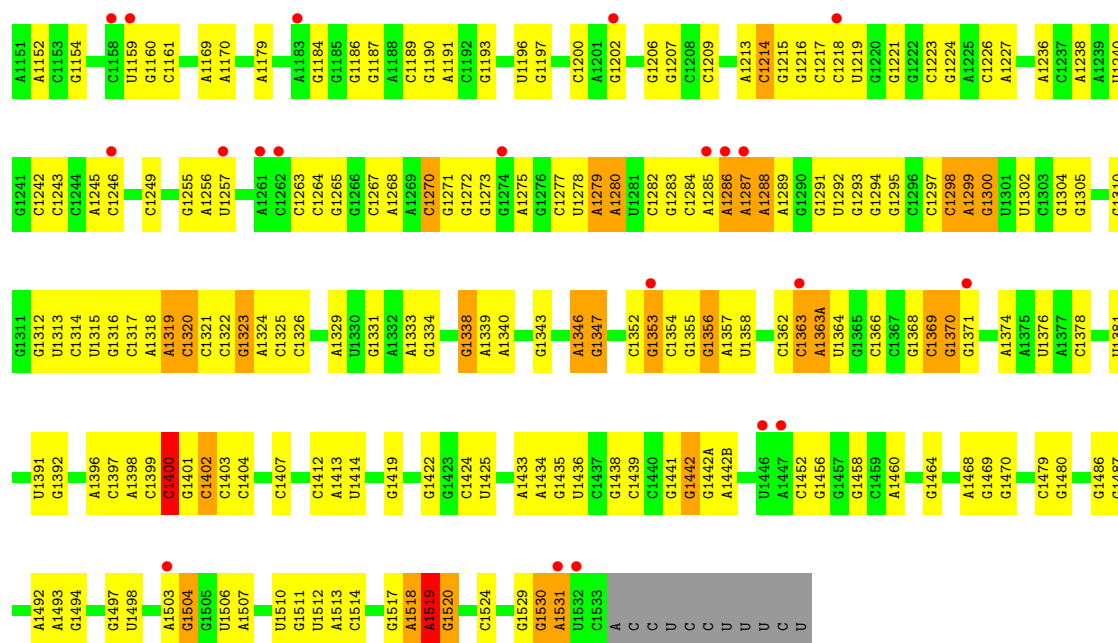


- Molecule 31: 50S ribosomal protein L36

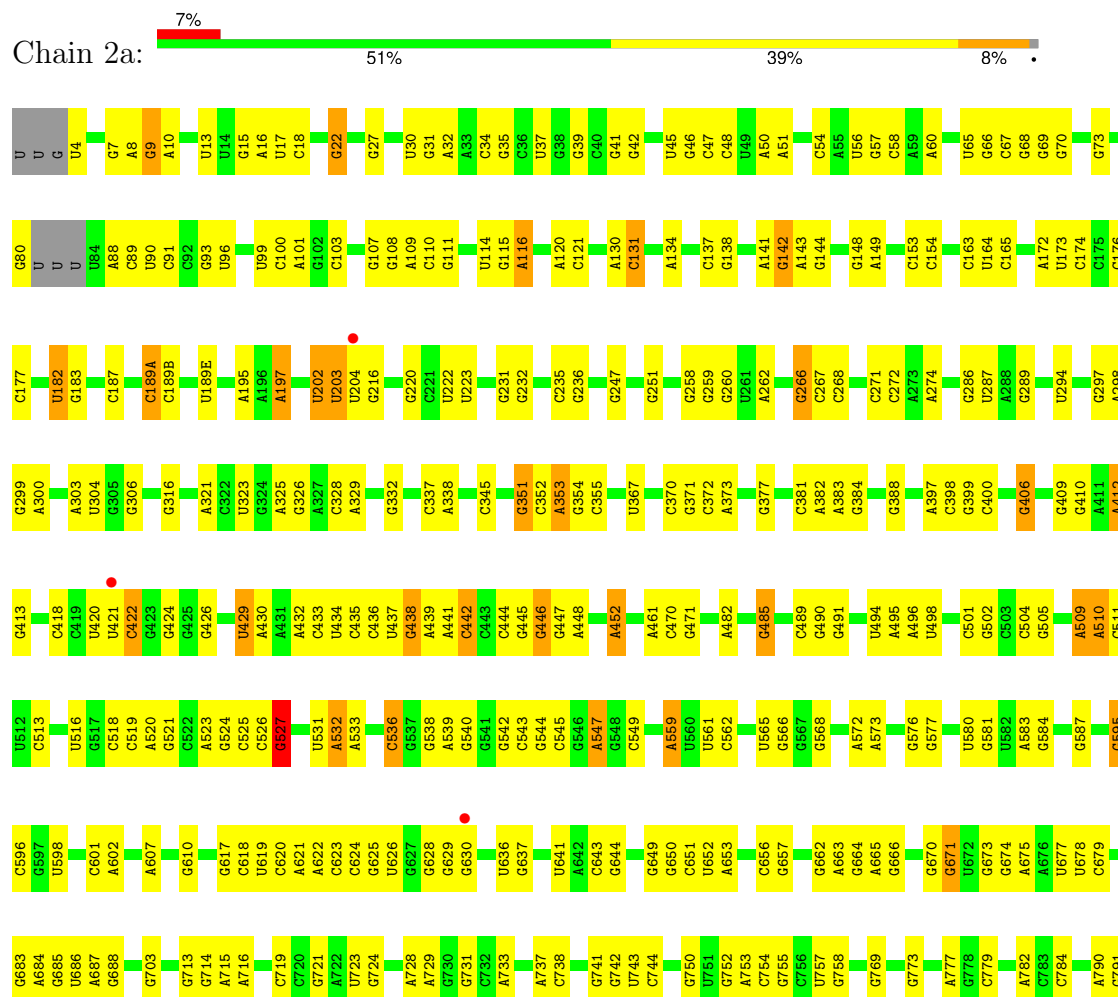


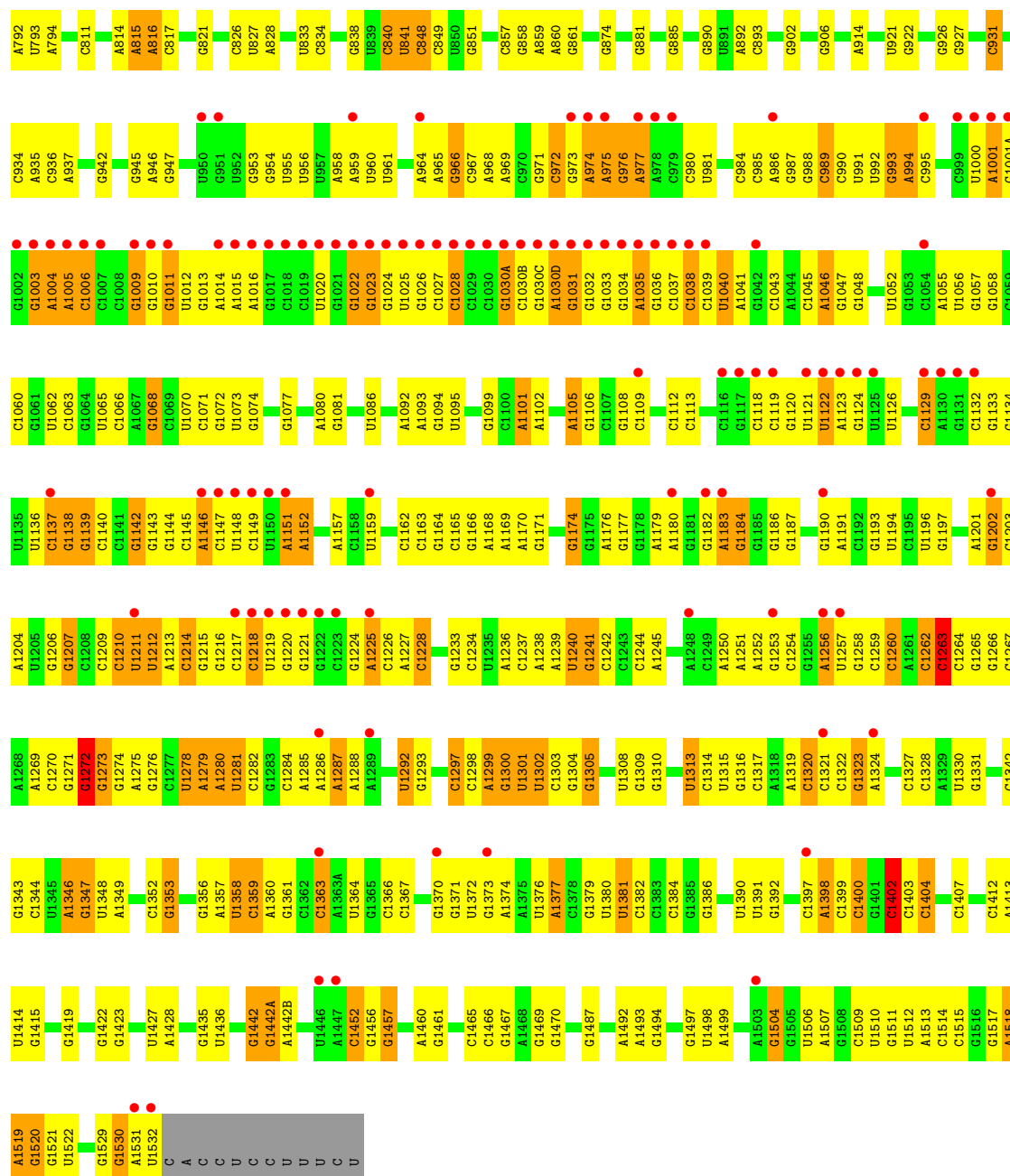
- Molecule 32: 16S Ribosomal RNA

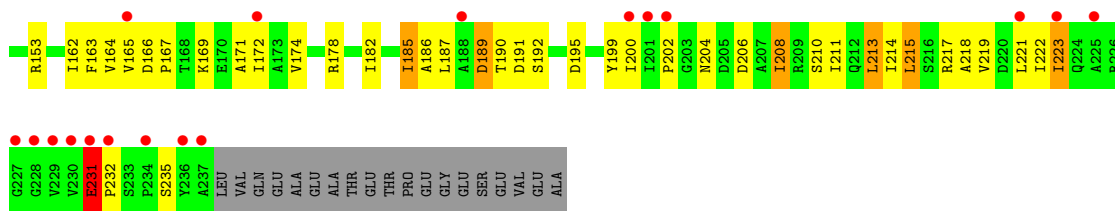




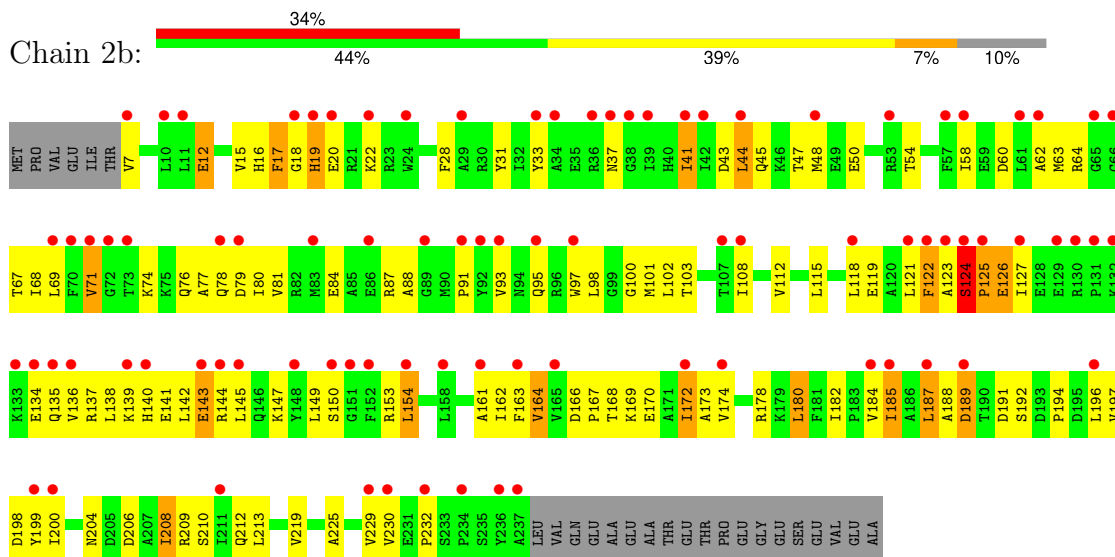
• Molecule 32: 16S Ribosomal RNA



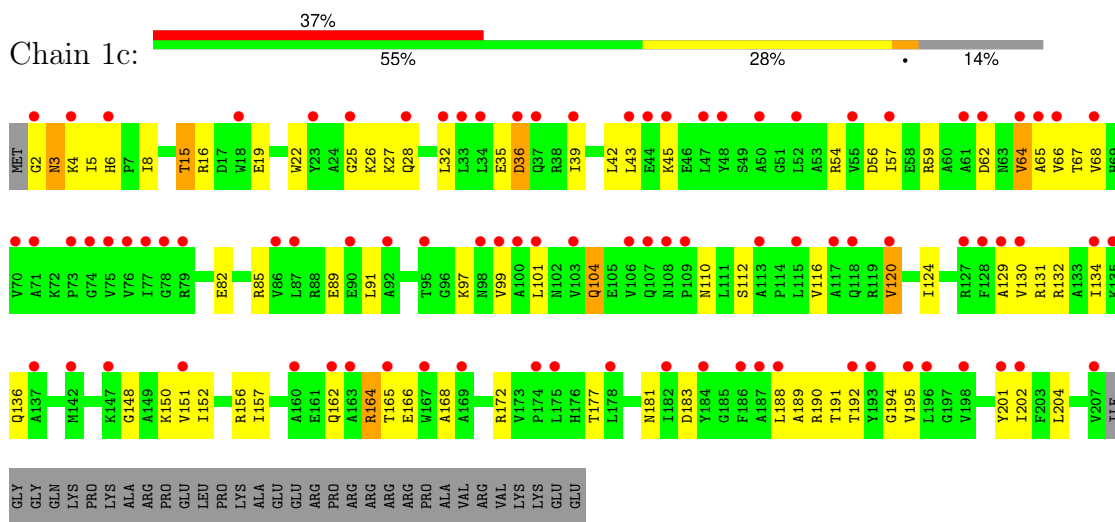




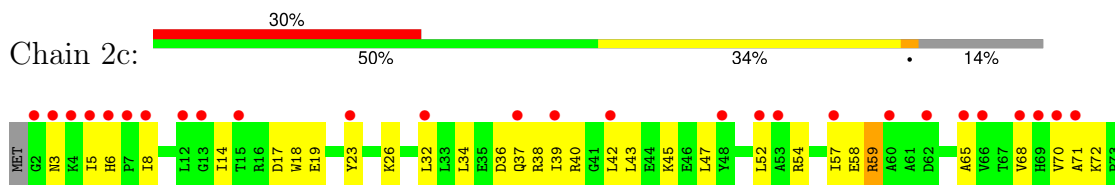
- Molecule 33: 30S ribosomal protein S2

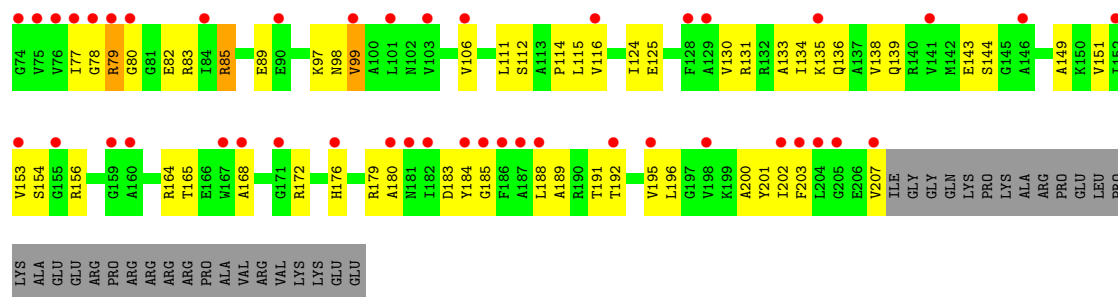


- Molecule 34: 30S ribosomal protein S3

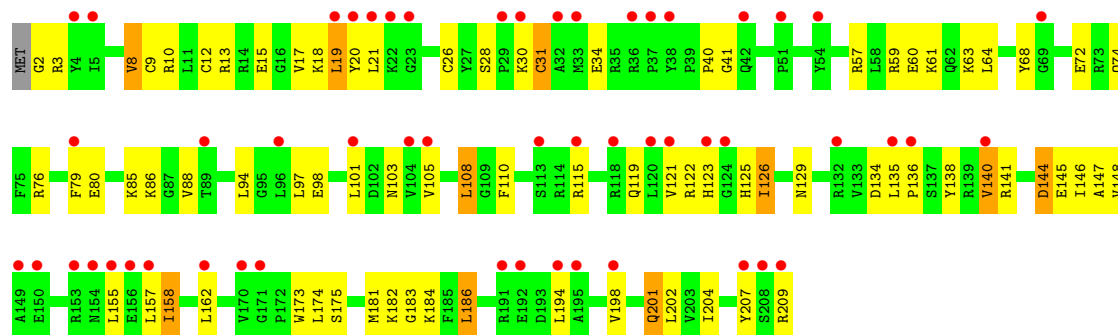


- Molecule 34: 30S ribosomal protein S3

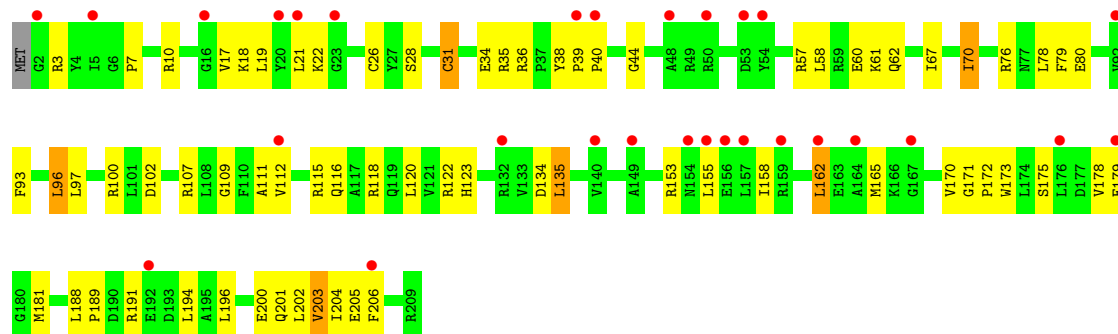




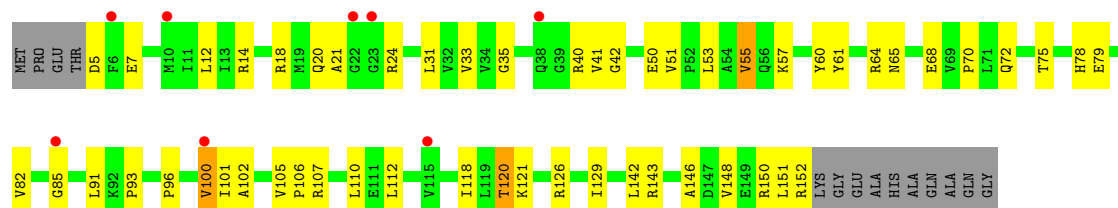
• Molecule 35: 30S ribosomal protein S4



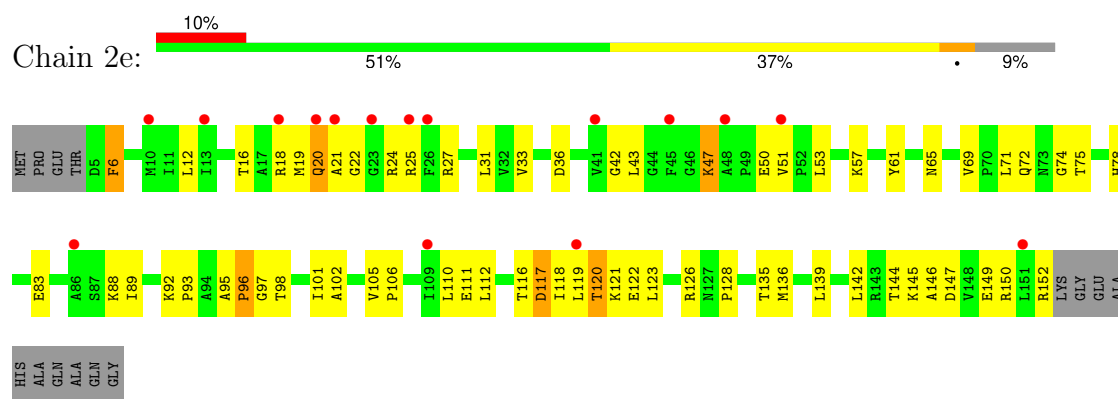
• Molecule 35: 30S ribosomal protein S4



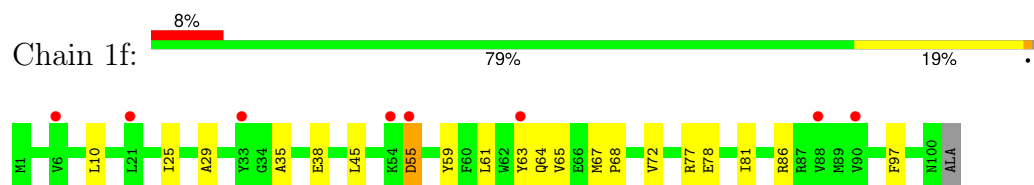
• Molecule 36: 30S ribosomal protein S5



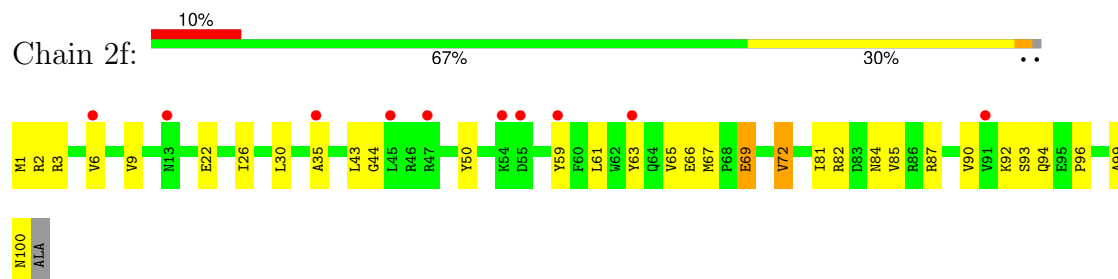
• Molecule 36: 30S ribosomal protein S5



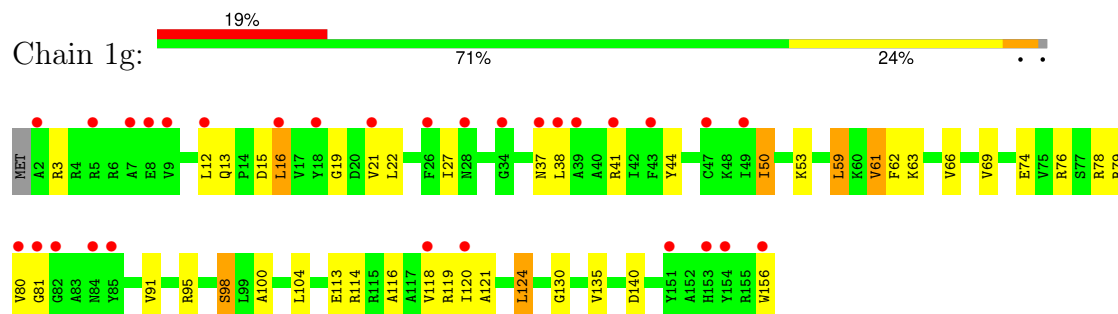
- Molecule 37: 30S ribosomal protein S6



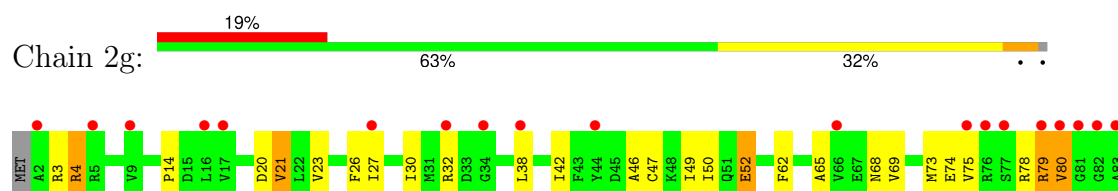
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

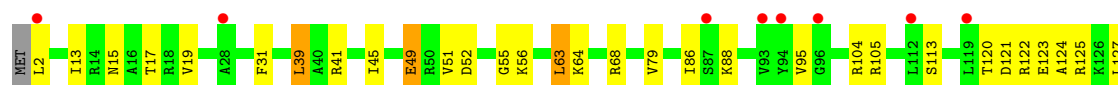
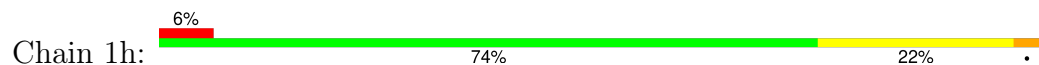


- Molecule 38: 30S ribosomal protein S7

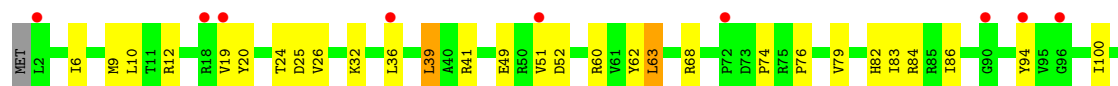




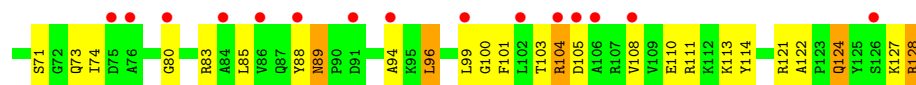
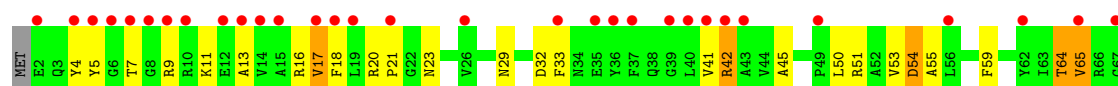
- Molecule 39: 30S ribosomal protein S8



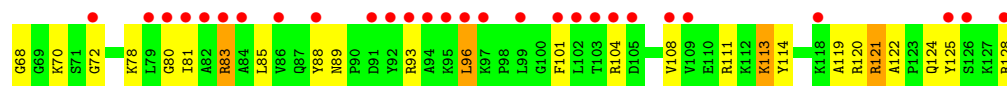
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9



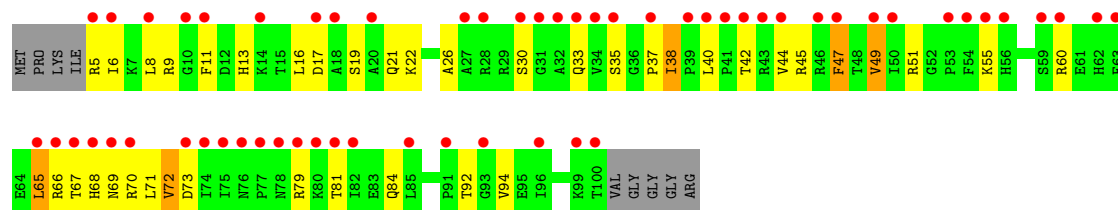
- Molecule 40: 30S ribosomal protein S9



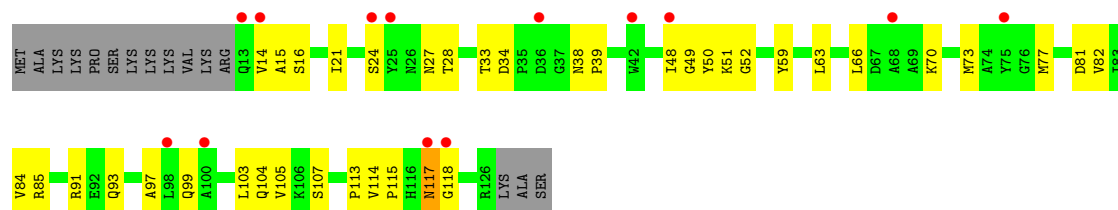
- Molecule 41: 30S ribosomal protein S10



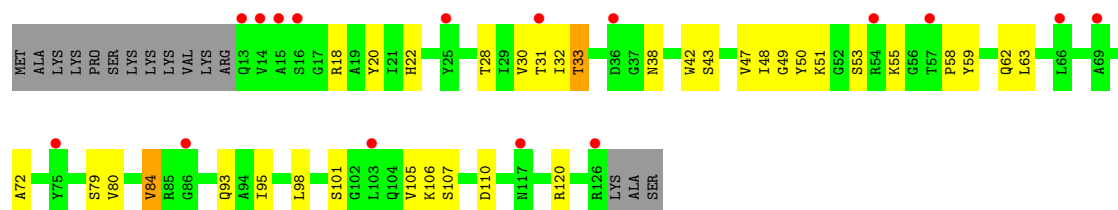
- Molecule 41: 30S ribosomal protein S10



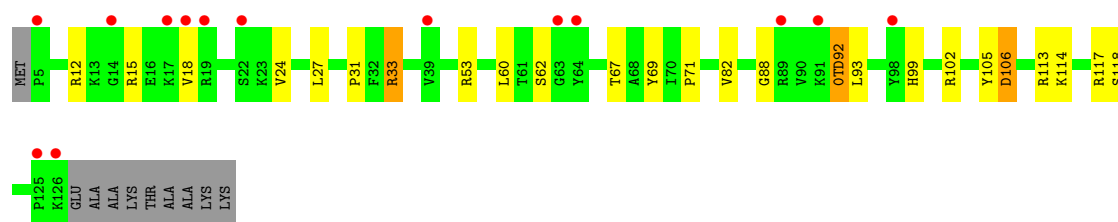
- Molecule 42: 30S ribosomal protein S11



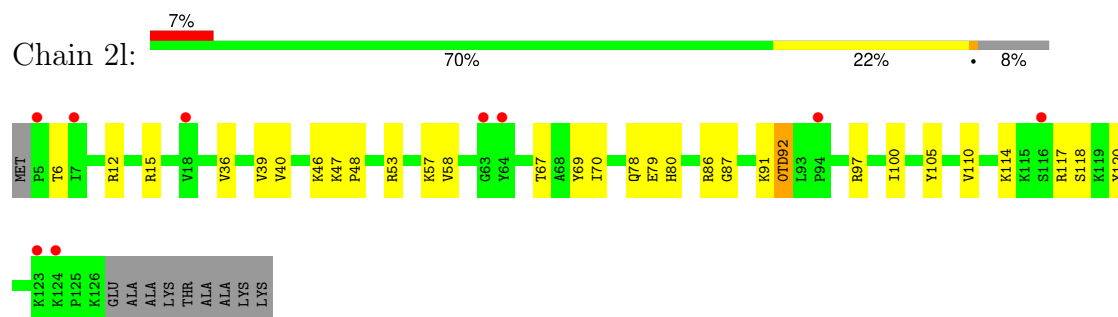
- Molecule 42: 30S ribosomal protein S11



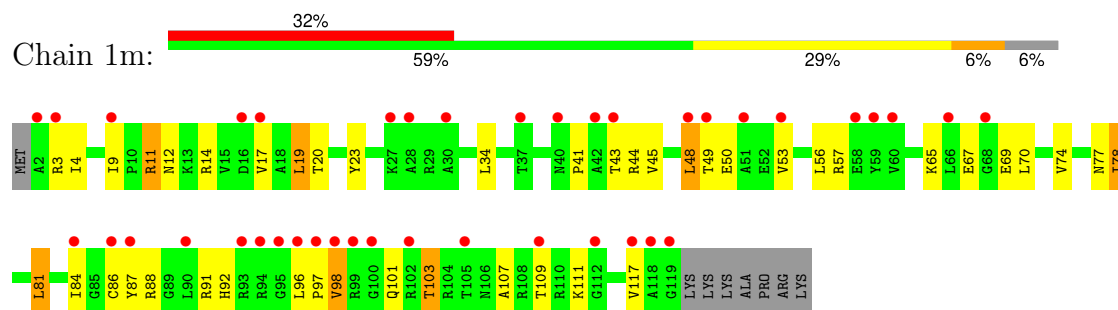
- Molecule 43: 30S ribosomal protein S12



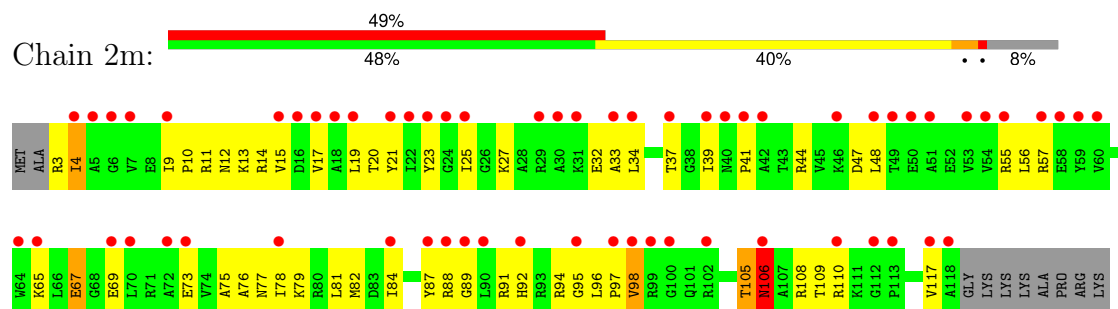
- Molecule 43: 30S ribosomal protein S12



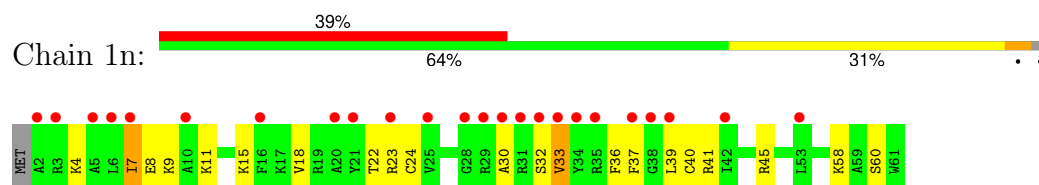
- Molecule 44: 30S ribosomal protein S13



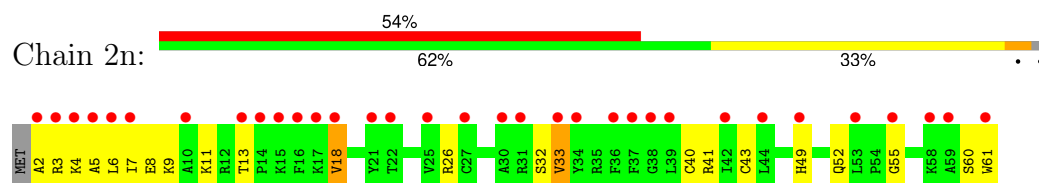
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



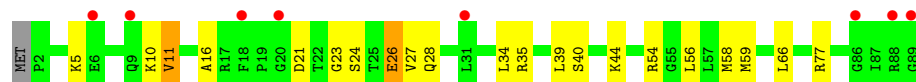
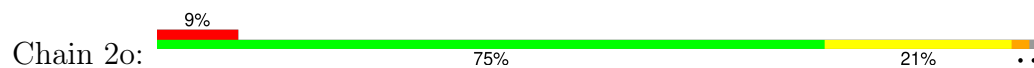
- Molecule 45: 30S ribosomal protein S14 type Z



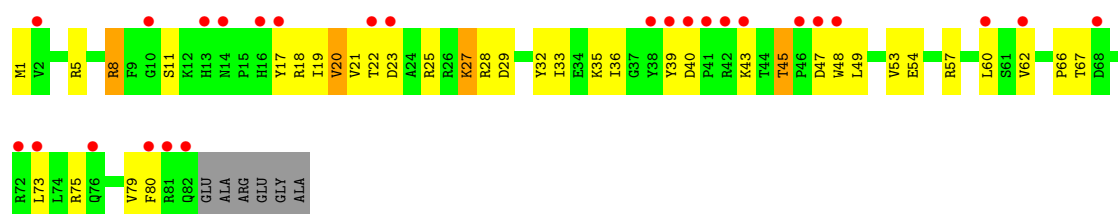
- Molecule 46: 30S ribosomal protein S15



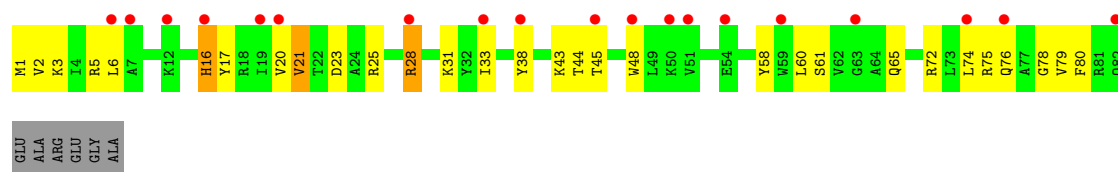
- Molecule 46: 30S ribosomal protein S15



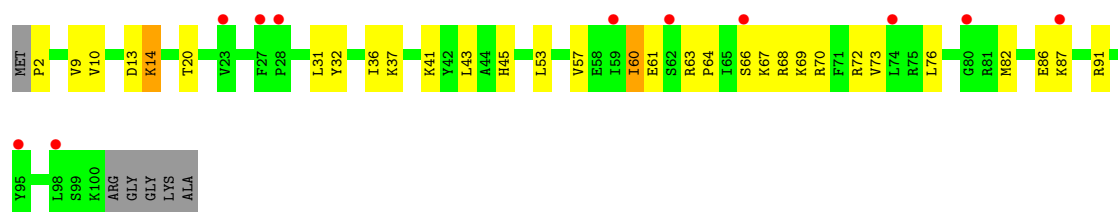
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16

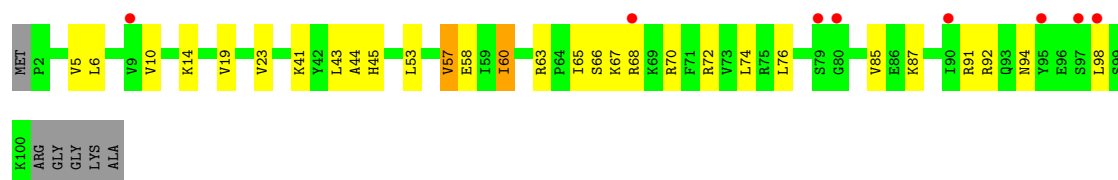


- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17





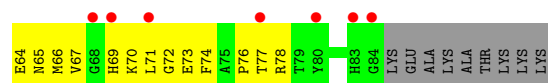
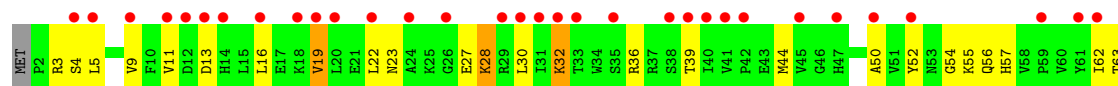
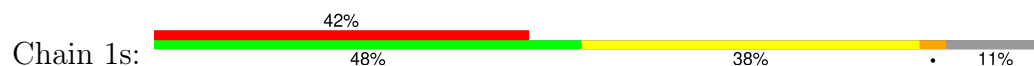
- Molecule 49: 30S ribosomal protein S18



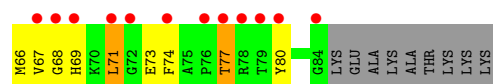
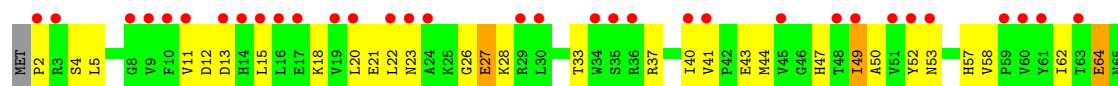
- Molecule 49: 30S ribosomal protein S18



- Molecule 50: 30S ribosomal protein S19

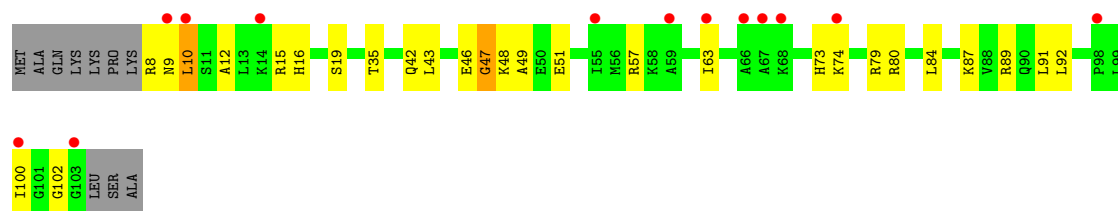


- Molecule 50: 30S ribosomal protein S19

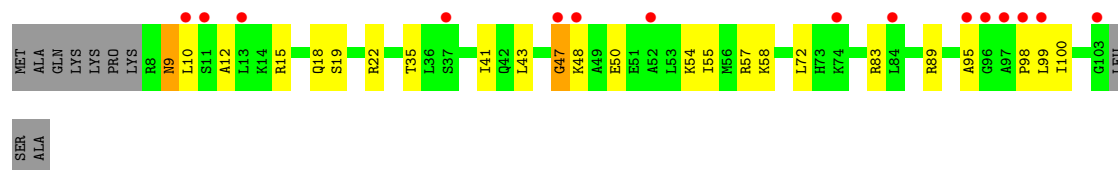


- Molecule 51: 30S ribosomal protein S20

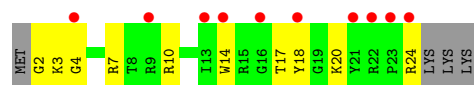




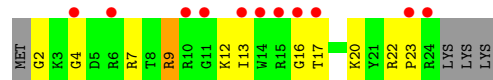
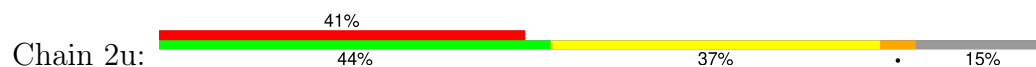
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: CYS-Stop mRNA

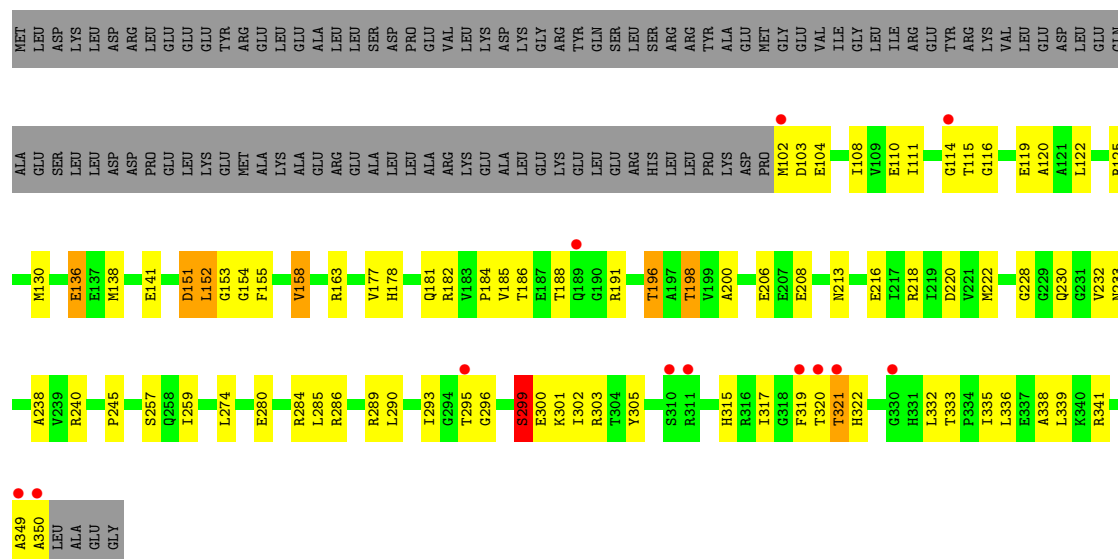


- Molecule 53: CYS-Stop mRNA

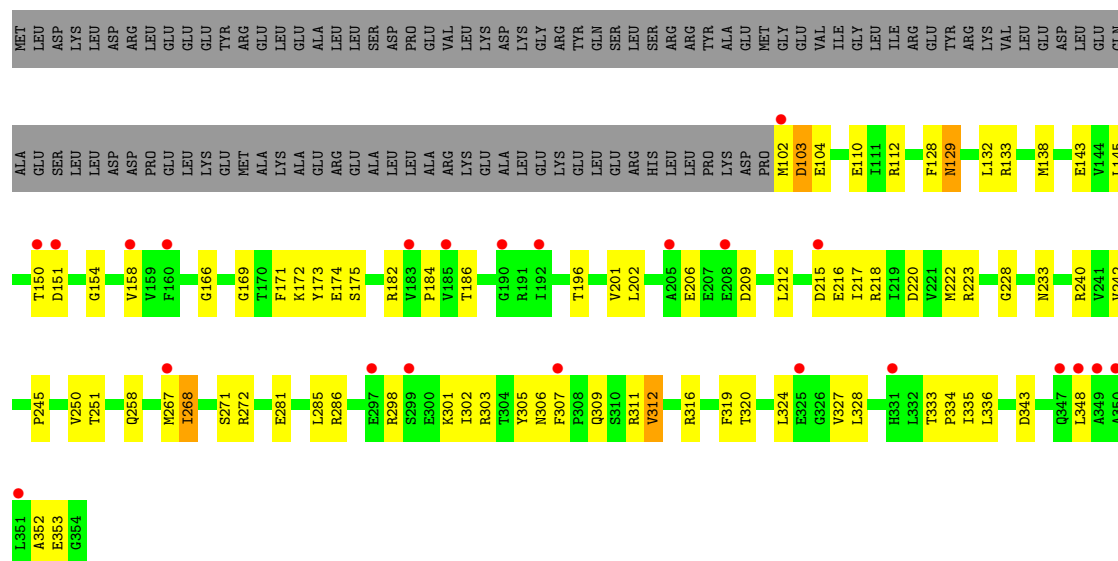


- Molecule 54: Peptide chain release factor 1

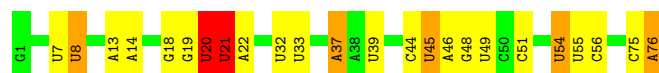




• Molecule 54: Peptide chain release factor 1

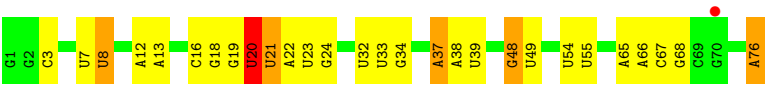


• Molecule 55: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys RNA-part



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

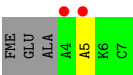




● Molecule 56: P-site Peptidyl-tRNA fMEAAAKC-tRNAcys Peptide-part



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.40Å 447.21Å 624.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.08 – 2.40 107.08 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (107.08-2.40) 94.3 (107.08-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.223 , 0.263 0.224 , 0.265	Depositor DCC
R_{free} test set	105915 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	297056	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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: MIA, MG, H2U, 5MU, OMU, 5MC, PSU, 2MA, UR3, G7M, 2MG, 4OC, MA6, 0TD, OMG, MEQ, ZN, K, 4SU, M2G, 8AN, SF4, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.30	0/69011	0.48	3/107720 (0.0%)
1	2A	0.22	1/67295 (0.0%)	0.41	1/105042 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.27	0/2186	0.52	1/2944 (0.0%)
3	2D	0.24	0/2186	0.46	0/2944
4	1E	0.28	0/1592	0.53	0/2149
4	2E	0.21	0/1592	0.45	0/2149
5	1F	0.27	0/1619	0.51	0/2193
5	2F	0.20	0/1615	0.41	0/2188
6	1G	0.20	0/1448	0.43	0/1957
6	2G	0.19	0/1453	0.42	0/1963
7	1H	0.21	0/1356	0.45	2/1834 (0.1%)
7	2H	0.18	0/1356	0.37	0/1834
8	1I	0.18	0/1112	0.41	0/1514
8	2I	0.19	0/1079	0.41	0/1475
9	1N	0.25	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.41	0/1543
10	1O	0.25	0/943	0.47	0/1269
10	2O	0.20	0/943	0.43	0/1269
11	1P	0.27	0/1152	0.53	0/1533
11	2P	0.21	0/1152	0.45	0/1533
12	1Q	0.29	0/1143	0.52	0/1527
12	2Q	0.20	0/1143	0.44	0/1527
13	1R	0.28	0/982	0.52	0/1312
13	2R	0.22	0/982	0.46	0/1312
14	1S	0.23	0/883	0.47	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.26	0/1105	0.46	0/1477
15	2T	0.21	0/1097	0.45	0/1468
16	1U	0.30	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.39	0/1301
17	1V	0.27	0/782	0.48	0/1049
17	2V	0.18	0/782	0.38	0/1049
18	1W	0.28	0/897	0.45	0/1205
18	2W	0.21	0/897	0.41	0/1205
19	1X	0.27	0/764	0.54	0/1025
19	2X	0.20	0/764	0.49	2/1025 (0.2%)
20	1Y	0.23	0/819	0.47	0/1095
20	2Y	0.19	0/819	0.41	0/1095
21	1Z	0.22	0/1267	0.50	0/1717
21	2Z	0.21	0/1299	0.46	0/1763
22	10	0.27	0/612	0.50	0/816
22	20	0.20	0/612	0.44	0/816
23	11	0.26	0/762	0.44	0/1014
23	21	0.21	0/762	0.40	0/1014
24	12	0.23	0/590	0.44	0/781
24	22	0.19	0/590	0.37	0/781
25	13	0.27	0/474	0.52	0/635
25	23	0.20	0/469	0.48	0/630
26	14	0.24	0/565	0.62	2/761 (0.3%)
26	24	0.24	0/545	0.56	0/737
27	15	0.28	0/469	0.54	0/635
27	25	0.24	0/469	0.53	0/635
28	16	0.27	0/460	0.52	0/613
28	26	0.18	0/456	0.42	0/608
29	17	0.33	0/426	0.53	0/561
29	27	0.23	0/426	0.48	0/561
30	18	0.26	0/525	0.50	0/691
30	28	0.20	0/525	0.40	0/691
31	19	0.29	0/310	0.48	0/407
31	29	0.19	0/310	0.43	0/407
32	1a	0.20	0/35795	0.39	0/55864
32	2a	0.20	0/35886	0.38	5/56005 (0.0%)
33	1b	0.23	0/1881	0.53	0/2542
33	2b	0.23	0/1860	0.46	0/2518
34	1c	0.21	0/1572	0.44	0/2126
34	2c	0.19	0/1566	0.42	0/2119
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.18	0/1704	0.41	0/2284
36	1e	0.20	0/1145	0.46	0/1543
36	2e	0.19	0/1149	0.44	0/1548
37	1f	0.20	0/823	0.41	0/1115
37	2f	0.19	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.47	0/1679
38	2g	0.18	0/1254	0.43	0/1683
39	1h	0.18	0/1108	0.41	0/1494
39	2h	0.20	0/1108	0.46	1/1494 (0.1%)
40	1i	0.20	0/1002	0.46	0/1346
40	2i	0.21	0/997	0.45	0/1343
41	1j	0.19	0/722	0.47	0/982
41	2j	0.25	0/727	0.48	0/988
42	1k	0.21	0/844	0.46	1/1145 (0.1%)
42	2k	0.19	0/848	0.40	0/1149
43	1l	0.21	0/937	0.45	0/1260
43	2l	0.19	0/937	0.42	0/1260
44	1m	0.20	0/929	0.49	0/1250
44	2m	0.21	0/917	0.44	0/1234
45	1n	0.17	0/501	0.46	0/664
45	2n	0.19	0/501	0.43	0/664
46	1o	0.20	0/739	0.39	0/985
46	2o	0.19	0/739	0.39	0/985
47	1p	0.19	0/697	0.42	0/939
47	2p	0.19	0/693	0.45	0/935
48	1q	0.19	0/836	0.41	0/1117
48	2q	0.18	0/836	0.40	0/1117
49	1r	0.18	0/560	0.38	0/746
49	2r	0.16	0/560	0.38	0/746
50	1s	0.21	0/667	0.50	0/900
50	2s	0.20	0/661	0.42	0/893
51	1t	0.19	0/730	0.48	0/965
51	2t	0.20	0/729	0.45	0/965
52	1u	0.21	0/203	0.44	0/266
52	2u	0.20	0/203	0.43	0/266
53	1v	0.22	0/213	0.46	0/329
53	2v	0.21	0/213	0.39	0/329
54	1w	0.21	0/1956	0.42	0/2634
54	2w	0.20	0/1974	0.44	0/2657
55	1x	0.22	1/1555 (0.1%)	0.36	0/2419
55	2x	0.21	0/1555	0.36	0/2419
56	1z	0.30	0/29	0.45	0/37
56	2z	0.28	0/24	0.48	0/30
All	All	0.24	2/313604 (0.0%)	0.43	18/468535 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
21	1Z	0	1
33	1b	0	2
33	2b	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	8	4SU	O3'-P	5.13	1.61	1.56
1	2A	2552	OMU	O3'-P	5.05	1.61	1.56

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	7.85	121.28	109.50
32	2a	1272	G	N1-C2-N2	-7.14	94.78	116.20
32	2a	1263	C	N1-C2-O2	6.83	139.38	118.90
1	2A	1992	G	C2'-C3'-O3'	6.82	119.73	109.50
32	2a	1272	G	N3-C2-N2	6.49	139.38	119.90
32	2a	1272	G	C5-C6-O6	6.20	147.20	128.60
3	1D	98	VAL	N-CA-C	-5.92	105.24	112.76
26	14	54	GLY	CA-C-N	5.73	132.48	121.54
26	14	54	GLY	C-N-CA	5.73	132.48	121.54
39	2h	79	VAL	N-CA-C	-5.64	107.33	111.90
7	1H	92	ILE	CA-C-N	-5.63	112.70	122.83
7	1H	92	ILE	C-N-CA	-5.63	112.70	122.83
19	2X	94	GLY	CA-C-N	5.29	131.23	121.70
19	2X	94	GLY	C-N-CA	5.29	131.23	121.70
1	1A	512	G	O4'-C1'-N9	5.19	115.98	108.20
42	1k	52	GLY	N-CA-C	5.18	119.76	110.95
1	1A	1210	A	C4'-C3'-O3'	5.05	116.98	109.40
32	2a	1263	C	N3-C2-O2	-5.03	106.80	121.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
21	1Z	136	PHE	Peptide
33	1b	122	PHE	Peptide
33	1b	9	GLU	Peptide
11	2P	35	HIS	Peptide
33	2b	124	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	622	0
1	2A	60322	0	30427	647	0
2	1B	2577	0	1304	20	0
2	2B	2575	0	1303	25	0
3	1D	2136	0	2218	45	0
3	2D	2136	0	2218	38	0
4	1E	1559	0	1618	24	0
4	2E	1559	0	1618	26	0
5	1F	1584	0	1625	37	0
5	2F	1580	0	1619	49	0
6	1G	1423	0	1436	35	0
6	2G	1428	0	1438	54	0
7	1H	1330	0	1407	33	0
7	2H	1330	0	1407	23	0
8	1I	1097	0	1140	27	0
8	2I	1064	0	1082	18	0
9	1N	1117	0	1184	18	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	15	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	32	0
11	2P	1135	0	1212	23	0
12	1Q	1122	0	1179	18	0
12	2Q	1122	0	1179	26	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	19	0
14	1S	873	0	927	18	0
14	2S	870	0	923	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	12	0
16	2U	959	0	1019	13	0
17	1V	771	0	830	6	0
17	2V	771	0	830	10	0
18	1W	886	0	939	6	0
18	2W	886	0	940	14	0
19	1X	750	0	814	13	0
19	2X	750	0	814	12	0
20	1Y	806	0	881	18	0
20	2Y	806	0	881	22	0
21	1Z	1240	0	1240	31	0
21	2Z	1271	0	1273	33	0
22	10	604	0	619	13	0
22	20	604	0	619	9	0
23	11	755	0	826	20	0
23	21	755	0	826	14	0
24	12	588	0	643	11	0
24	22	588	0	643	5	0
25	13	469	0	518	6	0
25	23	464	0	514	6	0
26	14	552	0	533	28	0
26	24	532	0	503	31	0
27	15	455	0	465	6	0
27	25	455	0	465	10	0
28	16	453	0	473	7	0
28	26	449	0	469	7	0
29	17	418	0	467	8	0
29	27	418	0	467	7	0
30	18	517	0	582	7	0
30	28	517	0	582	9	0
31	19	307	0	335	1	0
31	29	307	0	335	6	0
32	1a	32246	0	16294	484	0
32	2a	32327	0	16338	495	0
33	1b	1846	0	1867	70	0
33	2b	1825	0	1828	73	0
34	1c	1548	0	1535	53	0
34	2c	1542	0	1517	62	0
35	1d	1655	0	1672	61	0
35	2d	1674	0	1713	49	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	1e	1129	0	1185	45	0
36	2e	1133	0	1191	47	0
37	1f	810	0	804	11	0
37	2f	816	0	808	25	0
38	1g	1231	0	1238	32	0
38	2g	1235	0	1249	46	0
39	1h	1088	0	1126	23	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	40	0
40	2i	978	0	966	42	0
41	1j	709	0	650	29	0
41	2j	714	0	672	36	0
42	1k	829	0	825	18	0
42	2k	833	0	836	19	0
43	1l	932	0	981	18	0
43	2l	932	0	981	18	0
44	1m	919	0	951	30	0
44	2m	907	0	934	40	0
45	1n	492	0	529	15	0
45	2n	492	0	529	21	0
46	1o	728	0	760	16	0
46	2o	728	0	760	14	0
47	1p	681	0	697	24	0
47	2p	677	0	686	20	0
48	1q	823	0	891	18	0
48	2q	823	0	891	17	0
49	1r	555	0	618	13	0
49	2r	555	0	618	15	0
50	1s	652	0	662	27	0
50	2s	646	0	644	32	0
51	1t	728	0	798	20	0
51	2t	727	0	796	18	0
52	1u	199	0	208	9	0
52	2u	199	0	208	11	0
53	1v	191	0	97	4	0
53	2v	191	0	97	2	0
54	1w	1939	0	1925	51	0
54	2w	1957	0	1935	39	0
55	1x	1577	0	801	10	0
55	2x	1577	0	802	17	0
56	1z	30	0	32	3	0
56	2z	25	0	27	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	10	7	0	0	0	0
57	11	4	0	0	0	0
57	12	2	0	0	0	0
57	13	3	0	0	0	0
57	15	9	0	0	0	0
57	16	2	0	0	0	0
57	17	5	0	0	0	0
57	18	4	0	0	0	0
57	19	1	0	0	0	0
57	1A	1101	0	0	0	0
57	1B	38	0	0	0	0
57	1D	14	0	0	0	0
57	1E	13	0	0	0	0
57	1F	16	0	0	0	0
57	1G	5	0	0	0	0
57	1I	1	0	0	0	0
57	1N	4	0	0	0	0
57	1O	4	0	0	0	0
57	1P	7	0	0	0	0
57	1Q	7	0	0	0	0
57	1R	4	0	0	0	0
57	1S	3	0	0	0	0
57	1T	3	0	0	0	0
57	1U	11	0	0	0	0
57	1V	7	0	0	0	0
57	1W	5	0	0	0	0
57	1X	5	0	0	0	0
57	1Y	4	0	0	0	0
57	1Z	2	0	0	0	0
57	1a	215	0	0	0	0
57	1b	2	0	0	0	0
57	1d	1	0	0	0	0
57	1e	3	0	0	0	0
57	1f	1	0	0	0	0
57	1k	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	2	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	4	0	0	0	0
57	1w	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1x	12	0	0	0	0
57	20	1	0	0	0	0
57	21	2	0	0	0	0
57	23	4	0	0	0	0
57	25	7	0	0	0	0
57	26	1	0	0	0	0
57	28	3	0	0	0	0
57	29	1	0	0	0	0
57	2A	852	0	0	0	0
57	2B	19	0	0	0	0
57	2D	7	0	0	0	0
57	2E	8	0	0	0	0
57	2F	7	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	2	0	0	0	0
57	2P	2	0	0	0	0
57	2Q	4	0	0	0	0
57	2R	1	0	0	0	0
57	2T	3	0	0	0	0
57	2U	2	0	0	0	0
57	2V	2	0	0	0	0
57	2W	2	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	185	0	0	0	0
57	2d	1	0	0	0	0
57	2e	2	0	0	0	0
57	2f	1	0	0	0	0
57	2g	1	0	0	0	0
57	2i	1	0	0	0	0
57	2j	1	0	0	0	0
57	2l	2	0	0	0	0
57	2n	1	0	0	0	0
57	2q	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	1	0	0	0	0
57	2x	5	0	0	0	0
58	1A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	1	0
60	2d	8	0	0	0	0
61	10	10	0	0	0	0
61	11	10	0	0	0	0
61	12	4	0	0	0	0
61	13	5	0	0	0	0
61	15	6	0	0	0	0
61	16	2	0	0	0	0
61	17	8	0	0	0	0
61	18	13	0	0	0	0
61	1A	2078	0	0	73	0
61	1B	64	0	0	1	0
61	1D	26	0	0	1	0
61	1E	25	0	0	0	0
61	1F	14	0	0	1	0
61	1G	3	0	0	1	0
61	1H	4	0	0	0	0
61	1I	1	0	0	0	0
61	1N	3	0	0	0	0
61	1O	8	0	0	0	0
61	1P	22	0	0	2	0
61	1Q	10	0	0	0	0
61	1R	14	0	0	2	0
61	1S	4	0	0	0	0
61	1T	5	0	0	0	0
61	1U	12	0	0	0	0
61	1V	9	0	0	0	0
61	1W	12	0	0	1	0
61	1X	2	0	0	0	0
61	1Y	3	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	287	0	0	20	0
61	1d	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	1e	1	0	0	0	0
6l	1f	2	0	0	0	0
6l	1j	1	0	0	0	0
6l	1l	3	0	0	0	0
6l	1q	1	0	0	0	0
6l	1v	7	0	0	0	0
6l	1w	1	0	0	0	0
6l	1x	19	0	0	2	0
6l	20	5	0	0	0	0
6l	21	9	0	0	1	0
6l	22	1	0	0	0	0
6l	23	2	0	0	1	0
6l	25	1	0	0	0	0
6l	27	3	0	0	0	0
6l	28	4	0	0	0	0
6l	29	1	0	0	0	0
6l	2A	1124	0	0	67	0
6l	2B	19	0	0	1	0
6l	2D	23	0	0	0	0
6l	2E	17	0	0	0	0
6l	2F	14	0	0	0	0
6l	2I	1	0	0	0	0
6l	2N	2	0	0	0	0
6l	2O	2	0	0	0	0
6l	2P	13	0	0	1	0
6l	2Q	2	0	0	0	0
6l	2R	4	0	0	2	0
6l	2T	3	0	0	0	0
6l	2U	2	0	0	0	0
6l	2V	1	0	0	0	0
6l	2W	2	0	0	0	0
6l	2X	4	0	0	0	0
6l	2Y	1	0	0	0	0
6l	2Z	1	0	0	0	0
6l	2a	144	0	0	8	0
6l	2d	3	0	0	0	0
6l	2e	1	0	0	0	0
6l	2g	1	0	0	0	0
6l	2i	2	0	0	0	0
6l	2j	2	0	0	0	0
6l	2l	4	0	0	0	0
6l	2q	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2r	1	0	0	0	0
61	2t	3	0	0	0	0
61	2v	2	0	0	0	0
61	2w	5	0	0	0	0
61	2x	17	0	0	2	0
All	All	297056	0	197048	4059	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 (4059) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2104:G:H1	1:2A:2185:C:H42	1.03	1.03
1:2A:2129:C:H42	1:2A:2159:G:H1	1.11	0.96
32:1a:1035:A:H2'	32:1a:1036:G:H21	1.29	0.95
1:1A:1082:U:H3	1:1A:1086:A:N6	1.62	0.95
1:2A:1689:A:H62	1:2A:1698:A:H2	1.15	0.95
1:1A:2427:C:OP1	61:1A:4204:HOH:O	1.86	0.93
32:2a:1086:U:H3	32:2a:1099:G:H22	1.16	0.93
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.49	0.93
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.01	0.93
1:1A:1082:U:O4	1:1A:1086:A:N1	2.02	0.92
9:2N:123:TYR:HH	9:2N:130:HIS:HE2	1.10	0.90
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.53	0.90
1:1A:1082:U:H3	1:1A:1086:A:H61	1.13	0.89
14:1S:61:ASN:HD22	14:1S:64:GLU:H	1.16	0.88
1:2A:2589:A:OP1	61:2A:4803:HOH:O	1.91	0.88
1:2A:783:A:OP2	61:2A:4803:HOH:O	1.92	0.88
34:2c:78:GLY:HA3	34:2c:83:ARG:H	1.38	0.87
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.18	0.87
29:17:24:THR:HG22	29:17:27:GLY:H	1.37	0.87
32:1a:1401:G:OP1	61:1a:1901:HOH:O	1.91	0.86
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.58	0.86
33:2b:15:VAL:HG13	33:2b:209:ARG:HG2	1.57	0.85
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.40	0.85
32:1a:1086:U:H3	32:1a:1099:G:H22	1.25	0.85
1:1A:1082:U:N3	1:1A:1086:A:N6	2.19	0.85
32:1a:975:A:H4'	32:1a:976:G:H5''	1.59	0.85
32:1a:1441:G:H5''	32:1a:1442:G:H5'	1.57	0.84
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.11	0.84
1:1A:2107:C:H42	1:1A:2182:G:H1	1.25	0.84
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.59	0.84
1:1A:1082:U:C4	1:1A:1086:A:N1	2.46	0.83
1:2A:2104:G:H1	1:2A:2185:C:N4	1.77	0.83
1:2A:2129:C:N4	1:2A:2159:G:H1	1.76	0.83
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.60	0.83
25:13:3:ARG:NH1	25:13:60:GLU:OE2	2.11	0.83
41:1j:50:ILE:HA	41:1j:60:ARG:HG2	1.59	0.82
44:1m:74:VAL:HA	44:1m:77:ASN:HD22	1.44	0.82
1:1A:192:C:OP1	61:1A:4205:HOH:O	1.95	0.82
1:1A:1669:A:OP2	61:1A:4206:HOH:O	1.97	0.82
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.12	0.82
25:23:13:ILE:O	61:23:201:HOH:O	1.98	0.82
32:1a:664:G:H22	32:1a:741:G:H1	1.26	0.82
1:2A:1271:G:OP2	61:2A:4804:HOH:O	1.98	0.81
38:1g:69:VAL:HG21	38:1g:104:LEU:HD11	1.62	0.81
32:2a:975:A:H4'	32:2a:976:G:H5''	1.63	0.81
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.15	0.80
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.63	0.80
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.29	0.80
1:2A:784:A:OP2	61:2A:4803:HOH:O	1.99	0.80
1:1A:962:G:OP1	61:1A:4207:HOH:O	1.98	0.80
38:1g:78:ARG:HG3	38:1g:156:TRP:HZ3	1.47	0.80
1:1A:1993:U:OP2	61:1A:4211:HOH:O	2.00	0.80
1:1A:2181:G:H2'	1:1A:2182:G:C8	2.17	0.79
1:2A:2430:A:OP2	61:2A:4805:HOH:O	2.00	0.79
44:2m:33:ALA:HB1	44:2m:56:LEU:HD11	1.64	0.79
1:1A:1971:A:OP1	61:1A:4210:HOH:O	2.00	0.79
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.63	0.79
36:2e:92:LYS:HB3	36:2e:119:LEU:HB2	1.65	0.79
33:1b:112:VAL:HG12	33:1b:149:LEU:HD13	1.63	0.79
1:1A:1332:G:OP1	61:1A:4209:HOH:O	1.99	0.79
1:1A:1865:G:OP1	61:1A:4208:HOH:O	1.98	0.79
1:1A:2447:G:OP2	61:1A:4212:HOH:O	2.01	0.79
1:2A:2100:G:H1	1:2A:2189:U:H3	1.31	0.78
34:2c:32:LEU:HD23	34:2c:59:ARG:HD3	1.65	0.78
34:1c:150:LYS:HE3	34:1c:152:ILE:HD11	1.65	0.78
32:2a:1129:C:OP1	40:2i:66:ARG:NH1	2.17	0.78
1:2A:2448:A:OP1	61:2A:4806:HOH:O	2.01	0.78
1:1A:2121:G:O6	1:1A:2176:A:N6	2.16	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:948:G:OP1	61:2A:4807:HOH:O	2.01	0.78
32:2a:542:G:OP1	35:2d:10:ARG:NH2	2.17	0.78
42:1k:99:GLN:HG2	42:1k:105:VAL:HG21	1.65	0.78
1:2A:1204:A:H2	1:2A:1241:A:H62	1.32	0.78
32:2a:953:G:H5'	32:2a:965:A:H61	1.48	0.78
32:1a:683:G:N7	61:1a:1911:HOH:O	2.17	0.77
8:1I:54:GLN:HE21	8:1I:57:ARG:HH22	1.32	0.77
1:1A:1648:C:OP1	61:1A:4213:HOH:O	2.03	0.77
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.65	0.77
32:2a:266:G:H5''	32:2a:268:C:H41	1.50	0.77
1:1A:826:U:OP1	61:1A:4204:HOH:O	2.02	0.77
42:1k:48:ILE:O	42:1k:50:TYR:N	2.17	0.77
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.67	0.76
36:1e:78:HIS:HD2	39:1h:104:ARG:HD2	1.49	0.76
54:2w:348:LEU:HA	54:2w:352:ALA:HB3	1.68	0.76
1:1A:948:G:OP1	61:1A:4207:HOH:O	2.03	0.76
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.19	0.76
1:1A:1970:A:OP1	61:1A:4210:HOH:O	2.02	0.76
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.19	0.76
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.19	0.76
32:2a:677:U:H3	32:2a:713:G:H22	1.31	0.76
5:2F:155:LEU:HD11	5:2F:176:LEU:HD12	1.68	0.75
1:1A:2131:G:OP2	1:1A:2158:A:N6	2.19	0.75
1:2A:1890:A:OP2	61:2A:4810:HOH:O	2.05	0.75
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.69	0.75
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.68	0.75
32:2a:664:G:H22	32:2a:741:G:H1	1.35	0.75
1:1A:1072:C:H1'	1:1A:1092:C:H41	1.52	0.75
1:1A:1093:G:H3'	1:1A:1094:U:H5''	1.67	0.75
32:1a:677:U:H3	32:1a:713:G:H22	1.32	0.75
32:1a:1224:G:OP1	61:1a:1902:HOH:O	2.05	0.75
18:1W:92:ARG:NH2	61:1W:301:HOH:O	2.20	0.74
32:2a:1279:A:O2'	32:2a:1281:U:OP2	2.05	0.74
1:2A:981:A:OP1	61:2A:4808:HOH:O	2.04	0.74
1:1A:1342:A:OP2	61:1A:4214:HOH:O	2.04	0.74
1:2A:1670:C:OP1	61:2A:4811:HOH:O	2.05	0.74
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.69	0.74
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.36	0.74
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.70	0.74
32:1a:1399:C:H4'	32:1a:1400:5MC:H5''	1.69	0.74
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:568:U:O4	61:2A:4809:HOH:O	2.05	0.74
35:2d:102:ASP:OD2	35:2d:118:ARG:NH1	2.20	0.74
50:2s:28:LYS:HD3	50:2s:47:HIS:HA	1.67	0.74
1:1A:2355:C:H1'	22:10:39:ARG:HH21	1.53	0.74
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.70	0.74
33:2b:76:GLN:HB3	33:2b:208:ILE:HG12	1.70	0.73
32:1a:116:A:OP1	61:1a:1903:HOH:O	2.06	0.73
48:1q:13:ASP:H	48:1q:14:LYS:HZ2	1.33	0.73
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.20	0.73
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.52	0.73
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.70	0.73
1:2A:973:A:OP2	61:2A:4809:HOH:O	2.07	0.73
1:2A:1648:C:OP1	61:2A:4804:HOH:O	2.07	0.73
26:24:58:ARG:HD3	50:2s:67:VAL:H	1.51	0.73
6:1G:77:ILE:HG13	6:1G:82:LEU:HD23	1.69	0.73
1:1A:2107:C:N4	1:1A:2182:G:H1	1.86	0.73
33:1b:189:ASP:OD1	33:1b:189:ASP:N	2.20	0.73
6:2G:35:GLU:HG3	6:2G:36:LYS:HG3	1.71	0.73
1:1A:2250:G:OP1	12:1Q:85:LYS:NZ	2.21	0.72
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.21	0.72
38:1g:113:GLU:HB3	38:1g:118:VAL:HG13	1.69	0.72
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.71	0.72
54:1w:114:GLY:HA3	54:1w:196:THR:HG22	1.71	0.72
2:2B:66:A:H61	2:2B:109:C:H5'	1.54	0.72
1:1A:1013:C:OP2	61:1A:4215:HOH:O	2.07	0.72
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.72	0.72
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.21	0.72
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.53	0.72
1:2A:2751:G:H5'	7:2H:2:SER:HA	1.71	0.72
40:2i:28:VAL:HG12	40:2i:63:ILE:HB	1.71	0.72
32:1a:382:A:H2'	32:1a:383:A:C8	2.24	0.72
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.23	0.72
61:1a:1901:HOH:O	53:1v:19:U:OP1	2.06	0.72
1:2A:1124:C:OP1	61:2A:4812:HOH:O	2.07	0.72
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.23	0.72
1:2A:1833:U:OP1	61:2A:4814:HOH:O	2.08	0.72
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.70	0.72
2:2B:43:C:O2	6:2G:95:ARG:NH2	2.23	0.72
39:1h:113:SER:HB2	39:1h:134:ILE:HD11	1.72	0.71
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.71	0.71
18:1W:12:ILE:HD13	18:1W:17:VAL:HG13	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.24	0.71
32:2a:1162:C:H42	32:2a:1174:G:H1	1.38	0.71
41:2j:6:ILE:HB	41:2j:72:VAL:HG23	1.72	0.71
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.71	0.71
32:1a:945:G:OP1	61:1a:1905:HOH:O	2.08	0.71
32:1a:1108:G:O6	61:1a:1904:HOH:O	2.07	0.71
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.22	0.71
39:1h:120:THR:H	39:1h:123:GLU:HB2	1.55	0.71
20:2Y:11:ASP:N	20:2Y:11:ASP:OD1	2.22	0.71
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.24	0.71
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.26	0.71
7:2H:3:ARG:HG2	7:2H:6:ARG:HE	1.56	0.71
32:2a:532:A:H2	34:2c:156:ARG:HH22	1.39	0.71
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.73	0.71
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.73	0.71
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.20	0.70
4:2E:110:GLY:O	61:2R:301:HOH:O	2.09	0.70
32:1a:1083:U:OP1	61:1a:1907:HOH:O	2.09	0.70
38:1g:78:ARG:HG2	38:1g:79:ARG:H	1.57	0.70
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.72	0.70
1:2A:1342:A:OP2	61:2A:4813:HOH:O	2.08	0.70
40:2i:3:GLN:HG2	40:2i:20:ARG:HH21	1.56	0.70
32:1a:943:U:OP2	61:1a:1906:HOH:O	2.08	0.70
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.23	0.70
1:2A:1973:G:OP1	61:2A:4820:HOH:O	2.09	0.70
33:2b:63:MET:HG3	33:2b:225:ALA:HB1	1.71	0.70
1:2A:2104:G:N2	1:2A:2185:C:N3	2.39	0.70
1:2A:1024:G:OP2	61:2A:4818:HOH:O	2.09	0.70
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.72	0.70
22:20:10:THR:HG22	22:20:12:ASN:H	1.56	0.70
1:1A:2840:C:OP2	61:1A:4217:HOH:O	2.10	0.70
15:1T:41:ARG:NH2	32:1a:346:G:OP1	2.24	0.70
1:2A:588:U:OP2	61:2A:4815:HOH:O	2.08	0.70
1:1A:1647:G:OP1	61:1A:4213:HOH:O	2.10	0.70
1:2A:1647:G:OP1	61:2A:4804:HOH:O	2.09	0.70
1:1A:762:U:OP1	61:1A:4216:HOH:O	2.08	0.70
32:1a:1353:G:OP1	52:1u:10:ARG:NH2	2.24	0.70
1:2A:2504:U:OP2	61:2A:4819:HOH:O	2.09	0.70
41:1j:23:ILE:HD11	41:1j:72:VAL:HG21	1.74	0.70
1:2A:2822:G:OP2	61:2A:4821:HOH:O	2.10	0.70
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1622:G:OP2	61:1A:4219:HOH:O	2.10	0.69
34:1c:19:GLU:HG2	34:1c:54:ARG:HE	1.57	0.69
1:2A:2269:A:OP1	61:2A:4822:HOH:O	2.10	0.69
32:2a:1126:U:H3	41:2j:40:LEU:HD11	1.56	0.69
44:1m:81:LEU:HD22	44:1m:88:ARG:HB2	1.74	0.69
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.72	0.69
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.74	0.69
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.55	0.69
1:2A:1324:G:N7	61:2A:4867:HOH:O	2.25	0.69
38:2g:113:GLU:HB2	38:2g:119:ARG:HG2	1.74	0.69
25:13:7:LYS:HG3	25:13:34:GLU:HG2	1.75	0.69
44:1m:4:ILE:HD12	44:1m:57:ARG:HB2	1.75	0.69
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.74	0.69
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.25	0.69
3:1D:206:LEU:O	3:1D:211:ARG:HD3	1.92	0.69
26:14:61:ARG:HG2	26:14:62:ARG:N	2.08	0.69
1:2A:1021:A:H62	1:2A:1141:U:H3	1.39	0.69
32:1a:1055:A:H2'	34:1c:156:ARG:HD2	1.75	0.69
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.73	0.69
1:2A:827:U:OP1	61:2A:4805:HOH:O	2.10	0.69
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.23	0.69
39:2h:24:THR:HG22	39:2h:63:LEU:HD21	1.74	0.69
47:2p:74:LEU:HD23	47:2p:79:VAL:HG11	1.75	0.69
1:1A:1023:U:OP2	61:1A:4218:HOH:O	2.10	0.69
40:1i:53:VAL:O	40:1i:55:ALA:N	2.20	0.69
1:1A:1702:G:N7	61:1A:4259:HOH:O	2.25	0.69
1:1A:2099:U:H3	1:1A:2190:G:H1	1.40	0.69
27:15:40:LYS:HD3	27:15:46:CYS:HA	1.73	0.69
37:2f:35:ALA:HA	37:2f:67:MET:HB3	1.75	0.69
5:1F:123:LEU:HD13	5:1F:192:LEU:HD13	1.73	0.68
47:1p:18:ARG:NH1	47:1p:32:TYR:OH	2.26	0.68
1:2A:2063:C:OP1	61:2A:4823:HOH:O	2.11	0.68
32:2a:1256:A:OP2	34:2c:26:LYS:NZ	2.25	0.68
1:2A:399:G:OP2	61:2A:4817:HOH:O	2.09	0.68
1:1A:998:C:OP1	61:1A:4221:HOH:O	2.11	0.68
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.11	0.68
40:2i:17:VAL:HG22	40:2i:63:ILE:HD12	1.76	0.68
1:1A:1315:C:OP2	61:1A:4209:HOH:O	2.11	0.68
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.08	0.68
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.74	0.68
34:2c:139:GLN:HE21	34:2c:143:GLU:HG3	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:111:ALA:HB2	35:2d:120:LEU:HD22	1.75	0.68
33:1b:16:HIS:HD2	33:1b:18:GLY:H	1.42	0.68
5:2F:165:ARG:HG2	5:2F:168:ARG:HH21	1.58	0.68
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.27	0.68
32:2a:73:G:H1	32:2a:96:U:H3	1.41	0.68
3:1D:237:GLU:OE2	61:1D:401:HOH:O	2.11	0.68
32:2a:972:C:OP1	61:2a:1801:HOH:O	2.12	0.68
42:2k:62:GLN:OE1	42:2k:93:GLN:NE2	2.26	0.68
32:1a:953:G:H5'	32:1a:965:A:H61	1.58	0.68
32:2a:1193:G:O2'	36:2e:25:ARG:NH2	2.27	0.68
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.74	0.68
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.12	0.68
1:2A:2133:G:N2	1:2A:2157:G:N7	2.41	0.68
1:1A:2504:U:OP2	61:1A:4220:HOH:O	2.11	0.68
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.02	0.68
1:2A:2049:G:N7	61:2A:4877:HOH:O	2.26	0.68
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.27	0.68
32:2a:972:C:O2'	41:2j:55:LYS:O	2.12	0.68
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.12	0.67
32:1a:1402:4OC:OP2	61:1a:1901:HOH:O	2.11	0.67
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.76	0.67
26:24:62:ARG:HA	26:24:62:ARG:NE	2.09	0.67
36:2e:136:MET:HA	36:2e:139:LEU:HD12	1.76	0.67
35:1d:20:TYR:HD1	35:1d:26:CYS:HB3	1.60	0.67
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.28	0.67
1:2A:1311:G:H2'	29:27:47:ARG:HH22	1.59	0.67
15:2T:107:ASP:OD2	15:2T:111:ARG:NH1	2.26	0.67
32:2a:316:G:OP2	32:2a:351:G:O2'	2.11	0.67
42:2k:79:SER:HB2	42:2k:106:LYS:HD3	1.75	0.67
1:1A:2120:G:H1	1:1A:2178:C:H42	1.42	0.67
15:1T:111:ARG:NH2	32:1a:1464:G:OP2	2.27	0.67
32:2a:1521:G:N3	61:2a:1810:HOH:O	2.26	0.67
1:2A:422:A:OP2	61:2A:4826:HOH:O	2.12	0.67
1:2A:2099:U:H3	1:2A:2190:G:H1	1.41	0.67
1:1A:1072:C:O2	1:1A:1092:C:N4	2.28	0.67
34:2c:47:LEU:HB3	34:2c:52:LEU:HB2	1.77	0.67
1:1A:1453:U:OP1	13:1R:77:ARG:NH1	2.26	0.67
1:2A:582:G:OP2	61:2A:4825:HOH:O	2.12	0.67
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.76	0.67
1:2A:324:A:N6	1:2A:338:G:O2'	2.26	0.67
11:2P:27:HIS:NE2	61:2P:302:HOH:O	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:44:ILE:HG12	20:1Y:64:GLU:HG3	1.77	0.67
1:2A:2134:A:O2'	1:2A:2159:G:N2	2.27	0.67
1:2A:2198:A:OP1	8:2I:33:ARG:NH2	2.27	0.67
44:2m:106:ASN:OD1	44:2m:106:ASN:N	2.27	0.67
50:1s:36:ARG:HB3	50:1s:72:GLY:HA3	1.77	0.67
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.60	0.67
44:2m:76:ALA:HA	44:2m:79:LYS:HB3	1.76	0.67
1:2A:271(P):C:O3'	8:2I:42:SER:OG	2.13	0.67
1:2A:2518:A:OP2	61:2A:4824:HOH:O	2.11	0.67
1:1A:2612:C:OP2	27:15:2:ALA:N	2.27	0.66
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.61	0.66
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.12	0.66
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.28	0.66
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.77	0.66
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.27	0.66
1:2A:1395:A:OP1	61:2A:4827:HOH:O	2.13	0.66
38:2g:99:LEU:HD23	38:2g:102:ARG:HH12	1.60	0.66
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.76	0.66
54:2w:169:GLY:HA2	54:2w:172:LYS:HE3	1.77	0.66
32:1a:309:G:O2'	32:1a:607:A:N1	2.27	0.66
1:2A:1023:U:OP2	61:2A:4818:HOH:O	2.14	0.66
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.28	0.66
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.60	0.66
32:2a:377:G:OP1	47:2p:3:LYS:HD3	1.96	0.66
1:1A:530:G:N1	1:1A:2023:G:OP1	2.24	0.66
1:1A:1468:C:OP1	61:1A:4222:HOH:O	2.13	0.66
32:1a:1030(C):G:N7	32:1a:1031:G:N2	2.44	0.66
48:1q:45:HIS:HB3	48:1q:72:ARG:HG2	1.75	0.66
32:2a:673:G:H2'	32:2a:674:G:C8	2.30	0.66
42:1k:91:ARG:HH21	49:1r:87:ARG:HH21	1.43	0.66
44:2m:3:ARG:HG2	44:2m:4:ILE:HG22	1.77	0.66
1:2A:792:G:O6	61:2A:4816:HOH:O	2.09	0.66
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.77	0.66
2:2B:54:G:H21	6:2G:29:TRP:HE1	1.43	0.66
1:1A:1267:U:OP1	61:1A:4223:HOH:O	2.13	0.66
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.28	0.66
54:1w:141:GLU:O	54:1w:163:ARG:N	2.26	0.66
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.26	0.66
33:2b:54:THR:HG22	33:2b:199:TYR:HB3	1.78	0.66
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.27	0.65
1:1A:2550:G:OP1	61:1A:4206:HOH:O	2.14	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:969:A:OP1	41:1j:55:LYS:NZ	2.29	0.65
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.29	0.65
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	1.78	0.65
46:2o:5:LYS:H	46:2o:5:LYS:HD3	1.60	0.65
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.29	0.65
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.78	0.65
1:1A:84:A:H5''	20:1Y:8:LYS:HE3	1.78	0.65
35:2d:18:LYS:NZ	35:2d:31:CYS:SG	2.68	0.65
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.77	0.65
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.78	0.65
1:2A:962:G:OP1	61:2A:4807:HOH:O	2.14	0.65
6:2G:37:VAL:HG21	6:2G:103:LEU:HD11	1.78	0.65
33:2b:91:PRO:HG3	33:2b:154:LEU:HB3	1.78	0.65
1:1A:271(L):U:H4'	8:1I:50:ARG:HH22	1.62	0.65
8:1I:4:ILE:HG12	8:1I:18:VAL:HG12	1.78	0.65
21:1Z:146:ILE:N	21:1Z:148:ASP:H	1.94	0.65
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.77	0.65
2:2B:81:G:OP2	61:2B:301:HOH:O	2.15	0.65
22:20:11:ARG:O	22:20:14:ARG:NH2	2.30	0.65
13:1R:2:ARG:HG2	13:1R:5:LYS:HB2	1.78	0.65
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.32	0.65
32:1a:964:A:OP1	61:1a:1908:HOH:O	2.14	0.65
1:2A:72:U:OP1	61:2A:4830:HOH:O	2.15	0.65
1:2A:299:A:H5''	20:2Y:86:ARG:HH21	1.62	0.65
1:2A:1241:A:OP2	61:2A:4829:HOH:O	2.14	0.65
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.79	0.65
14:2S:71:ARG:NH1	14:2S:107:GLU:OE2	2.29	0.65
32:2a:1106:G:H5''	34:2c:172:ARG:HG2	1.79	0.65
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.28	0.65
1:1A:1091:G:N1	1:1A:1100:C:O2	2.29	0.65
1:1A:1469:A:OP2	61:1A:4225:HOH:O	2.15	0.65
51:1t:10:LEU:HG	51:1t:12:ALA:H	1.61	0.65
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.30	0.65
39:2h:12:ARG:HD3	39:2h:26:VAL:HG12	1.79	0.65
32:1a:1027:C:C2	32:1a:1034:G:N2	2.57	0.65
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.45	0.65
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.78	0.65
33:2b:87:ARG:NH2	33:2b:232:PRO:O	2.25	0.65
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.30	0.65
1:1A:1760:A:OP1	61:1A:4224:HOH:O	2.14	0.65
7:1H:41:MET:HE2	7:1H:65:HIS:HA	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:140:VAL:HG11	35:1d:146:ILE:HD11	1.78	0.64
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.30	0.64
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.79	0.64
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.30	0.64
33:1b:17:PHE:HA	33:1b:44:LEU:HD21	1.78	0.64
1:2A:2127:G:C2	1:2A:2161:C:C2	2.85	0.64
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.79	0.64
10:2O:49:ARG:NH2	32:2a:1423:G:OP1	2.29	0.64
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.80	0.64
32:1a:1209:C:O2'	32:1a:1214:C:N4	2.30	0.64
1:1A:2155:G:H3'	1:1A:2156:G:C8	2.32	0.64
26:14:61:ARG:C	26:14:63:TYR:H	2.06	0.64
1:2A:848:G:OP1	61:2A:4828:HOH:O	2.13	0.64
40:2i:88:TYR:HD2	40:2i:89:ASN:HD22	1.45	0.64
1:1A:1418:G:OP2	61:1A:4226:HOH:O	2.15	0.64
32:1a:574:A:OP2	61:1a:1909:HOH:O	2.15	0.64
2:2B:44:G:OP1	6:2G:98:ARG:NH2	2.30	0.64
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.79	0.64
1:1A:1091:G:O6	1:1A:1100:C:N3	2.31	0.64
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.80	0.64
1:2A:2133:G:O2'	1:2A:2157:G:N1	2.31	0.64
32:2a:509:A:N3	32:2a:543:C:O2'	2.31	0.64
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.33	0.64
1:1A:1072:C:H42	1:1A:1098:A:P	2.21	0.64
1:1A:1088:A:H5'	1:1A:1089:G:H8	1.63	0.64
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.21	0.64
54:1w:141:GLU:HB3	54:1w:163:ARG:HB2	1.80	0.64
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.31	0.64
1:2A:2305:A:H1'	6:2G:136:ARG:HG2	1.80	0.64
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.45	0.64
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.80	0.63
32:2a:1191:A:OP2	34:2c:3:ASN:ND2	2.31	0.63
32:1a:310:G:OP2	47:1p:27:LYS:NZ	2.31	0.63
38:1g:120:ILE:HG22	38:1g:124:LEU:HD11	1.79	0.63
32:2a:222:U:H2'	32:2a:223:U:C6	2.32	0.63
32:2a:297:G:N2	32:2a:300:A:OP2	2.28	0.63
32:2a:429:U:OP2	35:2d:36:ARG:NH2	2.32	0.63
32:1a:1035:A:H2'	32:1a:1036:G:N2	2.09	0.63
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	1.80	0.63
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.34	0.63
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.20	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:656:C:O2'	46:1o:28:GLN:OE1	2.10	0.63
36:1e:50:GLU:HB2	36:1e:53:LEU:HD13	1.80	0.63
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.46	0.63
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.45	0.63
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.80	0.63
40:1i:5:TYR:HH	40:1i:7:THR:HG1	1.47	0.63
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.78	0.63
38:2g:42:ILE:HD12	38:2g:116:ALA:HB3	1.81	0.63
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.31	0.63
32:1a:1025:U:H3	32:1a:1036:G:H1	1.46	0.63
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.30	0.63
1:2A:2169:A:H2'	1:2A:2170:A:C8	2.33	0.63
5:2F:70:THR:HG22	5:2F:72:ARG:H	1.63	0.63
21:1Z:7:ALA:HB2	21:1Z:59:LEU:HD22	1.81	0.63
54:1w:299:SER:O	54:1w:301:LYS:N	2.32	0.63
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.16	0.63
32:2a:519:C:O5'	54:2w:301:LYS:NZ	2.32	0.63
26:14:58:ARG:HG3	50:1s:67:VAL:HB	1.80	0.63
32:1a:976:G:H5'	32:1a:1358:U:O2'	1.98	0.63
1:1A:1056:G:H4'	1:1A:1086:A:H1'	1.80	0.63
44:1m:92:HIS:CE1	44:1m:98:VAL:HG21	2.33	0.63
1:2A:586:A:N1	1:2A:809:G:O2'	2.30	0.63
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.81	0.63
32:2a:17:U:H2'	32:2a:18:C:C6	2.34	0.63
32:2a:437:U:H5'	35:2d:155:LEU:HD21	1.81	0.63
34:2c:34:LEU:HD11	34:2c:38:ARG:HH21	1.64	0.63
3:1D:242:ARG:N	3:1D:242:ARG:HD3	2.14	0.62
32:1a:56:U:H2'	32:1a:57:G:C8	2.34	0.62
32:2a:580:U:OP2	61:2a:1803:HOH:O	2.16	0.62
7:1H:86:GLU:OE1	7:1H:132:ARG:NH2	2.32	0.62
33:2b:95:GLN:HE22	33:2b:147:LYS:HB3	1.63	0.62
1:1A:883:G:N2	1:1A:893:C:H42	1.96	0.62
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.63	0.62
12:1Q:32:TYR:OH	12:1Q:111:GLU:OE2	2.12	0.62
32:1a:1366:C:O2'	41:1j:60:ARG:NH1	2.32	0.62
32:2a:8:A:N6	35:2d:205:GLU:O	2.30	0.62
32:2a:1271:G:N2	32:2a:1272:G:N7	2.48	0.62
36:2e:144:THR:H	36:2e:147:ASP:HB2	1.64	0.62
54:1w:230:MEQ:HE2	56:1z:6:LYS:HD2	1.81	0.62
32:1a:1414:U:H3	32:1a:1486:G:H1	1.48	0.62
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2110:G:H1	1:2A:2179:C:H42	1.45	0.62
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.31	0.62
32:2a:504:C:OP1	61:2a:1804:HOH:O	2.16	0.62
49:2r:48:GLY:O	49:2r:74:ARG:NH2	2.33	0.62
1:1A:72:U:OP2	24:12:29:LYS:NZ	2.27	0.62
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.80	0.62
1:2A:336:C:O2'	20:2Y:35:TYR:OH	2.17	0.62
1:2A:2258:C:O2'	1:2A:2427:C:OP2	2.18	0.62
41:2j:38:ILE:HG12	41:2j:71:LEU:HB3	1.81	0.62
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.35	0.62
7:1H:97:ARG:NE	7:1H:104:GLU:OE2	2.30	0.62
32:1a:1298:C:OP2	38:1g:114:ARG:NH2	2.32	0.62
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.32	0.62
1:2A:299:A:N1	1:2A:322:A:O2'	2.31	0.62
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.35	0.62
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.34	0.62
1:2A:2849:U:O4	15:2T:23:ARG:NH1	2.31	0.62
32:2a:1263:C:N3	32:2a:1272:G:O6	2.33	0.62
1:1A:11:G:H2'	1:1A:12:U:H5'	1.82	0.62
1:1A:1493:C:N4	1:1A:2206:G:O2'	2.33	0.62
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.15	0.62
32:1a:1034:G:H3'	32:1a:1035:A:H8	1.63	0.62
1:2A:833:U:O2	11:2P:55:ARG:NH2	2.33	0.62
1:1A:1155:A:OP1	16:1U:55:ARG:HD3	2.00	0.62
7:1H:3:ARG:HE	7:1H:54:ARG:HH12	1.48	0.62
34:1c:36:ASP:HA	34:1c:39:ILE:HD12	1.81	0.62
1:2A:1993:U:OP2	61:2A:4831:HOH:O	2.15	0.62
32:2a:651:C:N4	32:2a:753:A:OP2	2.33	0.62
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.35	0.62
22:10:10:THR:HG22	22:10:12:ASN:H	1.64	0.62
32:1a:652:U:O4	32:1a:752:G:O2'	2.15	0.62
32:1a:972:C:O2'	41:1j:55:LYS:O	2.18	0.62
38:1g:16:LEU:HD21	40:1i:45:ALA:HB2	1.80	0.62
35:2d:7:PRO:HB2	35:2d:10:ARG:HD2	1.81	0.62
32:1a:142:G:H2'	32:1a:143:A:C8	2.35	0.61
32:2a:544:G:OP1	35:2d:62:GLN:NE2	2.27	0.61
37:2f:82:ARG:HB2	37:2f:85:VAL:HG23	1.82	0.61
32:2a:1133:G:H2'	32:2a:1134:G:H8	1.66	0.61
48:2q:53:LEU:HD23	48:2q:85:VAL:HG11	1.82	0.61
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.65	0.61
32:1a:1191:A:OP1	34:1c:4:LYS:NZ	2.29	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1396:A:H4'	32:1a:1397:C:H5''	1.82	0.61
1:2A:247:G:H4'	1:2A:386:G:C5	2.35	0.61
1:2A:2207:G:O2'	1:2A:2208:A:OP1	2.18	0.61
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.82	0.61
54:1w:228:GLY:HA3	54:1w:232:VAL:HB	1.82	0.61
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.34	0.61
1:2A:2499:C:OP1	61:2A:4806:HOH:O	2.16	0.61
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.34	0.61
32:1a:961:U:OP2	32:1a:1223:C:O2'	2.13	0.61
36:1e:142:LEU:O	36:1e:143:ARG:NH1	2.34	0.61
26:24:58:ARG:HE	50:2s:68:GLY:H	1.48	0.61
1:1A:205:G:O6	23:11:39:LYS:NZ	2.33	0.61
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.34	0.61
54:1w:130:MET:HE3	54:1w:332:LEU:HD11	1.82	0.61
32:2a:1272:G:N2	32:2a:1273:G:C5	2.69	0.61
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.33	0.61
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.32	0.61
32:2a:663:A:O3'	49:2r:64:ARG:NH2	2.32	0.61
33:2b:69:LEU:HD23	33:2b:91:PRO:HB2	1.83	0.61
34:2c:42:LEU:HA	34:2c:45:LYS:HD2	1.82	0.61
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.01	0.61
20:1Y:11:ASP:OD2	20:1Y:97:ARG:NH2	2.34	0.61
32:1a:444:C:H2'	32:1a:445:G:H8	1.65	0.61
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.81	0.61
1:2A:2313:C:H4'	6:2G:91:ARG:HG3	1.83	0.61
32:2a:959:A:HO2'	32:2a:984:C:HO2'	1.46	0.61
44:1m:88:ARG:O	44:1m:92:HIS:ND1	2.34	0.61
33:2b:33:TYR:HD2	33:2b:41:ILE:HD11	1.64	0.61
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.35	0.61
1:1A:1673:U:OP1	61:1A:4228:HOH:O	2.16	0.61
8:1I:75:LEU:HD22	8:1I:105:HIS:HD2	1.65	0.61
32:1a:966:M2G:HM13	32:1a:967:5MC:H1'	1.82	0.61
33:1b:13:ALA:HA	33:1b:17:PHE:HB3	1.83	0.61
1:2A:1453:U:O2'	1:2A:1455:G:N7	2.32	0.61
1:2A:1604:C:OP1	61:2A:4833:HOH:O	2.16	0.61
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.36	0.61
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.36	0.61
32:2a:674:G:H2'	32:2a:675:A:H8	1.65	0.61
32:2a:1359:C:O2'	32:2a:1361:G:N7	2.34	0.61
1:1A:821:A:H2'	1:1A:946:G:H5''	1.83	0.60
1:1A:982:C:OP2	61:1A:4230:HOH:O	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1N:42:TRP:HA	9:1N:48:MET:HE1	1.82	0.60
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.34	0.60
38:1g:16:LEU:HD23	40:1i:42:ARG:HA	1.82	0.60
1:2A:1456:G:OP2	61:2A:4832:HOH:O	2.16	0.60
14:2S:99:LYS:NZ	14:2S:103:GLU:OE2	2.30	0.60
37:1f:35:ALA:HB1	37:1f:65:VAL:HG11	1.82	0.60
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.15	0.60
34:2c:131:ARG:HH21	34:2c:135:LYS:HE3	1.64	0.60
1:1A:222:A:OP2	61:1A:4227:HOH:O	2.15	0.60
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.83	0.60
35:1d:57:ARG:HH22	36:1e:107:ARG:HD3	1.67	0.60
32:1a:17:U:H2'	32:1a:18:C:C6	2.35	0.60
32:1a:156:G:H3'	32:1a:157:G:H5''	1.84	0.60
34:1c:26:LYS:HB2	41:1j:45:ARG:HH12	1.66	0.60
38:1g:74:GLU:OE2	38:1g:76:ARG:NH1	2.34	0.60
1:2A:880:G:H1	1:2A:897:C:H42	1.49	0.60
1:2A:2166:G:N7	1:2A:2168:G:N2	2.49	0.60
32:2a:890:G:O2'	32:2a:906:G:O6	2.18	0.60
1:1A:2146:C:H4'	1:1A:2147:G:H5''	1.84	0.60
32:1a:642:A:N3	39:1h:113:SER:OG	2.30	0.60
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.36	0.60
47:1p:53:VAL:HG12	47:1p:79:VAL:HG22	1.83	0.60
32:2a:1308:U:H2'	32:2a:1309:G:H8	1.66	0.60
33:2b:45:GLN:HG3	33:2b:48:MET:HE2	1.84	0.60
1:1A:1101:U:H2'	1:1A:1102:C:C6	2.37	0.60
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.37	0.60
1:1A:2336:A:H61	22:10:43:THR:CG2	2.15	0.60
54:1w:317:ILE:HG13	54:1w:319:PHE:H	1.65	0.60
41:2j:22:LYS:O	41:2j:26:ALA:N	2.35	0.60
1:1A:271(H):G:H2'	1:1A:271(I):G:H8	1.67	0.60
29:17:5:TRP:NE1	29:17:7:PRO:HG3	2.17	0.60
1:2A:1223:G:N2	1:2A:1226:A:OP2	2.29	0.60
1:1A:1840:G:N7	61:1A:4288:HOH:O	2.31	0.60
14:1S:61:ASN:ND2	14:1S:64:GLU:H	1.96	0.60
42:1k:70:LYS:HA	42:1k:73:MET:HE2	1.83	0.60
1:2A:774:A:H2'	1:2A:774:A:N3	2.17	0.60
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.27	0.60
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.84	0.60
34:2c:19:GLU:O	34:2c:40:ARG:NH2	2.34	0.60
40:2i:48:GLU:HB3	40:2i:78:LYS:HE2	1.83	0.60
1:1A:604:G:OP2	11:1P:90:ARG:NH1	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:108:G:C6	51:1t:15:ARG:HG2	2.37	0.60
34:1c:82:GLU:OE2	34:1c:85:ARG:NH1	2.33	0.60
47:1p:19:ILE:HG22	47:1p:36:ILE:HG13	1.84	0.60
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.01	0.60
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.83	0.60
32:2a:619:U:N3	35:2d:134:ASP:OD1	2.33	0.60
5:2F:33:LEU:HD21	5:2F:112:MET:HB3	1.83	0.59
41:2j:44:VAL:HG13	41:2j:66:ARG:HG2	1.84	0.59
1:1A:1670:C:OP1	61:1A:4229:HOH:O	2.16	0.59
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.35	0.59
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	1.82	0.59
35:1d:28:SER:OG	35:1d:30:LYS:HG2	2.02	0.59
4:2E:34:VAL:HB	4:2E:48:GLN:HE21	1.67	0.59
38:2g:46:ALA:HB1	38:2g:121:ALA:HB2	1.84	0.59
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.34	0.59
38:1g:38:LEU:HA	38:1g:41:ARG:HD2	1.85	0.59
1:2A:796:C:H2'	1:2A:797:C:C6	2.37	0.59
1:2A:1376:C:OP2	61:2A:4835:HOH:O	2.17	0.59
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.85	0.59
23:11:77:ALA:HA	23:11:80:LEU:HD13	1.85	0.59
55:1x:20:H2U:O2'	55:1x:21:H2U:OP1	2.16	0.59
1:2A:821:A:H2'	1:2A:946:G:H5''	1.83	0.59
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.38	0.59
44:2m:82:MET:HE2	44:2m:92:HIS:HB3	1.82	0.59
1:1A:154(A):C:H42	1:1A:171:G:H1	1.49	0.59
32:1a:1027:C:C4	32:1a:1034:G:N1	2.66	0.59
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.85	0.59
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.68	0.59
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.38	0.59
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.35	0.59
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.37	0.59
2:1B:106:G:H5'	21:1Z:31:ARG:HB3	1.85	0.59
32:1a:159:G:H3'	32:1a:160:A:H5''	1.83	0.59
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.37	0.59
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.17	0.59
49:2r:73:ALA:HB1	49:2r:78:LEU:HB2	1.85	0.59
1:1A:1073:A:H2'	1:1A:1074:G:H8	1.67	0.59
1:1A:2189:U:H2'	1:1A:2190:G:H8	1.66	0.59
1:1A:2462:U:H1'	1:1A:2491:U:O4	2.02	0.59
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.85	0.59
26:14:43:TYR:O	26:14:45:GLY:N	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:643:A:N1	1:2A:2369:A:O2'	2.34	0.59
32:2a:583:A:O2'	48:2q:91:ARG:NH1	2.36	0.59
32:2a:1015:A:H2'	32:2a:1016:A:C8	2.38	0.59
32:2a:1316:G:H4'	45:2n:18:VAL:HG13	1.83	0.59
38:2g:78:ARG:HH12	38:2g:156:TRP:HB3	1.67	0.59
7:1H:3:ARG:HG2	7:1H:6:ARG:HG2	1.85	0.59
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.83	0.59
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.84	0.59
32:1a:455:C:H42	32:1a:476:G:H1	1.50	0.59
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.36	0.59
46:1o:26:GLU:HG3	46:1o:81:LEU:HD13	1.85	0.59
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.02	0.59
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.84	0.59
32:1a:1272:G:H2'	32:1a:1273:G:O4'	2.03	0.59
33:1b:21:ARG:HB3	33:1b:39:ILE:HG12	1.84	0.59
21:2Z:157:LEU:HB3	21:2Z:161:VAL:HG22	1.85	0.59
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.85	0.59
1:1A:2115:G:H2'	1:1A:2117:A:H62	1.68	0.58
1:1A:2428:G:OP1	61:1A:4204:HOH:O	2.17	0.58
32:1a:407:G:H5''	35:1d:115:ARG:HB3	1.85	0.58
32:1a:414:A:H2'	32:1a:415:A:H8	1.68	0.58
32:1a:1226:C:H2'	44:1m:103:THR:HB	1.85	0.58
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.38	0.58
35:1d:122:ARG:NH1	35:1d:134:ASP:O	2.36	0.58
1:2A:800:A:H8	1:2A:800:A:OP1	1.87	0.58
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.83	0.58
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.84	0.58
21:1Z:138:GLU:HB2	21:1Z:156:LYS:HZ2	1.68	0.58
32:1a:1240:U:OP1	38:1g:119:ARG:NH2	2.36	0.58
1:2A:2135:A:N1	1:2A:2156:G:O2'	2.36	0.58
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.39	0.58
1:1A:2206:G:H5''	1:1A:2207:G:N7	2.18	0.58
33:1b:15:VAL:HG11	33:1b:213:LEU:HD12	1.84	0.58
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.84	0.58
1:1A:1509(A):A:H3'	1:1A:1509(B):A:H8	1.68	0.58
28:26:12:GLU:OE1	28:26:19:ARG:NH1	2.36	0.58
1:1A:579:G:H2'	1:1A:580:C:C6	2.39	0.58
1:1A:1783:A:N7	61:1A:4298:HOH:O	2.32	0.58
1:1A:1971:A:OP2	3:1D:242:ARG:NH2	2.36	0.58
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.52	0.58
42:1k:33:THR:HA	42:1k:39:PRO:HA	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.03	0.58
32:2a:45:U:H2'	32:2a:46:G:C8	2.39	0.58
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.36	0.58
32:2a:452:A:OP1	47:2p:43:LYS:NZ	2.37	0.58
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.39	0.58
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.04	0.58
32:1a:501:C:H2'	32:1a:502:G:H8	1.68	0.58
1:2A:468:G:O2'	5:2F:62:ARG:NH2	2.35	0.58
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.84	0.58
38:2g:150:ALA:HA	42:2k:59:TYR:HB3	1.84	0.58
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.85	0.58
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.37	0.58
1:1A:2134:A:H1'	1:1A:2159:G:H1'	1.86	0.58
32:1a:352:C:O2'	32:1a:354:G:OP1	2.18	0.58
49:1r:26:LEU:HD21	49:1r:39:VAL:HG13	1.86	0.58
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.38	0.58
1:2A:1346:G:OP2	61:2A:4834:HOH:O	2.16	0.58
5:2F:148:LEU:HD21	5:2F:191:ARG:HE	1.69	0.58
18:2W:65:LEU:HB2	18:2W:68:ARG:HG3	1.85	0.58
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.68	0.58
33:2b:143:GLU:O	33:2b:147:LYS:HG3	2.03	0.58
50:2s:27:GLU:HG3	50:2s:28:LYS:HE3	1.85	0.58
54:1w:285:LEU:HG	54:1w:289:ARG:NH1	2.18	0.58
5:2F:122:LYS:HB3	5:2F:191:ARG:HG2	1.86	0.58
32:2a:538:G:H5''	43:2l:114:LYS:HB2	1.86	0.58
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.69	0.58
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.38	0.58
1:1A:747:U:O2	1:1A:2014:A:H1'	2.03	0.58
1:1A:1352:U:OP2	61:1A:4231:HOH:O	2.16	0.58
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.86	0.58
33:1b:32:ILE:HG21	33:1b:40:HIS:HD2	1.68	0.58
26:24:16:CYS:SG	26:24:17:GLY:N	2.76	0.58
35:2d:155:LEU:HB3	35:2d:158:ILE:HG22	1.86	0.58
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.67	0.58
40:2i:61:ALA:HB1	40:2i:63:ILE:HD11	1.85	0.58
1:1A:1071:G:H1'	1:1A:1089:G:C6	2.39	0.58
12:1Q:136:ALA:HB1	21:1Z:52:SER:HB2	1.86	0.58
26:14:56:VAL:O	26:14:60:GLN:HB2	2.04	0.58
32:1a:1005:A:OP2	32:1a:1006:C:N4	2.37	0.58
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.85	0.58
1:2A:1016:G:N7	61:2A:4902:HOH:O	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:71:ASP:CG	3:2D:103:ARG:HH22	2.11	0.58
15:2T:24:PRO:HA	15:2T:49:VAL:HG23	1.85	0.58
33:2b:124:SER:HB3	33:2b:125:PRO:CD	2.34	0.58
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	1.86	0.58
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.33	0.57
1:2A:2129:C:N3	1:2A:2159:G:N2	2.44	0.57
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.39	0.57
12:2Q:109:VAL:HG13	12:2Q:113:GLN:HB2	1.85	0.57
32:2a:652:U:O4	32:2a:752:G:O2'	2.19	0.57
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.86	0.57
50:2s:33:THR:HG21	50:2s:49:ILE:HD11	1.86	0.57
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.86	0.57
1:1A:2166:G:H2'	1:1A:2167:U:H5	1.67	0.57
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.39	0.57
10:1O:104:ARG:NE	15:1T:36:GLU:OE2	2.33	0.57
32:1a:56:U:H2'	32:1a:57:G:H8	1.68	0.57
32:1a:673:G:H2'	32:1a:674:G:C8	2.39	0.57
33:1b:88:ALA:HB2	33:1b:219:VAL:HG13	1.84	0.57
1:2A:307:G:N1	1:2A:310:A:OP2	2.36	0.57
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.36	0.57
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.18	0.57
40:2i:19:LEU:HD23	40:2i:61:ALA:HB2	1.86	0.57
1:1A:881:G:H2'	1:1A:882:G:O4'	2.04	0.57
1:1A:2079:U:O3'	23:11:35:THR:OG1	2.23	0.57
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.39	0.57
1:2A:1957:C:OP1	61:2A:4837:HOH:O	2.18	0.57
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.39	0.57
42:2k:98:LEU:O	42:2k:101:SER:OG	2.15	0.57
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.39	0.57
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.69	0.57
34:1c:59:ARG:HG2	34:1c:64:VAL:HB	1.85	0.57
55:1x:7:U:O2'	55:1x:49:U:OP2	2.22	0.57
1:2A:2112:G:C2	1:2A:2113:U:H1'	2.39	0.57
32:2a:946:A:H2'	32:2a:947:G:C8	2.39	0.57
33:2b:163:PHE:HD1	33:2b:185:ILE:HG13	1.69	0.57
32:1a:1325:C:H4'	52:1u:17:THR:HG21	1.85	0.57
1:2A:668:G:H5'	1:2A:669:G:OP2	2.05	0.57
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.87	0.57
7:2H:24:VAL:HG22	7:2H:35:VAL:HB	1.87	0.57
15:2T:127:ALA:C	15:2T:129:ARG:H	2.12	0.57
21:2Z:145:GLU:HG3	21:2Z:146:ILE:H	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	1.86	0.57
32:1a:41:G:H2'	32:1a:42:G:C8	2.39	0.57
36:1e:93:PRO:HG2	39:1h:105:ARG:NH1	2.19	0.57
32:2a:1297:C:OP1	44:2m:44:ARG:NH1	2.30	0.57
35:2d:189:PRO:HB2	35:2d:194:LEU:HD21	1.87	0.57
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.69	0.57
1:1A:1101:U:H2'	1:1A:1102:C:H6	1.70	0.57
2:1B:23:G:O6	61:1B:301:HOH:O	2.16	0.57
32:1a:445:G:H2'	32:1a:446:G:H8	1.70	0.57
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	1.85	0.57
49:1r:24:ALA:O	49:1r:26:LEU:N	2.36	0.57
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.39	0.57
11:2P:96:THR:HG23	11:2P:99:LEU:H	1.68	0.57
54:2w:182:ARG:HB3	54:2w:307:PHE:HB2	1.85	0.57
54:2w:250:VAL:HG11	54:2w:268:ILE:HG12	1.87	0.57
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.37	0.57
32:1a:7:G:H5'	32:1a:298:A:O4'	2.04	0.57
51:1t:42:GLN:NE2	51:1t:46:GLU:OE2	2.37	0.57
1:2A:1971:A:OP2	3:2D:242:ARG:NH2	2.35	0.57
14:2S:49:VAL:HG11	14:2S:77:ALA:HB2	1.85	0.57
32:2a:1060:C:H5''	41:2j:51:ARG:HG2	1.85	0.57
32:2a:1108:G:H5'	34:2c:176:HIS:HD2	1.69	0.57
54:2w:110:GLU:OE1	54:2w:112:ARG:NH1	2.37	0.57
1:1A:2175:C:H2'	1:1A:2176:A:C8	2.39	0.57
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.67	0.57
31:19:17:ILE:HD13	31:19:26:ILE:HD13	1.87	0.57
42:1k:15:ALA:HA	42:1k:77:MET:HA	1.87	0.57
1:2A:271(M):G:H4'	1:2A:271(N):U:OP1	2.04	0.57
1:2A:686:G:N2	1:2A:788:A:H61	2.03	0.57
1:2A:963:U:OP2	61:2A:4807:HOH:O	2.17	0.57
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.38	0.57
1:1A:1056:G:H5''	1:1A:1057:A:O4'	2.04	0.57
32:1a:952:U:H2'	32:1a:953:G:C8	2.40	0.57
41:1j:23:ILE:O	41:1j:27:ALA:N	2.36	0.57
3:2D:71:ASP:HB3	3:2D:103:ARG:HH12	1.70	0.57
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.86	0.57
32:2a:202:U:H5''	32:2a:203:U:H5	1.69	0.57
32:2a:620:C:C2	35:2d:135:LEU:HG	2.39	0.57
32:2a:1187:G:N2	45:2n:60:SER:OG	2.32	0.57
43:2l:47:LYS:NZ	53:2v:21:A:OP1	2.31	0.57
46:2o:26:GLU:OE1	46:2o:77:ARG:NH2	2.26	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:125:PHE:O	61:1G:301:HOH:O	2.17	0.56
32:1a:160:A:H2'	32:1a:161:A:O4'	2.05	0.56
1:2A:500:G:N1	1:2A:503:A:OP2	2.38	0.56
35:2d:153:ARG:HH11	35:2d:181:MET:HE3	1.70	0.56
54:2w:173:TYR:O	54:2w:316:ARG:NH2	2.37	0.56
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.40	0.56
4:1E:33:VAL:HG13	4:1E:47:VAL:HG23	1.86	0.56
16:2U:49:HIS:HA	16:2U:52:ARG:HG2	1.87	0.56
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.05	0.56
1:1A:1915:5MU:H1'	54:1w:286:ARG:HD2	1.87	0.56
1:1A:2070:G:OP2	61:1A:4234:HOH:O	2.18	0.56
1:1A:2239:G:OP2	61:1A:4236:HOH:O	2.18	0.56
1:1A:2494:G:O2'	12:1Q:80:GLU:HA	2.05	0.56
32:1a:1030(D):A:C8	32:1a:1031:G:H1'	2.40	0.56
32:1a:1129:C:H42	32:1a:1143:G:H1	1.54	0.56
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	1.87	0.56
1:2A:271(A):A:N1	1:2A:272(D):G:O2'	2.34	0.56
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.35	0.56
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.20	0.56
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.39	0.56
27:25:56:LYS:NZ	27:25:58:LEU:O	2.38	0.56
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.70	0.56
51:2t:57:ARG:NH2	51:2t:100:ILE:HD12	2.20	0.56
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.36	0.56
32:1a:524:G:H2'	32:1a:525:C:C6	2.41	0.56
47:1p:45:THR:HG23	47:1p:47:ASP:H	1.71	0.56
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.05	0.56
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.38	0.56
23:21:21:ARG:HD3	23:21:35:THR:HG21	1.87	0.56
33:2b:102:LEU:HD23	33:2b:182:ILE:HD12	1.87	0.56
34:2c:5:ILE:HD11	45:2n:49:HIS:HE1	1.70	0.56
39:2h:100:ILE:O	39:2h:125:ARG:NH1	2.38	0.56
1:1A:551:G:O2'	1:1A:1220:A:N3	2.34	0.56
1:1A:1057:A:C8	1:1A:1086:A:H2'	2.41	0.56
1:1A:1057:A:N7	1:1A:1086:A:H2'	2.20	0.56
1:1A:1354:A:H5''	3:1D:38:LYS:HD3	1.87	0.56
32:1a:45:U:H2'	32:1a:46:G:C8	2.41	0.56
37:1f:45:LEU:HD12	37:1f:59:TYR:HD1	1.70	0.56
32:2a:1224:G:OP1	61:2a:1805:HOH:O	2.18	0.56
40:2i:7:THR:HB	40:2i:83:ARG:HE	1.70	0.56
44:2m:34:LEU:HD22	44:2m:39:ILE:HB	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:2u:17:THR:O	52:2u:22:ARG:NH1	2.39	0.56
55:2x:67:C:H2'	55:2x:68:G:C8	2.39	0.56
7:1H:41:MET:HE1	7:1H:54:ARG:HB3	1.88	0.56
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.06	0.56
32:1a:59:A:N1	61:1a:1932:HOH:O	2.32	0.56
32:1a:60:A:N1	32:1a:107:G:O2'	2.36	0.56
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.39	0.56
37:1f:38:GLU:HB2	37:1f:64:GLN:HG2	1.87	0.56
50:1s:69:HIS:HB3	50:1s:73:GLU:OE1	2.05	0.56
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.20	0.56
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.05	0.56
6:1G:107:LEU:HA	6:1G:111:LEU:HD12	1.87	0.56
11:1P:96:THR:HG23	11:1P:99:LEU:H	1.70	0.56
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.05	0.56
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.39	0.56
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.38	0.56
5:2F:28:ILE:HD12	5:2F:119:ARG:HH21	1.70	0.56
20:2Y:85:VAL:HG13	20:2Y:97:ARG:HB3	1.87	0.56
32:2a:137:C:H2'	32:2a:138:G:H8	1.70	0.56
32:2a:958:A:N6	50:2s:77:THR:O	2.39	0.56
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.41	0.56
33:2b:12:GLU:HB2	33:2b:213:LEU:HD21	1.87	0.56
36:2e:102:ALA:HB1	36:2e:106:PRO:HG2	1.87	0.56
43:2l:40:VAL:HG21	43:2l:78:GLN:HA	1.88	0.56
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.41	0.56
1:1A:2014:A:OP1	61:1A:4237:HOH:O	2.18	0.56
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.37	0.56
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.40	0.56
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.39	0.56
32:2a:56:U:H2'	32:2a:57:G:H8	1.70	0.56
32:2a:587:G:N2	32:2a:754:C:OP2	2.34	0.56
1:1A:883:G:H22	1:1A:893:C:H42	1.54	0.56
1:1A:2100:G:H2'	1:1A:2101:G:O4'	2.06	0.56
32:1a:624:C:H2'	32:1a:625:G:H8	1.70	0.56
32:1a:1353:G:H2'	32:1a:1354:C:H6	1.71	0.56
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.87	0.56
35:2d:122:ARG:NH1	35:2d:134:ASP:O	2.39	0.56
8:1I:54:GLN:HG3	8:1I:57:ARG:HH12	1.70	0.56
12:1Q:38:GLU:HA	12:1Q:99:PRO:HG3	1.87	0.56
1:2A:657:U:H2'	1:2A:658:C:C6	2.41	0.56
1:2A:900:A:H2'	1:2A:901:A:H8	1.71	0.56

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	1.68	0.56
8:2I:77:LEU:HD23	8:2I:142:VAL:HG13	1.86	0.56
32:2a:1148:U:O2'	40:2i:66:ARG:NH2	2.39	0.56
1:1A:2658:C:OP1	7:1H:160:LYS:NZ	2.39	0.55
32:1a:100:C:H2'	32:1a:101:A:C8	2.41	0.55
32:1a:1064:G:H1'	32:1a:1190:G:N2	2.20	0.55
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.42	0.55
34:2c:43:LEU:HB3	34:2c:47:LEU:HD12	1.87	0.55
35:2d:76:ARG:NH2	35:2d:80:GLU:OE2	2.34	0.55
1:1A:2133:G:O2'	1:1A:2157:G:N2	2.39	0.55
32:1a:324:G:N7	61:1a:1935:HOH:O	2.33	0.55
48:1q:53:LEU:HB3	48:1q:82:MET:HE1	1.87	0.55
32:2a:532:A:H2'	32:2a:532:A:N3	2.22	0.55
33:2b:77:ALA:HA	33:2b:80:ILE:HG22	1.89	0.55
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.14	0.55
51:2t:57:ARG:HH22	51:2t:100:ILE:HD12	1.71	0.55
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.26	0.55
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.89	0.55
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.06	0.55
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.23	0.55
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.38	0.55
23:21:50:ARG:HG2	23:21:59:THR:HG23	1.87	0.55
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.87	0.55
32:1a:1288:A:N3	32:1a:1352:C:O2'	2.39	0.55
1:2A:223:A:O2'	1:2A:420:C:O2	2.25	0.55
13:2R:2:ARG:HG2	13:2R:5:LYS:HB2	1.88	0.55
32:2a:448:A:P	32:2a:485:G:H22	2.29	0.55
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.21	0.55
33:1b:21:ARG:HA	33:1b:39:ILE:HA	1.88	0.55
41:1j:54:PHE:O	41:1j:56:HIS:N	2.40	0.55
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.87	0.55
32:2a:625:G:H4'	47:2p:16:HIS:CD2	2.42	0.55
1:1A:2689:U:H4'	1:1A:2690:C:H5'	1.89	0.55
7:1H:27:LYS:HG2	7:1H:32:GLU:HG2	1.87	0.55
32:1a:601:C:H2'	32:1a:602:A:C8	2.41	0.55
32:1a:1073:U:O2'	33:1b:104:ASN:OD1	2.22	0.55
33:1b:127:ILE:HG22	33:1b:130:ARG:H	1.71	0.55
46:1o:3:ILE:HG21	46:1o:34:LEU:HD21	1.89	0.55
1:2A:2188:C:H2'	1:2A:2189:U:O4'	2.07	0.55
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.88	0.55
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.07	0.55
32:1a:702:A:OP2	61:1a:1912:HOH:O	2.18	0.55
8:2I:86:THR:OG1	8:2I:87:LYS:NZ	2.38	0.55
32:2a:56:U:H2'	32:2a:57:G:C8	2.41	0.55
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.42	0.55
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.42	0.55
54:2w:129:ASN:O	54:2w:133:ARG:HG3	2.06	0.55
1:1A:1068:G:H2'	1:1A:1096:A:O2'	2.07	0.55
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.89	0.55
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.89	0.55
21:1Z:7:ALA:HB3	21:1Z:61:LEU:HD12	1.88	0.55
32:1a:920:U:H2'	32:1a:921:U:C6	2.42	0.55
32:1a:946:A:H2'	32:1a:947:G:C8	2.41	0.55
32:1a:1320:C:O2	50:1s:36:ARG:NH2	2.40	0.55
36:1e:102:ALA:HB1	36:1e:106:PRO:HB2	1.87	0.55
38:1g:22:LEU:HG	38:1g:62:PHE:HE2	1.71	0.55
38:1g:78:ARG:HG3	38:1g:156:TRP:CZ3	2.36	0.55
47:1p:60:LEU:HD21	47:1p:66:PRO:HD3	1.89	0.55
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.41	0.55
5:2F:140:LEU:HD11	5:2F:170:LEU:HD11	1.88	0.55
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.07	0.55
32:2a:433:C:H2'	32:2a:434:U:H6	1.71	0.55
32:2a:814:A:H2'	32:2a:816:A:H5''	1.88	0.55
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.87	0.55
50:2s:22:LEU:HD22	50:2s:27:GLU:HA	1.89	0.55
1:1A:2839:G:OP1	61:1A:4238:HOH:O	2.18	0.55
18:1W:1:MET:HE3	18:1W:2:GLU:H	1.71	0.55
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.89	0.55
32:1a:1319:A:OP2	50:1s:3:ARG:NH1	2.40	0.55
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.71	0.55
11:2P:89:ALA:O	11:2P:121:LYS:NZ	2.36	0.55
32:2a:719:C:H1'	49:2r:49:LYS:HG2	1.89	0.55
32:2a:1108:G:H5'	34:2c:176:HIS:CD2	2.42	0.55
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.06	0.55
32:2a:1209:C:O2'	32:2a:1214:C:N4	2.37	0.55
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.35	0.55
38:2g:78:ARG:HB2	38:2g:87:VAL:HG21	1.89	0.55
41:2j:30:SER:HB2	41:2j:81:THR:HB	1.88	0.55
1:1A:752:A:H3'	29:17:1:MET:HE1	1.88	0.55
1:1A:774:A:N3	1:1A:774:A:H2'	2.22	0.55
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.25	0.55
54:1w:110:GLU:HB2	54:1w:200:ALA:HB3	1.88	0.55
1:2A:606:U:H4'	1:2A:658:C:H4'	1.89	0.55
26:24:59:PHE:O	26:24:62:ARG:NH1	2.39	0.55
32:2a:757:U:H2'	32:2a:758:G:O4'	2.07	0.55
32:2a:840:C:H4'	32:2a:841:U:OP1	2.06	0.55
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.72	0.55
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.42	0.55
38:2g:38:LEU:O	38:2g:42:ILE:HG12	2.07	0.55
6:1G:16:ARG:HB2	6:1G:17:PRO:HD3	1.88	0.54
32:1a:1144:G:N2	32:1a:1146:A:H62	2.05	0.54
54:1w:285:LEU:HG	54:1w:289:ARG:HH12	1.71	0.54
1:2A:323:G:O2'	1:2A:1205:U:N3	2.37	0.54
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.25	0.54
1:2A:1815:A:P	3:2D:54:ARG:HH22	2.30	0.54
1:2A:2639:A:O3'	9:2N:97:ARG:NH2	2.40	0.54
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.24	0.54
33:2b:44:LEU:HD23	33:2b:44:LEU:H	1.71	0.54
1:1A:833:U:O2	11:1P:55:ARG:NH2	2.41	0.54
1:1A:2155:G:H3'	1:1A:2156:G:H8	1.72	0.54
13:1R:87:TYR:OH	13:1R:117:VAL:O	2.22	0.54
32:1a:601:C:H2'	32:1a:602:A:H8	1.73	0.54
32:1a:1006:C:H2'	32:1a:1007:C:C6	2.42	0.54
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.42	0.54
35:1d:57:ARG:NH2	36:1e:107:ARG:HD3	2.22	0.54
38:1g:59:LEU:HD11	38:1g:63:LYS:HE2	1.89	0.54
7:2H:59:ARG:O	7:2H:63:SER:OG	2.25	0.54
32:2a:9:G:H2'	32:2a:10:A:H8	1.72	0.54
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.07	0.54
1:1A:1814:G:C4'	3:1D:51:VAL:HG21	2.38	0.54
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.89	0.54
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.71	0.54
32:1a:501:C:H1'	32:1a:549:C:H1'	1.89	0.54
32:1a:1286:A:H8	32:1a:1287:A:H4'	1.72	0.54
33:1b:48:MET:HA	33:1b:51:LEU:HB2	1.90	0.54
1:2A:746:A:H2'	1:2A:2612:C:H5''	1.89	0.54
3:2D:206:LEU:O	3:2D:211:ARG:HD3	2.07	0.54
32:2a:1314:C:N4	50:2s:2:PRO:O	2.40	0.54
38:2g:75:VAL:HG13	38:2g:145:ALA:HA	1.90	0.54
41:2j:16:LEU:O	41:2j:19:SER:N	2.40	0.54
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:62:ARG:O	26:14:64:GLY:N	2.39	0.54
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.42	0.54
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.42	0.54
1:2A:2138:C:N4	1:2A:2153:G:H1	2.06	0.54
9:2N:46:VAL:HG23	9:2N:48:MET:HG2	1.89	0.54
32:2a:931:C:H42	32:2a:1386:G:H1	1.54	0.54
32:2a:1048:G:OP1	45:2n:3:ARG:HB3	2.06	0.54
55:2x:67:C:H2'	55:2x:68:G:H8	1.71	0.54
32:1a:923:A:OP1	36:1e:21:ALA:HB2	2.07	0.54
1:2A:1490:A:O2'	3:2D:99:ASP:OD1	2.22	0.54
6:2G:114:ILE:HB	6:2G:117:PHE:HB2	1.89	0.54
32:2a:1162:C:N4	32:2a:1174:G:H1	2.05	0.54
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.22	0.54
32:2a:1492:A:O2'	54:2w:298:ARG:NH2	2.40	0.54
36:2e:89:ILE:HG12	36:2e:135:THR:HG22	1.89	0.54
48:2q:6:LEU:HD22	48:2q:23:VAL:HG11	1.89	0.54
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.43	0.54
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.89	0.54
23:11:14:VAL:HG11	23:11:39:LYS:HE2	1.88	0.54
32:1a:381:C:H2'	32:1a:382:A:O4'	2.08	0.54
32:1a:1270:C:H2'	32:1a:1271:G:C8	2.42	0.54
35:1d:141:ARG:N	35:1d:144:ASP:OD2	2.37	0.54
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.90	0.54
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.43	0.54
35:2d:111:ALA:HB1	35:2d:116:GLN:HG2	1.88	0.54
1:1A:1055:G:H2'	1:1A:1056:G:O4'	2.07	0.54
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.72	0.54
3:1D:211:ARG:HG2	3:1D:214:TRP:CE3	2.43	0.54
33:1b:178:ARG:HH22	39:1h:68:ARG:HH12	1.55	0.54
47:1p:5:ARG:HE	47:1p:22:THR:HG23	1.72	0.54
1:2A:108:U:H2'	1:2A:109:G:C8	2.43	0.54
1:2A:1611:C:OP1	61:2A:4839:HOH:O	2.19	0.54
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.90	0.54
37:2f:99:ALA:HB1	49:2r:23:LYS:HE3	1.90	0.54
39:2h:9:MET:HB2	39:2h:32:LYS:HD3	1.89	0.54
1:1A:247:G:H4'	1:1A:386:G:C5	2.43	0.54
1:1A:588:U:H2'	1:1A:589:C:C6	2.43	0.54
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.42	0.54
10:1O:104:ARG:CZ	15:1T:34:VAL:HG11	2.38	0.54
32:1a:532:A:N6	32:1a:1206:G:O2'	2.41	0.54
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:191:THR:OG1	34:1c:194:GLY:O	2.22	0.54
1:2A:1721:G:H8	1:2A:1741:A:H62	1.56	0.54
33:2b:115:LEU:HD13	33:2b:145:LEU:HB2	1.89	0.54
1:1A:305:U:H2'	1:1A:306:U:C6	2.42	0.54
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.42	0.54
32:1a:460:G:N2	32:1a:471:G:N7	2.55	0.54
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.41	0.54
34:1c:26:LYS:HA	45:1n:36:PHE:HE1	1.72	0.54
1:2A:307:G:H21	1:2A:330:A:H62	1.55	0.54
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.90	0.54
1:2A:2579:C:H4'	4:2E:134:ILE:HG12	1.90	0.54
7:2H:3:ARG:HG2	7:2H:6:ARG:NE	2.23	0.54
27:25:41:PRO:O	27:25:44:THR:OG1	2.25	0.54
1:1A:2306:C:O2	61:1A:4232:HOH:O	2.17	0.54
19:1X:92:LEU:O	19:1X:94:GLY:N	2.41	0.54
32:1a:739:C:O2'	46:1o:42:HIS:ND1	2.38	0.54
54:1w:196:THR:HG21	54:1w:296:GLY:O	2.08	0.54
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.25	0.54
1:2A:839:U:H2'	1:2A:840:C:C6	2.42	0.54
1:2A:2657:A:O3'	7:2H:160:LYS:NZ	2.40	0.54
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	1.90	0.54
32:2a:975:A:H5'	32:2a:975:A:H8	1.72	0.54
47:2p:3:LYS:HZ1	47:2p:65:GLN:HB2	1.73	0.54
1:1A:185:U:H4'	1:1A:218:A:H4'	1.90	0.53
1:1A:2010:G:H5''	18:1W:42:ARG:HB2	1.90	0.53
1:1A:2130:U:H2'	1:1A:2158:A:H61	1.73	0.53
1:1A:2336:A:H61	22:10:43:THR:HG22	1.74	0.53
32:1a:1264:C:H2'	32:1a:1265:G:C8	2.42	0.53
40:1i:50:LEU:HD23	40:1i:85:LEU:HD11	1.89	0.53
50:1s:19:VAL:O	50:1s:23:ASN:ND2	2.38	0.53
1:2A:947:G:H2'	1:2A:948:G:C8	2.42	0.53
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.32	0.53
1:2A:1547:C:H2'	1:2A:1548:C:C6	2.43	0.53
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.90	0.53
32:2a:437:U:O2'	35:2d:123:HIS:HD2	1.91	0.53
32:2a:1348:U:H2'	32:2a:1349:A:H8	1.72	0.53
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.43	0.53
38:2g:69:VAL:HG12	38:2g:135:VAL:HG12	1.89	0.53
43:2l:47:LYS:HG2	43:2l:48:PRO:HA	1.90	0.53
6:1G:62:LEU:HA	26:14:27:THR:HG21	1.90	0.53
32:1a:250:A:H4'	32:1a:251:G:O5'	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:390:C:H2'	32:1a:391:G:C8	2.43	0.53
32:1a:507:C:OP2	32:1a:508:C:O2'	2.23	0.53
41:1j:8:LEU:H	41:1j:8:LEU:HD12	1.72	0.53
1:2A:295:G:H5'	20:2Y:1:MET:HG2	1.89	0.53
1:2A:2129:C:H3'	1:2A:2130:U:C6	2.42	0.53
1:2A:2365:G:O6	30:28:43:GLN:NE2	2.30	0.53
26:24:26:SER:OG	26:24:27:THR:N	2.40	0.53
32:2a:838:G:H1	32:2a:848:C:H42	1.56	0.53
32:2a:1038:C:H2'	32:2a:1039:C:C6	2.42	0.53
37:2f:3:ARG:HB3	37:2f:93:SER:HB2	1.90	0.53
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.16	0.53
1:1A:957:A:H5'	12:1Q:76:LYS:HD2	1.89	0.53
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.22	0.53
1:1A:1753:G:N1	1:1A:1756:G:OP2	2.42	0.53
1:1A:2304:G:H22	1:1A:2312:U:H3	1.56	0.53
7:1H:72:ILE:O	7:1H:76:VAL:HG23	2.08	0.53
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.28	0.53
39:1h:13:ILE:O	39:1h:17:THR:HG23	2.08	0.53
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.43	0.53
1:2A:958:U:OP2	12:2Q:14:ARG:NE	2.40	0.53
1:2A:2127:G:O2'	1:2A:2173:A:N3	2.41	0.53
26:24:34:GLU:HB2	44:2m:57:ARG:HD3	1.91	0.53
32:2a:1093:A:N3	32:2a:1109:C:O2'	2.40	0.53
32:2a:1272:G:N2	32:2a:1273:G:C8	2.76	0.53
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.23	0.53
47:2p:3:LYS:NZ	47:2p:65:GLN:HB2	2.22	0.53
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.07	0.53
1:2A:570:G:H2'	1:2A:2030:A:C5	2.42	0.53
1:2A:602:G:O2'	1:2A:655:A:N6	2.41	0.53
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.91	0.53
1:2A:2174:C:H2'	1:2A:2175:C:C6	2.44	0.53
6:2G:60:LEU:HD23	6:2G:68:PRO:HG3	1.89	0.53
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.73	0.53
33:2b:163:PHE:HA	33:2b:185:ILE:O	2.08	0.53
34:2c:116:VAL:HG21	34:2c:202:ILE:HD11	1.91	0.53
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.90	0.53
38:1g:74:GLU:OE2	38:1g:95:ARG:NE	2.41	0.53
1:2A:271(F):C:H2'	1:2A:271(G):C:O4'	2.07	0.53
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.43	0.53
1:2A:2110:G:H1	1:2A:2179:C:N4	2.07	0.53
1:2A:2371:G:O2'	28:26:46:HIS:ND1	2.35	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.91	0.53
4:2E:52:LEU:HB2	4:2E:76:ARG:HB2	1.91	0.53
4:2E:52:LEU:O	4:2E:76:ARG:N	2.33	0.53
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.33	0.53
38:2g:153:HIS:HA	38:2g:155:ARG:NH1	2.23	0.53
39:2h:51:VAL:HG21	39:2h:60:ARG:HB2	1.91	0.53
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.08	0.53
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.44	0.53
5:1F:18:ARG:NH2	5:1F:127:GLU:OE2	2.37	0.53
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.73	0.53
32:1a:159:G:H5'	32:1a:160:A:OP2	2.09	0.53
32:1a:1316:G:N2	32:1a:1318:A:H3'	2.24	0.53
34:1c:42:LEU:HA	34:1c:45:LYS:HG2	1.89	0.53
2:2B:14:U:H1'	2:2B:108:U:O2'	2.08	0.53
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.73	0.53
26:24:58:ARG:HH21	50:2s:68:GLY:HA3	1.73	0.53
32:2a:137:C:H2'	32:2a:138:G:C8	2.44	0.53
1:1A:271(H):G:H2'	1:1A:271(I):G:C8	2.43	0.53
14:1S:61:ASN:ND2	14:1S:64:GLU:HG3	2.24	0.53
1:2A:687:C:OP2	61:2A:4840:HOH:O	2.19	0.53
1:2A:856:C:H2'	1:2A:857:C:C6	2.44	0.53
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.90	0.53
15:2T:122:ASP:OD2	32:2a:1442(A):G:O2'	2.27	0.53
21:2Z:7:ALA:O	21:2Z:62:PRO:HD3	2.09	0.53
1:1A:2549:G:N7	61:1A:4312:HOH:O	2.34	0.53
4:1E:13:ARG:HD2	4:1E:20:ALA:HB1	1.90	0.53
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.42	0.53
32:1a:444:C:H2'	32:1a:445:G:C8	2.44	0.53
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.06	0.53
54:1w:338:ALA:HA	54:1w:341:ARG:HG2	1.90	0.53
1:2A:1203:G:O6	61:2A:4829:HOH:O	2.17	0.53
1:2A:2130:U:H5''	1:2A:2133:G:H5'	1.90	0.53
1:2A:2138:C:H42	1:2A:2153:G:H1	1.54	0.53
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.55	0.53
26:24:40:HIS:HB3	26:24:43:TYR:CD2	2.43	0.53
32:2a:438:G:O2'	32:2a:494:U:O4	2.24	0.53
42:2k:110:ASP:HB3	49:2r:85:LEU:HB3	1.90	0.53
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.42	0.53
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.06	0.53
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.44	0.53
11:2P:121:LYS:O	11:2P:123:LEU:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.09	0.53
26:24:48:ARG:O	26:24:50:VAL:N	2.41	0.53
31:29:10:ILE:HD12	31:29:32:HIS:HA	1.90	0.53
37:2f:44:GLY:HA2	37:2f:59:TYR:CZ	2.44	0.53
6:1G:12:TYR:HA	6:1G:16:ARG:HG3	1.90	0.53
6:1G:79:ASN:OD1	6:1G:79:ASN:N	2.42	0.53
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	1.92	0.53
21:1Z:138:GLU:H	21:1Z:156:LYS:HZ3	1.55	0.53
26:14:14:ILE:HD13	26:14:31:ILE:HB	1.90	0.53
32:1a:473:G:H2'	32:1a:474:G:H8	1.73	0.53
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.44	0.53
32:1a:1270:C:H2'	32:1a:1271:G:H8	1.73	0.53
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.26	0.53
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.43	0.53
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.25	0.53
1:2A:1943:U:OP1	54:2w:272:ARG:NH1	2.33	0.53
1:2A:2462:U:H1'	1:2A:2491:U:O4	2.08	0.53
1:2A:2680:C:H5'	4:2E:189:PRO:HA	1.91	0.53
6:2G:15:VAL:HB	6:2G:175:LEU:HB3	1.90	0.53
13:2R:62:ALA:O	13:2R:66:VAL:HG23	2.09	0.53
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.09	0.53
34:2c:124:ILE:HG22	34:2c:130:VAL:HG22	1.91	0.53
34:2c:188:LEU:HG	34:2c:195:VAL:HG13	1.90	0.53
41:2j:42:THR:HG22	41:2j:68:HIS:HA	1.91	0.53
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.43	0.52
15:1T:19:LEU:HD13	15:1T:86:ILE:HD12	1.91	0.52
32:1a:1304:G:OP1	52:1u:2:GLY:N	2.43	0.52
33:1b:138:LEU:O	33:1b:142:LEU:N	2.37	0.52
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.91	0.52
26:24:57:GLU:CB	26:24:58:ARG:HG2	2.39	0.52
32:2a:7:G:H5'	32:2a:298:A:O4'	2.09	0.52
1:1A:1859:A:N6	1:1A:1883:G:O2'	2.42	0.52
8:1I:40:THR:HG23	8:1I:42:SER:H	1.75	0.52
32:1a:266:G:O3'	48:1q:67:LYS:HB2	2.09	0.52
32:1a:1187:G:N3	45:1n:60:SER:OG	2.42	0.52
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.74	0.52
34:1c:131:ARG:NE	36:1e:50:GLU:OE2	2.39	0.52
39:1h:124:ALA:O	39:1h:128:GLY:N	2.41	0.52
40:1i:4:TYR:CZ	40:1i:88:TYR:HD1	2.27	0.52
1:2A:327:G:N2	20:2Y:70:SER:OG	2.42	0.52
1:2A:831:G:O2'	11:2P:38:GLN:OE1	2.26	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1636:C:OP2	61:2A:4841:HOH:O	2.19	0.52
32:2a:58:C:O2'	32:2a:388:G:N7	2.38	0.52
32:2a:176:C:H2'	32:2a:177:C:C6	2.44	0.52
32:2a:773:G:N7	61:2a:1815:HOH:O	2.33	0.52
32:2a:1244:C:H2'	32:2a:1245:A:H8	1.74	0.52
40:2i:6:GLY:HA3	40:2i:80:GLY:O	2.09	0.52
1:1A:1309:G:H4'	29:17:7:PRO:HB2	1.92	0.52
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.73	0.52
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.44	0.52
34:1c:148:GLY:HA3	34:1c:172:ARG:H	1.74	0.52
44:1m:65:LYS:HG2	44:1m:69:GLU:HB3	1.90	0.52
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.24	0.52
38:2g:153:HIS:CE1	42:2k:58:PRO:HD2	2.44	0.52
41:2j:11:PHE:HE1	41:2j:67:THR:HG22	1.74	0.52
1:1A:826:U:H4'	11:1P:55:ARG:HB3	1.91	0.52
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.09	0.52
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.21	0.52
15:1T:39:ARG:NH2	32:1a:345:C:OP2	2.43	0.52
32:1a:262:A:H2'	32:1a:263:A:C8	2.44	0.52
32:1a:447:G:O6	32:1a:485:G:O2'	2.26	0.52
34:1c:35:GLU:OE2	34:1c:59:ARG:NH2	2.33	0.52
46:1o:68:ARG:O	46:1o:72:ARG:HG3	2.09	0.52
7:2H:11:VAL:HG13	7:2H:15:VAL:HB	1.91	0.52
7:2H:124:GLU:HB2	7:2H:132:ARG:HB3	1.90	0.52
34:2c:183:ASP:N	34:2c:202:ILE:O	2.41	0.52
36:2e:74:GLY:HA3	36:2e:116:THR:HG22	1.92	0.52
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.24	0.52
1:1A:1670:C:OP2	61:1A:4206:HOH:O	2.18	0.52
1:1A:2062:A:H2	56:1z:5:ALA:HB1	1.74	0.52
1:1A:2166:G:H2'	1:1A:2167:U:C5	2.45	0.52
5:1F:187:VAL:HG11	11:1P:6:LEU:HD11	1.92	0.52
9:1N:14:VAL:HG12	9:1N:52:VAL:HA	1.92	0.52
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.44	0.52
32:1a:538:G:H5''	43:1l:114:LYS:HB2	1.92	0.52
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.44	0.52
35:1d:76:ARG:NH2	35:1d:80:GLU:OE2	2.33	0.52
38:1g:79:ARG:NH1	38:1g:81:GLY:H	2.07	0.52
41:1j:5:ARG:HD3	41:1j:71:LEU:HD11	1.91	0.52
54:1w:119:GLU:OE2	54:1w:182:ARG:NE	2.41	0.52
32:2a:973:G:H3'	32:2a:974:A:H5''	1.90	0.52
32:2a:1073:U:H2'	32:2a:1074:G:C8	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:40:LEU:HB2	41:2j:69:ASN:HB2	1.91	0.52
1:1A:548:A:N6	17:1V:19:LYS:H	2.08	0.52
1:1A:626:U:O4	11:1P:107:LYS:HE2	2.10	0.52
1:1A:1914:C:H1'	54:1w:290:LEU:HD11	1.92	0.52
1:1A:1991:U:H2'	1:1A:1992:G:H5''	1.92	0.52
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.10	0.52
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.10	0.52
1:2A:1200:C:H1'	16:2U:2:PRO:HG3	1.91	0.52
1:2A:1364:G:P	23:21:3:LYS:HG3	2.49	0.52
14:2S:38:GLN:OE1	14:2S:47:THR:OG1	2.19	0.52
21:2Z:8:TYR:HB2	21:2Z:38:TYR:CE2	2.44	0.52
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.91	0.52
33:2b:134:GLU:O	33:2b:138:LEU:HG	2.09	0.52
34:2c:139:GLN:NE2	34:2c:143:GLU:HG3	2.23	0.52
41:2j:9:ARG:HG2	41:2j:69:ASN:HA	1.90	0.52
54:2w:102:MET:HG3	54:2w:103:ASP:H	1.74	0.52
1:1A:2184:G:H2'	1:1A:2185:C:O4'	2.10	0.52
2:1B:75:G:H22	21:1Z:73:GLN:HE21	1.58	0.52
4:1E:7:VAL:HG13	4:1E:27:LEU:HB3	1.91	0.52
11:1P:124:LYS:HE3	11:1P:146:VAL:HG21	1.92	0.52
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.10	0.52
1:2A:466:A:N1	1:2A:795:C:O2'	2.41	0.52
1:2A:1038:C:H42	1:2A:1117:G:H1	1.56	0.52
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.09	0.52
32:2a:412:A:O4'	35:2d:35:ARG:NH2	2.43	0.52
32:2a:1118:C:O3'	40:2i:83:ARG:NH2	2.43	0.52
33:2b:58:ILE:O	33:2b:62:ALA:N	2.30	0.52
1:1A:667:U:O2	30:18:2:PRO:HD2	2.09	0.52
1:1A:2469:A:H4'	12:1Q:56:ARG:HG2	1.91	0.52
10:1O:86:ILE:HG22	10:1O:94:ARG:HD3	1.91	0.52
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.45	0.52
32:1a:986:A:H1'	50:1s:54:GLY:O	2.09	0.52
33:1b:131:PRO:O	33:1b:134:GLU:N	2.42	0.52
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.41	0.52
1:2A:829:A:N7	1:2A:2248:C:H5'	2.25	0.52
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.25	0.52
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.36	0.52
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.27	0.52
32:2a:60:A:N1	32:2a:107:G:O2'	2.39	0.52
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.10	0.52
1:1A:1580:A:OP2	1:1A:1580:A:H8	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.28	0.52
23:11:5:CYS:SG	23:11:62:VAL:HG23	2.50	0.52
32:1a:881:G:P	43:11:12:ARG:HH22	2.33	0.52
32:1a:952:U:H2'	32:1a:953:G:H8	1.73	0.52
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.09	0.52
33:1b:16:HIS:HB3	33:1b:210:SER:CB	2.40	0.52
51:1t:16:HIS:O	51:1t:19:SER:OG	2.23	0.52
5:2F:148:LEU:HD21	5:2F:191:ARG:NE	2.24	0.52
6:2G:103:LEU:HD22	6:2G:178:PHE:HZ	1.73	0.52
32:2a:624:C:H2'	32:2a:625:G:H8	1.75	0.52
38:2g:78:ARG:HG2	38:2g:79:ARG:H	1.75	0.52
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.35	0.52
8:1I:38:LEU:O	8:1I:40:THR:N	2.41	0.52
38:1g:118:VAL:HA	38:1g:121:ALA:HB3	1.90	0.52
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.74	0.52
6:2G:72:ARG:NH1	6:2G:87:PRO:HG3	2.25	0.52
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.92	0.52
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.45	0.52
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.10	0.52
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.93	0.52
32:2a:1133:G:H2'	32:2a:1134:G:C8	2.45	0.52
32:2a:1342:C:H2'	32:2a:1343:G:H8	1.74	0.52
34:2c:134:ILE:HG22	34:2c:168:ALA:HB3	1.92	0.52
1:1A:274:G:H2'	1:1A:275:G:C8	2.45	0.51
1:1A:2134:A:H4'	1:1A:2159:G:H21	1.75	0.51
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.45	0.51
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.45	0.51
32:1a:300:A:O2'	32:1a:564:C:N3	2.40	0.51
32:1a:620:C:H2'	32:1a:621:A:O4'	2.09	0.51
32:1a:757:U:H2'	32:1a:758:G:O4'	2.11	0.51
32:1a:959:A:HO2'	32:1a:984:C:HO2'	1.56	0.51
41:1j:81:THR:C	41:1j:83:GLU:H	2.17	0.51
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.75	0.51
6:2G:151:ALA:HB3	6:2G:153:ARG:HH12	1.75	0.51
22:20:70:GLN:HG2	22:20:72:ARG:HG3	1.92	0.51
32:2a:1262:C:C2'	32:2a:1263:C:H5'	2.40	0.51
32:2a:1308:U:H2'	32:2a:1309:G:C8	2.45	0.51
32:2a:1530:G:OP1	32:2a:1530:G:H4'	2.10	0.51
1:1A:839:U:H1'	1:1A:1191:G:H1'	1.92	0.51
1:1A:2850:A:N7	1:1A:2868:A:O2'	2.40	0.51
2:1B:51:G:N7	14:1S:62:LYS:NZ	2.48	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1065:U:H4'	32:1a:1066:C:O5'	2.10	0.51
35:1d:88:VAL:HG12	36:1e:96:PRO:HB2	1.91	0.51
42:1k:66:LEU:HG	42:1k:97:ALA:HB1	1.91	0.51
1:2A:674:G:O2'	5:2F:74:ARG:HD3	2.09	0.51
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.44	0.51
32:2a:353:A:H5'	32:2a:353:A:H8	1.74	0.51
32:2a:1275:A:H2'	32:2a:1276:G:O4'	2.10	0.51
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.44	0.51
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.45	0.51
48:2q:57:VAL:HG12	48:2q:76:LEU:HA	1.92	0.51
1:1A:271(L):U:H4'	8:1I:50:ARG:NH2	2.23	0.51
1:1A:2130:U:H2'	1:1A:2158:A:N1	2.26	0.51
1:1A:2577:A:OP2	27:15:3:LYS:NZ	2.41	0.51
4:1E:170:LEU:HB3	4:1E:184:VAL:HG22	1.93	0.51
5:1F:122:LYS:HB3	5:1F:191:ARG:HG3	1.92	0.51
6:1G:41:GLN:NE2	6:1G:154:GLY:O	2.36	0.51
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.93	0.51
32:1a:1249:C:O2'	40:1i:73:GLN:NE2	2.43	0.51
34:1c:124:ILE:HD11	34:1c:189:ALA:HB3	1.92	0.51
35:1d:9:CYS:O	35:1d:13:ARG:HG3	2.10	0.51
45:1n:8:GLU:HA	45:1n:11:LYS:HE3	1.93	0.51
32:2a:936:C:H2'	32:2a:937:A:O4'	2.09	0.51
34:2c:39:ILE:O	34:2c:43:LEU:HG	2.11	0.51
1:1A:523:C:H4'	1:1A:540:C:O2	2.10	0.51
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.46	0.51
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.10	0.51
3:1D:175:LEU:HD12	3:1D:185:VAL:HG21	1.91	0.51
22:10:11:ARG:O	22:10:14:ARG:NH2	2.31	0.51
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.07	0.51
32:1a:1064:G:H1'	32:1a:1190:G:H21	1.75	0.51
40:1i:5:TYR:OH	40:1i:7:THR:OG1	2.22	0.51
50:1s:27:GLU:HG2	50:1s:28:LYS:HG2	1.93	0.51
54:1w:119:GLU:HG3	54:1w:184:PRO:HB3	1.92	0.51
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.35	0.51
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.45	0.51
32:2a:1225:A:H2'	32:2a:1225:A:N3	2.25	0.51
34:2c:134:ILE:HG23	34:2c:151:VAL:HB	1.92	0.51
1:1A:1187:G:N2	1:1A:1188:U:O4	2.44	0.51
1:2A:108:U:H2'	1:2A:109:G:H8	1.76	0.51
1:2A:212:G:H2'	1:2A:213:A:O4'	2.10	0.51
1:2A:1354:A:H5''	3:2D:38:LYS:HD3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1740:G:H2'	1:2A:1741:A:C8	2.46	0.51
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.27	0.51
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.27	0.51
1:2A:2321:G:H5''	1:2A:2322:A:OP2	2.10	0.51
1:2A:2336:A:H61	22:20:43:THR:HG22	1.75	0.51
12:2Q:31:ASP:HA	12:2Q:134:ARG:HH11	1.76	0.51
32:2a:9:G:H2'	32:2a:10:A:C8	2.45	0.51
32:2a:959:A:O2'	32:2a:984:C:O2'	2.22	0.51
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.26	0.51
39:2h:36:LEU:HD23	39:2h:39:LEU:HD23	1.93	0.51
1:1A:8:A:H2'	1:1A:9:U:H6	1.75	0.51
1:1A:102:G:OP1	24:12:7:ARG:NH2	2.43	0.51
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.46	0.51
1:1A:2116:G:H2'	1:1A:2117:A:C5	2.46	0.51
5:1F:135:LYS:HB2	5:1F:138:GLU:CD	2.34	0.51
26:14:34:GLU:HB2	44:1m:57:ARG:CZ	2.41	0.51
50:1s:36:ARG:NH2	50:1s:72:GLY:O	2.43	0.51
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.76	0.51
1:2A:893:C:H2'	1:2A:894:C:C5	2.46	0.51
1:2A:1992:G:H1'	61:2A:4831:HOH:O	2.11	0.51
1:2A:2469:A:H4'	12:2Q:56:ARG:HG2	1.90	0.51
20:2Y:5:MET:HG2	20:2Y:30:VAL:HG11	1.93	0.51
32:2a:881:G:P	43:2l:12:ARG:HH22	2.34	0.51
33:2b:80:ILE:HD11	33:2b:212:GLN:HB2	1.92	0.51
36:2e:145:LYS:O	36:2e:149:GLU:HB2	2.09	0.51
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.46	0.51
1:1A:1250:G:N7	11:1P:18:ARG:NH2	2.59	0.51
1:1A:1420:U:O2'	1:1A:1421:G:OP1	2.27	0.51
1:1A:1920:OMC:HM22	1:1A:1921:G:O4'	2.10	0.51
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.46	0.51
1:1A:2122:U:H2'	1:1A:2123:G:O4'	2.11	0.51
32:1a:1118:C:OP1	40:1i:104:ARG:NH1	2.44	0.51
7:2H:83:TYR:CE2	7:2H:138:LYS:HB2	2.46	0.51
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.43	0.51
32:2a:1347:G:H22	32:2a:1374:A:P	2.34	0.51
41:2j:9:ARG:HE	41:2j:69:ASN:ND2	2.09	0.51
1:1A:184:C:H2'	1:1A:185:U:C6	2.46	0.51
1:1A:226:G:H21	1:1A:228:A:H62	1.59	0.51
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.11	0.51
36:1e:118:ILE:HG12	36:1e:120:THR:HG22	1.92	0.51
55:1x:44:C:H2'	55:1x:45:U:C6	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.45	0.51
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.25	0.51
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.34	0.51
32:2a:1009:G:H1	32:2a:1020:U:H3	1.58	0.51
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.32	0.51
34:2c:78:GLY:O	34:2c:80:GLY:N	2.43	0.51
38:2g:111:ARG:HB3	38:2g:113:GLU:OE1	2.10	0.51
45:2n:32:SER:O	45:2n:40:CYS:HA	2.11	0.51
50:2s:50:ALA:HA	50:2s:58:VAL:O	2.11	0.51
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.09	0.51
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.93	0.51
32:1a:1129:C:N4	32:1a:1143:G:H1	2.09	0.51
41:1j:9:ARG:NH2	41:1j:95:GLU:OE2	2.43	0.51
1:2A:2640:G:P	9:2N:97:ARG:HH22	2.33	0.51
2:2B:49:C:OP2	14:2S:30:ARG:NH1	2.44	0.51
34:2c:164:ARG:HG2	34:2c:165:THR:H	1.75	0.51
37:2f:100:ASN:ND2	49:2r:23:LYS:HE2	2.26	0.51
42:2k:43:SER:HA	42:2k:47:VAL:HG21	1.93	0.51
32:1a:1226:C:O2'	44:1m:111:LYS:NZ	2.44	0.51
47:1p:23:ASP:OD1	47:1p:25:ARG:NH1	2.45	0.51
1:2A:1352:U:OP2	61:2A:4835:HOH:O	2.19	0.51
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.46	0.51
2:2B:72:G:O2'	2:2B:105:A:N6	2.44	0.51
32:2a:176:C:H2'	32:2a:177:C:H6	1.76	0.51
36:2e:93:PRO:HG2	39:2h:105:ARG:CZ	2.40	0.51
1:1A:236:C:H2'	1:1A:237:C:C6	2.46	0.50
1:1A:1082:U:O4	1:1A:1086:A:C6	2.63	0.50
1:1A:1271:G:OP2	61:1A:4213:HOH:O	2.20	0.50
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.24	0.50
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	1.93	0.50
32:1a:1131:G:H2'	32:1a:1132:C:C6	2.46	0.50
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	1.91	0.50
40:1i:18:PHE:HB3	40:1i:20:ARG:HH21	1.76	0.50
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.25	0.50
47:1p:49:LEU:HD11	47:1p:73:LEU:HB3	1.92	0.50
32:2a:1163:C:H2'	32:2a:1164:G:C8	2.45	0.50
32:2a:1342:C:H4'	40:2i:125:TYR:HB3	1.93	0.50
33:2b:28:PHE:CD1	33:2b:194:PRO:HG3	2.46	0.50
33:2b:97:TRP:CH2	33:2b:173:ALA:HA	2.46	0.50
33:2b:98:LEU:HG	33:2b:101:MET:HE3	1.93	0.50
50:2s:22:LEU:O	50:2s:26:GLY:N	2.38	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:272(H):C:H2'	1:1A:272(I):U:C6	2.46	0.50
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.46	0.50
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.76	0.50
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.76	0.50
32:1a:456:C:H2'	32:1a:457:C:C6	2.47	0.50
32:1a:755:G:OP2	46:1o:65:ARG:HD2	2.11	0.50
33:1b:55:PHE:HE1	33:1b:218:ALA:HA	1.77	0.50
35:1d:119:GLN:HG3	35:1d:123:HIS:CD2	2.46	0.50
40:1i:100:GLY:O	40:1i:103:THR:HG22	2.11	0.50
47:1p:8:ARG:HG2	47:1p:17:TYR:CE1	2.47	0.50
1:2A:11:G:C2'	1:2A:12:U:H5'	2.41	0.50
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.24	0.50
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.11	0.50
32:2a:1145:C:O2	32:2a:1147:C:N4	2.44	0.50
33:2b:138:LEU:HA	33:2b:141:GLU:HB3	1.93	0.50
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.26	0.50
36:2e:33:VAL:HG22	36:2e:112:LEU:HD12	1.94	0.50
1:1A:271(K):U:O2	8:1I:50:ARG:HG3	2.11	0.50
1:1A:760:G:OP1	61:1A:4239:HOH:O	2.20	0.50
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.12	0.50
1:1A:2120:G:H1	1:1A:2178:C:N4	2.07	0.50
8:1I:65:ALA:HB1	8:1I:132:PRO:HG2	1.92	0.50
32:1a:113:G:OP1	61:1a:1913:HOH:O	2.20	0.50
32:1a:1355:G:H2'	32:1a:1356:G:C8	2.47	0.50
41:1j:30:SER:HB3	41:1j:81:THR:HG23	1.93	0.50
1:2A:315:G:H2'	1:2A:316:C:C6	2.46	0.50
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.44	0.50
32:2a:222:U:H2'	32:2a:223:U:H6	1.73	0.50
32:2a:993:G:H4'	32:2a:994:A:OP2	2.11	0.50
32:2a:1233:G:H2'	32:2a:1234:C:C6	2.47	0.50
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.11	0.50
41:2j:45:ARG:HG2	41:2j:47:PHE:CE1	2.47	0.50
1:1A:548:A:H1'	1:1A:549:G:OP1	2.11	0.50
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.77	0.50
1:1A:2107:C:N3	1:1A:2182:G:N2	2.58	0.50
1:1A:2130:U:O2'	1:1A:2133:G:H4'	2.12	0.50
15:1T:127:ALA:C	15:1T:129:ARG:H	2.19	0.50
16:1U:69:CYS:HB3	16:1U:74:LEU:HD13	1.93	0.50
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.93	0.50
26:14:58:ARG:O	26:14:61:ARG:HD3	2.11	0.50
32:1a:562:C:H1'	43:1l:15:ARG:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:987:G:H1	32:1a:1218:C:H42	1.60	0.50
32:1a:1005:A:C2	32:1a:1025:U:H1'	2.45	0.50
32:1a:1051:C:H2'	32:1a:1052:U:C6	2.46	0.50
54:1w:125:ARG:HD3	54:1w:153:GLY:O	2.11	0.50
1:2A:391:G:O2'	1:2A:410:G:OP1	2.20	0.50
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.12	0.50
2:2B:24:G:N7	2:2B:56:G:H2'	2.26	0.50
32:2a:9:G:OP2	36:2e:121:LYS:NZ	2.28	0.50
34:2c:184:TYR:HA	34:2c:200:ALA:O	2.12	0.50
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.45	0.50
1:1A:784:A:C8	1:1A:792:G:C5	2.99	0.50
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.11	0.50
4:1E:109:LYS:O	4:1E:111:ARG:NH1	2.43	0.50
25:13:3:ARG:HD3	25:13:60:GLU:OE2	2.11	0.50
32:1a:297:G:N2	32:1a:300:A:OP2	2.40	0.50
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.42	0.50
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.77	0.50
1:2A:2176:A:H2'	1:2A:2177:C:H6	1.76	0.50
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.11	0.50
2:2B:9:G:P	14:2S:25:ARG:HH22	2.34	0.50
19:2X:54:VAL:HG22	19:2X:81:VAL:HG12	1.93	0.50
32:2a:1112:C:H1'	34:2c:179:ARG:HH11	1.76	0.50
32:2a:1271:G:N2	32:2a:1272:G:C8	2.79	0.50
32:2a:1314:C:H2'	32:2a:1315:U:C6	2.46	0.50
34:2c:97:LYS:O	34:2c:99:VAL:N	2.45	0.50
54:2w:202:LEU:HD22	54:2w:285:LEU:HD23	1.93	0.50
1:1A:436:C:H2'	1:1A:437:G:C8	2.46	0.50
1:1A:2124:G:H3'	1:1A:2125:G:H8	1.75	0.50
7:1H:46:GLU:HB2	7:1H:49:VAL:HG12	1.92	0.50
8:1I:54:GLN:HG3	8:1I:57:ARG:NH1	2.26	0.50
32:1a:263:A:OP1	51:1t:79:ARG:NH1	2.45	0.50
32:1a:946:A:O2'	32:1a:1333:A:N3	2.43	0.50
2:2B:115:G:H2'	2:2B:116:G:C8	2.45	0.50
21:2Z:129:SER:HB3	21:2Z:132:ASN:ND2	2.26	0.50
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.40	0.50
36:2e:98:THR:HB	36:2e:117:ASP:HB3	1.93	0.50
55:2x:23:U:H2'	55:2x:24:G:C8	2.47	0.50
1:1A:1889:A:N1	1:1A:2234:G:H1'	2.27	0.50
26:14:54:GLY:C	26:14:56:VAL:HA	2.36	0.50
32:1a:35:G:O2'	43:1l:118:SER:O	2.29	0.50
32:1a:403:C:H5''	35:1d:136:PRO:HD2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:434:U:H2'	32:1a:435:C:C6	2.46	0.50
32:1a:445:G:H2'	32:1a:446:G:C8	2.47	0.50
32:1a:1063:C:OP2	32:1a:1064:G:O2'	2.25	0.50
33:1b:102:LEU:HD23	33:1b:182:ILE:HD12	1.92	0.50
35:1d:31:CYS:HB2	60:1d:302:SF4:S3	2.52	0.50
39:1h:17:THR:HG22	39:1h:63:LEU:HG	1.93	0.50
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.93	0.50
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.45	0.50
5:2F:165:ARG:HG2	5:2F:168:ARG:NH2	2.25	0.50
26:24:40:HIS:HB3	26:24:43:TYR:HD2	1.77	0.50
29:27:24:THR:HG22	29:27:26:GLY:H	1.77	0.50
32:2a:565:U:OP2	32:2a:566:G:O2'	2.27	0.50
32:2a:811:C:N4	61:2a:1826:HOH:O	2.43	0.50
1:1A:2552:OMU:OP2	61:1A:4228:HOH:O	2.19	0.50
1:1A:2556:C:O2'	54:1w:240:ARG:NH2	2.44	0.50
7:1H:11:VAL:HG13	7:1H:15:VAL:HB	1.93	0.50
32:1a:254:G:H5''	48:1q:69:LYS:HD2	1.93	0.50
1:2A:603:A:N1	1:2A:625:G:O2'	2.38	0.50
1:2A:2116:G:N7	1:2A:2166:G:N2	2.59	0.50
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.27	0.50
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.46	0.50
1:2A:2396:G:OP1	23:21:25:LYS:NZ	2.37	0.50
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.46	0.50
1:2A:2839:G:H5'	13:2R:46:GLY:CA	2.40	0.50
32:2a:601:C:H2'	32:2a:602:A:C8	2.47	0.50
44:2m:15:VAL:O	44:2m:19:LEU:HG	2.12	0.50
47:2p:21:VAL:HG22	47:2p:33:ILE:HB	1.94	0.50
55:2x:19:G:H3'	55:2x:20:H2U:O2	2.11	0.50
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.12	0.50
8:1I:77:LEU:HB3	8:1I:142:VAL:HG22	1.94	0.50
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.93	0.50
54:1w:125:ARG:HD2	54:1w:155:PHE:CE2	2.46	0.50
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.57	0.50
1:2A:892:G:N2	1:2A:894:C:OP1	2.45	0.50
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.46	0.50
1:2A:2682:U:OP2	61:2A:4842:HOH:O	2.20	0.50
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.94	0.50
8:2I:12:LEU:O	8:2I:19:VAL:HG11	2.11	0.50
31:29:12:ASP:OD1	31:29:12:ASP:N	2.42	0.50
35:2d:100:ARG:HH22	35:2d:118:ARG:HH22	1.60	0.50
50:2s:20:LEU:HD21	50:2s:43:GLU:HG2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:52:TYR:HB2	50:2s:57:HIS:CE1	2.47	0.50
1:1A:286:C:H2'	1:1A:287:C:C6	2.47	0.49
1:1A:686:G:OP1	29:17:11:LYS:NZ	2.43	0.49
1:1A:2507:C:H4'	54:1w:233:ASN:O	2.12	0.49
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.47	0.49
6:1G:103:LEU:HD23	6:1G:106:LEU:HD23	1.94	0.49
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.94	0.49
26:14:53:GLU:HB3	26:14:55:ARG:H	1.77	0.49
32:1a:1015:A:H4'	45:1n:15:LYS:NZ	2.27	0.49
33:1b:133:LYS:O	33:1b:136:VAL:HG22	2.11	0.49
1:2A:1451:C:H4'	1:2A:1452:A:C8	2.46	0.49
15:2T:83:ILE:HD13	15:2T:86:ILE:HD11	1.93	0.49
23:21:60:PHE:HZ	23:21:94:LEU:HD12	1.77	0.49
33:2b:33:TYR:HB2	33:2b:43:ASP:HA	1.94	0.49
34:2c:79:ARG:H	34:2c:82:GLU:HB3	1.77	0.49
1:1A:226:G:N2	1:1A:228:A:H62	2.10	0.49
1:1A:592:G:O6	61:1A:4233:HOH:O	2.17	0.49
1:1A:1253:A:OP1	61:1A:4235:HOH:O	2.18	0.49
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.44	0.49
6:1G:37:VAL:HG23	6:1G:99:MET:HG3	1.93	0.49
32:1a:389:A:C6	32:1a:390:C:H1'	2.47	0.49
55:1x:75:C:H2'	55:1x:76:8AN:H1'	1.95	0.49
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.48	0.49
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.11	0.49
1:2A:2494:G:O2'	12:2Q:80:GLU:HA	2.12	0.49
6:2G:41:GLN:O	6:2G:43:LEU:N	2.45	0.49
24:22:10:LEU:HD21	24:22:59:ARG:HG2	1.93	0.49
32:2a:833:U:H2'	32:2a:834:C:H6	1.77	0.49
41:2j:81:THR:HA	41:2j:84:GLN:HB3	1.95	0.49
48:2q:67:LYS:O	48:2q:68:ARG:HB3	2.11	0.49
1:1A:1364:G:P	23:11:3:LYS:HG3	2.52	0.49
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.24	0.49
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.27	0.49
1:1A:2879:C:OP2	61:1A:4240:HOH:O	2.20	0.49
32:1a:501:C:H2'	32:1a:502:G:C8	2.46	0.49
32:1a:713:G:H2'	32:1a:714:G:C8	2.47	0.49
32:1a:1030:C:N4	32:1a:1030(A):G:N3	2.60	0.49
32:1a:1189:C:H5''	34:1c:5:ILE:HD12	1.93	0.49
34:1c:22:TRP:CH2	34:1c:32:LEU:HB2	2.48	0.49
36:1e:35:GLY:HA3	36:1e:112:LEU:HB3	1.94	0.49
38:1g:50:ILE:HG12	38:1g:61:VAL:HG11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.12	0.49
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.47	0.49
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.11	0.49
14:2S:3:ARG:NH1	14:2S:4:LEU:O	2.46	0.49
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD21	1.94	0.49
35:2d:158:ILE:HG12	35:2d:162:LEU:HD12	1.94	0.49
1:1A:8:A:H2'	1:1A:9:U:C6	2.47	0.49
1:1A:213:A:H2'	1:1A:214:G:O4'	2.12	0.49
1:1A:796:C:H2'	1:1A:797:C:C6	2.47	0.49
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.12	0.49
1:1A:2185:C:H2'	1:1A:2186:G:C8	2.48	0.49
32:1a:148:G:H2'	32:1a:149:A:C8	2.47	0.49
32:1a:618:C:H5'	32:1a:619:U:H5''	1.94	0.49
36:1e:51:VAL:O	36:1e:55:VAL:HG23	2.11	0.49
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.44	0.49
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.77	0.49
10:2O:87:ILE:HD12	10:2O:91:LEU:HA	1.94	0.49
32:2a:683:G:H2'	32:2a:684:A:C8	2.47	0.49
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.46	0.49
32:2a:1239:A:H62	32:2a:1299:A:N6	2.11	0.49
32:2a:1252:A:H2'	32:2a:1253:G:O4'	2.10	0.49
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.12	0.49
3:1D:211:ARG:HG2	3:1D:214:TRP:CZ3	2.48	0.49
26:14:44:THR:O	26:14:47:GLN:HB2	2.12	0.49
32:1a:269:C:H2'	32:1a:270:A:C8	2.48	0.49
32:1a:903:G:OP1	61:1a:1914:HOH:O	2.20	0.49
44:1m:87:TYR:CE2	44:1m:91:ARG:HD2	2.48	0.49
1:2A:93:G:H2'	1:2A:94:C:C6	2.48	0.49
1:2A:581:C:H2'	1:2A:582:G:C8	2.47	0.49
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.47	0.49
9:2N:10:GLU:HG2	9:2N:11:PRO:HD2	1.94	0.49
32:2a:628:G:H2'	32:2a:629:G:C8	2.47	0.49
32:2a:685:G:C2	32:2a:686:U:C4	3.00	0.49
32:2a:728:A:H2'	32:2a:729:A:C8	2.48	0.49
32:2a:1272:G:N2	32:2a:1273:G:N7	2.58	0.49
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.45	0.49
1:1A:2125:G:H2'	1:1A:2173:A:H61	1.78	0.49
11:1P:42:SER:O	61:1P:301:HOH:O	2.20	0.49
32:1a:1187:G:H5'	40:1i:113:LYS:HE2	1.95	0.49
32:1a:1369:C:H2'	32:1a:1370:G:C8	2.48	0.49
33:1b:59:GLU:HB2	33:1b:221:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:61:LYS:NZ	35:1d:72:GLU:OE1	2.39	0.49
1:2A:493:G:OP1	61:2A:4845:HOH:O	2.20	0.49
10:2O:35:VAL:HG13	10:2O:65:THR:HG23	1.95	0.49
10:2O:105:GLU:O	10:2O:109:LYS:HG3	2.13	0.49
28:26:6:ARG:HH11	28:26:26:ASN:HB2	1.77	0.49
32:2a:1228:C:P	44:2m:108:ARG:HH22	2.36	0.49
32:2a:1259:C:N4	32:2a:1260:C:O2	2.46	0.49
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.93	0.49
44:2m:14:ARG:HB2	44:2m:17:VAL:HG23	1.93	0.49
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.46	0.49
32:1a:222:U:H2'	32:1a:223:U:C6	2.48	0.49
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.47	0.49
47:1p:43:LYS:HA	47:1p:48:TRP:CD1	2.47	0.49
1:2A:959:A:N3	1:2A:2457:U:O2'	2.44	0.49
1:2A:1420:U:O2'	1:2A:1421:G:O5'	2.25	0.49
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.13	0.49
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.27	0.49
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.74	0.49
32:2a:1030(D):A:H8	32:2a:1031:G:C8	2.30	0.49
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.47	0.49
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.77	0.49
32:2a:1380:U:C4	38:2g:3:ARG:HG2	2.48	0.49
51:2t:18:GLN:O	51:2t:22:ARG:HG2	2.13	0.49
33:1b:16:HIS:CD2	33:1b:18:GLY:H	2.25	0.49
33:1b:21:ARG:O	33:1b:23:ARG:N	2.44	0.49
38:1g:22:LEU:HG	38:1g:62:PHE:CE2	2.47	0.49
40:1i:96:LEU:HD22	40:1i:101:PHE:HD2	1.76	0.49
54:1w:111:ILE:HB	54:1w:158:VAL:HG23	1.95	0.49
1:2A:579:G:H2'	1:2A:580:C:C6	2.48	0.49
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.47	0.49
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.48	0.49
1:2A:1827:C:OP2	3:2D:222:ARG:HD2	2.13	0.49
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.38	0.49
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.28	0.49
21:2Z:124:ILE:HD11	21:2Z:165:VAL:HG21	1.93	0.49
32:2a:790:A:OP1	55:2x:38:A:O2'	2.29	0.49
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.48	0.49
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.95	0.49
50:2s:12:ASP:OD1	50:2s:37:ARG:NH2	2.46	0.49
51:2t:50:GLU:HB2	51:2t:99:LEU:HD13	1.94	0.49
1:1A:922:U:H2'	1:1A:923:C:C6	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:13:55:ARG:NH1	25:13:57:GLU:OE1	2.46	0.49
32:1a:277:C:H5''	48:1q:68:ARG:HH21	1.78	0.49
32:1a:1030:C:C4	32:1a:1030(A):G:H1'	2.48	0.49
32:1a:1035:A:C2'	32:1a:1036:G:H21	2.15	0.49
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.48	0.49
35:1d:98:GLU:OE2	35:1d:103:ASN:ND2	2.39	0.49
51:1t:9:ASN:O	51:1t:10:LEU:HB2	2.12	0.49
1:2A:1633:G:OP2	61:2A:4844:HOH:O	2.20	0.49
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	1.94	0.49
24:22:51:ARG:O	24:22:55:ARG:HG2	2.13	0.49
32:2a:130:A:C8	48:2q:63:ARG:HG3	2.47	0.49
32:2a:1163:C:H2'	32:2a:1164:G:H8	1.78	0.49
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.53	0.49
47:2p:75:ARG:HB2	47:2p:80:PHE:HD2	1.78	0.49
1:1A:1139:G:OP1	9:1N:101:HIS:ND1	2.33	0.49
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.13	0.49
1:2A:30:G:H2'	1:2A:31:C:C6	2.47	0.49
1:2A:236:C:H2'	1:2A:237:C:H6	1.78	0.49
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.11	0.49
32:2a:841:U:H6	32:2a:841:U:P	2.35	0.49
1:1A:1054:A:H2'	1:1A:1055:G:C8	2.48	0.48
26:14:24:THR:OG1	26:14:25:TYR:N	2.45	0.48
35:1d:8:VAL:HG22	35:1d:21:LEU:HD13	1.95	0.48
46:1o:5:LYS:H	46:1o:5:LYS:HD2	1.78	0.48
1:2A:184:C:H2'	1:2A:185:U:C6	2.48	0.48
1:2A:484:C:H2'	1:2A:485:C:H6	1.77	0.48
1:2A:623:G:H2'	1:2A:624:C:C6	2.49	0.48
1:2A:1420:U:HO2'	1:2A:1421:G:P	2.36	0.48
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.48	0.48
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.13	0.48
4:2E:96:PHE:O	4:2E:175:VAL:HG21	2.13	0.48
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.95	0.48
21:2Z:52:SER:C	21:2Z:54:HIS:H	2.20	0.48
32:2a:110:C:H2'	32:2a:111:G:O4'	2.13	0.48
32:2a:1070:U:H2'	32:2a:1071:C:C6	2.48	0.48
32:2a:1266:G:N2	32:2a:1269:A:OP2	2.36	0.48
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.48	0.48
35:2d:109:GLY:HA3	35:2d:165:MET:HG3	1.95	0.48
38:2g:68:ASN:ND2	38:2g:128:ALA:HA	2.27	0.48
1:1A:286:C:H2'	1:1A:287:C:H6	1.78	0.48
1:1A:1754:C:OP1	15:1T:96:ARG:NH1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:1A:5808:HOH:O	9:1N:28:THR:HG23	2.12	0.48
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	1.96	0.48
28:16:13:CYS:SG	28:16:47:THR:HG21	2.53	0.48
32:1a:156:G:H5'	32:1a:157:G:OP2	2.13	0.48
32:1a:376:G:O3'	47:1p:5:ARG:HD2	2.13	0.48
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.31	0.48
34:1c:56:ASP:HB2	34:1c:67:THR:HB	1.95	0.48
36:1e:78:HIS:HE1	36:1e:142:LEU:HA	1.77	0.48
40:1i:16:ARG:NH1	40:1i:64:THR:HG21	2.27	0.48
1:2A:65:C:H5'	19:2X:71:GLY:HA3	1.94	0.48
1:2A:1253:A:OP1	61:2A:4843:HOH:O	2.20	0.48
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.45	0.48
1:2A:2127:G:C6	1:2A:2161:C:C4	3.01	0.48
1:2A:2336:A:H61	22:20:43:THR:CG2	2.27	0.48
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.45	0.48
1:2A:2391:G:O6	1:2A:2425:A:H8	1.97	0.48
6:2G:54:GLU:HA	6:2G:57:ALA:HB3	1.95	0.48
10:2O:15:GLY:O	10:2O:47:ILE:HG13	2.13	0.48
12:2Q:43:THR:N	12:2Q:46:GLN:OE1	2.39	0.48
32:2a:532:A:N6	32:2a:1206:G:O2'	2.46	0.48
32:2a:1014:A:C2	32:2a:1219:U:H1'	2.49	0.48
32:2a:1292:U:H2'	32:2a:1293:G:C8	2.48	0.48
32:2a:1327:C:H5''	52:2u:20:LYS:HB3	1.94	0.48
33:2b:19:HIS:HE2	33:2b:206:ASP:HB2	1.78	0.48
35:2d:112:VAL:HG22	35:2d:116:GLN:NE2	2.29	0.48
42:2k:84:VAL:HG21	42:2k:95:ILE:HD11	1.94	0.48
44:2m:14:ARG:HH21	44:2m:41:PRO:HB2	1.78	0.48
1:1A:2100:G:H1	1:1A:2189:U:H3	1.61	0.48
2:1B:103:G:H21	21:1Z:73:GLN:NE2	2.07	0.48
23:11:44:PRO:HB2	23:11:46:LEU:HD13	1.94	0.48
32:1a:109:A:C6	32:1a:326:G:C6	3.01	0.48
32:1a:376:G:H5''	47:1p:5:ARG:HB2	1.94	0.48
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.95	0.48
35:1d:101:LEU:HD23	35:1d:121:VAL:HG13	1.96	0.48
36:1e:91:LEU:HB3	36:1e:118:ILE:HD11	1.95	0.48
1:2A:1184:G:OP1	25:23:30:ARG:NH1	2.44	0.48
1:2A:2238:G:H5''	61:2A:5471:HOH:O	2.13	0.48
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.95	0.48
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.42	0.48
32:2a:441:A:H3'	32:2a:442:C:C6	2.49	0.48
32:2a:490:G:H2'	32:2a:491:G:H8	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:524:G:H2'	32:2a:525:C:C6	2.48	0.48
32:2a:841:U:OP1	32:2a:841:U:H6	1.96	0.48
32:2a:1055:A:N3	34:2c:156:ARG:NH1	2.61	0.48
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.78	0.48
33:2b:134:GLU:O	33:2b:137:ARG:HG3	2.13	0.48
1:1A:228:A:H3'	1:1A:229:A:C5'	2.42	0.48
1:1A:1607:C:N4	1:1A:1622:G:OP2	2.35	0.48
8:1I:31:LEU:HD21	8:1I:38:LEU:HG	1.96	0.48
32:1a:165:C:H2'	32:1a:166:G:H8	1.78	0.48
32:1a:692:U:O2'	32:1a:694:A:N7	2.36	0.48
36:1e:91:LEU:HD23	36:1e:120:THR:HB	1.94	0.48
44:1m:84:ILE:HD11	44:1m:86:CYS:HB2	1.95	0.48
54:1w:216:GLU:HB2	54:1w:245:PRO:HD3	1.95	0.48
1:2A:370:G:OP1	1:2A:403:U:N3	2.34	0.48
1:2A:646:A:H2'	1:2A:647:G:O4'	2.14	0.48
1:2A:882:G:H1	1:2A:894:C:H42	1.62	0.48
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.49	0.48
7:2H:3:ARG:NH2	7:2H:65:HIS:HB3	2.28	0.48
32:2a:1216:G:OP1	45:2n:2:ALA:HA	2.13	0.48
32:2a:1304:G:OP1	52:2u:2:GLY:N	2.47	0.48
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.48	0.48
41:2j:11:PHE:CE1	41:2j:67:THR:HG22	2.48	0.48
42:2k:31:THR:HG22	42:2k:42:TRP:HB2	1.94	0.48
53:2v:20:A:N6	54:2w:186:THR:OG1	2.47	0.48
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.11	0.48
1:1A:2188:C:H2'	1:1A:2189:U:O4'	2.13	0.48
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.96	0.48
26:14:34:GLU:HB2	44:1m:57:ARG:NH1	2.27	0.48
32:1a:189(B):C:H2'	32:1a:189(C):C:C6	2.49	0.48
32:1a:1298:C:H2'	38:1g:114:ARG:NH2	2.28	0.48
32:1a:1376:U:OP1	38:1g:98:SER:HB3	2.13	0.48
33:1b:167:PRO:HG2	33:1b:192:SER:HB3	1.95	0.48
35:1d:121:VAL:O	35:1d:134:ASP:HA	2.14	0.48
39:1h:64:LYS:HG2	39:1h:79:VAL:HG21	1.96	0.48
39:1h:86:ILE:HG12	39:1h:135:CYS:HA	1.96	0.48
43:1l:24:VAL:HB	43:1l:27:LEU:HD12	1.96	0.48
1:2A:910:A:N3	1:2A:2264:C:O2'	2.44	0.48
1:2A:1187:G:H5''	17:2V:81:TYR:CE1	2.49	0.48
1:2A:1858:G:N2	1:2A:1883:G:H2'	2.28	0.48
15:2T:26:ASP:O	15:2T:49:VAL:HG22	2.13	0.48
21:2Z:93:ASP:HA	21:2Z:130:PRO:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1137:C:H5''	32:2a:1138:G:OP1	2.13	0.48
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.48	0.48
32:2a:1187:G:H5'	40:2i:113:LYS:NZ	2.29	0.48
48:2q:5:VAL:HG22	48:2q:60:ILE:HD12	1.95	0.48
54:2w:319:PHE:HE2	54:2w:335:ILE:HG12	1.77	0.48
1:1A:1914:C:OP1	61:1A:4241:HOH:O	2.20	0.48
11:1P:65:ARG:HD2	30:18:25:MET:SD	2.54	0.48
32:1a:316:G:OP2	32:1a:351:G:O2'	2.28	0.48
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.31	0.48
36:1e:148:VAL:O	36:1e:152:ARG:HG2	2.13	0.48
1:2A:2255:G:O2'	55:2x:3:C:H5'	2.14	0.48
15:2T:88:ILE:HG21	15:2T:91:ARG:NE	2.29	0.48
35:2d:153:ARG:NH1	35:2d:181:MET:HE3	2.29	0.48
40:2i:20:ARG:O	40:2i:60:ASP:N	2.42	0.48
44:2m:11:ARG:HB2	44:2m:12:ASN:HD22	1.79	0.48
1:1A:2052:G:H4'	4:1E:143:ASN:O	2.14	0.48
1:1A:2206:G:H3'	1:1A:2207:G:H8	1.78	0.48
6:1G:126:ASP:HB2	6:1G:130:ASN:O	2.13	0.48
11:1P:121:LYS:O	11:1P:123:LEU:N	2.46	0.48
26:14:57:GLU:OE1	26:14:58:ARG:NH1	2.46	0.48
32:1a:127:G:HO2'	48:1q:2:PRO:N	2.12	0.48
32:1a:1127:G:H5'	32:1a:1280:A:O2'	2.14	0.48
39:1h:39:LEU:HB3	39:1h:45:ILE:HG12	1.95	0.48
44:1m:3:ARG:HG2	44:1m:4:ILE:HG12	1.95	0.48
1:2A:271(M):G:N3	1:2A:271(M):G:H5'	2.28	0.48
1:2A:536:A:H2'	1:2A:537:C:C6	2.49	0.48
1:2A:588:U:H2'	1:2A:589:C:C6	2.49	0.48
8:2I:114:LEU:HD22	8:2I:130:TYR:HB2	1.95	0.48
15:2T:49:VAL:HG12	15:2T:63:VAL:HG22	1.96	0.48
26:24:16:CYS:HA	26:24:33:VAL:O	2.13	0.48
32:2a:153:C:H2'	32:2a:154:C:C6	2.49	0.48
32:2a:1052:U:O2'	32:2a:1055:A:OP2	2.20	0.48
55:2x:7:U:O2'	55:2x:49:U:OP2	2.29	0.48
1:1A:478:A:N1	1:1A:500:G:H4'	2.28	0.48
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.55	0.48
4:1E:181:LEU:HD21	15:1T:6:LEU:HD12	1.96	0.48
21:1Z:45:ASP:O	21:1Z:49:ARG:HB2	2.14	0.48
32:1a:77:G:H1	32:1a:92:C:H42	1.62	0.48
32:1a:1347:G:N7	40:1i:11:LYS:HE2	2.28	0.48
33:1b:40:HIS:HB3	33:1b:190:THR:HG21	1.95	0.48
33:1b:76:GLN:HG2	33:1b:206:ASP:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.78	0.48
41:1j:81:THR:O	41:1j:83:GLU:N	2.47	0.48
47:1p:20:VAL:HG23	47:1p:35:LYS:HA	1.95	0.48
1:2A:2014:A:H2'	1:2A:2015:A:C8	2.49	0.48
6:2G:28:VAL:O	6:2G:31:VAL:HG13	2.13	0.48
9:2N:30:ILE:O	9:2N:34:LEU:HG	2.14	0.48
14:2S:18:ILE:O	14:2S:21:THR:HG23	2.14	0.48
32:2a:1123:A:H4'	41:2j:37:PRO:HD2	1.96	0.48
32:2a:1151:A:H5''	41:2j:40:LEU:O	2.14	0.48
32:2a:1210:C:H2'	32:2a:1211:U:H5''	1.95	0.48
38:2g:23:VAL:HG12	38:2g:62:PHE:CE2	2.49	0.48
38:2g:101:LEU:HA	38:2g:104:LEU:HD12	1.94	0.48
47:2p:48:TRP:HH2	47:2p:76:GLN:HE22	1.62	0.48
54:2w:312:VAL:HG11	54:2w:327:VAL:HG21	1.95	0.48
1:1A:2245:U:O2'	1:1A:2436:G:OP2	2.30	0.48
5:1F:9:ILE:HD13	5:1F:123:LEU:HD23	1.96	0.48
27:15:40:LYS:HE2	27:15:44:THR:O	2.14	0.48
32:1a:1096:C:HO2'	32:1a:1170:A:HO2'	1.60	0.48
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.49	0.48
42:1k:14:VAL:HG22	42:1k:16:SER:H	1.79	0.48
53:1v:22:U:OP2	54:1w:191:ARG:NH1	2.45	0.48
1:2A:2314:C:H2'	1:2A:2315:G:H8	1.79	0.48
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.27	0.48
1:2A:2821:A:OP2	61:2R:301:HOH:O	2.19	0.48
5:2F:113:ALA:HB1	5:2F:186:ILE:HG21	1.95	0.48
32:2a:986:A:N3	50:2s:52:TYR:OH	2.33	0.48
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.29	0.48
33:2b:140:HIS:O	33:2b:144:ARG:N	2.47	0.48
1:1A:436:C:H2'	1:1A:437:G:H8	1.78	0.48
1:1A:491:G:H2'	1:1A:492:A:C8	2.49	0.48
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.49	0.48
2:1B:73:A:N1	21:1Z:34:ASN:ND2	2.61	0.48
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.79	0.48
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.61	0.48
12:1Q:7:MET:HE3	12:1Q:7:MET:HB3	1.74	0.48
32:1a:1310:G:OP2	44:1m:88:ARG:NH2	2.43	0.48
32:1a:1343:G:O2'	40:1i:121:ARG:HD2	2.14	0.48
34:1c:130:VAL:HG21	34:1c:157:ILE:HG23	1.96	0.48
5:2F:36:VAL:O	5:2F:40:GLN:HG3	2.13	0.48
32:2a:410:G:O6	35:2d:22:LYS:NZ	2.46	0.48
32:2a:1521:G:H2'	32:2a:1522:U:C6	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:71:VAL:HB	33:2b:164:VAL:HG13	1.96	0.48
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.14	0.48
1:1A:1179:C:H2'	1:1A:1180:C:H6	1.79	0.47
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.96	0.47
1:1A:2390:U:P	30:18:35:GLN:HE22	2.37	0.47
5:1F:170:LEU:HD13	5:1F:172:TRP:CZ2	2.49	0.47
20:1Y:12:THR:OG1	20:1Y:26:LYS:HE3	2.14	0.47
32:1a:303:A:HO2'	32:1a:555:C:HO2'	1.62	0.47
32:1a:737:A:H2'	32:1a:738:C:C6	2.49	0.47
1:2A:468:G:N7	29:27:39:ARG:NH2	2.52	0.47
1:2A:752:A:H3'	29:27:1:MET:HE1	1.96	0.47
6:2G:146:TYR:O	6:2G:149:VAL:HG12	2.14	0.47
27:25:33:CYS:HB2	27:25:40:LYS:HD3	1.95	0.47
32:2a:130:A:O2'	32:2a:131:C:O5'	2.29	0.47
32:2a:617:G:H4'	47:2p:44:THR:O	2.13	0.47
32:2a:1273:G:C6	32:2a:1274:G:C4	3.01	0.47
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.29	0.47
32:2a:1347:G:HO2'	32:2a:1373:G:H1	1.61	0.47
32:2a:1376:U:OP1	38:2g:98:SER:OG	2.15	0.47
54:2w:212:LEU:HB3	54:2w:217:ILE:HD11	1.96	0.47
1:1A:743:G:O2'	1:1A:1659:U:OP1	2.30	0.47
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.48	0.47
1:2A:912:C:OP1	12:2Q:9:TYR:OH	2.30	0.47
1:2A:2107:C:H2'	1:2A:2108:C:O4'	2.14	0.47
1:2A:2869:G:H2'	1:2A:2870:C:O4'	2.13	0.47
10:2O:63:VAL:HG11	10:2O:85:VAL:HG23	1.96	0.47
26:24:56:VAL:O	26:24:60:GLN:HB2	2.14	0.47
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.79	0.47
32:2a:1360:A:H8	32:2a:1360:A:OP1	1.97	0.47
40:2i:26:VAL:HG12	40:2i:61:ALA:H	1.79	0.47
1:1A:531:C:H4'	1:1A:532:A:H5''	1.95	0.47
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.46	0.47
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.13	0.47
1:1A:2716:U:O2'	61:1A:4242:HOH:O	2.20	0.47
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.13	0.47
5:1F:32:LEU:HD22	5:1F:112:MET:HE2	1.96	0.47
32:1a:719:C:N4	49:1r:71:LYS:HE2	2.29	0.47
49:1r:35:ARG:O	49:1r:37:VAL:N	2.46	0.47
54:1w:257:SER:OG	54:1w:259:ILE:HG22	2.15	0.47
1:2A:288:C:H2'	1:2A:289:A:H8	1.78	0.47
1:2A:493:G:H2'	1:2A:494:G:O4'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.95	0.47
26:24:53:GLU:H	26:24:53:GLU:HG3	1.50	0.47
32:2a:1057:G:OP1	34:2c:154:SER:OG	2.32	0.47
32:2a:1072:G:H2'	32:2a:1073:U:C6	2.50	0.47
32:2a:1292:U:H2'	32:2a:1293:G:H8	1.78	0.47
34:2c:47:LEU:HD13	34:2c:68:VAL:HG11	1.96	0.47
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.79	0.47
37:2f:65:VAL:HG21	37:2f:67:MET:HE2	1.95	0.47
40:2i:55:ALA:HA	40:2i:58:HIS:CD2	2.49	0.47
1:1A:807:U:O2'	1:1A:2060:A:N1	2.42	0.47
1:1A:1309:G:OP1	29:17:9:ARG:HG3	2.14	0.47
1:1A:2161:C:HO2'	1:1A:2162:G:H8	1.60	0.47
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.49	0.47
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.14	0.47
32:1a:160:A:H1'	32:1a:344:A:C5	2.49	0.47
32:1a:473:G:H2'	32:1a:474:G:C8	2.49	0.47
32:1a:738:C:H2'	32:1a:739:C:H6	1.80	0.47
32:1a:911:U:H2'	32:1a:912:C:C6	2.50	0.47
32:1a:1009:G:H2'	32:1a:1010:G:H5'	1.95	0.47
32:1a:1284:C:H3'	32:1a:1285:A:H8	1.80	0.47
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.97	0.47
47:1p:40:ASP:HB3	47:1p:48:TRP:HB2	1.95	0.47
1:2A:784:A:C8	1:2A:792:G:C5	3.02	0.47
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.12	0.47
1:2A:1419:A:H5'	1:2A:1579:A:H61	1.79	0.47
1:2A:1532:C:H3'	1:2A:1533:G:H8	1.80	0.47
1:2A:2548:G:O6	61:2A:4838:HOH:O	2.18	0.47
5:2F:148:LEU:HD11	5:2F:193:VAL:HG11	1.96	0.47
10:2O:63:VAL:HG23	10:2O:64:ARG:HG3	1.95	0.47
15:2T:74:ARG:HG2	15:2T:76:PHE:CZ	2.49	0.47
18:2W:68:ARG:HB2	18:2W:109:GLU:HG2	1.97	0.47
32:2a:35:G:O2'	43:2l:118:SER:O	2.25	0.47
35:2d:78:LEU:HD23	35:2d:97:LEU:HD23	1.96	0.47
40:2i:56:LEU:H	40:2i:56:LEU:HG	1.45	0.47
1:1A:1056:G:H4'	1:1A:1086:A:C8	2.50	0.47
2:1B:22:U:H2'	2:1B:23:G:C8	2.50	0.47
24:12:64:LEU:HD11	24:12:68:ARG:NH2	2.29	0.47
32:1a:175:C:H2'	32:1a:176:C:H6	1.80	0.47
1:2A:458:G:O2'	1:2A:469:G:O6	2.33	0.47
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.30	0.47
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:34:GLU:HG2	26:24:35:VAL:HG23	1.95	0.47
32:2a:448:A:OP2	32:2a:485:G:N1	2.42	0.47
32:2a:1239:A:H62	32:2a:1299:A:H62	1.62	0.47
36:2e:6:PHE:HE1	36:2e:36:ASP:HB3	1.80	0.47
39:2h:49:GLU:OE2	39:2h:62:TYR:OH	2.24	0.47
1:1A:173:G:H2'	1:1A:174:C:C6	2.49	0.47
1:1A:1057:A:N6	1:1A:1087:G:OP2	2.39	0.47
1:1A:1507:A:O2'	1:1A:1509(A):A:N6	2.47	0.47
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.14	0.47
3:1D:169:GLU:OE2	3:1D:184:LYS:NZ	2.36	0.47
14:1S:67:ARG:O	14:1S:71:ARG:HG3	2.15	0.47
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.49	0.47
25:13:4:LEU:O	25:13:36:VAL:HA	2.14	0.47
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.95	0.47
33:1b:56:ARG:HB2	33:1b:56:ARG:HH11	1.79	0.47
54:1w:299:SER:C	54:1w:301:LYS:H	2.22	0.47
1:2A:593:G:H4'	30:28:63:PRO:HB3	1.95	0.47
1:2A:629:G:H5''	1:2A:650:C:O2'	2.14	0.47
1:2A:870:A:OP1	12:2Q:6:ARG:NH1	2.48	0.47
1:2A:890:A:H2'	1:2A:892:G:C8	2.50	0.47
1:2A:1353:A:O4'	1:2A:1569:A:H2	1.98	0.47
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.15	0.47
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.97	0.47
18:2W:11:ARG:HD3	18:2W:82:LEU:HD12	1.95	0.47
22:20:50:ASN:HB3	22:20:63:VAL:HG22	1.96	0.47
32:2a:1492:A:N6	43:2l:48:PRO:O	2.48	0.47
34:2c:111:LEU:HD11	34:2c:144:SER:O	2.15	0.47
36:2e:88:LYS:HB3	36:2e:123:LEU:HB2	1.97	0.47
40:2i:111:ARG:O	40:2i:113:LYS:HD2	2.13	0.47
52:2u:9:ARG:HE	52:2u:9:ARG:HB3	1.44	0.47
1:1A:55:G:O2'	1:1A:127:A:N1	2.38	0.47
1:1A:323:G:H1'	1:1A:1205:U:O2	2.15	0.47
1:1A:1266:G:H3'	61:1A:4223:HOH:O	2.14	0.47
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.14	0.47
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.50	0.47
1:1A:1800:C:OP1	3:1D:264:LYS:NZ	2.44	0.47
1:1A:1805:U:O2	3:1D:50:THR:HB	2.14	0.47
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.14	0.47
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.14	0.47
1:1A:2110:G:H5''	1:1A:2111:C:H5	1.80	0.47
1:1A:2506:U:C2	1:1A:2585:U:O4	2.68	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.14	0.47
3:1D:108:PRO:HG3	3:1D:143:HIS:CE1	2.49	0.47
5:1F:12:LEU:HB3	5:1F:126:VAL:HG12	1.96	0.47
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.30	0.47
32:1a:160:A:HO2'	32:1a:344:A:N6	2.13	0.47
32:1a:181:G:N2	32:1a:182:U:O4	2.45	0.47
32:1a:392:G:H2'	32:1a:393:A:C8	2.50	0.47
32:1a:735:C:H2'	32:1a:736:C:C6	2.50	0.47
32:1a:944:G:N1	32:1a:1338:G:OP2	2.42	0.47
32:1a:1008:C:H2'	32:1a:1009:G:O4'	2.14	0.47
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.63	0.47
33:1b:119:GLU:OE2	33:1b:153:ARG:NH1	2.46	0.47
34:1c:36:ASP:OD1	34:1c:57:ILE:HG21	2.14	0.47
35:1d:15:GLU:OE2	35:1d:59:ARG:NH2	2.41	0.47
1:2A:271(L):U:OP1	8:2I:50:ARG:NH2	2.46	0.47
1:2A:300:A:N6	61:2A:4934:HOH:O	2.37	0.47
1:2A:1169:G:H1	1:2A:1180:C:H42	1.62	0.47
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.50	0.47
1:2A:1915:5MU:O2	54:2w:286:ARG:NH1	2.46	0.47
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.97	0.47
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.30	0.47
28:26:35:GLU:OE2	28:26:50:ARG:NH1	2.48	0.47
29:27:24:THR:HG22	29:27:26:GLY:N	2.30	0.47
32:2a:10:A:OP2	36:2e:126:ARG:HD2	2.15	0.47
32:2a:109:A:C6	32:2a:326:G:C6	3.02	0.47
32:2a:187:C:O2'	51:2t:89:ARG:HD3	2.15	0.47
32:2a:643:C:H2'	32:2a:644:G:H8	1.79	0.47
32:2a:953:G:H5'	32:2a:965:A:N6	2.25	0.47
32:2a:1327:C:OP1	52:2u:12:LYS:NZ	2.30	0.47
42:2k:48:ILE:O	42:2k:50:TYR:N	2.43	0.47
44:2m:10:PRO:HG3	44:2m:21:TYR:CD2	2.50	0.47
54:2w:217:ILE:HA	54:2w:242:VAL:O	2.14	0.47
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.50	0.47
9:1N:73:THR:OG1	9:1N:82:LEU:HD11	2.15	0.47
32:1a:9:G:OP2	36:1e:121:LYS:NZ	2.32	0.47
32:1a:406:G:O3'	35:1d:3:ARG:NH2	2.47	0.47
34:1c:132:ARG:HH11	34:1c:136:GLN:NE2	2.11	0.47
1:2A:567:A:OP2	11:2P:29:LYS:NZ	2.33	0.47
1:2A:2127:G:N2	1:2A:2161:C:C2	2.83	0.47
1:2A:2867:G:OP2	15:2T:119:LYS:NZ	2.46	0.47
6:2G:96:ARG:N	6:2G:99:MET:HE2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:35:ILE:HD13	14:2S:66:ALA:HB2	1.97	0.47
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.15	0.47
21:2Z:36:LYS:HB2	21:2Z:36:LYS:HE3	1.60	0.47
26:24:43:TYR:O	26:24:45:GLY:N	2.48	0.47
32:2a:664:G:P	49:2r:64:ARG:HH21	2.38	0.47
32:2a:1404:5MC:O2	32:2a:1519:MA6:O2'	2.30	0.47
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.76	0.47
38:2g:26:PHE:CE2	38:2g:30:ILE:HD11	2.50	0.47
40:2i:81:ILE:O	40:2i:85:LEU:HG	2.15	0.47
1:1A:218:A:C2	1:1A:235:U:H4'	2.49	0.47
1:1A:800:A:H8	1:1A:800:A:OP1	1.98	0.47
1:1A:1056:G:H5''	1:1A:1086:A:H8	1.79	0.47
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.30	0.47
32:1a:189(C):C:H2'	32:1a:189(D):C:O4'	2.15	0.47
32:1a:401:C:H2'	32:1a:402:G:H8	1.80	0.47
34:1c:150:LYS:HB3	34:1c:201:TYR:HB2	1.96	0.47
39:1h:121:ASP:HB2	39:1h:125:ARG:HH22	1.79	0.47
45:1n:24:CYS:HB2	45:1n:40:CYS:HB3	1.96	0.47
1:2A:647:G:N3	1:2A:2350:C:O2'	2.48	0.47
1:2A:1779:U:H2'	61:2A:4998:HOH:O	2.15	0.47
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.50	0.47
32:2a:108:G:N1	51:2t:15:ARG:HG2	2.29	0.47
32:2a:662:G:H2'	32:2a:663:A:C8	2.50	0.47
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.50	0.47
36:2e:71:LEU:O	36:2e:72:GLN:NE2	2.48	0.47
36:2e:96:PRO:HA	36:2e:117:ASP:OD2	2.15	0.47
38:2g:78:ARG:HH21	38:2g:79:ARG:NH2	2.13	0.47
44:2m:19:LEU:HD11	44:2m:56:LEU:HD21	1.97	0.47
54:2w:309:GLN:CD	54:2w:311:ARG:HE	2.22	0.47
1:1A:493:G:H2'	1:1A:494:G:O4'	2.14	0.47
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.97	0.47
9:1N:36:GLY:HA2	9:1N:38:HIS:CE1	2.50	0.47
14:1S:83:LYS:HB3	14:1S:111:GLU:HG3	1.97	0.47
32:1a:750:G:N3	46:1o:23:GLY:HA3	2.30	0.47
34:1c:15:THR:HG22	34:1c:16:ARG:HG2	1.96	0.47
35:1d:72:GLU:OE2	35:1d:76:ARG:HG3	2.15	0.47
42:1k:81:ASP:OD1	42:1k:107:SER:OG	2.26	0.47
47:1p:75:ARG:HG3	47:1p:80:PHE:HB2	1.96	0.47
48:1q:66:SER:HB3	48:1q:69:LYS:HB2	1.96	0.47
1:2A:639:U:H2'	1:2A:640:C:C6	2.50	0.47
6:2G:167:GLU:H	6:2G:167:GLU:CD	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:179:PRO:HB2	26:24:42:PHE:CE2	2.49	0.47
32:2a:15:G:H21	36:2e:18:ARG:HA	1.80	0.47
32:2a:523:A:H61	43:2l:92:OTD:CG	2.28	0.47
32:2a:664:G:N2	32:2a:741:G:H1	2.09	0.47
32:2a:1240:U:OP2	38:2g:116:ALA:N	2.48	0.47
32:2a:1457:G:H5''	51:2t:35:THR:HG21	1.97	0.47
32:2a:1504:G:OP1	32:2a:1507:A:H4'	2.15	0.47
38:2g:26:PHE:HB2	38:2g:101:LEU:HD22	1.96	0.47
1:1A:864:G:OP2	12:1Q:22:LYS:HE3	2.16	0.46
1:1A:1557:C:H5''	1:1A:1558:A:OP2	2.15	0.46
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.28	0.46
1:1A:1924:C:H4'	55:1x:13:A:H4'	1.97	0.46
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.51	0.46
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.64	0.46
32:1a:137:C:H1'	47:1p:62:VAL:O	2.15	0.46
35:1d:12:CYS:HA	35:1d:19:LEU:HD12	1.96	0.46
39:1h:121:ASP:HB2	39:1h:125:ARG:NH2	2.30	0.46
50:1s:11:VAL:HG12	50:1s:13:ASP:H	1.80	0.46
6:2G:133:LEU:HG	6:2G:157:ILE:HB	1.97	0.46
32:2a:922:G:N3	32:2a:1398:A:H2	2.13	0.46
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.50	0.46
32:2a:1264:C:C4	32:2a:1272:G:O6	2.68	0.46
37:2f:6:VAL:HG22	37:2f:90:VAL:HG13	1.96	0.46
45:2n:6:LEU:HD23	45:2n:9:LYS:HD2	1.96	0.46
1:1A:265:A:N1	1:1A:427:U:O2'	2.43	0.46
1:1A:1012:U:C5	9:1N:28:THR:HG21	2.51	0.46
1:1A:1060:U:O2	1:1A:1062:G:H1'	2.15	0.46
1:1A:1091:G:C2	1:1A:1101:U:H1'	2.50	0.46
1:1A:2138:C:H42	1:1A:2153:G:H1	1.62	0.46
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.30	0.46
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.51	0.46
1:1A:2836:U:C4	1:1A:2883:A:N6	2.83	0.46
3:1D:3:VAL:HG13	3:1D:17:THR:HB	1.96	0.46
5:1F:181:LEU:O	5:1F:205:ARG:NH2	2.37	0.46
8:1I:123:LEU:HA	8:1I:144:VAL:HG23	1.97	0.46
23:11:52:ARG:NH1	23:11:55:GLY:O	2.48	0.46
32:1a:202:U:O2'	32:1a:203:U:O5'	2.31	0.46
35:1d:146:ILE:O	35:1d:183:GLY:N	2.49	0.46
35:1d:175:SER:HB3	35:1d:186:LEU:HD21	1.97	0.46
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.97	0.46
1:2A:302:C:OP2	20:2Y:73:ARG:NH1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.15	0.46
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.16	0.46
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.45	0.46
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.97	0.46
32:2a:337:C:H2'	32:2a:338:A:C8	2.50	0.46
38:2g:46:ALA:HA	38:2g:49:ILE:HG22	1.96	0.46
44:2m:20:THR:HA	44:2m:25:ILE:O	2.15	0.46
54:2w:103:ASP:OD2	54:2w:172:LYS:NZ	2.32	0.46
1:1A:284:U:H2'	1:1A:285:C:C6	2.51	0.46
6:1G:167:GLU:CD	6:1G:167:GLU:H	2.22	0.46
32:1a:838:G:H1	32:1a:848:C:N4	2.14	0.46
36:1e:146:ALA:O	36:1e:150:ARG:HG3	2.14	0.46
54:1w:321:THR:OG1	54:1w:322:HIS:N	2.49	0.46
1:2A:1354:A:H2'	1:2A:1355:G:O4'	2.15	0.46
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.80	0.46
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.52	0.46
12:2Q:110:THR:HG23	12:2Q:113:GLN:NE2	2.30	0.46
32:2a:433:C:H2'	32:2a:434:U:C6	2.50	0.46
38:2g:115:ARG:HH11	38:2g:118:VAL:HG21	1.80	0.46
44:2m:105:THR:HG22	44:2m:106:ASN:H	1.80	0.46
48:2q:14:LYS:NZ	48:2q:53:LEU:HD11	2.30	0.46
55:2x:12:A:OP2	61:2x:201:HOH:O	2.20	0.46
1:1A:1041:C:H42	1:1A:1114:G:H1	1.64	0.46
1:1A:2189:U:H2'	1:1A:2190:G:C8	2.47	0.46
4:1E:175:VAL:O	4:1E:177:PRO:HD3	2.14	0.46
7:1H:3:ARG:HH22	7:1H:66:GLY:H	1.64	0.46
10:1O:64:ARG:NH1	10:1O:81:ASP:OD2	2.48	0.46
13:1R:56:LYS:HB3	13:1R:56:LYS:HE3	1.83	0.46
32:1a:60:A:H4'	32:1a:61:G:H5'	1.97	0.46
32:1a:438:G:O2'	32:1a:494:U:O4	2.32	0.46
32:1a:892:A:H2'	32:1a:893:C:C6	2.50	0.46
32:1a:1010:G:N2	32:1a:1020:U:H1'	2.31	0.46
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.16	0.46
32:1a:1023:G:H8	32:1a:1023:G:OP2	1.98	0.46
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.98	0.46
32:1a:1255:G:C2	32:1a:1283:G:C2	3.03	0.46
32:1a:1343:G:H4'	40:1i:122:ALA:HB3	1.97	0.46
36:1e:57:LYS:HG2	36:1e:61:TYR:HE2	1.80	0.46
37:1f:97:PHE:HD2	49:1r:31:LEU:HD12	1.80	0.46
38:1g:15:ASP:OD1	38:1g:19:GLY:N	2.48	0.46
1:2A:764:A:O4'	3:2D:213:ARG:HG3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.51	0.46
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.50	0.46
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.15	0.46
32:2a:625:G:H4'	47:2p:16:HIS:CG	2.51	0.46
34:2c:189:ALA:HB3	34:2c:196:LEU:HB2	1.97	0.46
44:2m:3:ARG:NH2	44:2m:9:ILE:O	2.42	0.46
47:2p:58:TYR:O	47:2p:61:SER:OG	2.21	0.46
1:1A:717:G:H2'	1:1A:718:A:O4'	2.15	0.46
1:1A:1364:G:N7	23:11:3:LYS:HD2	2.30	0.46
1:1A:2117:A:O2'	1:1A:2118:U:H5''	2.15	0.46
2:1B:66:A:H61	2:1B:108:U:H2'	1.80	0.46
8:1I:135:GLU:O	8:1I:137:PRO:HD3	2.15	0.46
12:1Q:1:MET:HE3	12:1Q:1:MET:HB2	1.90	0.46
26:14:59:PHE:CE2	50:1s:64:GLU:HB3	2.51	0.46
32:1a:189(F):U:O2	48:1q:63:ARG:NH2	2.48	0.46
32:1a:671:G:H5'	37:1f:77:ARG:HH21	1.80	0.46
32:1a:997:U:H3'	32:1a:998:G:C8	2.50	0.46
33:1b:42:ILE:HG21	33:1b:202:PRO:O	2.16	0.46
33:1b:223:ILE:H	33:1b:223:ILE:HG12	1.59	0.46
35:1d:138:TYR:HD2	35:1d:140:VAL:HG22	1.80	0.46
44:1m:23:TYR:HE2	44:1m:70:LEU:HB3	1.79	0.46
1:2A:658:C:H2'	1:2A:659:C:C6	2.49	0.46
1:2A:715:G:C4	46:2o:56:LEU:HD21	2.51	0.46
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.15	0.46
2:2B:54:G:H21	6:2G:29:TRP:NE1	2.11	0.46
5:2F:53:THR:HG22	5:2F:56:GLU:CD	2.41	0.46
10:2O:48:PRO:CB	32:2a:1422:G:H5''	2.44	0.46
14:2S:38:GLN:HG3	14:2S:40:ILE:HD11	1.98	0.46
18:2W:1:MET:HE2	18:2W:2:GLU:H	1.80	0.46
32:2a:715:A:H2'	32:2a:716:A:C8	2.51	0.46
33:2b:178:ARG:HH12	39:2h:68:ARG:HH22	1.62	0.46
36:2e:93:PRO:HG2	39:2h:105:ARG:NH1	2.30	0.46
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.96	0.46
54:2w:174:GLU:OE1	54:2w:303:ARG:NH1	2.43	0.46
1:1A:657:U:H2'	1:1A:658:C:C6	2.51	0.46
1:1A:668:G:H5'	1:1A:669:G:OP2	2.16	0.46
2:1B:55:U:H2'	2:1B:56:G:O4'	2.14	0.46
4:1E:170:LEU:HB3	4:1E:184:VAL:CG2	2.45	0.46
21:1Z:1:MET:HE1	21:1Z:133:ILE:O	2.15	0.46
32:1a:8:A:H5'	36:1e:101:ILE:HG22	1.97	0.46
32:1a:302:G:O2'	32:1a:556:C:H5''	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:79:PHE:CE1	35:1d:204:ILE:HD13	2.51	0.46
46:1o:9:GLN:NE2	46:1o:12:ILE:HD12	2.30	0.46
1:2A:2702:U:H4'	1:2A:2703:C:OP1	2.16	0.46
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.96	0.46
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.96	0.46
11:2P:138:LEU:HD23	11:2P:145:PRO:HB3	1.97	0.46
19:2X:44:GLU:O	19:2X:48:LYS:N	2.47	0.46
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.15	0.46
32:2a:435:C:H2'	32:2a:436:C:C6	2.51	0.46
32:2a:583:A:N6	32:2a:758:G:O2'	2.48	0.46
33:2b:93:VAL:HG21	33:2b:97:TRP:HD1	1.80	0.46
1:1A:61:G:OP1	24:12:51:ARG:NH2	2.49	0.46
1:1A:207:A:H2'	1:1A:208:C:O4'	2.15	0.46
1:1A:264:C:O2'	1:1A:265:A:H2'	2.16	0.46
1:1A:328:U:H4'	20:1Y:68:HIS:CG	2.51	0.46
1:1A:886:C:H2'	1:1A:887:A:H5''	1.98	0.46
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.29	0.46
14:1S:61:ASN:HD21	14:1S:63:THR:HB	1.80	0.46
32:1a:142:G:H2'	32:1a:143:A:H8	1.80	0.46
32:1a:334:C:H2'	32:1a:335:C:C6	2.51	0.46
32:1a:382:A:H2'	32:1a:383:A:H8	1.78	0.46
37:1f:38:GLU:OE1	37:1f:64:GLN:NE2	2.33	0.46
39:1h:86:ILE:HG21	39:1h:133:LEU:HD13	1.98	0.46
40:1i:11:LYS:C	40:1i:13:ALA:H	2.23	0.46
43:1l:27:LEU:HD23	43:1l:33:ARG:HB2	1.98	0.46
1:2A:981:A:N1	1:2A:2027:G:O2'	2.41	0.46
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.15	0.46
1:2A:2162:G:H2'	1:2A:2163:C:O4'	2.16	0.46
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.16	0.46
3:2D:96:HIS:NE2	3:2D:102:LYS:HE2	2.31	0.46
32:2a:297:G:O2'	32:2a:299:G:N7	2.47	0.46
32:2a:947:G:O3'	44:2m:109:THR:OG1	2.34	0.46
32:2a:1003:G:H4'	32:2a:1003:G:OP1	2.16	0.46
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.51	0.46
1:1A:272(H):C:H2'	1:1A:272(I):U:H6	1.80	0.46
1:1A:621:A:OP2	11:1P:108:LYS:NZ	2.46	0.46
1:1A:1176:G:H1'	1:1A:1177:A:H5''	1.97	0.46
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.51	0.46
1:1A:2116:G:H2'	1:1A:2117:A:C4	2.50	0.46
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.80	0.46
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:2:ARG:HD2	61:1R:310:HOH:O	2.15	0.46
28:16:14:THR:HG21	28:16:48:VAL:HG13	1.98	0.46
32:1a:224:C:OP1	51:1t:74:LYS:HE3	2.16	0.46
32:1a:718:G:H5'	42:1k:117:ASN:HB2	1.98	0.46
32:1a:865:A:H2	32:1a:918:A:H4'	1.80	0.46
32:1a:1226:C:OP2	44:1m:91:ARG:NH2	2.49	0.46
32:1a:1268:A:N3	32:1a:1326:C:O2'	2.45	0.46
40:1i:29:ASN:HD21	40:1i:65:VAL:HG12	1.80	0.46
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.40	0.46
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.14	0.46
1:2A:441:U:H2'	1:2A:442:G:C8	2.50	0.46
1:2A:1261:C:OP2	18:2W:83:LYS:NZ	2.35	0.46
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.51	0.46
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.30	0.46
1:2A:2508:G:OP1	54:2w:223:ARG:NH1	2.48	0.46
1:2A:2785:C:OP1	4:2E:41:LYS:HE3	2.16	0.46
2:2B:75:G:H22	21:2Z:73:GLN:HE22	1.64	0.46
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.32	0.46
32:2a:1250:A:O3'	40:2i:67:GLY:HA2	2.16	0.46
1:1A:321:G:O4'	5:1F:165:ARG:HD2	2.16	0.46
1:1A:848:G:O6	1:1A:928:G:H2'	2.16	0.46
1:1A:1071:G:N2	1:1A:1100:C:H42	2.14	0.46
1:1A:2818:G:O2'	1:1A:2819:G:H5'	2.16	0.46
6:1G:59:GLU:CD	6:1G:153:ARG:HH21	2.24	0.46
7:1H:113:VAL:HG11	7:1H:151:ILE:HD13	1.97	0.46
32:1a:448:A:P	32:1a:485:G:H22	2.38	0.46
32:1a:624:C:H5'	47:1p:11:SER:HB3	1.98	0.46
44:1m:50:GLU:HA	44:1m:53:VAL:HB	1.96	0.46
54:1w:336:LEU:HA	54:1w:339:LEU:HD12	1.98	0.46
55:1x:13:A:N6	61:1x:201:HOH:O	2.19	0.46
1:2A:218:A:C2	1:2A:235:U:H4'	2.50	0.46
1:2A:484:C:H2'	1:2A:485:C:C6	2.51	0.46
1:2A:900:A:H2'	1:2A:901:A:C8	2.49	0.46
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.15	0.46
1:2A:2206:G:H3'	1:2A:2207:G:N7	2.29	0.46
1:2A:2376:A:N6	14:2S:89:ARG:HD3	2.30	0.46
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.97	0.46
23:21:37:ILE:O	61:21:201:HOH:O	2.20	0.46
26:24:41:PRO:HG3	26:24:49:PHE:CE1	2.51	0.46
27:25:16:ARG:HG3	27:25:17:ASP:N	2.31	0.46
32:2a:16:A:O2'	36:2e:16:THR:HB	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1280:A:H5'	41:2j:40:LEU:HD22	1.98	0.46
32:2a:1358:U:H5''	45:2n:33:VAL:O	2.16	0.46
33:2b:60:ASP:O	33:2b:64:ARG:N	2.48	0.46
34:2c:180:ALA:HB1	34:2c:203:PHE:CE1	2.50	0.46
50:2s:44:MET:HB3	50:2s:62:ILE:HD13	1.97	0.46
54:2w:104:GLU:HA	54:2w:166:GLY:H	1.81	0.46
1:1A:773:U:H2'	1:1A:774:A:H5'	1.98	0.46
1:1A:996:A:H4'	16:1U:91:ASP:OD2	2.17	0.46
1:1A:1045:A:H1'	1:1A:1047:G:C4	2.52	0.46
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.97	0.46
7:1H:152:ARG:HD3	7:1H:152:ARG:HA	1.56	0.46
21:1Z:155:LEU:HD12	21:1Z:155:LEU:HA	1.85	0.46
32:1a:44:G:O6	61:1a:1915:HOH:O	2.20	0.46
32:1a:443:C:O2'	32:1a:444:C:H5'	2.15	0.46
32:1a:486:U:H2'	32:1a:487:A:H8	1.80	0.46
32:1a:1061:G:OP1	41:1j:59:SER:OG	2.22	0.46
32:1a:1317:C:H2'	32:1a:1318:A:O4'	2.16	0.46
34:1c:5:ILE:HG12	34:1c:6:HIS:H	1.80	0.46
34:1c:36:ASP:OD2	34:1c:57:ILE:HG13	2.16	0.46
35:1d:64:LEU:HB2	35:1d:198:VAL:HG11	1.98	0.46
50:1s:44:MET:HE1	50:1s:71:LEU:HD11	1.97	0.46
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.50	0.46
1:2A:2134:A:OP2	1:2A:2157:G:N2	2.49	0.46
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.49	0.46
1:2A:2788:C:O2'	1:2A:2809:A:N3	2.48	0.46
2:2B:14:U:OP2	2:2B:70:C:O2'	2.31	0.46
11:2P:94:GLU:HG3	11:2P:124:LYS:HD3	1.96	0.46
32:2a:114:U:H2'	32:2a:115:G:C8	2.51	0.46
33:2b:97:TRP:CZ3	33:2b:172:ILE:HB	2.51	0.46
35:2d:57:ARG:HB3	35:2d:206:PHE:HB2	1.98	0.46
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.98	0.46
40:2i:40:LEU:HD21	40:2i:70:LYS:HD2	1.98	0.46
1:1A:1210:A:H5''	1:1A:1212:G:O4'	2.16	0.45
1:1A:1745(A):C:H5'	1:1A:1746:G:OP2	2.16	0.45
1:1A:2302:G:N2	6:1G:126:ASP:OD1	2.43	0.45
2:1B:103:G:N2	21:1Z:73:GLN:HE22	2.07	0.45
24:12:2:LYS:HB2	24:12:5:GLU:HG3	1.98	0.45
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.16	0.45
41:1j:27:ALA:HA	41:1j:81:THR:HG21	1.97	0.45
54:1w:177:VAL:HG22	54:1w:198:THR:HG22	1.98	0.45
1:2A:265:A:C8	1:2A:266:G:H1'	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.49	0.45
1:2A:2592:G:OP2	61:2A:4847:HOH:O	2.21	0.45
6:2G:108:ASN:HA	26:24:37:SER:HB2	1.98	0.45
8:2I:38:LEU:HB2	8:2I:40:THR:HG22	1.98	0.45
33:2b:15:VAL:HG21	33:2b:213:LEU:HD22	1.98	0.45
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.81	0.45
36:2e:101:ILE:O	36:2e:120:THR:HB	2.17	0.45
1:1A:182:A:H2'	1:1A:183:C:O4'	2.15	0.45
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.31	0.45
3:1D:25:THR:HG21	3:1D:113:VAL:HG11	1.98	0.45
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.49	0.45
21:1Z:138:GLU:HB2	21:1Z:156:LYS:NZ	2.30	0.45
32:1a:300:A:H2'	32:1a:301:G:O4'	2.16	0.45
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.98	0.45
35:1d:68:TYR:OH	35:1d:98:GLU:OE1	2.19	0.45
35:1d:148:VAL:HG23	35:1d:181:MET:O	2.17	0.45
36:1e:53:LEU:H	36:1e:53:LEU:HD12	1.81	0.45
1:2A:479:A:N3	1:2A:481:G:H5''	2.31	0.45
1:2A:631:A:H2'	1:2A:632:A:O4'	2.15	0.45
1:2A:1651:G:H4'	13:2R:39:PRO:HG2	1.98	0.45
1:2A:1739:U:O2'	1:2A:1740:G:H8	1.99	0.45
12:2Q:109:VAL:HG22	12:2Q:113:GLN:NE2	2.32	0.45
25:23:26:LEU:HD21	25:23:46:ASN:HB2	1.98	0.45
32:2a:1203:C:H2'	32:2a:1204:A:O4'	2.16	0.45
32:2a:1265:G:C2	32:2a:1271:G:C2	3.04	0.45
32:2a:1359:C:H2'	32:2a:1361:G:OP2	2.16	0.45
37:2f:61:LEU:HB3	37:2f:63:TYR:CE2	2.51	0.45
1:1A:274:G:H2'	1:1A:275:G:H8	1.81	0.45
1:1A:606:U:H4'	1:1A:658:C:H4'	1.98	0.45
1:1A:857:C:N4	1:1A:858:U:O4	2.50	0.45
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.37	0.45
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.51	0.45
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.82	0.45
28:16:12:GLU:HB2	28:16:19:ARG:HG3	1.99	0.45
32:1a:110:C:H2'	32:1a:111:G:O4'	2.16	0.45
32:1a:396:G:O2'	32:1a:398:C:OP1	2.31	0.45
32:1a:865:A:C2	32:1a:918:A:H4'	2.52	0.45
32:1a:890:G:O2'	32:1a:906:G:O6	2.31	0.45
33:1b:56:ARG:HB2	33:1b:56:ARG:NH1	2.32	0.45
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.99	0.45
1:2A:295:G:O5'	20:2Y:1:MET:HE3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1683:C:H2'	1:2A:1684:C:C6	2.51	0.45
1:2A:2845:G:H5''	15:2T:54:ARG:O	2.16	0.45
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	1.98	0.45
25:23:59:VAL:HG12	25:23:60:GLU:H	1.81	0.45
32:2a:1121:U:O2'	32:2a:1122:U:H5'	2.16	0.45
32:2a:1256:A:N6	32:2a:1278:U:H1'	2.31	0.45
32:2a:1403:C:C2	32:2a:1404:5MC:HM52	2.50	0.45
36:2e:78:HIS:NE2	36:2e:142:LEU:HA	2.31	0.45
48:2q:41:LYS:HZ2	48:2q:92:ARG:HH21	1.65	0.45
1:1A:1068:G:C8	1:1A:1096:A:H1'	2.52	0.45
1:1A:1800:C:OP2	3:1D:183:ARG:NH2	2.50	0.45
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.81	0.45
3:1D:68:LYS:HB2	3:1D:70:TRP:CE2	2.52	0.45
21:1Z:79:ARG:HD2	21:1Z:80:ARG:NH1	2.32	0.45
32:1a:159:G:C3'	32:1a:160:A:H5''	2.47	0.45
32:1a:674:G:H2'	32:1a:675:A:C8	2.51	0.45
32:1a:763:G:H2'	32:1a:764:C:C6	2.51	0.45
32:1a:877:C:OP1	39:1h:88:LYS:NZ	2.25	0.45
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.52	0.45
41:1j:5:ARG:HG3	41:1j:73:ASP:OD1	2.17	0.45
1:2A:995:C:O2	9:2N:3:THR:OG1	2.32	0.45
1:2A:1204:A:H2	1:2A:1241:A:N6	2.07	0.45
5:2F:11:VAL:HG21	5:2F:20:LEU:HB2	1.99	0.45
10:2O:53:LYS:HG2	10:2O:56:ASP:OD2	2.16	0.45
32:2a:406:G:O3'	35:2d:3:ARG:NH2	2.48	0.45
32:2a:539:A:H2'	32:2a:540:G:C8	2.52	0.45
32:2a:656:C:HO2'	46:2o:28:GLN:CD	2.22	0.45
32:2a:1212:U:H4'	32:2a:1213:A:C8	2.52	0.45
32:2a:1313:U:OP1	50:2s:5:LEU:HB2	2.16	0.45
33:2b:100:GLY:O	33:2b:108:ILE:HG13	2.16	0.45
34:2c:70:VAL:HG12	34:2c:72:LYS:H	1.81	0.45
34:2c:82:GLU:HA	34:2c:85:ARG:NH1	2.31	0.45
41:2j:8:LEU:HG	41:2j:70:ARG:HB2	1.98	0.45
55:2x:12:A:H2'	55:2x:13:A:O4'	2.16	0.45
1:1A:1014:U:OP2	61:1A:4215:HOH:O	2.20	0.45
1:1A:2557:G:H2'	1:1A:2558:C:C6	2.51	0.45
1:1A:2678:C:H2'	1:1A:2679:A:O4'	2.16	0.45
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.17	0.45
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.52	0.45
7:1H:96:ALA:HB2	7:1H:105:LEU:HD23	1.98	0.45
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:235:C:H2'	32:1a:236:G:H8	1.81	0.45
54:1w:125:ARG:HB2	54:1w:154:GLY:HA2	1.97	0.45
1:2A:807:U:O2'	1:2A:2060:A:N1	2.43	0.45
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.32	0.45
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.52	0.45
19:2X:94:GLY:H	19:2X:95:LEU:C	2.25	0.45
32:2a:148:G:H2'	32:2a:149:A:C8	2.50	0.45
32:2a:1221:G:OP1	32:2a:1320:C:N4	2.48	0.45
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.16	0.45
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.17	0.45
39:2h:20:TYR:CE1	39:2h:76:PRO:HG2	2.52	0.45
51:2t:43:LEU:HD12	51:2t:55:ILE:HG13	1.99	0.45
51:2t:54:LYS:HE2	51:2t:54:LYS:HB3	1.70	0.45
54:2w:171:PHE:O	54:2w:201:VAL:HG21	2.16	0.45
1:1A:614(C):A:C4	5:1F:180:GLY:HA2	2.52	0.45
1:1A:1268:A:C2	1:1A:2013:A:C4	3.05	0.45
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.29	0.45
4:1E:27:LEU:HD12	4:1E:180:ASN:O	2.16	0.45
24:12:51:ARG:O	24:12:55:ARG:HG2	2.17	0.45
32:1a:997:U:H3'	32:1a:998:G:H8	1.81	0.45
32:1a:1169:A:H2'	32:1a:1170:A:C8	2.52	0.45
32:1a:1218:C:OP2	45:1n:9:LYS:NZ	2.48	0.45
32:1a:1456:G:N2	51:1t:43:LEU:HD11	2.32	0.45
36:1e:68:GLU:HG3	36:1e:70:PRO:HD3	1.98	0.45
45:1n:37:PHE:HB3	45:1n:39:LEU:HD12	1.98	0.45
45:1n:58:LYS:HE2	45:1n:58:LYS:HB3	1.63	0.45
48:1q:20:THR:HG21	48:1q:41:LYS:HD2	1.98	0.45
53:1v:22:U:H6	53:1v:22:U:H2'	1.56	0.45
1:2A:359:A:H2'	1:2A:360:G:O4'	2.17	0.45
1:2A:699:A:H2'	1:2A:700:G:O4'	2.17	0.45
1:2A:1815:A:H8	1:2A:1815:A:OP1	1.99	0.45
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.49	0.45
5:2F:34:TRP:CZ3	11:2P:8:PRO:HB3	2.52	0.45
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.35	0.45
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.17	0.45
13:2R:9:LYS:O	13:2R:17:ARG:HD3	2.17	0.45
26:24:24:THR:OG1	26:24:25:TYR:N	2.49	0.45
32:2a:598:U:H4'	39:2h:94:TYR:CD2	2.51	0.45
32:2a:815:A:N7	32:2a:1509:C:O2'	2.43	0.45
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.16	0.45
34:2c:37:GLN:HE22	45:2n:52:GLN:HB3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:91:ARG:HB2	44:2m:98:VAL:HG13	1.97	0.45
1:1A:251:A:C5	1:1A:252:G:H1'	2.51	0.45
1:1A:879:G:H2'	1:1A:880:G:H8	1.82	0.45
1:1A:954:G:H5''	12:1Q:13:GLN:HB3	1.99	0.45
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.51	0.45
1:1A:2785:C:OP1	4:1E:41:LYS:HE3	2.17	0.45
1:1A:2790:A:H2'	1:1A:2790:A:N3	2.32	0.45
15:1T:41:ARG:HH22	32:1a:346:G:P	2.37	0.45
21:1Z:1:MET:N	21:1Z:2:GLU:HA	2.32	0.45
21:1Z:146:ILE:N	21:1Z:147:GLY:HA2	2.31	0.45
32:1a:67:C:H2'	32:1a:68:G:C8	2.51	0.45
32:1a:192:U:H2'	32:1a:193:C:H6	1.82	0.45
32:1a:826:C:H2'	32:1a:827:U:C6	2.52	0.45
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.17	0.45
35:1d:20:TYR:CD1	35:1d:26:CYS:HB3	2.45	0.45
36:1e:31:LEU:HD11	36:1e:129:ILE:HA	1.98	0.45
40:1i:53:VAL:C	40:1i:55:ALA:H	2.20	0.45
45:1n:4:LYS:O	45:1n:7:ILE:HG22	2.16	0.45
50:1s:70:LYS:N	50:1s:73:GLU:OE1	2.50	0.45
1:2A:529:A:H62	1:2A:2041:U:H3	1.65	0.45
9:2N:61:ARG:HD3	9:2N:61:ARG:HA	1.77	0.45
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.99	0.45
21:2Z:95:PRO:HA	21:2Z:129:SER:HA	1.98	0.45
32:2a:90:U:H2'	32:2a:91:C:C6	2.52	0.45
54:2w:281:GLU:O	54:2w:285:LEU:HD12	2.16	0.45
1:1A:27:G:N2	1:1A:512:G:H1'	2.32	0.45
1:1A:479:A:N3	1:1A:481:G:H5''	2.31	0.45
1:1A:709:U:H2'	1:1A:710:G:C8	2.52	0.45
1:1A:1026:U:OP1	61:1A:4218:HOH:O	2.21	0.45
1:1A:1054:A:H2'	1:1A:1055:G:H8	1.82	0.45
1:1A:1426:G:N7	3:1D:31:LYS:NZ	2.57	0.45
11:1P:46:LYS:HE3	11:1P:46:LYS:HB3	1.73	0.45
21:1Z:93:ASP:CB	21:1Z:131:ARG:HH22	2.29	0.45
23:11:67:ILE:N	23:11:68:PRO:HD2	2.31	0.45
32:1a:828:A:H2'	32:1a:829:G:O4'	2.16	0.45
32:1a:1438:G:H2'	32:1a:1439:C:C6	2.52	0.45
40:1i:89:ASN:HD22	40:1i:89:ASN:N	2.15	0.45
1:2A:1263:U:C4	1:2A:1264:G:C6	3.04	0.45
4:2E:5:LEU:HD21	4:2E:79:ARG:HB2	1.98	0.45
9:2N:38:HIS:NE2	9:2N:50:ASP:OD2	2.34	0.45
11:2P:92:GLU:OE2	11:2P:121:LYS:NZ	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:2:PHE:CZ	17:2V:41:GLY:HA3	2.52	0.45
32:2a:713:G:H2'	32:2a:714:G:C8	2.52	0.45
32:2a:737:A:H5'	37:2f:90:VAL:O	2.16	0.45
32:2a:922:G:H1'	36:2e:19:MET:HB2	1.99	0.45
32:2a:1047:G:H5''	45:2n:4:LYS:HD2	1.99	0.45
32:2a:1101:A:H4'	32:2a:1102:A:O5'	2.17	0.45
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.52	0.45
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.17	0.45
41:2j:17:ASP:CG	41:2j:70:ARG:HH21	2.25	0.45
44:2m:95:GLY:O	44:2m:110:ARG:HG3	2.17	0.45
1:1A:324:A:H2'	1:1A:325:G:O4'	2.17	0.45
1:1A:414:C:H2'	1:1A:415:A:C8	2.52	0.45
1:1A:839:U:H2'	1:1A:840:C:C6	2.52	0.45
1:1A:1082:U:C4	1:1A:1086:A:C6	3.03	0.45
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.17	0.45
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.52	0.45
1:1A:2131:G:H5'	1:1A:2133:G:O4'	2.17	0.45
1:1A:2464:C:H1'	61:1A:5568:HOH:O	2.16	0.45
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.52	0.45
13:1R:98:LEU:HB2	13:1R:113:LEU:HD11	1.99	0.45
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.52	0.45
21:1Z:16:SER:HB2	21:1Z:20:ARG:HH21	1.82	0.45
32:1a:115:G:H4'	32:1a:116:A:O5'	2.16	0.45
32:1a:192:U:H2'	32:1a:193:C:C6	2.51	0.45
32:1a:583:A:H2'	32:1a:584:G:O4'	2.17	0.45
32:1a:1264:C:H2'	32:1a:1265:G:H8	1.81	0.45
34:1c:116:VAL:O	34:1c:120:VAL:HG23	2.17	0.45
35:1d:19:LEU:HD21	35:1d:63:LYS:HG3	1.98	0.45
41:1j:81:THR:C	41:1j:83:GLU:N	2.75	0.45
43:1l:82:VAL:O	43:1l:106:ASP:HB2	2.17	0.45
54:1w:280:GLU:CD	54:1w:284:ARG:HE	2.25	0.45
1:2A:686:G:H21	1:2A:788:A:H61	1.65	0.45
3:2D:141:VAL:HG13	3:2D:162:SER:HB2	1.99	0.45
4:2E:170:LEU:HB3	4:2E:184:VAL:HG22	1.99	0.45
32:2a:743:U:H2'	32:2a:744:C:C6	2.52	0.45
32:2a:954:G:H2'	32:2a:955:U:C6	2.52	0.45
32:2a:1126:U:O4	41:2j:71:LEU:HD13	2.17	0.45
32:2a:1390:U:H2'	32:2a:1391:U:C6	2.52	0.45
34:2c:134:ILE:HD11	34:2c:153:VAL:HG12	1.98	0.45
38:2g:47:CYS:O	38:2g:50:ILE:HG22	2.17	0.45
39:2h:51:VAL:HG12	39:2h:52:ASP:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:73:GLU:O	44:2m:77:ASN:HB2	2.17	0.45
1:1A:93:G:H2'	1:1A:94:C:C6	2.52	0.45
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.16	0.45
1:1A:2115:G:H1'	1:1A:2171:A:H61	1.82	0.45
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.80	0.45
61:1A:4339:HOH:O	19:1X:40:LYS:HE2	2.17	0.45
6:1G:5:VAL:HG12	6:1G:104:GLU:OE1	2.18	0.45
13:1R:59:ASP:OD1	13:1R:59:ASP:N	2.43	0.45
21:1Z:46:LYS:HB3	21:1Z:46:LYS:HE2	1.83	0.45
32:1a:414:A:H2'	32:1a:415:A:C8	2.48	0.45
32:1a:508:C:OP1	35:1d:209:ARG:NH2	2.50	0.45
32:1a:1143:G:H2'	32:1a:1144:G:H8	1.82	0.45
34:1c:22:TRP:HB3	34:1c:59:ARG:HB2	1.99	0.45
50:1s:39:THR:HA	50:1s:70:LYS:HD3	1.99	0.45
1:2A:1026:U:H4'	1:2A:1027:A:OP1	2.15	0.45
1:2A:2062:A:H2	56:2z:5:ALA:HB1	1.82	0.45
1:2A:2740:A:C6	1:2A:2764:A:C8	3.05	0.45
14:2S:41:ASP:HB3	14:2S:46:VAL:HG23	1.99	0.45
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	1.99	0.45
26:24:64:GLY:O	26:24:66:SER:N	2.45	0.45
32:2a:649:G:H2'	32:2a:650:G:O4'	2.17	0.45
32:2a:1244:C:H2'	32:2a:1245:A:C8	2.51	0.45
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.52	0.45
35:2d:196:LEU:H	35:2d:196:LEU:HD12	1.82	0.45
38:2g:27:ILE:HA	38:2g:30:ILE:HD12	1.99	0.45
40:2i:8:GLY:O	40:2i:14:VAL:HA	2.17	0.45
1:1A:236:C:H2'	1:1A:237:C:H6	1.82	0.44
1:1A:581:C:H2'	1:1A:582:G:C8	2.52	0.44
1:1A:1339:G:H5''	19:1X:16:LYS:HD3	1.99	0.44
12:1Q:12:GLN:NE2	12:1Q:72:LYS:HG3	2.32	0.44
16:1U:18:LEU:HD23	16:1U:18:LEU:HA	1.82	0.44
32:1a:453:A:N6	32:1a:480:U:O2	2.50	0.44
32:1a:748:C:H4'	32:1a:749:C:O5'	2.17	0.44
32:1a:1368:G:OP1	40:1i:111:ARG:NH2	2.50	0.44
33:1b:164:VAL:O	33:1b:186:ALA:HA	2.17	0.44
34:1c:64:VAL:O	34:1c:99:VAL:HA	2.16	0.44
36:1e:100:VAL:O	36:1e:107:ARG:NH2	2.50	0.44
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.51	0.44
54:1w:349:ALA:HA	54:1w:350:ALA:HA	1.69	0.44
1:2A:373:U:H2'	1:2A:374:A:H8	1.83	0.44
1:2A:614(C):A:C4	5:2F:180:GLY:HA2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:910:A:N1	1:2A:2277:G:H1'	2.31	0.44
1:2A:911:A:N6	12:2Q:11:LYS:O	2.44	0.44
1:2A:1509(B):A:H2'	1:2A:1510:G:H8	1.83	0.44
1:2A:1547:C:H2'	1:2A:1548:C:H6	1.82	0.44
12:2Q:18:LYS:HE3	12:2Q:18:LYS:HB2	1.85	0.44
32:2a:381:C:H2'	32:2a:382:A:O4'	2.17	0.44
35:2d:10:ARG:HB2	35:2d:40:PRO:HG3	1.98	0.44
35:2d:39:PRO:O	35:2d:44:GLY:HA3	2.17	0.44
48:2q:41:LYS:NZ	48:2q:92:ARG:HH21	2.15	0.44
1:1A:1071:G:H22	1:1A:1100:C:H42	1.65	0.44
1:1A:1882:C:H2'	1:1A:1883:G:O4'	2.16	0.44
1:1A:2506:U:O4	56:1z:4:ALA:HB3	2.16	0.44
5:1F:14:PRO:C	5:1F:16:GLY:H	2.25	0.44
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.52	0.44
32:1a:864:A:H2'	32:1a:865:A:C8	2.52	0.44
32:1a:1131:G:H2'	32:1a:1132:C:H6	1.82	0.44
32:1a:1149:C:H2'	32:1a:1150:U:O4'	2.17	0.44
33:1b:48:MET:HA	33:1b:51:LEU:HD12	1.98	0.44
37:1f:25:ILE:O	37:1f:29:ALA:N	2.50	0.44
47:1p:39:TYR:CD1	47:1p:49:LEU:HD12	2.53	0.44
48:1q:10:VAL:HA	48:1q:20:THR:O	2.17	0.44
1:2A:1426:G:N7	3:2D:31:LYS:NZ	2.58	0.44
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.97	0.44
4:2E:52:LEU:HB3	4:2E:76:ARG:HD3	1.99	0.44
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.52	0.44
21:2Z:45:ASP:O	21:2Z:49:ARG:HG2	2.17	0.44
26:24:58:ARG:NE	50:2s:68:GLY:H	2.13	0.44
31:29:18:ARG:NH1	31:29:21:GLY:HA2	2.33	0.44
32:2a:189(A):C:H2'	32:2a:189(B):C:C6	2.52	0.44
32:2a:203:U:H2'	32:2a:203:U:OP2	2.17	0.44
32:2a:737:A:H2'	32:2a:738:C:C6	2.52	0.44
32:2a:1092:A:H5''	38:2g:4:ARG:CZ	2.47	0.44
32:2a:1239:A:H4'	32:2a:1240:U:C5'	2.47	0.44
32:2a:1327:C:H2'	32:2a:1328:C:H6	1.82	0.44
37:2f:26:ILE:O	37:2f:30:LEU:HG	2.17	0.44
41:2j:49:VAL:O	41:2j:60:ARG:HB3	2.17	0.44
1:1A:1067:A:H2'	1:1A:1068:G:H5'	1.99	0.44
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.52	0.44
1:1A:2706:G:N7	61:1A:4327:HOH:O	2.36	0.44
5:1F:196:LEU:HD23	5:1F:196:LEU:HA	1.79	0.44
6:1G:82:LEU:HD12	6:1G:86:MET:SD	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:57:ARG:HA	8:1I:60:GLU:HB3	2.00	0.44
14:1S:25:ARG:HD3	14:1S:42:ASP:OD1	2.18	0.44
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.52	0.44
24:12:3:LEU:HA	24:12:3:LEU:HD23	1.84	0.44
32:1a:389:A:C5	32:1a:390:C:H1'	2.52	0.44
34:1c:104:GLN:NE2	34:1c:104:GLN:HA	2.32	0.44
35:1d:61:LYS:HD2	35:1d:207:TYR:OH	2.18	0.44
44:1m:78:ILE:HG22	44:1m:92:HIS:CE1	2.52	0.44
54:1w:299:SER:C	54:1w:301:LYS:N	2.72	0.44
1:2A:103:A:H4'	24:22:3:LEU:HD11	1.99	0.44
1:2A:224:G:H2'	1:2A:225:A:O4'	2.18	0.44
1:2A:586:A:H5'	5:2F:89:VAL:HG21	2.00	0.44
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.51	0.44
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.82	0.44
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.33	0.44
1:2A:2748:A:H2'	1:2A:2749:A:O4'	2.16	0.44
2:2B:58:A:H2'	2:2B:59:A:O4'	2.17	0.44
32:2a:601:C:H2'	32:2a:602:A:H8	1.82	0.44
32:2a:1014:A:H2	32:2a:1219:U:H1'	1.82	0.44
32:2a:1186:G:H21	45:2n:61:TRP:C	2.26	0.44
32:2a:1264:C:O2	32:2a:1272:G:N7	2.50	0.44
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.86	0.44
33:2b:184:VAL:HG13	33:2b:198:ASP:H	1.82	0.44
36:2e:116:THR:HG23	36:2e:117:ASP:OD2	2.17	0.44
38:2g:152:ALA:O	38:2g:155:ARG:HD3	2.17	0.44
1:1A:428:A:H8	1:1A:428:A:OP2	2.01	0.44
1:1A:1056:G:C5'	1:1A:1086:A:H8	2.30	0.44
1:1A:1425:G:H2'	1:1A:1426:G:C8	2.52	0.44
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.17	0.44
1:1A:2090:G:N2	23:11:45:ASN:OD1	2.34	0.44
2:1B:2:C:H2'	2:1B:3:C:C6	2.53	0.44
9:1N:21:LYS:NZ	9:1N:140:VAL:HG23	2.32	0.44
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.18	0.44
32:1a:881:G:OP2	43:1l:12:ARG:NH2	2.51	0.44
32:1a:1053:G:N7	32:1a:1200:C:H5''	2.33	0.44
32:1a:1279:A:H5'	41:1j:7:LYS:NZ	2.32	0.44
32:1a:1370:G:C2	32:1a:1371:G:C8	3.06	0.44
33:1b:28:PHE:CD2	33:1b:190:THR:HA	2.52	0.44
35:1d:110:PHE:N	35:1d:110:PHE:CD1	2.85	0.44
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.52	0.44
46:1o:4:THR:HG1	46:1o:7:GLU:HG3	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:151:ASP:OD1	54:1w:151:ASP:N	2.33	0.44
1:2A:297:C:H2'	1:2A:298:G:O4'	2.18	0.44
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.31	0.44
1:2A:2145:C:O2'	1:2A:2147:G:N7	2.40	0.44
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.53	0.44
4:2E:1:MET:HE1	4:2E:199:ARG:HB3	1.99	0.44
6:2G:145:THR:HG22	6:2G:147:ASP:H	1.81	0.44
16:2U:86:ALA:HB2	16:2U:116:ALA:HB2	1.99	0.44
26:24:1:MET:HE2	26:24:6:HIS:CD2	2.53	0.44
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.50	0.44
32:2a:1145:C:H4'	32:2a:1146:A:H5'	1.98	0.44
32:2a:1216:G:H5''	45:2n:5:ALA:CB	2.47	0.44
32:2a:1267:C:O2	52:2u:20:LYS:HE3	2.18	0.44
34:2c:125:GLU:HA	34:2c:191:THR:HG22	1.99	0.44
38:2g:49:ILE:HA	38:2g:52:GLU:HB2	2.00	0.44
41:2j:5:ARG:HA	41:2j:73:ASP:OD1	2.17	0.44
43:2l:86:ARG:HG3	43:2l:87:GLY:O	2.17	0.44
47:2p:76:GLN:C	47:2p:78:GLY:H	2.25	0.44
1:1A:95:G:O2'	24:12:48:HIS:ND1	2.35	0.44
1:1A:1540:U:H2'	1:1A:1541:G:O4'	2.17	0.44
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.17	0.44
28:16:11:LEU:HD23	28:16:11:LEU:HA	1.80	0.44
32:1a:1243:C:C2	32:1a:1295:G:N2	2.86	0.44
32:1a:1287:A:H2'	32:1a:1288:A:C8	2.52	0.44
32:1a:1288:A:H2'	32:1a:1289:A:C8	2.52	0.44
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.18	0.44
33:1b:60:ASP:OD1	33:1b:64:ARG:NH2	2.42	0.44
39:1h:55:GLY:O	39:1h:56:LYS:HD3	2.17	0.44
43:1l:53:ARG:CB	43:1l:93:LEU:HD11	2.48	0.44
54:1w:119:GLU:HA	54:1w:122:LEU:HD12	1.98	0.44
1:2A:323:G:H1'	1:2A:1205:U:O2	2.17	0.44
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.52	0.44
1:2A:2745:C:H2'	1:2A:2746:U:O4'	2.17	0.44
5:2F:148:LEU:HD13	5:2F:154:VAL:HG21	2.00	0.44
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.17	0.44
14:2S:34:HIS:C	14:2S:35:ILE:HG13	2.43	0.44
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.82	0.44
32:2a:985:C:H2'	32:2a:986:A:C8	2.52	0.44
32:2a:1034:G:C6	32:2a:1035:A:H1'	2.53	0.44
34:2c:114:PRO:HA	34:2c:185:GLY:HA3	1.99	0.44
39:2h:121:ASP:HB2	39:2h:125:ARG:NH2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:2l:70:ILE:HG12	43:2l:100:ILE:HG13	1.99	0.44
54:2w:324:LEU:HA	54:2w:327:VAL:HG22	1.99	0.44
1:1A:646:A:H2'	1:1A:647:G:O4'	2.18	0.44
1:1A:862:G:H2'	1:1A:863:A:O4'	2.17	0.44
1:1A:1645:G:H5''	1:1A:1646:C:H5'	1.99	0.44
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.52	0.44
11:1P:52:GLU:HB3	11:1P:55:ARG:NH1	2.33	0.44
32:1a:401:C:H2'	32:1a:402:G:C8	2.52	0.44
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.53	0.44
32:1a:1479:C:H2'	32:1a:1480:G:C8	2.53	0.44
33:1b:132:LYS:O	33:1b:136:VAL:HG13	2.18	0.44
34:1c:91:LEU:HD22	34:1c:101:LEU:HD12	1.99	0.44
44:1m:45:VAL:HA	44:1m:48:LEU:HD11	2.00	0.44
51:1t:49:ALA:HA	51:1t:92:LEU:HD22	1.99	0.44
54:1w:319:PHE:CE2	54:1w:335:ILE:HG12	2.52	0.44
55:1x:8:4SU:O2'	55:1x:46:A:N3	2.45	0.44
1:2A:656:G:H2'	1:2A:657:U:O4'	2.17	0.44
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.32	0.44
1:2A:2103:C:H2'	1:2A:2104:G:O4'	2.18	0.44
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.53	0.44
7:2H:75:ALA:O	7:2H:78:GLY:N	2.51	0.44
21:2Z:44:PHE:O	21:2Z:47:VAL:HG23	2.17	0.44
32:2a:266:G:N3	32:2a:266:G:H2'	2.32	0.44
32:2a:966:M2G:HM22	55:2x:34:G:H5'	2.00	0.44
32:2a:1452:C:H5'	32:2a:1457:G:C4	2.53	0.44
38:2g:69:VAL:HG11	38:2g:104:LEU:HD21	2.00	0.44
40:2i:96:LEU:HD22	40:2i:101:PHE:CD2	2.52	0.44
43:2l:79:GLU:HG2	43:2l:80:HIS:CD2	2.52	0.44
52:2u:9:ARG:HD2	52:2u:13:ILE:HD11	1.99	0.44
54:2w:128:PHE:CZ	54:2w:132:LEU:HD11	2.53	0.44
1:1A:336:C:O2'	20:1Y:35:TYR:OH	2.33	0.44
1:1A:1429:G:H2'	1:1A:1430:C:H6	1.83	0.44
1:1A:1720:U:H2'	1:1A:1721:G:O4'	2.18	0.44
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.17	0.44
1:1A:2319:G:C2	14:1S:3:ARG:HA	2.52	0.44
9:1N:1:MET:HE3	9:1N:1:MET:HB2	1.89	0.44
11:1P:8:PRO:HB2	11:1P:12:ALA:HB3	2.00	0.44
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.25	0.44
15:1T:126:ALA:O	15:1T:129:ARG:HB2	2.17	0.44
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.52	0.44
16:1U:85:LYS:HB3	16:1U:85:LYS:HE2	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:96:U:H2'	32:1a:97:G:H8	1.82	0.44
33:1b:47:THR:O	33:1b:51:LEU:N	2.44	0.44
33:1b:127:ILE:HG22	33:1b:130:ARG:N	2.32	0.44
34:1c:181:ASN:ND2	34:1c:204:LEU:HB2	2.33	0.44
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.99	0.44
42:1k:21:ILE:HB	42:1k:84:VAL:HG12	2.00	0.44
1:2A:644:A:H4'	1:2A:645:C:C4	2.53	0.44
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.53	0.44
1:2A:2303:G:O2'	6:2G:132:ASN:HB2	2.18	0.44
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.81	0.44
1:2A:2882:A:H5'	13:2R:96:ARG:HG3	2.00	0.44
6:2G:179:PRO:HB2	26:24:42:PHE:HE2	1.82	0.44
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.33	0.44
32:2a:595:G:O2'	32:2a:641:U:O4	2.29	0.44
33:2b:122:PHE:HD2	33:2b:142:LEU:HD13	1.83	0.44
37:2f:9:VAL:HA	37:2f:59:TYR:O	2.16	0.44
48:2q:10:VAL:HG13	48:2q:19:VAL:HB	2.00	0.44
51:2t:72:LEU:HD23	51:2t:72:LEU:HA	1.90	0.44
54:2w:150:THR:HB	54:2w:154:GLY:H	1.81	0.44
1:1A:586:A:N1	1:1A:809:G:O2'	2.46	0.44
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.17	0.44
1:1A:1954:G:N3	1:1A:2551:C:H5''	2.33	0.44
1:1A:2439:A:N6	55:1x:76:8AN:O1P	2.51	0.44
1:1A:2504:U:O5'	1:1A:2504:U:H6	2.00	0.44
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.43	0.44
11:1P:126:VAL:HG12	11:1P:148:LEU:HD13	1.99	0.44
32:1a:735:C:H2'	32:1a:736:C:H6	1.81	0.44
32:1a:1095:U:P	32:1a:1108:G:H1	2.41	0.44
41:1j:55:LYS:HE3	41:1j:56:HIS:CE1	2.52	0.44
1:2A:280:C:H2'	1:2A:281:G:O4'	2.17	0.44
1:2A:320:A:H4'	1:2A:322:A:C8	2.53	0.44
1:2A:862:G:H2'	1:2A:863:A:O4'	2.17	0.44
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.32	0.44
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.18	0.44
1:2A:1426:G:O2'	1:2A:1572:A:N6	2.45	0.44
1:2A:2053:G:OP1	4:2E:144:ARG:HG3	2.18	0.44
1:2A:2136:C:O2'	1:2A:2137:C:O4'	2.35	0.44
1:2A:2469:A:O2'	12:2Q:56:ARG:NE	2.41	0.44
2:2B:17:C:H2'	2:2B:18:G:O4'	2.17	0.44
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.38	0.44
32:2a:714:G:H2'	32:2a:715:A:C8	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:76:GLN:CD	33:2b:76:GLN:H	2.26	0.44
33:2b:174:VAL:O	33:2b:178:ARG:HG3	2.17	0.44
38:2g:75:VAL:HA	38:2g:87:VAL:O	2.18	0.44
38:2g:114:ARG:HB2	38:2g:115:ARG:NH2	2.33	0.44
1:1A:460:A:OP1	29:17:41:ARG:NH2	2.49	0.44
1:1A:1017:G:N7	61:1A:4324:HOH:O	2.36	0.44
1:1A:1359:A:C2	1:1A:1372:U:O4	2.71	0.44
61:1A:4759:HOH:O	5:1F:70:THR:HG23	2.17	0.44
6:1G:148:MET:H	6:1G:148:MET:HG3	1.45	0.44
32:1a:165:C:H2'	32:1a:166:G:C8	2.53	0.44
32:1a:243:A:C2	32:1a:246:A:C8	3.06	0.44
32:1a:523:A:H61	43:1l:92:OTD:CG	2.30	0.44
34:1c:134:ILE:HG22	34:1c:168:ALA:HB3	2.00	0.44
1:2A:42:G:H2'	1:2A:43:A:O4'	2.18	0.44
1:2A:336:C:HO2'	20:2Y:35:TYR:HH	1.57	0.44
1:2A:2171:A:N3	1:2A:2172:U:N3	2.65	0.44
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.18	0.44
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.53	0.44
7:2H:140:LYS:HB2	7:2H:140:LYS:HE3	1.77	0.44
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.81	0.44
20:2Y:5:MET:HE2	20:2Y:5:MET:HB2	1.80	0.44
26:24:64:GLY:C	26:24:66:SER:H	2.26	0.44
32:2a:298:A:C6	32:2a:299:G:C2	3.06	0.44
32:2a:490:G:H2'	32:2a:491:G:C8	2.52	0.44
32:2a:684:A:H1'	42:2k:38:ASN:HB3	2.00	0.44
33:2b:122:PHE:CD2	33:2b:142:LEU:HD13	2.53	0.44
33:2b:145:LEU:O	33:2b:149:LEU:HB2	2.17	0.44
35:2d:191:ARG:NH2	35:2d:200:GLU:OE1	2.50	0.44
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.53	0.43
32:1a:767:A:H2'	32:1a:768:A:O4'	2.19	0.43
32:1a:1005:A:H5''	32:1a:1006:C:C5	2.53	0.43
34:1c:164:ARG:HG2	34:1c:165:THR:N	2.33	0.43
44:1m:84:ILE:HG13	44:1m:86:CYS:H	1.82	0.43
54:1w:141:GLU:HG2	54:1w:163:ARG:HE	1.83	0.43
1:2A:330:A:H2	1:2A:1210:A:H2'	1.83	0.43
1:2A:483:A:O4'	20:2Y:48:ALA:HB1	2.18	0.43
1:2A:824:A:H1'	1:2A:2358:G:N7	2.33	0.43
1:2A:1973:G:OP2	61:2A:4848:HOH:O	2.21	0.43
1:2A:2117:A:O2'	1:2A:2118:U:H5''	2.18	0.43
4:2E:89:ASP:OD1	4:2E:89:ASP:N	2.40	0.43
5:2F:32:LEU:HD22	5:2F:112:MET:HE1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:34:HIS:ND1	14:2S:53:SER:OG	2.49	0.43
17:2V:24:LYS:HA	17:2V:92:THR:OG1	2.18	0.43
32:2a:22:G:H4'	32:2a:885:G:C8	2.53	0.43
32:2a:399:G:H2'	32:2a:400:C:C6	2.53	0.43
32:2a:526:C:C4	32:2a:527:G7M:H1'	2.53	0.43
32:2a:990:C:H2'	32:2a:991:U:O4'	2.18	0.43
32:2a:1469:G:H2'	32:2a:1470:G:H8	1.83	0.43
33:2b:16:HIS:CD2	33:2b:18:GLY:H	2.36	0.43
37:2f:96:PRO:HB3	49:2r:30:ASP:OD2	2.18	0.43
44:2m:14:ARG:NH2	44:2m:41:PRO:HB2	2.33	0.43
51:2t:98:PRO:O	51:2t:100:ILE:N	2.46	0.43
1:1A:35:G:H2'	1:1A:36:G:O4'	2.19	0.43
1:1A:359:A:H2'	1:1A:360:G:O4'	2.18	0.43
1:1A:1056:G:H4'	1:1A:1086:A:H8	1.82	0.43
1:1A:2336:A:H61	22:10:43:THR:HG21	1.83	0.43
1:1A:2563:U:O2	1:1A:2565:A:H8	2.01	0.43
5:1F:107:LYS:HE2	5:1F:205:ARG:O	2.18	0.43
32:1a:932:C:H2'	32:1a:933:G:C8	2.53	0.43
32:1a:1424:C:H2'	32:1a:1425:U:O4'	2.18	0.43
36:1e:5:ASP:OD1	36:1e:5:ASP:N	2.51	0.43
40:1i:18:PHE:HB3	40:1i:20:ARG:NH2	2.33	0.43
40:1i:121:ARG:NH1	40:1i:122:ALA:O	2.51	0.43
54:1w:152:LEU:HD12	54:1w:152:LEU:HA	1.90	0.43
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.33	0.43
1:2A:1359:A:H2'	1:2A:1360:A:H5'	2.00	0.43
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.53	0.43
1:2A:2012:G:O3'	18:2W:96:ILE:HG23	2.18	0.43
1:2A:2477:C:N4	31:29:10:ILE:HG23	2.33	0.43
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.53	0.43
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.17	0.43
14:2S:65:VAL:O	14:2S:69:VAL:HG12	2.18	0.43
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.18	0.43
32:2a:519:C:OP1	54:2w:301:LYS:NZ	2.51	0.43
32:2a:526:C:OP2	43:2l:91:LYS:HE3	2.17	0.43
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	1.99	0.43
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.53	0.43
32:2a:1381:U:H2'	32:2a:1382:C:C6	2.53	0.43
32:2a:1511:G:H2'	32:2a:1512:U:O4'	2.17	0.43
34:2c:6:HIS:CD2	34:2c:8:ILE:H	2.37	0.43
35:2d:78:LEU:HB3	35:2d:93:PHE:HE1	1.82	0.43
44:2m:11:ARG:O	44:2m:13:LYS:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2p:23:ASP:OD1	47:2p:25:ARG:NH1	2.51	0.43
1:1A:1448:G:H1'	1:1A:1528:A:N1	2.34	0.43
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.18	0.43
2:1B:14:U:O2	2:1B:108:U:H4'	2.19	0.43
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.53	0.43
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.18	0.43
11:1P:2:LYS:HE3	11:1P:4:SER:OG	2.18	0.43
23:11:73:LEU:HD22	23:11:97:LEU:HB2	1.99	0.43
32:1a:515:G:H2'	32:1a:516:PSU:O4'	2.19	0.43
32:1a:584:G:H5'	48:1q:91:ARG:HH22	1.82	0.43
32:1a:945:G:C2	32:1a:946:A:C8	3.05	0.43
32:1a:1034:G:H3'	32:1a:1035:A:C8	2.50	0.43
32:1a:1118:C:P	40:1i:104:ARG:HH11	2.42	0.43
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.99	0.43
1:2A:26:G:C6	1:2A:27:G:N1	2.86	0.43
1:2A:118:A:N3	1:2A:178:G:H1'	2.33	0.43
1:2A:242:G:C8	30:28:5:LYS:HG2	2.52	0.43
1:2A:280:C:C2	1:2A:361:G:C2	3.06	0.43
1:2A:947:G:H2'	1:2A:948:G:H8	1.82	0.43
1:2A:2113:U:H3'	1:2A:2115:G:N1	2.34	0.43
1:2A:2484:G:C2	1:2A:2485:G:C8	3.07	0.43
1:2A:2629:A:H1'	1:2A:2630:G:H5''	1.99	0.43
2:2B:12:C:O2	22:20:74:ARG:NH2	2.47	0.43
21:2Z:3:TYR:CD2	21:2Z:51:ALA:HB2	2.53	0.43
32:2a:501:C:H2'	32:2a:502:G:H8	1.83	0.43
32:2a:501:C:H2'	32:2a:502:G:C8	2.53	0.43
32:2a:1262:C:H2'	32:2a:1263:C:H5'	2.00	0.43
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.53	0.43
33:2b:76:GLN:HG2	33:2b:206:ASP:O	2.18	0.43
39:2h:105:ARG:HD2	39:2h:105:ARG:HA	1.78	0.43
1:1A:883:G:H2'	1:1A:884:C:C5	2.53	0.43
1:1A:910:A:N1	1:1A:2277:G:H1'	2.33	0.43
1:1A:1313:U:H2'	1:1A:1610:A:C2	2.53	0.43
1:1A:2101:G:H3'	1:1A:2102:U:C6	2.53	0.43
1:1A:2251:OMG:H1'	1:1A:2251:OMG:HM23	1.74	0.43
4:1E:110:GLY:O	61:1R:301:HOH:O	2.21	0.43
32:1a:308:C:H2'	32:1a:309:G:H8	1.82	0.43
32:1a:363:A:C5	43:1l:31:PRO:HD2	2.53	0.43
32:1a:540:G:H2'	32:1a:541:G:O4'	2.18	0.43
33:1b:54:THR:O	33:1b:58:ILE:HG13	2.19	0.43
48:1q:31:LEU:HD23	48:1q:32:TYR:CZ	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:213:ASN:O	54:1w:216:GLU:HG2	2.19	0.43
1:2A:645:C:H5''	1:2A:646:A:OP2	2.17	0.43
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.54	0.43
3:2D:242:ARG:HG2	3:2D:246:PRO:HG3	2.01	0.43
6:2G:20:ILE:H	6:2G:20:ILE:HG13	1.69	0.43
6:2G:71:THR:O	6:2G:71:THR:OG1	2.32	0.43
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.18	0.43
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.99	0.43
26:24:61:ARG:HH12	50:2s:41:VAL:HG12	1.83	0.43
32:2a:34:C:H2'	32:2a:35:G:C8	2.54	0.43
32:2a:182:U:C4	32:2a:183:G:H1'	2.53	0.43
32:2a:303:A:H2'	32:2a:304:U:O4'	2.19	0.43
32:2a:382:A:H2'	32:2a:383:A:C8	2.53	0.43
32:2a:848:C:H2'	32:2a:849:C:O4'	2.19	0.43
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.80	0.43
33:2b:50:GLU:HB3	33:2b:200:ILE:O	2.17	0.43
34:2c:6:HIS:HB3	45:2n:49:HIS:ND1	2.33	0.43
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.18	0.43
40:2i:9:ARG:HB3	40:2i:104:ARG:NH1	2.34	0.43
42:2k:18:ARG:HB2	42:2k:33:THR:HG23	1.99	0.43
49:2r:40:LEU:HB3	49:2r:79:LEU:HD11	2.01	0.43
1:1A:601:C:O2'	1:1A:605:C:H5''	2.18	0.43
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.19	0.43
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.33	0.43
3:1D:70:TRP:HB3	3:1D:190:TYR:CZ	2.53	0.43
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.51	0.43
27:15:16:ARG:HG3	27:15:17:ASP:N	2.32	0.43
32:1a:41:G:H2'	32:1a:42:G:H8	1.82	0.43
32:1a:487:A:H2'	32:1a:488:C:O4'	2.17	0.43
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.30	0.43
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	2.00	0.43
35:1d:158:ILE:HD13	35:1d:158:ILE:HA	1.82	0.43
50:1s:74:PHE:C	50:1s:76:PRO:HD3	2.43	0.43
1:2A:1154:G:O5'	1:2A:1154:G:H8	2.02	0.43
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.54	0.43
1:2A:2207:G:H2'	1:2A:2208:A:C2	2.53	0.43
3:2D:258:LYS:HE2	3:2D:273:ARG:CZ	2.48	0.43
32:2a:622:A:C8	32:2a:623:C:C6	3.06	0.43
32:2a:1285:A:H5'	32:2a:1286:A:C2	2.54	0.43
32:2a:1316:G:N1	32:2a:1319:A:OP2	2.50	0.43
34:2c:77:ILE:HG13	34:2c:78:GLY:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:43:LEU:H	36:2e:65:ASN:HD22	1.66	0.43
54:2w:328:LEU:HD23	54:2w:328:LEU:HA	1.83	0.43
1:1A:672:C:OP2	11:1P:42:SER:OG	2.35	0.43
1:1A:1311:G:OP2	29:17:47:ARG:NH2	2.50	0.43
7:1H:121:ILE:HD13	7:1H:121:ILE:HA	1.83	0.43
12:1Q:58:PHE:CE1	12:1Q:109:VAL:HG21	2.54	0.43
15:1T:15:VAL:HG13	15:1T:79:HIS:CE1	2.54	0.43
32:1a:419:C:H2'	32:1a:420:U:O4'	2.18	0.43
32:1a:458:C:H2'	32:1a:460:G:O4'	2.19	0.43
32:1a:865:A:H2'	32:1a:866:C:C6	2.54	0.43
32:1a:1267:C:O2	52:1u:20:LYS:HE3	2.19	0.43
32:1a:1334:G:OP2	61:1a:1916:HOH:O	2.20	0.43
33:1b:7:VAL:O	33:1b:217:ARG:HD2	2.18	0.43
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.52	0.43
49:1r:40:LEU:HD22	49:1r:70:ILE:HG12	2.01	0.43
1:2A:875:G:H2'	1:2A:876:C:O4'	2.18	0.43
1:2A:1414:G:C6	1:2A:1415:U:C4	3.06	0.43
1:2A:2080:G:H5'	23:21:35:THR:OG1	2.19	0.43
1:2A:2514:U:H2'	1:2A:2515:C:C6	2.54	0.43
5:2F:148:LEU:HA	5:2F:148:LEU:HD23	1.73	0.43
16:2U:43:GLY:HA3	17:2V:73:SER:HB3	1.99	0.43
16:2U:90:VAL:HG12	16:2U:95:LEU:HG	2.00	0.43
32:2a:1005:A:H1'	32:2a:1036:G:N1	2.34	0.43
35:2d:173:TRP:CD1	35:2d:189:PRO:HG3	2.53	0.43
35:2d:181:MET:HE3	35:2d:181:MET:HB2	1.96	0.43
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.18	0.43
37:2f:69:GLU:O	37:2f:72:VAL:HG12	2.19	0.43
40:2i:23:ASN:OD1	40:2i:23:ASN:N	2.42	0.43
40:2i:93:ARG:HD3	40:2i:93:ARG:HA	1.65	0.43
42:2k:32:ILE:HD12	42:2k:72:ALA:HB2	2.00	0.43
1:1A:2461:C:H2'	1:1A:2462:U:C6	2.54	0.43
2:1B:13:A:N1	2:1B:69:G:O2'	2.46	0.43
10:1O:63:VAL:HA	10:1O:106:LEU:HD11	1.99	0.43
11:1P:55:ARG:H	11:1P:55:ARG:HG3	1.58	0.43
12:1Q:10:ARG:HH12	12:1Q:90:VAL:H	1.67	0.43
30:18:4:MET:HE2	30:18:4:MET:HB3	1.81	0.43
32:1a:976:G:OP2	32:1a:1358:U:O2'	2.29	0.43
33:1b:115:LEU:C	33:1b:117:GLU:H	2.27	0.43
1:2A:34:C:N4	1:2A:447:A:H61	2.17	0.43
1:2A:480:A:O2'	20:2Y:46:LYS:O	2.34	0.43
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.53	0.43
1:2A:2705:A:H2'	1:2A:2706:G:O4'	2.18	0.43
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.51	0.43
19:2X:1:MET:HE3	19:2X:1:MET:HB3	1.85	0.43
27:25:8:LYS:O	27:25:9:LYS:HD2	2.19	0.43
28:26:35:GLU:HG2	28:26:50:ARG:HG2	2.00	0.43
32:2a:532:A:H2	34:2c:156:ARG:NH2	2.11	0.43
32:2a:833:U:H2'	32:2a:834:C:C6	2.53	0.43
32:2a:1003:G:C6	32:2a:1004:A:C6	3.06	0.43
32:2a:1217:C:OP1	45:2n:9:LYS:NZ	2.52	0.43
32:2a:1265:G:C4	32:2a:1271:G:N2	2.87	0.43
33:2b:97:TRP:CZ2	33:2b:173:ALA:HA	2.54	0.43
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	2.00	0.43
34:2c:133:ALA:HA	34:2c:136:GLN:HG2	2.00	0.43
39:2h:120:THR:H	39:2h:123:GLU:HB2	1.83	0.43
48:2q:58:GLU:O	48:2q:74:LEU:N	2.41	0.43
55:2x:8:4SU:O5'	55:2x:8:4SU:H6	2.19	0.43
1:1A:375:C:H5''	61:1A:4437:HOH:O	2.18	0.43
1:1A:432:A:N6	61:1A:4455:HOH:O	2.48	0.43
1:1A:686:G:N2	1:1A:788:A:H61	2.16	0.43
1:1A:831:G:N2	11:1P:53:GLY:O	2.52	0.43
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.83	0.43
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.53	0.43
1:1A:2615:U:H2'	1:1A:2616:C:C6	2.54	0.43
6:1G:108:ASN:HD22	26:14:22:ILE:HD13	1.84	0.43
9:1N:21:LYS:NZ	9:1N:140:VAL:OXT	2.48	0.43
32:1a:404:U:H2'	32:1a:405:U:C6	2.54	0.43
32:1a:741:G:H2'	32:1a:742:G:O4'	2.18	0.43
32:1a:1223:C:OP2	50:1s:78:ARG:NH2	2.42	0.43
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.54	0.43
32:1a:1362:C:H2'	32:1a:1363:C:H5''	2.01	0.43
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.47	0.43
34:1c:129:ALA:HB3	34:1c:132:ARG:HB3	2.00	0.43
35:1d:121:VAL:HG11	35:1d:136:PRO:HA	1.99	0.43
35:1d:173:TRP:O	35:1d:186:LEU:N	2.48	0.43
37:1f:55:ASP:HB2	37:1f:86:ARG:HH12	1.84	0.43
38:1g:113:GLU:HB2	38:1g:119:ARG:HG2	2.00	0.43
41:1j:61:GLU:OE1	45:1n:45:ARG:NE	2.52	0.43
49:1r:34:TYR:CD1	49:1r:35:ARG:HG3	2.54	0.43
1:2A:740:U:H2'	1:2A:741:G:C8	2.54	0.43
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1889:A:N1	1:2A:2234:G:H1'	2.34	0.43
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.54	0.43
1:2A:2633:G:H2'	1:2A:2634:G:O4'	2.19	0.43
1:2A:2788:C:P	4:2E:61:ARG:HH21	2.41	0.43
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	2.01	0.43
8:2I:84:GLY:C	8:2I:86:THR:H	2.26	0.43
21:2Z:141:VAL:O	21:2Z:144:LEU:HB2	2.19	0.43
21:2Z:146:ILE:HA	21:2Z:147:GLY:HA2	1.59	0.43
32:2a:986:A:H2'	32:2a:987:G:C8	2.54	0.43
32:2a:1237:C:HO2'	32:2a:1300:G:H1	1.64	0.43
32:2a:1264:C:N4	32:2a:1265:G:O6	2.50	0.43
32:2a:1323:G:H4'	32:2a:1363:C:N3	2.34	0.43
32:2a:1519:MA6:H102	32:2a:1520:G:O2'	2.19	0.43
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.83	0.43
50:2s:23:ASN:HA	50:2s:27:GLU:OE1	2.18	0.43
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.54	0.43
1:1A:1466:G:O2'	1:1A:1546:C:O2'	2.21	0.43
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.54	0.43
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	2.00	0.43
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	2.01	0.43
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.19	0.43
10:1O:63:VAL:HG11	10:1O:85:VAL:HG23	2.01	0.43
24:12:51:ARG:HD3	24:12:55:ARG:NH1	2.34	0.43
32:1a:262:A:C6	32:1a:263:A:C6	3.07	0.43
32:1a:420:U:H1'	32:1a:424:G:N2	2.33	0.43
32:1a:437:U:O2'	35:1d:125:HIS:HE1	2.01	0.43
32:1a:1027:C:N1	32:1a:1034:G:N2	2.67	0.43
32:1a:1313:U:P	50:1s:5:LEU:HB2	2.58	0.43
34:1c:62:ASP:O	34:1c:97:LYS:HB2	2.19	0.43
42:1k:59:TYR:CE2	42:1k:63:LEU:HD11	2.54	0.43
54:1w:218:ARG:NH1	54:1w:220:ASP:OD2	2.50	0.43
1:2A:271(X):G:C2	1:2A:271(Y):U:O4	2.72	0.43
1:2A:302:C:P	20:2Y:73:ARG:HH12	2.42	0.43
1:2A:2740:A:C6	1:2A:2741:A:C6	3.07	0.43
2:2B:105:A:H5'	2:2B:106:G:OP2	2.18	0.43
3:2D:182:LEU:O	3:2D:271:ILE:N	2.46	0.43
32:2a:8:A:H5'	36:2e:101:ILE:HG22	2.00	0.43
32:2a:99:U:H2'	32:2a:100:C:C6	2.54	0.43
32:2a:294:U:OP1	32:2a:610:G:O2'	2.30	0.43
32:2a:489:C:H2'	32:2a:490:G:H8	1.84	0.43
35:2d:61:LYS:HA	35:2d:203:VAL:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:72:GLN:O	36:2e:75:THR:HG22	2.19	0.43
43:2l:110:VAL:HG23	43:2l:120:TYR:HB3	2.00	0.43
50:2s:53:ASN:HB2	50:2s:77:THR:HA	2.01	0.43
54:2w:218:ARG:NH1	54:2w:220:ASP:OD2	2.52	0.43
1:1A:22:C:H2'	1:1A:23:G:O4'	2.19	0.43
1:1A:491:G:H2'	1:1A:492:A:H8	1.84	0.43
1:1A:924:C:H2'	1:1A:925:C:C6	2.53	0.43
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.54	0.43
1:1A:2006:C:OP2	61:1A:4243:HOH:O	2.21	0.43
5:1F:72:ARG:HE	5:1F:72:ARG:HB3	1.55	0.43
5:1F:117:ARG:NH2	5:1F:189:THR:O	2.52	0.43
6:1G:114:ILE:HG12	6:1G:140:ILE:HG12	1.99	0.43
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	2.01	0.43
25:13:39:ASP:OD2	25:13:44:ARG:NH2	2.52	0.43
32:1a:15:G:H21	36:1e:18:ARG:HA	1.84	0.43
32:1a:1118:C:OP1	40:1i:9:ARG:HD2	2.18	0.43
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.19	0.43
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.53	0.43
33:1b:116:GLU:HA	33:1b:119:GLU:HG3	2.00	0.43
33:1b:138:LEU:HA	33:1b:141:GLU:HB3	2.01	0.43
35:1d:140:VAL:HG12	35:1d:144:ASP:HB2	2.01	0.43
35:1d:147:ALA:HA	35:1d:182:LYS:HA	2.01	0.43
51:1t:8:ARG:HA	51:1t:8:ARG:HD2	1.78	0.43
1:2A:415:A:H2'	1:2A:416:C:O4'	2.19	0.43
1:2A:1434:A:H61	1:2A:1558:A:H62	1.66	0.43
15:2T:127:ALA:C	15:2T:129:ARG:N	2.77	0.43
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.34	0.43
17:2V:40:LEU:HD12	17:2V:46:VAL:HG21	2.00	0.43
22:20:43:THR:HG23	22:20:43:THR:O	2.19	0.43
26:24:3:GLU:H	26:24:3:GLU:HG2	1.43	0.43
32:2a:860:A:H2'	32:2a:861:G:O4'	2.19	0.43
32:2a:1342:C:H2'	32:2a:1343:G:C8	2.54	0.43
32:2a:1372:U:OP1	40:2i:72:GLY:N	2.45	0.43
32:2a:1414:U:H2'	32:2a:1415:G:H8	1.84	0.43
33:2b:162:ILE:HG13	33:2b:162:ILE:O	2.19	0.43
34:2c:23:TYR:HA	41:2j:11:PHE:CD2	2.54	0.43
34:2c:57:ILE:HG21	34:2c:59:ARG:HH21	1.84	0.43
39:2h:104:ARG:HD3	39:2h:104:ARG:HA	1.84	0.43
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	2.00	0.43
42:2k:22:HIS:O	42:2k:28:THR:HA	2.19	0.43
44:2m:81:LEU:C	44:2m:89:GLY:HA3	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:38:A:H2'	1:1A:39:C:C6	2.54	0.42
1:1A:144:C:H5'	19:1X:2:LYS:HD3	2.00	0.42
1:1A:2406:U:H2'	1:1A:2406:U:OP2	2.19	0.42
4:1E:79:ARG:HD3	4:1E:79:ARG:HA	1.89	0.42
19:1X:88:LYS:HD3	19:1X:90:GLU:OE1	2.18	0.42
32:1a:1114:C:H42	32:1a:1186:G:H1	1.65	0.42
32:1a:1304:G:C5	32:1a:1305:G:C6	3.07	0.42
35:1d:94:LEU:HA	35:1d:97:LEU:HD12	2.01	0.42
37:1f:97:PHE:CD2	49:1r:31:LEU:HD12	2.54	0.42
47:1p:43:LYS:HG2	47:1p:48:TRP:CE2	2.54	0.42
48:1q:60:ILE:HG13	48:1q:61:GLU:N	2.34	0.42
1:2A:982:C:OP1	61:2A:4852:HOH:O	2.22	0.42
1:2A:2250:G:O2'	1:2A:2496:C:OP1	2.32	0.42
1:2A:2275:C:H6	1:2A:2275:C:H5'	1.84	0.42
2:2B:42:C:O2'	6:2G:67:LYS:O	2.34	0.42
13:2R:31:HIS:C	13:2R:33:ARG:H	2.27	0.42
13:2R:98:LEU:HB2	13:2R:113:LEU:HD11	2.01	0.42
20:2Y:38:ILE:HD11	20:2Y:66:PRO:HG3	2.01	0.42
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.34	0.42
32:2a:509:A:H2'	32:2a:510:A:C8	2.53	0.42
32:2a:620:C:H2'	32:2a:621:A:O4'	2.19	0.42
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.34	0.42
32:2a:1092:A:H8	32:2a:1092:A:OP1	2.03	0.42
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.19	0.42
44:2m:13:LYS:HD3	44:2m:17:VAL:HG11	1.99	0.42
1:1A:945:A:C4	1:1A:2448:A:C2	3.07	0.42
1:1A:1923:U:H2'	1:1A:1924:C:C6	2.54	0.42
1:1A:2848:G:H3'	15:1T:95:ARG:O	2.19	0.42
2:1B:28:C:H2'	2:1B:29:A:O4'	2.19	0.42
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	2.01	0.42
6:1G:131:TYR:HB3	6:1G:159:VAL:CG1	2.49	0.42
6:1G:151:ALA:HB3	6:1G:153:ARG:NH1	2.34	0.42
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.67	0.42
7:1H:3:ARG:CG	7:1H:6:ARG:HG2	2.48	0.42
10:1O:7:TYR:CZ	10:1O:44:LYS:HG3	2.55	0.42
32:1a:405:U:O4	35:1d:2:GLY:N	2.52	0.42
32:1a:418:C:H1'	32:1a:540:G:O2'	2.19	0.42
32:1a:1080:A:H5'	36:1e:14:ARG:NH2	2.34	0.42
32:1a:1292:U:OP2	38:1g:41:ARG:NH2	2.52	0.42
33:1b:35:GLU:HB2	33:1b:40:HIS:HA	2.01	0.42
33:1b:211:ILE:O	33:1b:215:LEU:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:98:GLU:HA	35:1d:103:ASN:ND2	2.34	0.42
53:1v:20:A:N6	54:1w:186:THR:OG1	2.51	0.42
54:1w:222:MET:HG2	54:1w:238:ALA:HB3	2.00	0.42
1:2A:118:A:H1'	1:2A:178:G:O4'	2.19	0.42
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.19	0.42
1:2A:565:C:H2'	1:2A:566:U:O4'	2.19	0.42
1:2A:1740:G:H2'	1:2A:1741:A:H8	1.82	0.42
1:2A:2443:C:OP1	5:2F:68:LYS:HD3	2.19	0.42
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.20	0.42
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	2.00	0.42
6:2G:51:ARG:O	6:2G:52:ILE:C	2.63	0.42
14:2S:5:THR:OG1	14:2S:8:GLU:HG3	2.18	0.42
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.99	0.42
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.19	0.42
38:2g:79:ARG:NH1	38:2g:80:VAL:HA	2.34	0.42
44:2m:27:LYS:HA	44:2m:27:LYS:HD2	1.65	0.42
54:2w:303:ARG:HD2	54:2w:305:TYR:OH	2.19	0.42
1:1A:272:G:O2'	1:1A:421:U:OP2	2.23	0.42
1:1A:272(F):C:H2'	1:1A:272(G):C:C6	2.54	0.42
1:1A:882:G:H1	1:1A:894:C:N4	2.17	0.42
1:1A:1042:G:C6	1:1A:1043:C:C4	3.08	0.42
1:1A:1078:U:H3	1:1A:1089:G:H5'	1.84	0.42
1:1A:2106:G:H2'	1:1A:2107:C:C6	2.54	0.42
1:1A:2161:C:O2'	1:1A:2162:G:H8	2.01	0.42
4:1E:143:ASN:HD22	4:1E:147:PRO:CD	2.33	0.42
10:1O:97:ARG:HH12	32:1a:338:A:P	2.42	0.42
32:1a:73:G:C6	32:1a:76:C:C4	3.08	0.42
32:1a:229:U:H5''	47:1p:33:ILE:HD13	2.00	0.42
32:1a:730:G:C5	32:1a:731:G:H1'	2.55	0.42
32:1a:1305:G:H1	32:1a:1331:G:H1'	1.85	0.42
33:1b:24:TRP:H	33:1b:24:TRP:HD1	1.67	0.42
34:1c:131:ARG:NH1	34:1c:166:GLU:HG3	2.33	0.42
35:1d:68:TYR:CE1	35:1d:97:LEU:HB3	2.54	0.42
42:1k:85:ARG:HD3	42:1k:113:PRO:HD3	2.02	0.42
54:1w:178:HIS:NE2	54:1w:302:ILE:HD11	2.34	0.42
1:2A:876:C:H2'	1:2A:877:U:O4'	2.18	0.42
1:2A:922:U:H2'	1:2A:923:C:C6	2.54	0.42
1:2A:1472:A:H2'	1:2A:1473:G:O4'	2.19	0.42
1:2A:1802:A:N1	1:2A:1822:G:H1'	2.34	0.42
2:2B:22:U:H2'	2:2B:23:G:C8	2.54	0.42
6:2G:135:LEU:HB2	6:2G:155:MET:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:137:TYR:HB3	21:2Z:76:LEU:HD21	2.01	0.42
32:2a:624:C:H2'	32:2a:625:G:C8	2.53	0.42
32:2a:991:U:C4	32:2a:1212:U:H1'	2.54	0.42
33:2b:136:VAL:O	33:2b:139:LYS:HB2	2.18	0.42
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	2.01	0.42
38:2g:14:PRO:HG3	38:2g:21:VAL:HG12	2.01	0.42
1:1A:118:A:C8	1:1A:119:A:C8	3.08	0.42
1:1A:969:U:H2'	1:1A:970:C:C6	2.54	0.42
1:1A:1022:G:OP2	9:1N:65:LYS:NZ	2.53	0.42
1:1A:2787:C:H2'	1:1A:2788:C:H6	1.84	0.42
1:1A:2833:G:H21	4:1E:57:LYS:CB	2.32	0.42
3:1D:38:LYS:HA	3:1D:38:LYS:HD2	1.86	0.42
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.49	0.42
5:1F:179:GLU:CD	5:1F:179:GLU:H	2.27	0.42
19:1X:4:ALA:HB1	19:1X:42:ALA:HA	2.01	0.42
32:1a:434:U:H2'	32:1a:435:C:H6	1.83	0.42
32:1a:439:A:C5	32:1a:441:A:H1'	2.54	0.42
32:1a:688:G:H2'	32:1a:689:C:H6	1.84	0.42
32:1a:838:G:H1	32:1a:848:C:H42	1.66	0.42
32:1a:1064:G:H4'	32:1a:1065:U:OP1	2.19	0.42
32:1a:1226:C:P	44:1m:91:ARG:HH22	2.42	0.42
32:1a:1314:C:H2'	32:1a:1315:U:C6	2.54	0.42
33:1b:171:ALA:HA	33:1b:174:VAL:HG22	2.02	0.42
1:2A:942:G:O2'	1:2A:1189:A:N3	2.51	0.42
1:2A:1019:U:O2'	1:2A:1021:A:H2	2.02	0.42
1:2A:2164:C:H41	1:2A:2165:G:H21	1.68	0.42
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.55	0.42
15:2T:27:THR:HB	15:2T:89:VAL:HG22	2.00	0.42
32:2a:202:U:H3'	32:2a:203:U:C6	2.55	0.42
32:2a:489:C:H2'	32:2a:490:G:C8	2.54	0.42
33:2b:12:GLU:O	33:2b:15:VAL:HB	2.19	0.42
33:2b:178:ARG:HH22	39:2h:74:PRO:HB3	1.84	0.42
40:2i:13:ALA:HB2	40:2i:68:GLY:HA3	2.01	0.42
1:1A:337:C:H2'	1:1A:338:G:O4'	2.20	0.42
1:1A:389:G:O6	11:1P:70:GLN:HB2	2.20	0.42
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.20	0.42
1:1A:2119:A:H61	1:1A:2168:G:H8	1.65	0.42
8:1I:114:LEU:HD12	8:1I:115:ALA:H	1.84	0.42
9:1N:29:LYS:HD2	9:1N:140:VAL:HB	2.02	0.42
15:1T:27:THR:HB	15:1T:90:GLN:HB3	2.01	0.42
15:1T:39:ARG:HH22	32:1a:345:C:P	2.42	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.18	0.42
28:16:44:ARG:HG2	28:16:44:ARG:HH11	1.85	0.42
32:1a:1111:A:N1	34:1c:177:THR:OG1	2.46	0.42
32:1a:1397:C:OP2	36:1e:24:ARG:NH2	2.50	0.42
33:1b:16:HIS:O	33:1b:18:GLY:N	2.53	0.42
35:1d:122:ARG:NH1	35:1d:134:ASP:OD2	2.43	0.42
36:1e:72:GLN:O	36:1e:75:THR:HG22	2.19	0.42
44:1m:101:GLN:OE1	44:1m:101:GLN:N	2.48	0.42
54:1w:303:ARG:HD2	54:1w:305:TYR:CZ	2.54	0.42
54:1w:303:ARG:HD2	54:1w:305:TYR:OH	2.19	0.42
55:1x:48:G:N2	61:1x:203:HOH:O	2.52	0.42
1:2A:58:G:O2'	1:2A:73:A:N1	2.42	0.42
1:2A:253:C:O2'	61:2A:4851:HOH:O	2.22	0.42
1:2A:494:G:OP1	18:2W:8:ARG:NH1	2.51	0.42
1:2A:1639:U:H4'	1:2A:2699:C:H4'	2.01	0.42
1:2A:2728:U:H2'	1:2A:2729:G:C8	2.55	0.42
8:2I:26:ALA:HA	8:2I:30:LEU:HB2	2.01	0.42
12:2Q:57:HIS:NE2	12:2Q:116:GLU:HB3	2.35	0.42
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.19	0.42
21:2Z:97:GLU:HB3	21:2Z:125:LEU:HD11	2.01	0.42
25:23:8:LEU:HD13	25:23:23:LEU:HD21	2.01	0.42
32:2a:370:C:H2'	32:2a:371:G:H8	1.85	0.42
32:2a:580:U:H2'	32:2a:581:G:O4'	2.19	0.42
32:2a:583:A:H2'	32:2a:584:G:O4'	2.19	0.42
32:2a:678:U:H2'	32:2a:679:C:C6	2.55	0.42
32:2a:977:A:O3'	32:2a:980:C:N4	2.53	0.42
32:2a:1022:G:H2'	32:2a:1023:G:C8	2.54	0.42
34:2c:58:GLU:HB2	34:2c:65:ALA:HB3	2.01	0.42
38:2g:20:ASP:HB3	38:2g:23:VAL:HG13	2.00	0.42
39:2h:82:HIS:CE1	39:2h:84:ARG:HD2	2.55	0.42
43:2l:53:ARG:HB3	43:2l:69:TYR:HE1	1.84	0.42
44:2m:65:LYS:HG3	44:2m:69:GLU:CD	2.45	0.42
1:1A:1665:A:H2'	1:1A:1666:G:O4'	2.20	0.42
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.34	0.42
1:1A:1891:G:H2'	1:1A:1892:C:O4'	2.20	0.42
1:1A:2121:G:H1	1:1A:2177:C:H42	1.67	0.42
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.54	0.42
2:1B:29:A:H2'	2:1B:30:C:O4'	2.19	0.42
15:1T:96:ARG:CZ	15:1T:96:ARG:HB3	2.49	0.42
21:1Z:3:TYR:CD2	21:1Z:51:ALA:HB2	2.54	0.42
28:16:47:THR:HG22	28:16:48:VAL:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:374:A:C6	32:1a:375:U:C4	3.08	0.42
32:1a:580:U:H2'	32:1a:581:G:O4'	2.20	0.42
32:1a:1433:A:C6	32:1a:1468:A:C4	3.08	0.42
38:1g:44:TYR:HE2	40:1i:41:VAL:HG11	1.84	0.42
1:2A:71:A:H5''	1:2A:73:A:C8	2.54	0.42
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.54	0.42
1:2A:127:A:H5''	1:2A:128:C:C6	2.55	0.42
1:2A:272:G:H4'	1:2A:272(A):U:H5''	2.01	0.42
1:2A:1029:A:N1	1:2A:2465:C:O2'	2.48	0.42
1:2A:1495:A:H8	1:2A:1495:A:O5'	2.03	0.42
1:2A:2303:G:C2'	1:2A:2304:G:H5'	2.49	0.42
1:2A:2390:U:P	30:28:35:GLN:HE22	2.42	0.42
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.52	0.42
2:2B:89:G:H2'	2:2B:90:A:C8	2.54	0.42
6:2G:138:GLN:OE1	6:2G:138:GLN:N	2.53	0.42
14:2S:38:GLN:HB2	14:2S:47:THR:HG23	2.01	0.42
23:21:50:ARG:HD2	23:21:57:GLU:OE2	2.20	0.42
32:2a:173:U:H5''	32:2a:197:A:O4'	2.20	0.42
32:2a:432:A:N7	32:2a:433:C:C4	2.88	0.42
32:2a:921:U:O2'	36:2e:19:MET:O	2.33	0.42
32:2a:1254:C:OP1	41:2j:45:ARG:HA	2.19	0.42
36:2e:12:LEU:HB3	36:2e:31:LEU:HB2	2.01	0.42
36:2e:149:GLU:HB3	36:2e:150:ARG:NH1	2.34	0.42
44:2m:84:ILE:HB	50:2s:74:PHE:HE1	1.84	0.42
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	2.00	0.42
46:2o:58:MET:HE3	46:2o:58:MET:HB2	1.88	0.42
47:2p:3:LYS:HE3	47:2p:3:LYS:HB3	1.83	0.42
1:1A:9:U:N3	1:1A:2629:A:C2	2.86	0.42
1:1A:675:A:C8	1:1A:804:A:C6	3.08	0.42
1:1A:1069:A:H4'	1:1A:1070:A:H5''	2.01	0.42
1:1A:2581:G:H2'	1:1A:2581:G:N3	2.34	0.42
4:1E:40:GLU:CD	4:1E:40:GLU:H	2.27	0.42
6:1G:11:TYR:HA	6:1G:15:VAL:HB	2.01	0.42
6:1G:76:SER:C	6:1G:77:ILE:HG12	2.45	0.42
20:1Y:5:MET:HG2	20:1Y:30:VAL:HG11	2.00	0.42
32:1a:113:G:H2'	32:1a:114:U:C6	2.55	0.42
32:1a:164:U:H2'	32:1a:165:C:C6	2.54	0.42
32:1a:371:G:H1'	32:1a:482:A:H1'	2.02	0.42
32:1a:512:U:H2'	32:1a:513:C:C6	2.55	0.42
32:1a:682:G:H2'	32:1a:683:G:O4'	2.19	0.42
32:1a:922:G:H4'	36:1e:20:GLN:HA	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.85	0.42
32:1a:1400:5MC:O2	54:1w:188:THR:HG21	2.20	0.42
33:1b:32:ILE:HD13	33:1b:40:HIS:CD2	2.54	0.42
33:1b:172:ILE:H	33:1b:172:ILE:HG13	1.56	0.42
1:2A:629:G:H4'	1:2A:650:C:O2	2.20	0.42
1:2A:647:G:H2'	1:2A:648:G:O4'	2.20	0.42
1:2A:902:C:H2'	1:2A:903:C:C6	2.55	0.42
1:2A:1809:A:H2'	1:2A:1810:A:C8	2.55	0.42
1:2A:2227:A:OP1	3:2D:263:ARG:HD2	2.20	0.42
3:2D:106:ILE:HD11	3:2D:144:ALA:HB2	2.02	0.42
5:2F:70:THR:CG2	5:2F:72:ARG:H	2.31	0.42
5:2F:182:ASN:O	5:2F:186:ILE:HD12	2.20	0.42
16:2U:76:TYR:CE2	16:2U:80:ILE:HG13	2.55	0.42
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.19	0.42
32:2a:93:G:H2'	32:2a:96:U:O4'	2.19	0.42
32:2a:202:U:H3'	32:2a:203:U:H6	1.84	0.42
32:2a:235:C:H2'	32:2a:236:G:H8	1.85	0.42
32:2a:892:A:H2'	32:2a:893:C:C6	2.55	0.42
32:2a:1057:G:H2'	32:2a:1058:G:O4'	2.19	0.42
32:2a:1206:G:C6	32:2a:1207:2MG:C5	3.08	0.42
33:2b:31:TYR:CE2	33:2b:200:ILE:HG21	2.55	0.42
33:2b:184:VAL:HG13	33:2b:197:VAL:HA	2.01	0.42
44:2m:87:TYR:O	44:2m:91:ARG:HG3	2.18	0.42
50:2s:49:ILE:HD11	50:2s:71:LEU:HD21	2.01	0.42
1:1A:444:C:H5''	61:1A:5337:HOH:O	2.19	0.42
1:1A:724:U:H2'	1:1A:725:G:O4'	2.20	0.42
1:1A:833:U:OP1	11:1P:45:LEU:HD13	2.19	0.42
61:1A:4601:HOH:O	3:1D:14:ARG:HD2	2.18	0.42
4:1E:89:ASP:OD1	4:1E:89:ASP:N	2.40	0.42
4:1E:111:ARG:HB2	4:1E:160:TYR:HB3	2.01	0.42
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.19	0.42
9:1N:4:TYR:CE2	16:1U:100:VAL:HG11	2.54	0.42
23:11:18:ILE:HG12	23:11:37:ILE:HG23	2.02	0.42
26:14:46:GLN:HG2	26:14:47:GLN:N	2.35	0.42
32:1a:499:A:H4'	32:1a:500:G:OP1	2.20	0.42
32:1a:670:G:H2'	32:1a:671:G:O4'	2.19	0.42
32:1a:1292:U:P	38:1g:41:ARG:HH22	2.42	0.42
32:1a:1358:U:H5''	45:1n:33:VAL:O	2.19	0.42
33:1b:218:ALA:O	33:1b:222:ILE:HG13	2.20	0.42
35:1d:108:LEU:HD21	35:1d:183:GLY:HA3	2.01	0.42
39:1h:31:PHE:HZ	39:1h:134:ILE:HD13	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:94:ALA:C	40:1i:96:LEU:H	2.28	0.42
41:1j:47:PHE:CE1	45:1n:37:PHE:HE2	2.37	0.42
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.35	0.42
1:2A:116:C:H2'	1:2A:117:G:O4'	2.20	0.42
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.84	0.42
1:2A:340:A:H2'	1:2A:341:G:O4'	2.19	0.42
1:2A:392:C:H5''	1:2A:409:C:H5''	2.02	0.42
1:2A:531:C:OP1	1:2A:561:G:N1	2.43	0.42
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.55	0.42
1:2A:1297:C:H5''	61:2A:5150:HOH:O	2.19	0.42
1:2A:1357:U:H2'	1:2A:1358:G:O4'	2.20	0.42
1:2A:1766:U:H2'	1:2A:1767:C:C6	2.55	0.42
5:2F:119:ARG:CZ	5:2F:119:ARG:HB3	2.50	0.42
17:2V:69:LYS:HA	17:2V:88:ARG:HG2	2.01	0.42
32:2a:37:U:O2'	32:2a:547:A:N1	2.49	0.42
32:2a:67:C:H2'	32:2a:68:G:C8	2.55	0.42
32:2a:69:G:H2'	32:2a:70:G:H8	1.84	0.42
32:2a:1190:G:O2'	34:2c:3:ASN:HB2	2.19	0.42
33:2b:68:ILE:HG12	33:2b:161:ALA:HB3	2.00	0.42
42:2k:51:LYS:HD3	42:2k:51:LYS:HA	1.80	0.42
51:2t:43:LEU:O	51:2t:47:GLY:N	2.53	0.42
1:1A:608:A:C4	1:1A:621:A:C6	3.08	0.42
1:1A:811:U:H2'	11:1P:21:ARG:HA	2.02	0.42
1:1A:2721:A:H2'	1:1A:2722:G:O4'	2.19	0.42
1:1A:2749:A:H3'	1:1A:2750:A:H2'	2.02	0.42
5:1F:44:ARG:NH1	61:1F:401:HOH:O	2.35	0.42
7:1H:3:ARG:HH22	7:1H:66:GLY:N	2.17	0.42
16:1U:17:ILE:HD13	16:1U:17:ILE:HA	1.91	0.42
32:1a:408:A:H2'	32:1a:409:G:O4'	2.19	0.42
32:1a:413:G:N2	32:1a:428:G:H1'	2.34	0.42
32:1a:768:A:H5'	32:1a:1524:C:H1'	2.02	0.42
32:1a:1020:U:H2'	32:1a:1021:G:H5'	2.01	0.42
1:2A:361:G:O2'	1:2A:362:U:H5'	2.19	0.42
1:2A:403:U:H4'	1:2A:404:C:H5'	2.02	0.42
1:2A:1558:A:H4'	1:2A:1559:G:O5'	2.19	0.42
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.53	0.42
12:2Q:133:ARG:HG2	12:2Q:134:ARG:N	2.33	0.42
32:2a:826:C:H2'	32:2a:827:U:C6	2.54	0.42
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	2.02	0.42
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.31	0.42
32:2a:1466:C:H2'	32:2a:1467:G:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2x:65:A:H2'	55:2x:66:A:O4'	2.20	0.42
1:1A:372:G:H8	23:11:65:SER:O	2.03	0.42
1:1A:735:A:N7	1:1A:761:A:H2	2.18	0.42
1:1A:749:C:H4'	1:1A:1271:G:N3	2.35	0.42
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.20	0.42
1:1A:2722:G:H5''	1:1A:2820:A:N7	2.34	0.42
1:1A:2785:C:H2'	1:1A:2786:U:O4'	2.20	0.42
14:1S:3:ARG:HA	14:1S:3:ARG:HD3	1.81	0.42
26:14:64:GLY:C	26:14:66:SER:H	2.28	0.42
32:1a:1293:G:H2'	32:1a:1294:G:C8	2.54	0.42
32:1a:1320:C:H2'	32:1a:1321:C:O4'	2.20	0.42
33:1b:54:THR:HG22	33:1b:58:ILE:HD11	2.02	0.42
36:1e:42:GLY:HA2	36:1e:65:ASN:O	2.20	0.42
1:2A:241:A:H8	1:2A:241:A:OP1	2.02	0.42
1:2A:448:U:O4	1:2A:583:G:H1'	2.20	0.42
1:2A:527:C:C5	1:2A:2779:U:H2'	2.55	0.42
1:2A:609:A:H2'	1:2A:610:G:O4'	2.20	0.42
1:2A:909:A:C6	1:2A:912:C:C2	3.08	0.42
1:2A:2110:G:H5''	1:2A:2111:C:C6	2.55	0.42
5:2F:126:VAL:O	5:2F:196:LEU:HG	2.20	0.42
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	2.01	0.42
10:2O:36:GLY:HA3	10:2O:109:LYS:HD3	2.02	0.42
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	2.02	0.42
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.37	0.42
32:2a:232:G:H1'	32:2a:262:A:N1	2.34	0.42
32:2a:964:A:O2'	41:2j:55:LYS:NZ	2.33	0.42
33:2b:121:LEU:HD11	33:2b:126:GLU:O	2.20	0.42
34:2c:149:ALA:HA	34:2c:201:TYR:O	2.19	0.42
54:2w:306:ASN:OD1	54:2w:309:GLN:HG2	2.20	0.42
1:1A:637:A:H2'	11:1P:117:GLU:OE1	2.20	0.41
1:1A:813:U:H2'	1:1A:814:C:C6	2.55	0.41
1:1A:817:C:H4'	1:1A:932:G:C5	2.55	0.41
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.55	0.41
1:1A:1683:C:H2'	1:1A:1684:C:C6	2.55	0.41
1:1A:2801(A):A:H5''	1:1A:2802:G:C8	2.55	0.41
8:1I:101:LEU:HD22	8:1I:140:LEU:HD11	2.02	0.41
26:14:26:SER:OG	26:14:27:THR:N	2.53	0.41
32:1a:143:A:H2	32:1a:220:G:H1	1.68	0.41
32:1a:537:G:H5''	43:1l:113:ARG:NH1	2.35	0.41
32:1a:857:C:H2'	32:1a:858:G:O4'	2.20	0.41
32:1a:994:A:N1	32:1a:1047:G:H4'	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1003:G:OP1	32:1a:1003:G:H4'	2.19	0.41
38:1g:69:VAL:HG22	38:1g:135:VAL:HG22	2.01	0.41
40:1i:16:ARG:HB2	40:1i:64:THR:HG23	2.01	0.41
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.43	0.41
1:2A:1310:G:OP2	29:27:9:ARG:NE	2.42	0.41
1:2A:2302:G:C6	1:2A:2315:G:C6	3.08	0.41
6:2G:72:ARG:HH12	6:2G:87:PRO:HG3	1.85	0.41
7:2H:7:LEU:HD12	7:2H:7:LEU:HA	1.94	0.41
13:2R:31:HIS:O	13:2R:33:ARG:N	2.49	0.41
14:2S:67:ARG:O	14:2S:71:ARG:HB2	2.20	0.41
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.55	0.41
32:2a:103:C:O2'	32:2a:172:A:N1	2.46	0.41
32:2a:259:G:H2'	32:2a:260:G:O4'	2.20	0.41
32:2a:955:U:H2'	32:2a:956:U:O4'	2.20	0.41
32:2a:1144:G:N2	32:2a:1146:A:H62	2.18	0.41
32:2a:1145:C:H4'	32:2a:1146:A:H8	1.85	0.41
32:2a:1298:C:N4	38:2g:114:ARG:HB3	2.34	0.41
32:2a:1414:U:O2	32:2a:1487:G:N2	2.53	0.41
34:2c:112:SER:HB3	34:2c:115:LEU:HD12	2.02	0.41
35:2d:107:ARG:HA	35:2d:107:ARG:HD2	1.81	0.41
35:2d:200:GLU:O	35:2d:204:ILE:HG12	2.20	0.41
36:2e:31:LEU:HD22	36:2e:43:LEU:HD11	2.01	0.41
40:2i:17:VAL:HG21	40:2i:80:GLY:HA3	2.02	0.41
42:2k:53:SER:C	42:2k:55:LYS:H	2.28	0.41
52:2u:12:LYS:O	52:2u:16:GLY:N	2.53	0.41
1:1A:234:C:H2'	1:1A:235:U:C6	2.56	0.41
1:1A:818:G:H4'	1:1A:838:C:O3'	2.19	0.41
1:1A:1802:A:N1	1:1A:1822:G:H1'	2.35	0.41
1:1A:2451:A:C2	54:1w:230:MEQ:HE1	2.55	0.41
1:1A:2789:C:H1'	1:1A:2892:A:H2	1.85	0.41
32:1a:177:C:H2'	32:1a:178:C:C6	2.55	0.41
32:1a:691:G:H2'	32:1a:692:U:C6	2.55	0.41
32:1a:814:A:H2'	32:1a:816:A:H5''	2.02	0.41
32:1a:1221:G:OP1	32:1a:1320:C:N4	2.41	0.41
32:1a:1284:C:H3'	32:1a:1285:A:C8	2.55	0.41
32:1a:1402:4OC:H2'	32:1a:1403:C:O4'	2.20	0.41
35:1d:129:ASN:OD1	35:1d:145:GLU:N	2.53	0.41
39:1h:49:GLU:O	39:1h:51:VAL:HG23	2.20	0.41
40:1i:21:PRO:HA	40:1i:59:PHE:HA	2.02	0.41
1:2A:84:A:OP2	20:2Y:8:LYS:NZ	2.51	0.41
1:2A:211:A:H2'	1:2A:212:G:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1530:C:H42	1:2A:1539:G:H1	1.67	0.41
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.20	0.41
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.20	0.41
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.20	0.41
1:2A:2689:U:H4'	1:2A:2690:C:H5'	2.02	0.41
14:2S:101:LEU:O	14:2S:101:LEU:HD23	2.20	0.41
14:2S:110:LEU:HD12	14:2S:110:LEU:HA	1.79	0.41
32:2a:34:C:H2'	32:2a:35:G:H8	1.85	0.41
32:2a:1264:C:N3	32:2a:1265:G:N7	2.68	0.41
32:2a:1367:C:H5'	41:2j:60:ARG:CZ	2.50	0.41
32:2a:1400:5MC:N4	55:2x:34:G:H1'	2.36	0.41
34:2c:71:ALA:HA	34:2c:106:VAL:HB	2.01	0.41
36:2e:6:PHE:CE1	36:2e:36:ASP:HB3	2.55	0.41
36:2e:19:MET:SD	36:2e:24:ARG:HB3	2.60	0.41
37:2f:1:MET:HA	37:2f:67:MET:O	2.20	0.41
38:2g:74:GLU:HG2	38:2g:91:VAL:HG22	2.00	0.41
41:2j:65:LEU:HD12	45:2n:55:GLY:O	2.20	0.41
44:2m:97:PRO:N	44:2m:110:ARG:HG2	2.35	0.41
54:2w:240:ARG:HB2	54:2w:251:THR:HG22	2.02	0.41
1:1A:639:U:H2'	1:1A:640:C:C6	2.55	0.41
1:1A:746:A:H2'	1:1A:2612:C:H5''	2.03	0.41
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.35	0.41
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.34	0.41
1:1A:1997:G:O2'	1:1A:1998:G:H5'	2.20	0.41
1:1A:2162:G:O2'	1:1A:2163:C:H5'	2.20	0.41
1:1A:2854:G:H2'	1:1A:2855:C:C6	2.55	0.41
3:1D:34:VAL:HA	3:1D:62:TYR:O	2.20	0.41
11:1P:59:LEU:HD21	30:18:10:ALA:HB2	2.01	0.41
17:1V:71:LEU:HD23	17:1V:71:LEU:HA	1.91	0.41
22:10:43:THR:O	22:10:43:THR:HG23	2.20	0.41
32:1a:982:U:H4'	32:1a:983:A:O5'	2.21	0.41
32:1a:1286:A:N6	32:1a:1354:C:O3'	2.54	0.41
37:1f:67:MET:HB2	37:1f:68:PRO:HD2	2.02	0.41
41:1j:44:VAL:HG11	41:1j:46:ARG:HH21	1.85	0.41
44:1m:14:ARG:HG2	44:1m:44:ARG:NH2	2.36	0.41
1:2A:859:G:O2'	1:2A:916:G:O6	2.35	0.41
1:2A:1016:G:H2'	1:2A:1017:G:O4'	2.20	0.41
1:2A:1036:G:P	7:2H:59:ARG:HD2	2.60	0.41
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.19	0.41
1:2A:1409:C:H2'	1:2A:1410:G:C8	2.54	0.41
1:2A:2695:C:H2'	1:2A:2696:U: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:2729:G:O2'	4:2E:186:GLY:HA3	2.21	0.41
5:2F:93:LYS:HD3	5:2F:93:LYS:HA	1.93	0.41
9:2N:28:THR:HG22	9:2N:29:LYS:HG3	2.02	0.41
11:2P:6:LEU:HD23	11:2P:6:LEU:HA	1.91	0.41
14:2S:67:ARG:HD2	14:2S:71:ARG:HH22	1.85	0.41
32:2a:164:U:H2'	32:2a:165:C:C6	2.55	0.41
32:2a:409:G:H1	32:2a:433:C:H42	1.68	0.41
32:2a:441:A:H3'	32:2a:442:C:H6	1.85	0.41
32:2a:1308:U:H5''	44:2m:98:VAL:CG2	2.50	0.41
33:2b:16:HIS:HB2	33:2b:204:ASN:CB	2.50	0.41
34:2c:82:GLU:HA	34:2c:85:ARG:HH11	1.84	0.41
35:2d:21:LEU:HD21	35:2d:67:ILE:HA	2.02	0.41
38:2g:111:ARG:NH2	38:2g:122:HIS:HB3	2.35	0.41
1:1A:1056:G:C2'	1:1A:1103:A:H61	2.33	0.41
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.56	0.41
1:1A:1412:A:H2'	1:1A:1413:G:C8	2.55	0.41
1:1A:1417:C:H2'	1:1A:1418:G:O4'	2.20	0.41
1:1A:1449:A:H2'	1:1A:1450:G:O4'	2.21	0.41
1:1A:2235:G:H2'	1:1A:2236:C:C6	2.56	0.41
2:1B:96:U:H2'	2:1B:97:G:C8	2.56	0.41
3:1D:92:ILE:HD12	3:1D:104:TYR:CD1	2.55	0.41
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.19	0.41
15:1T:41:ARG:CZ	32:1a:345:C:H3'	2.50	0.41
22:10:82:ARG:HE	22:10:82:ARG:HB2	1.47	0.41
26:14:53:GLU:CB	26:14:55:ARG:H	2.33	0.41
32:1a:1058:G:C6	32:1a:1059:C:C4	3.09	0.41
32:1a:1305:G:H5''	52:1u:4:GLY:HA3	2.01	0.41
34:1c:164:ARG:HD2	34:1c:166:GLU:OE1	2.21	0.41
38:1g:100:ALA:O	38:1g:104:LEU:HD13	2.19	0.41
42:1k:115:PRO:C	42:1k:117:ASN:H	2.29	0.41
48:1q:57:VAL:HG12	48:1q:76:LEU:HA	2.02	0.41
1:2A:1022:G:N2	1:2A:1023:U:O4	2.45	0.41
1:2A:1319:G:C6	1:2A:1320:C:N4	2.88	0.41
1:2A:1902:C:H5'	3:2D:246:PRO:HD3	2.03	0.41
1:2A:2182:G:H2'	1:2A:2183:C:C6	2.55	0.41
1:2A:2851:A:H2'	1:2A:2852:G:O4'	2.21	0.41
3:2D:16:MET:HE3	3:2D:16:MET:HB2	1.89	0.41
7:2H:24:VAL:HG21	7:2H:72:ILE:HG12	2.02	0.41
15:2T:19:LEU:HD22	15:2T:86:ILE:HD12	2.02	0.41
15:2T:41:ARG:HD2	32:2a:345:C:OP1	2.20	0.41
32:2a:41:G:H2'	32:2a:42:G:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:298:A:H8	32:2a:298:A:OP1	2.03	0.41
32:2a:520:A:N1	32:2a:536:C:H1'	2.35	0.41
32:2a:670:G:H2'	32:2a:671:G:O4'	2.20	0.41
32:2a:741:G:H5''	46:2o:59:MET:HE1	2.03	0.41
32:2a:1309:G:OP1	44:2m:88:ARG:NH2	2.47	0.41
32:2a:1356:G:H2'	32:2a:1357:A:C8	2.55	0.41
32:2a:1460:A:H2'	32:2a:1461:G:O4'	2.21	0.41
34:2c:85:ARG:O	34:2c:89:GLU:HB2	2.20	0.41
36:2e:27:ARG:HD3	36:2e:47:LYS:HB3	2.01	0.41
37:2f:22:GLU:OE2	37:2f:84:ASN:ND2	2.42	0.41
37:2f:92:LYS:HB2	37:2f:92:LYS:HE3	1.86	0.41
38:2g:126:ASP:HB3	38:2g:131:LYS:HB2	2.02	0.41
40:2i:113:LYS:HD3	40:2i:119:ALA:O	2.20	0.41
46:2o:40:SER:O	46:2o:44:LYS:HG3	2.21	0.41
54:2w:216:GLU:HB3	54:2w:245:PRO:HD3	2.02	0.41
54:2w:228:GLY:C	55:2x:76:8AN:H5'A	2.46	0.41
1:1A:27:G:C2	1:1A:512:G:N3	2.89	0.41
1:1A:1092:C:H2'	1:1A:1093:G:H8	1.85	0.41
1:1A:1668:A:H4'	1:1A:1669:A:O5'	2.20	0.41
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.20	0.41
6:1G:108:ASN:O	6:1G:112:PRO:HG2	2.19	0.41
8:1I:109:ILE:HD12	8:1I:109:ILE:HA	1.89	0.41
11:1P:95:VAL:HG23	11:1P:123:LEU:HD12	2.02	0.41
26:14:46:GLN:HB2	26:14:48:ARG:HG2	2.02	0.41
32:1a:192:U:O3'	51:1t:57:ARG:HD2	2.20	0.41
32:1a:358:U:H2'	32:1a:359:U:H6	1.86	0.41
32:1a:690:G:C6	32:1a:691:G:C6	3.09	0.41
32:1a:719:C:O2'	49:1r:50:ILE:O	2.36	0.41
32:1a:776:G:HO2'	32:1a:777:A:H8	1.64	0.41
32:1a:1006:C:H42	32:1a:1023:G:H1	1.68	0.41
32:1a:1277:C:O2'	32:1a:1279:A:H8	2.04	0.41
34:1c:112:SER:O	34:1c:116:VAL:HG23	2.20	0.41
36:1e:78:HIS:CE1	36:1e:142:LEU:HA	2.55	0.41
47:1p:57:ARG:HG3	47:1p:79:VAL:HG13	2.01	0.41
1:2A:637:A:H2'	11:2P:117:GLU:OE1	2.20	0.41
1:2A:890:A:H2'	1:2A:892:G:H8	1.85	0.41
7:2H:126:PRO:HB2	7:2H:127:GLU:H	1.70	0.41
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	2.01	0.41
32:2a:90:U:H2'	32:2a:91:C:H6	1.84	0.41
32:2a:418:C:H1'	32:2a:540:G:O2'	2.19	0.41
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:103:VAL:HG11	39:2h:136:GLU:HB2	2.02	0.41
42:2k:20:TYR:O	42:2k:30:VAL:HA	2.21	0.41
50:2s:15:LEU:HD13	50:2s:33:THR:HB	2.02	0.41
52:2u:20:LYS:O	52:2u:23:PRO:HD3	2.21	0.41
1:1A:139(A):G:O2'	1:1A:140:G:H5'	2.20	0.41
1:1A:222:A:H3'	1:1A:421:U:H5'	2.02	0.41
1:1A:373:U:H2'	1:1A:374:A:H8	1.86	0.41
1:1A:444:C:H4'	5:1F:49:ALA:HB2	2.03	0.41
1:1A:706:A:H2'	1:1A:707:G:O4'	2.20	0.41
1:1A:715:G:C4	46:1o:56:LEU:HD21	2.55	0.41
1:1A:1803:A:H2'	1:1A:1804:C:O4'	2.21	0.41
1:1A:2059:A:OP2	61:1A:4244:HOH:O	2.21	0.41
1:1A:2134:A:HO2'	1:1A:2135:A:P	2.39	0.41
1:1A:2185:C:H2'	1:1A:2186:G:H8	1.83	0.41
1:1A:2787:C:H2'	1:1A:2788:C:C6	2.56	0.41
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.21	0.41
15:1T:91:ARG:NE	15:1T:124:ASP:OD2	2.53	0.41
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	2.02	0.41
22:10:10:THR:HG22	22:10:12:ASN:N	2.33	0.41
32:1a:141:A:H1'	32:1a:182:U:O2	2.20	0.41
32:1a:152:A:H3'	32:1a:153:C:H6	1.86	0.41
32:1a:1277:C:H1'	32:1a:1282:C:O2	2.20	0.41
34:1c:134:ILE:HG23	34:1c:151:VAL:HB	2.03	0.41
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.21	0.41
1:2A:748:G:O6	18:2W:90:ARG:NH1	2.54	0.41
1:2A:910:A:C6	1:2A:911:A:C6	3.08	0.41
1:2A:1359:A:C2	1:2A:1372:U:O4	2.74	0.41
1:2A:1570:A:H2'	1:2A:1571:A:C8	2.56	0.41
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.56	0.41
1:2A:2080:G:H5''	23:21:19:GLN:HG3	2.03	0.41
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.21	0.41
3:2D:38:LYS:HE2	3:2D:39:LYS:N	2.36	0.41
6:2G:41:GLN:HE22	6:2G:153:ARG:HG3	1.85	0.41
9:2N:73:THR:HA	9:2N:83:LYS:O	2.20	0.41
10:2O:70:LYS:HB3	10:2O:70:LYS:HE2	1.84	0.41
21:2Z:151:HIS:HA	21:2Z:170:THR:HA	2.01	0.41
27:25:41:PRO:HG2	27:25:44:THR:OG1	2.20	0.41
32:2a:134:A:H1'	32:2a:325:A:C5	2.56	0.41
32:2a:857:C:H2'	32:2a:858:G:O4'	2.20	0.41
32:2a:881:G:OP2	43:2l:12:ARG:NH2	2.53	0.41
32:2a:1001:A:H2'	32:2a:1001(A):G:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1038:C:H2'	32:2a:1039:C:H6	1.82	0.41
32:2a:1040:U:H3'	32:2a:1041:A:H8	1.86	0.41
32:2a:1213:A:C4	32:2a:1215:G:C8	3.09	0.41
32:2a:1240:U:H3'	32:2a:1241:G:H5'	2.02	0.41
32:2a:1321:C:H4'	44:2m:87:TYR:CZ	2.56	0.41
38:2g:73:MET:SD	38:2g:90:GLU:HG2	2.61	0.41
40:2i:114:TYR:HE1	41:2j:60:ARG:H	1.68	0.41
43:2l:46:LYS:HE3	43:2l:46:LYS:HB2	1.81	0.41
1:1A:127:A:H5''	1:1A:128:C:C6	2.55	0.41
1:1A:590:A:H2'	1:1A:591:C:O4'	2.21	0.41
1:1A:2123:G:O2'	1:1A:2124:G:H8	2.02	0.41
1:1A:2200:C:O2	1:1A:2226:C:N4	2.52	0.41
1:1A:2375:G:O2'	1:1A:2377:A:N7	2.45	0.41
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.55	0.41
15:1T:108:ARG:NH2	15:1T:112:ARG:HD3	2.35	0.41
21:1Z:62:PRO:C	21:1Z:64:GLY:H	2.29	0.41
26:14:61:ARG:HG2	26:14:62:ARG:H	1.85	0.41
32:1a:5:U:C4	35:1d:86:LYS:HE2	2.56	0.41
32:1a:119:A:H4'	32:1a:120:A:C8	2.56	0.41
32:1a:443:C:H2'	32:1a:444:C:C6	2.55	0.41
32:1a:688:G:O2'	32:1a:704:A:N1	2.40	0.41
32:1a:977:A:H1'	32:1a:982:U:O4	2.20	0.41
32:1a:994:A:N7	32:1a:1216:G:H4'	2.36	0.41
32:1a:995:C:O2'	32:1a:996:A:H5'	2.21	0.41
32:1a:1047:G:H1'	32:1a:1215:G:O2'	2.20	0.41
32:1a:1245:A:H2'	32:1a:1246:C:O4'	2.21	0.41
33:1b:231:GLU:HB3	33:1b:232:PRO:HD3	2.02	0.41
43:1l:33:ARG:HD2	43:1l:33:ARG:HA	1.99	0.41
46:1o:4:THR:OG1	46:1o:7:GLU:HG3	2.21	0.41
1:2A:494:G:H4'	18:2W:6:ILE:HB	2.02	0.41
1:2A:637:A:OP1	11:2P:133:SER:OG	2.22	0.41
1:2A:875:G:H5''	21:2Z:149:SER:HB3	2.02	0.41
1:2A:1028:A:N3	1:2A:2486:G:O2'	2.52	0.41
1:2A:1339:G:H5''	19:2X:16:LYS:HD3	2.03	0.41
1:2A:1470:G:H5''	1:2A:1471:A:OP1	2.20	0.41
1:2A:1799:G:C2	3:2D:155:LEU:HD13	2.56	0.41
1:2A:1942:5MC:C4	1:2A:1943:U:C4	3.09	0.41
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.55	0.41
3:2D:182:LEU:HB3	3:2D:271:ILE:HB	2.01	0.41
5:2F:112:MET:HE3	5:2F:112:MET:HB2	1.83	0.41
11:2P:93:GLY:O	11:2P:123:LEU:HD13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:163:LEU:HD23	21:2Z:163:LEU:HA	1.83	0.41
32:2a:107:G:C2	32:2a:108:G:H1'	2.55	0.41
32:2a:286:G:C6	32:2a:287:U:C4	3.09	0.41
32:2a:626:U:H5''	47:2p:38:TYR:CD2	2.56	0.41
32:2a:1005:A:P	32:2a:1006:C:H41	2.44	0.41
32:2a:1074:G:O2'	32:2a:1101:A:N1	2.48	0.41
32:2a:1169:A:H2'	32:2a:1170:A:C8	2.55	0.41
32:2a:1234:C:H1'	32:2a:1364:U:O2	2.21	0.41
32:2a:1320:C:H1'	50:2s:73:GLU:HG3	2.01	0.41
33:2b:170:GLU:O	33:2b:174:VAL:HG23	2.21	0.41
34:2c:85:ARG:CZ	34:2c:85:ARG:HB2	2.50	0.41
35:2d:78:LEU:HG	35:2d:96:LEU:HB3	2.02	0.41
41:2j:44:VAL:HG21	41:2j:66:ARG:NH1	2.36	0.41
45:2n:8:GLU:HA	45:2n:11:LYS:HE2	2.02	0.41
50:2s:27:GLU:HB2	50:2s:28:LYS:HB3	2.03	0.41
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.56	0.41
1:1A:412:A:OP1	61:1A:4245:HOH:O	2.22	0.41
1:1A:744:G:OP1	4:1E:132:HIS:ND1	2.45	0.41
1:1A:2049:G:N7	61:1A:4332:HOH:O	2.37	0.41
1:1A:2098:U:H3	1:1A:2191:G:H1	1.67	0.41
1:1A:2126:A:C5	1:1A:2163:C:H1'	2.55	0.41
5:1F:29:ASN:HB3	5:1F:112:MET:HE1	2.03	0.41
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.85	0.41
12:1Q:103:MET:HE1	12:1Q:125:LEU:HD13	2.02	0.41
13:1R:8:ARG:HE	13:1R:43:GLU:CG	2.34	0.41
17:1V:98:GLU:CD	17:1V:100:ARG:HH11	2.29	0.41
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.39	0.41
20:1Y:30:VAL:O	20:1Y:32:PRO:HD3	2.20	0.41
21:1Z:99:TYR:HA	21:1Z:124:ILE:O	2.21	0.41
32:1a:149:A:H2'	32:1a:150:C:C6	2.56	0.41
32:1a:474:G:H2'	32:1a:475:G:C8	2.56	0.41
32:1a:976:G:OP1	45:1n:32:SER:N	2.38	0.41
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.34	0.41
34:1c:25:GLY:C	34:1c:27:LYS:H	2.28	0.41
35:1d:174:LEU:HD23	35:1d:174:LEU:HA	1.94	0.41
44:1m:74:VAL:O	44:1m:78:ILE:HG12	2.21	0.41
1:2A:117:G:OP2	1:2A:119:A:O2'	2.25	0.41
1:2A:582:G:H2'	1:2A:583:G:C8	2.56	0.41
1:2A:2582:G:C2	1:2A:2583:G:C8	3.08	0.41
1:2A:2748:A:N3	7:2H:63:SER:HB3	2.35	0.41
1:2A:2752:C:H2'	1:2A:2753:A:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2854:G:H2'	1:2A:2855:C:C6	2.56	0.41
6:2G:103:LEU:HD22	6:2G:178:PHE:CZ	2.55	0.41
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.20	0.41
13:2R:92:GLY:HA2	13:2R:94:TYR:CZ	2.55	0.41
32:2a:636:U:H2'	32:2a:637:G:C8	2.56	0.41
32:2a:758:G:O6	61:2a:1806:HOH:O	2.21	0.41
32:2a:1304:G:C6	32:2a:1305:G:N1	2.89	0.41
35:2d:58:LEU:O	35:2d:62:GLN:HG2	2.21	0.41
36:2e:95:ALA:O	36:2e:97:GLY:N	2.54	0.41
38:2g:78:ARG:HH21	38:2g:79:ARG:HH22	1.67	0.41
38:2g:79:ARG:H	38:2g:79:ARG:HG3	1.58	0.41
40:2i:16:ARG:HB2	40:2i:64:THR:HG23	2.03	0.41
44:2m:23:TYR:HD2	44:2m:67:GLU:HA	1.86	0.41
48:2q:19:VAL:HG23	48:2q:44:ALA:HB3	2.02	0.41
48:2q:87:LYS:H	48:2q:87:LYS:HG3	1.70	0.41
48:2q:94:ASN:O	48:2q:98:LEU:HD13	2.21	0.41
1:1A:228:A:H8	1:1A:229:A:H5'	1.85	0.41
1:1A:465:G:C6	1:1A:466:A:N6	2.89	0.41
1:1A:570:G:C6	1:1A:2030:A:C2	3.09	0.41
1:1A:605:C:H2'	1:1A:606:U:O4'	2.20	0.41
1:1A:1173:G:N1	1:1A:1176:G:OP2	2.53	0.41
1:1A:1197:G:H2'	1:1A:1198:U:C6	2.55	0.41
1:1A:1299:G:N7	61:1A:4323:HOH:O	2.36	0.41
1:1A:1448:G:O2'	1:1A:1528(A):A:N1	2.48	0.41
1:1A:1837:C:OP1	32:1a:784:C:H4'	2.20	0.41
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.21	0.41
1:1A:2155:G:N3	1:1A:2155:G:H2'	2.36	0.41
1:1A:2203:U:O2'	1:1A:2205:C:H5'	2.21	0.41
1:1A:2352:A:C4	1:1A:2366:A:C2	3.09	0.41
1:1A:2532:G:O2'	1:1A:2657:A:N1	2.52	0.41
1:1A:2852:G:H2'	1:1A:2853:C:O4'	2.21	0.41
7:1H:3:ARG:HE	7:1H:54:ARG:NH1	2.17	0.41
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.18	0.41
7:1H:38:SER:HB3	7:1H:41:MET:HG2	2.01	0.41
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.90	0.41
20:1Y:20:TYR:HB3	20:1Y:23:ARG:HG3	2.03	0.41
26:14:57:GLU:HA	26:14:58:ARG:HA	1.55	0.41
32:1a:262:A:H5'	51:1t:73:HIS:HB3	2.03	0.41
32:1a:271:C:H2'	32:1a:272:C:C6	2.56	0.41
32:1a:384:G:H2'	32:1a:385:C:C6	2.56	0.41
32:1a:402:G:OP1	35:1d:74:GLN:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:630:G:H2'	32:1a:631:G:C8	2.56	0.41
32:1a:631:G:H2'	32:1a:632:A:C8	2.56	0.41
32:1a:864:A:OP1	61:1a:1917:HOH:O	2.21	0.41
32:1a:943:U:H1'	40:1i:124:GLN:HE22	1.85	0.41
32:1a:966:M2G:CM1	40:1i:127:LYS:HD3	2.51	0.41
32:1a:1007:C:H42	32:1a:1022:G:H1	1.67	0.41
32:1a:1032:G:H2'	32:1a:1033:G:C8	2.56	0.41
32:1a:1117:G:H5''	40:1i:104:ARG:NH1	2.36	0.41
32:1a:1242:C:H42	32:1a:1295:G:H1	1.68	0.41
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.51	0.41
32:1a:1364:U:C6	52:1u:14:TRP:HH2	2.39	0.41
36:1e:31:LEU:HD23	36:1e:31:LEU:HA	1.96	0.41
37:1f:61:LEU:HD13	37:1f:63:TYR:OH	2.20	0.41
42:1k:34:ASP:OD1	42:1k:38:ASN:N	2.54	0.41
43:1l:60:LEU:HD23	43:1l:60:LEU:HA	1.84	0.41
44:1m:96:LEU:HB3	44:1m:97:PRO:HD2	2.03	0.41
52:1u:18:TYR:CZ	52:1u:24:ARG:HD3	2.56	0.41
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.63	0.41
1:2A:528:A:H8	9:2N:114:ARG:NH2	2.19	0.41
1:2A:627:A:C6	1:2A:637:A:C8	3.09	0.41
1:2A:679:C:H2'	1:2A:680:G:C8	2.55	0.41
1:2A:784:A:C5	3:2D:229:VAL:HG21	2.56	0.41
1:2A:839:U:H1'	1:2A:1191:G:H1'	2.02	0.41
1:2A:1419:A:C8	1:2A:1421:G:C6	3.09	0.41
1:2A:2316:C:H4'	6:2G:128:ARG:NH1	2.35	0.41
1:2A:2510:C:C4	1:2A:2511:U:C4	3.08	0.41
1:2A:2812:G:H2'	1:2A:2813:A:C8	2.55	0.41
1:2A:2821:A:C2	1:2A:2822:G:C4	3.08	0.41
1:2A:2872:G:C2	1:2A:2873:A:N6	2.88	0.41
5:2F:130:ALA:H	5:2F:142:TRP:CD1	2.38	0.41
6:2G:44:GLY:N	6:2G:88:ILE:O	2.52	0.41
6:2G:179:PRO:HG3	26:24:43:TYR:CZ	2.55	0.41
7:2H:71:LEU:HD12	7:2H:71:LEU:HA	1.93	0.41
9:2N:30:ILE:HG21	9:2N:120:LEU:HD13	2.03	0.41
13:2R:26:LYS:HE2	13:2R:70:LEU:O	2.20	0.41
16:2U:110:VAL:HG12	16:2U:114:LYS:HE3	2.02	0.41
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	2.03	0.41
32:2a:115:G:H4'	32:2a:116:A:O5'	2.20	0.41
32:2a:271:C:H2'	32:2a:272:C:C6	2.56	0.41
32:2a:420:U:H2'	32:2a:422:C:C5	2.56	0.41
32:2a:545:C:O2'	32:2a:549:C:OP1	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:946:A:H2'	32:2a:947:G:H8	1.86	0.41
32:2a:995:C:N3	32:2a:1046:A:O2'	2.45	0.41
32:2a:1265:G:C6	32:2a:1266:G:C5	3.09	0.41
33:2b:103:THR:HA	33:2b:180:LEU:HD21	2.03	0.41
34:2c:18:TRP:O	34:2c:54:ARG:NH2	2.54	0.41
35:2d:31:CYS:O	35:2d:35:ARG:HG3	2.21	0.41
36:2e:31:LEU:HD23	36:2e:31:LEU:HA	1.92	0.41
47:2p:6:LEU:HD23	47:2p:17:TYR:CG	2.55	0.41
49:2r:58:LEU:HD23	49:2r:58:LEU:HA	1.93	0.41
50:2s:18:LYS:HA	50:2s:21:GLU:HB2	2.02	0.41
54:2w:184:PRO:C	54:2w:186:THR:N	2.79	0.41
1:1A:128:C:H2'	1:1A:129:C:O4'	2.21	0.41
1:1A:581:C:H2'	1:1A:582:G:H8	1.86	0.41
1:1A:878:A:H2'	1:1A:879:G:H5'	2.03	0.41
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.54	0.41
26:14:13:ARG:O	26:14:30:GLU:HA	2.21	0.41
32:1a:130:A:C8	48:1q:63:ARG:HG3	2.55	0.41
32:1a:188:C:H4'	51:1t:89:ARG:CZ	2.51	0.41
32:1a:622:A:C8	32:1a:623:C:C6	3.09	0.41
32:1a:674:G:H2'	32:1a:675:A:H8	1.86	0.41
32:1a:1092:A:C6	32:1a:1093:A:C6	3.09	0.41
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.56	0.41
32:1a:1456:G:H1	51:1t:51:GLU:CD	2.29	0.41
33:1b:213:LEU:HB3	33:1b:214:ILE:HD12	2.02	0.41
34:1c:39:ILE:O	34:1c:43:LEU:HG	2.21	0.41
34:1c:85:ARG:O	34:1c:89:GLU:N	2.48	0.41
34:1c:110:ASN:OD1	34:1c:110:ASN:N	2.52	0.41
47:1p:28:ARG:HG3	47:1p:29:ASP:N	2.35	0.41
54:1w:136:GLU:C	54:1w:138:MET:H	2.29	0.41
1:2A:271(S):G:C6	1:2A:271(T):C:C4	3.08	0.41
1:2A:286:C:H2'	1:2A:287:C:C6	2.56	0.41
1:2A:581:C:H2'	1:2A:582:G:H8	1.84	0.41
1:2A:635:C:O2'	1:2A:639:U:OP1	2.38	0.41
1:2A:900:A:HO2'	1:2A:901:A:P	2.43	0.41
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.56	0.41
1:2A:1859:A:N6	1:2A:1883:G:O2'	2.53	0.41
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.56	0.41
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.56	0.41
1:2A:2469:A:HO2'	12:2Q:56:ARG:HE	1.62	0.41
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.21	0.41
4:2E:151:TYR:HB3	9:2N:79:PRO:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:11:TYR:O	6:2G:15:VAL:HG22	2.21	0.41
23:21:64:ALA:HA	23:21:67:ILE:HG13	2.03	0.41
24:22:25:VAL:HG13	24:22:57:ILE:HG23	2.03	0.41
32:2a:4:U:O4	39:2h:105:ARG:HD2	2.21	0.41
32:2a:826:C:H4'	39:2h:12:ARG:HG2	2.03	0.41
33:2b:119:GLU:CD	33:2b:153:ARG:HH12	2.29	0.41
35:2d:70:ILE:HD12	35:2d:100:ARG:HD2	2.02	0.41
40:2i:15:ALA:CB	40:2i:65:VAL:HG23	2.51	0.41
43:2l:57:LYS:HG2	43:2l:67:THR:HG22	2.04	0.41
51:2t:58:LYS:HA	51:2t:58:LYS:HD2	1.79	0.41
52:2u:12:LYS:HB3	52:2u:22:ARG:HH11	1.86	0.41
54:2w:319:PHE:CE2	54:2w:335:ILE:HG12	2.55	0.41
1:1A:295:G:H4'	20:1Y:1:MET:HE3	2.03	0.40
1:1A:488:G:O2'	18:1W:49:LYS:NZ	2.44	0.40
1:1A:709:U:H2'	1:1A:710:G:H8	1.86	0.40
1:1A:1445:A:H4'	1:1A:1445(A):C:OP2	2.21	0.40
1:1A:1550:C:OP1	1:1A:1720:U:O2'	2.25	0.40
1:1A:2109:U:O4	1:1A:2179:C:N4	2.54	0.40
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.54	0.40
1:1A:2691:C:O3'	1:1A:2871:C:H4'	2.21	0.40
3:1D:97:TYR:C	3:1D:99:ASP:N	2.79	0.40
5:1F:107:LYS:HG3	5:1F:206:ILE:HA	2.02	0.40
20:1Y:43:ASN:HA	20:1Y:43:ASN:HD22	1.50	0.40
32:1a:130:A:N3	32:1a:263:A:O2'	2.46	0.40
32:1a:738:C:H2'	32:1a:739:C:C6	2.55	0.40
32:1a:986:A:H1'	50:1s:55:LYS:HA	2.03	0.40
32:1a:1007:C:N4	32:1a:1022:G:H1	2.19	0.40
32:1a:1036:G:H3'	32:1a:1037:C:H6	1.84	0.40
32:1a:1338:G:C6	32:1a:1339:A:C6	3.10	0.40
32:1a:1381:U:H1'	38:1g:79:ARG:HB3	2.02	0.40
32:1a:1519:MA6:H5''	32:1a:1520:G:OP2	2.20	0.40
33:1b:101:MET:HA	33:1b:108:ILE:HG13	2.03	0.40
33:1b:208:ILE:HA	33:1b:211:ILE:HD12	2.02	0.40
35:1d:17:VAL:HG12	35:1d:18:LYS:H	1.85	0.40
36:1e:7:GLU:N	36:1e:35:GLY:O	2.50	0.40
42:1k:103:LEU:HA	42:1k:103:LEU:HD23	1.83	0.40
48:1q:63:ARG:HG2	48:1q:64:PRO:HD2	2.03	0.40
50:1s:52:TYR:HA	50:1s:56:GLN:O	2.20	0.40
1:2A:263:C:H2'	1:2A:264:C:O4'	2.21	0.40
1:2A:303:U:H2'	1:2A:304:G:C8	2.56	0.40
1:2A:445:C:H5''	16:2U:3:ARG:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:760:G:H2'	1:2A:761:A:O4'	2.21	0.40
1:2A:945:A:C4	1:2A:2448:A:C2	3.08	0.40
1:2A:1200:C:H5'	61:2A:4949:HOH:O	2.20	0.40
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.21	0.40
1:2A:2405:G:H5'	11:2P:75:ILE:HD13	2.02	0.40
6:2G:124:SER:HB2	6:2G:131:TYR:CE1	2.56	0.40
8:2I:12:LEU:HD23	8:2I:12:LEU:HA	1.90	0.40
14:2S:36:TYR:OH	14:2S:54:LEU:HD22	2.21	0.40
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.23	0.40
32:2a:977:A:O2'	32:2a:981:U:N3	2.54	0.40
33:2b:16:HIS:HD2	33:2b:18:GLY:H	1.69	0.40
33:2b:97:TRP:HZ2	33:2b:102:LEU:HD13	1.85	0.40
35:2d:171:GLY:HA2	35:2d:172:PRO:HD3	1.96	0.40
1:1A:68:G:H2'	1:1A:69:C:O4'	2.21	0.40
1:1A:527:C:C4	1:1A:2779:U:H2'	2.56	0.40
1:1A:631:A:H2'	1:1A:632:A:O4'	2.21	0.40
1:1A:676:A:N1	1:1A:2069:G:O2'	2.52	0.40
1:1A:983:A:C6	1:1A:984:A:N1	2.89	0.40
1:1A:2145:C:H6	1:1A:2145:C:H2'	1.77	0.40
1:1A:2162:G:C2'	1:1A:2163:C:H5'	2.52	0.40
2:1B:57:A:H1'	6:1G:29:TRP:HB2	2.04	0.40
6:1G:11:TYR:O	6:1G:16:ARG:HG2	2.21	0.40
7:1H:22:GLY:HA2	7:1H:37:VAL:O	2.21	0.40
9:1N:96:GLU:CD	9:1N:96:GLU:H	2.30	0.40
11:1P:27:HIS:HB2	61:1P:309:HOH:O	2.21	0.40
12:1Q:8:LYS:HB3	12:1Q:8:LYS:HE2	1.90	0.40
21:1Z:158:PRO:O	21:1Z:161:VAL:HG13	2.22	0.40
23:11:82:LEU:HA	23:11:85:LEU:HD12	2.03	0.40
32:1a:96:U:H2'	32:1a:97:G:C8	2.56	0.40
32:1a:716:A:N3	42:1k:118:GLY:HA2	2.36	0.40
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	2.03	0.40
35:1d:63:LYS:HB2	35:1d:63:LYS:HE3	1.76	0.40
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.46	0.40
54:1w:349:ALA:HB1	54:1w:350:ALA:HB2	2.02	0.40
1:2A:357:A:H2'	1:2A:358:U:C6	2.56	0.40
1:2A:1466:G:O2'	1:2A:1546:C:O2'	2.38	0.40
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.56	0.40
1:2A:2592:G:H2'	1:2A:2593:U:O4'	2.21	0.40
6:2G:62:LEU:O	6:2G:143:GLU:HG2	2.21	0.40
9:2N:111:PRO:HA	9:2N:114:ARG:NH1	2.35	0.40
12:2Q:27:VAL:HB	12:2Q:134:ARG:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	2.03	0.40
21:2Z:29:TYR:HA	21:2Z:34:ASN:HA	2.02	0.40
28:26:38:LYS:HE3	28:26:38:LYS:HB3	1.69	0.40
32:2a:782:A:O3'	32:2a:1515:C:H4'	2.21	0.40
32:2a:838:G:H3'	32:2a:840:C:H41	1.86	0.40
32:2a:1015:A:O2'	32:2a:1218:C:O2'	2.37	0.40
32:2a:1168:A:C6	32:2a:1169:A:C6	3.10	0.40
37:2f:2:ARG:O	37:2f:66:GLU:HA	2.22	0.40
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.21	0.40
44:2m:33:ALA:O	44:2m:37:THR:OG1	2.22	0.40
1:1A:409:C:O2'	1:1A:410:G:H5'	2.22	0.40
1:1A:620:G:N3	1:1A:620:G:H2'	2.35	0.40
1:1A:720:C:H2'	1:1A:721:C:C6	2.55	0.40
1:1A:754:C:H2'	1:1A:755:C:C6	2.56	0.40
1:1A:1197:G:H2'	1:1A:1198:U:H6	1.86	0.40
1:1A:2104:G:H1	1:1A:2185:C:H42	1.69	0.40
1:1A:2115:G:H1	1:1A:2119:A:P	2.43	0.40
1:1A:2156:G:H8	1:1A:2156:G:OP2	2.05	0.40
1:1A:2235:G:N7	61:1A:4334:HOH:O	2.37	0.40
1:1A:2348:U:O4	1:1A:2382:G:N1	2.55	0.40
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.22	0.40
1:1A:2439:A:H5'	1:1A:2439:A:C8	2.56	0.40
3:1D:68:LYS:HB2	3:1D:70:TRP:CZ2	2.57	0.40
5:1F:64:ILE:HG23	5:1F:76:GLY:O	2.21	0.40
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.78	0.40
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.22	0.40
13:1R:38:VAL:HB	13:1R:39:PRO:HD3	2.03	0.40
24:12:62:THR:O	24:12:66:GLU:HG3	2.22	0.40
32:1a:271:C:H2'	32:1a:272:C:H6	1.86	0.40
32:1a:1038:C:H2'	32:1a:1039:C:C6	2.56	0.40
32:1a:1139:G:N2	32:1a:1143:G:C6	2.90	0.40
32:1a:1299:A:O2'	32:1a:1300:G:H4'	2.21	0.40
32:1a:1312:G:H5'	50:1s:5:LEU:HD12	2.03	0.40
32:1a:1434:A:H2'	32:1a:1435:G:O4'	2.22	0.40
33:1b:16:HIS:C	33:1b:17:PHE:HD2	2.30	0.40
34:1c:16:ARG:NH1	34:1c:183:ASP:OD1	2.54	0.40
35:1d:105:VAL:HG21	35:1d:126:ILE:HD13	2.03	0.40
40:1i:114:TYR:HE1	41:1j:59:SER:HA	1.86	0.40
49:1r:26:LEU:HD23	49:1r:29:PHE:CD2	2.56	0.40
51:1t:87:LYS:O	51:1t:91:LEU:HG	2.21	0.40
54:1w:116:GLY:HA3	54:1w:120:ALA:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:248:G:C2	1:2A:2431:U:H4'	2.57	0.40
1:2A:320:A:H4'	1:2A:322:A:N7	2.36	0.40
1:2A:657:U:H2'	1:2A:658:C:H6	1.84	0.40
1:2A:679:C:H2'	1:2A:680:G:H8	1.86	0.40
1:2A:729:G:O2'	1:2A:763:G:H4'	2.21	0.40
1:2A:814:C:H2'	1:2A:815:C:H6	1.85	0.40
1:2A:1420:U:HO2'	1:2A:1421:G:H8	1.70	0.40
1:2A:2100:G:H2'	1:2A:2101:G:O4'	2.21	0.40
1:2A:2316:C:H2'	1:2A:2317:C:H6	1.87	0.40
1:2A:2378:A:C5	1:2A:2379:G:H1'	2.56	0.40
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.21	0.40
15:2T:119:LYS:O	15:2T:123:GLN:HG3	2.21	0.40
32:2a:17:U:H2'	32:2a:18:C:H6	1.85	0.40
32:2a:779:C:O2'	42:2k:120:ARG:HD3	2.21	0.40
32:2a:790:A:C6	32:2a:791:G:C6	3.09	0.40
32:2a:1060:C:C5'	41:2j:51:ARG:HG2	2.49	0.40
37:2f:35:ALA:CA	37:2f:67:MET:HB3	2.49	0.40
40:2i:23:ASN:HB2	40:2i:25:LYS:HZ2	1.87	0.40
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.46	0.40
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.83	0.40
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.03	0.40
8:1I:40:THR:HG22	8:1I:43:ASN:OD1	2.21	0.40
8:1I:79:ILE:HB	8:1I:144:VAL:HG12	2.04	0.40
32:1a:875:C:H1'	39:1h:15:ASN:OD1	2.22	0.40
32:1a:1027:C:H5	32:1a:1028:C:C4	2.40	0.40
32:1a:1286:A:C8	32:1a:1287:A:H4'	2.53	0.40
32:1a:1312:G:C2	32:1a:1326:C:C2	3.10	0.40
35:1d:10:ARG:HB2	35:1d:40:PRO:HG3	2.02	0.40
36:1e:35:GLY:HA2	36:1e:40:ARG:O	2.20	0.40
44:1m:34:LEU:HD23	44:1m:56:LEU:HD11	2.03	0.40
1:2A:192:C:O2'	1:2A:802:A:N3	2.51	0.40
1:2A:702:G:C2	1:2A:731:C:C2	3.09	0.40
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.21	0.40
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.09	0.40
1:2A:1359:A:H2	1:2A:1372:U:O4	2.04	0.40
1:2A:2131:G:H5''	1:2A:2133:G:O4'	2.21	0.40
1:2A:2507:C:H4'	54:2w:233:ASN:O	2.21	0.40
12:2Q:41:TRP:HB3	12:2Q:94:VAL:HB	2.03	0.40
30:28:32:LEU:O	30:28:36:LYS:HE3	2.22	0.40
32:2a:16:A:N3	32:2a:1080:A:O2'	2.45	0.40
32:2a:141:A:H2'	32:2a:142:G:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:444:C:H2'	32:2a:445:G:H8	1.86	0.40
32:2a:607:A:C2	47:2p:31:LYS:HG3	2.56	0.40
32:2a:685:G:N1	32:2a:686:U:O4	2.54	0.40
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.37	0.40
32:2a:976:G:C8	32:2a:1358:U:C2	3.09	0.40
32:2a:1027:C:H3'	32:2a:1028:C:H6	1.85	0.40
32:2a:1165:C:H2'	32:2a:1166:G:H8	1.86	0.40
32:2a:1183:A:O2'	32:2a:1184:G:OP1	2.36	0.40
32:2a:1240:U:H3'	32:2a:1241:G:C5'	2.51	0.40
32:2a:1465:C:H2'	32:2a:1466:C:O4'	2.22	0.40
38:2g:46:ALA:O	38:2g:50:ILE:N	2.46	0.40
51:2t:10:LEU:HB3	51:2t:12:ALA:H	1.87	0.40
55:2x:48:G:H3'	61:2x:202:HOH:O	2.20	0.40
1:1A:609:A:H2'	1:1A:610:G:O4'	2.21	0.40
1:1A:1243:G:OP2	61:1A:4246:HOH:O	2.22	0.40
1:1A:1759:A:H1'	1:1A:2711:A:C2	2.56	0.40
1:1A:2152:G:H2'	1:1A:2153:G:H8	1.86	0.40
5:1F:136:THR:HA	5:1F:166:ALA:O	2.21	0.40
20:1Y:19:LYS:HB3	20:1Y:19:LYS:HE2	1.76	0.40
23:11:50:ARG:HD2	23:11:57:GLU:OE2	2.21	0.40
32:1a:175:C:H2'	32:1a:176:C:C6	2.57	0.40
32:1a:413:G:H21	32:1a:428:G:H1'	1.86	0.40
32:1a:629:G:H2'	32:1a:630:G:O4'	2.21	0.40
32:1a:971:G:N1	32:1a:1363(A):A:OP2	2.52	0.40
34:1c:188:LEU:HD12	34:1c:188:LEU:HA	1.96	0.40
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	2.03	0.40
35:1d:201:GLN:HE21	35:1d:201:GLN:HB3	1.58	0.40
36:1e:60:TYR:CE1	36:1e:64:ARG:HD2	2.57	0.40
51:1t:63:ILE:HD13	51:1t:80:ARG:HB3	2.03	0.40
54:1w:102:MET:O	54:1w:104:GLU:N	2.55	0.40
1:2A:265:A:H1'	1:2A:266:G:O4'	2.21	0.40
1:2A:288:C:H2'	1:2A:289:A:C8	2.56	0.40
1:2A:448:U:C4	1:2A:583:G:H1'	2.56	0.40
1:2A:698:C:O2'	1:2A:734:A:N6	2.54	0.40
1:2A:1908:C:O2	55:2x:12:A:H4'	2.22	0.40
1:2A:2845:G:H2'	1:2A:2846:G:C8	2.56	0.40
3:2D:52:ARG:O	3:2D:54:ARG:HG2	2.21	0.40
3:2D:146:GLU:HB2	3:2D:189:CYS:HB3	2.03	0.40
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.46	0.40
8:2I:79:ILE:N	8:2I:143:SER:O	2.49	0.40
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.61	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:59:ALA:HB1	17:2V:94:LEU:HB3	2.04	0.40
21:2Z:27:VAL:HG13	21:2Z:29:TYR:HD2	1.86	0.40
21:2Z:153:SER:OG	21:2Z:154:ASP:N	2.55	0.40
32:2a:323:U:H4'	51:2t:22:ARG:HB2	2.03	0.40
32:2a:446:G:H3'	32:2a:447:G:H8	1.86	0.40
32:2a:988:G:C2	32:2a:989:C:H1'	2.56	0.40
35:2d:162:LEU:HD13	35:2d:181:MET:HG2	2.04	0.40
36:2e:105:VAL:HG21	36:2e:128:PRO:HB3	2.04	0.40
37:2f:96:PRO:HB3	49:2r:30:ASP:CG	2.47	0.40
42:2k:48:ILE:HD13	42:2k:63:LEU:HB2	2.04	0.40
44:2m:94:ARG:HB3	44:2m:96:LEU:HG	2.03	0.40
45:2n:11:LYS:H	45:2n:11:LYS:HG3	1.67	0.40
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	261 (96%)	12 (4%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	37
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	37
5	1F	201/210 (96%)	193 (96%)	6 (3%)	2 (1%)	12	20
5	2F	201/210 (96%)	188 (94%)	12 (6%)	1 (0%)	24	37
6	1G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	21	32
6	2G	179/182 (98%)	157 (88%)	18 (10%)	4 (2%)	5	6
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	21	32
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	21	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	1I	144/148 (97%)	125 (87%)	17 (12%)	2 (1%)	9	13
8	2I	144/148 (97%)	127 (88%)	15 (10%)	2 (1%)	9	13
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16	25
11	1P	147/150 (98%)	139 (95%)	7 (5%)	1 (1%)	18	28
11	2P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	28
12	1Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	18	28
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	18	28
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	22
14	1S	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	14	22
14	2S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	14	22
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	25
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	20
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	18
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	18
20	1Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
20	2Y	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
21	1Z	148/206 (72%)	132 (89%)	13 (9%)	3 (2%)	6	7
21	2Z	156/206 (76%)	141 (90%)	12 (8%)	3 (2%)	6	8
22	10	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
22	20	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	18
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	49 (73%)	11 (16%)	7 (10%)	0	0
26	24	67/71 (94%)	51 (76%)	9 (13%)	7 (10%)	0	0
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	194 (85%)	28 (12%)	7 (3%)	3	3
33	2b	229/256 (90%)	203 (89%)	19 (8%)	7 (3%)	3	3
34	1c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	12	20
34	2c	204/239 (85%)	174 (85%)	27 (13%)	3 (2%)	8	12
35	1d	206/209 (99%)	185 (90%)	21 (10%)	0	100	100
35	2d	206/209 (99%)	187 (91%)	19 (9%)	0	100	100
36	1e	146/162 (90%)	129 (88%)	16 (11%)	1 (1%)	18	28
36	2e	146/162 (90%)	138 (94%)	6 (4%)	2 (1%)	9	13
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	134 (88%)	17 (11%)	2 (1%)	9	14
38	2g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	6	7
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	1i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16	25
40	2i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	25
41	1j	95/105 (90%)	82 (86%)	9 (10%)	4 (4%)	2	2
41	2j	94/105 (90%)	76 (81%)	16 (17%)	2 (2%)	5	7
42	1k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	6	9
42	2k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	14	22
43	1l	119/132 (90%)	113 (95%)	5 (4%)	1 (1%)	16	25
43	2l	119/132 (90%)	112 (94%)	6 (5%)	1 (1%)	16	25
44	1m	116/126 (92%)	100 (86%)	14 (12%)	2 (2%)	7	10
44	2m	114/126 (90%)	94 (82%)	18 (16%)	2 (2%)	6	9
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
47	1p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	61 (92%)	3 (4%)	2 (3%)	3	3
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	12
50	1s	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
50	2s	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	10	16
51	1t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	3	3
51	2t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	5	7
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	16 (76%)	5 (24%)	0	100	100
54	1w	246/354 (70%)	228 (93%)	14 (6%)	4 (2%)	7	11
54	2w	250/354 (71%)	235 (94%)	13 (5%)	2 (1%)	16	25
56	1z	3/7 (43%)	3 (100%)	0	0	100	100
56	2z	2/7 (29%)	2 (100%)	0	0	100	100
All	All	11846/12850 (92%)	10950 (92%)	787 (7%)	109 (1%)	14	22

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	1Z	53	ILE
23	11	3	LYS
26	14	44	THR
26	14	55	ARG
26	14	62	ARG
26	14	63	TYR
33	1b	17	PHE
33	1b	126	GLU
34	1c	66	VAL
38	1g	80	VAL
40	1i	54	ASP
44	1m	67	GLU
44	1m	107	ALA
49	1r	25	THR
51	1t	10	LEU
54	1w	299	SER
5	2F	130	ALA
7	2H	126	PRO
11	2P	29	LYS
26	24	56	VAL
33	2b	17	PHE
33	2b	22	LYS
33	2b	78	GLN
38	2g	80	VAL
44	2m	106	ASN
5	1F	130	ALA
12	1Q	16	ARG
19	1X	93	GLU
26	14	49	PHE
34	1c	65	ALA
41	1j	55	LYS
42	1k	49	GLY
49	1r	36	ASN
51	1t	47	GLY
54	1w	103	ASP
54	1w	300	GLU
6	2G	42	GLY
6	2G	47	LYS
6	2G	52	ILE
14	2S	96	GLY
17	2V	79	VAL
26	24	62	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	79	ARG
34	2c	98	ASN
38	2g	52	GLU
50	2s	13	ASP
51	2t	95	ALA
54	2w	334	PRO
4	1E	52	LEU
8	1I	39	ALA
11	1P	29	LYS
33	1b	22	LYS
33	1b	123	ALA
33	1b	125	PRO
36	1e	85	GLY
38	1g	130	GLY
43	1l	105	TYR
4	2E	52	LEU
8	2I	117	GLU
10	2O	29	ASN
19	2X	93	GLU
21	2Z	52	SER
21	2Z	159	PRO
23	2l	3	LYS
26	24	44	THR
33	2b	20	GLU
5	1F	207	GLY
6	1G	43	LEU
14	1S	94	TYR
26	14	47	GLN
26	14	57	GLU
41	1j	33	GLN
41	1j	82	ILE
42	1k	104	GLN
51	1t	102	GLY
54	1w	206	GLU
12	2Q	60	ARG
21	2Z	142	SER
26	24	29	PRO
26	24	49	PHE
26	24	65	ASP
38	2g	4	ARG
40	2i	121	ARG
41	2j	33	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	79	ARG
43	2l	105	TYR
54	2w	209	ASP
21	1Z	156	LYS
33	1b	20	GLU
33	1b	231	GLU
41	1j	77	PRO
6	2G	43	LEU
33	2b	123	ALA
33	2b	124	SER
33	2b	125	PRO
36	2e	69	VAL
44	2m	75	ALA
51	2t	47	GLY
15	1T	37	GLY
26	24	47	GLN
42	2k	49	GLY
49	2r	25	THR
7	1H	126	PRO
21	1Z	157	LEU
8	1I	34	GLY
13	2R	32	GLY
34	2c	99	VAL
36	2e	96	PRO
8	2I	80	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	203 (94%)	12 (6%)	19	33
3	2D	215/218 (99%)	206 (96%)	9 (4%)	26	45
4	1E	164/166 (99%)	152 (93%)	12 (7%)	13	22
4	2E	164/166 (99%)	152 (93%)	12 (7%)	13	22
5	1F	160/166 (96%)	148 (92%)	12 (8%)	12	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	143 (90%)	16 (10%)	7	11
6	1G	143/156 (92%)	131 (92%)	12 (8%)	10	17
6	2G	143/156 (92%)	125 (87%)	18 (13%)	4	6
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	21
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6	9
8	1I	113/124 (91%)	100 (88%)	13 (12%)	5	8
8	2I	105/124 (85%)	90 (86%)	15 (14%)	3	4
9	1N	118/119 (99%)	110 (93%)	8 (7%)	14	25
9	2N	118/119 (99%)	106 (90%)	12 (10%)	7	11
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68	84
10	2O	100/100 (100%)	93 (93%)	7 (7%)	14	24
11	1P	115/116 (99%)	108 (94%)	7 (6%)	17	30
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26	44
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	20	35
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	24	42
13	1R	101/101 (100%)	94 (93%)	7 (7%)	14	24
13	2R	101/101 (100%)	98 (97%)	3 (3%)	36	58
14	1S	86/88 (98%)	77 (90%)	9 (10%)	6	10
14	2S	85/88 (97%)	78 (92%)	7 (8%)	10	18
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	24
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11	19
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26	44
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	35
17	1V	80/82 (98%)	79 (99%)	1 (1%)	61	80
17	2V	80/82 (98%)	76 (95%)	4 (5%)	22	38
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	26
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19	33
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61	80
19	2X	77/78 (99%)	72 (94%)	5 (6%)	15	27
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5	7
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	13	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	135/179 (75%)	117 (87%)	18 (13%)	4	5
21	2Z	137/179 (76%)	113 (82%)	24 (18%)	2	2
22	10	61/67 (91%)	60 (98%)	1 (2%)	55	76
22	20	61/67 (91%)	61 (100%)	0	100	100
23	11	80/83 (96%)	75 (94%)	5 (6%)	16	29
23	21	80/83 (96%)	73 (91%)	7 (9%)	9	15
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	57
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	14
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	20
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	31
26	14	59/63 (94%)	52 (88%)	7 (12%)	5	7
26	24	53/63 (84%)	47 (89%)	6 (11%)	5	8
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	11
27	25	50/52 (96%)	45 (90%)	5 (10%)	7	11
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	12
28	26	50/52 (96%)	46 (92%)	4 (8%)	11	19
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	22
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	22
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	33
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	51
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	60
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	60
33	1b	192/220 (87%)	161 (84%)	31 (16%)	2	3
33	2b	187/220 (85%)	155 (83%)	32 (17%)	2	2
34	1c	142/188 (76%)	129 (91%)	13 (9%)	8	14
34	2c	140/188 (74%)	132 (94%)	8 (6%)	18	33
35	1d	169/181 (93%)	151 (89%)	18 (11%)	6	10
35	2d	173/181 (96%)	156 (90%)	17 (10%)	7	12
36	1e	113/123 (92%)	106 (94%)	7 (6%)	16	29
36	2e	114/123 (93%)	104 (91%)	10 (9%)	9	15
37	1f	84/90 (93%)	79 (94%)	5 (6%)	17	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23	41
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5	7
38	2g	120/127 (94%)	115 (96%)	5 (4%)	26	45
39	1h	114/119 (96%)	104 (91%)	10 (9%)	9	15
39	2h	114/119 (96%)	106 (93%)	8 (7%)	14	24
40	1i	90/99 (91%)	73 (81%)	17 (19%)	1	2
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6	9
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6	10
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	8
42	1k	82/99 (83%)	76 (93%)	6 (7%)	13	22
42	2k	83/99 (84%)	78 (94%)	5 (6%)	17	31
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21	36
43	2l	96/108 (89%)	90 (94%)	6 (6%)	16	29
44	1m	89/101 (88%)	76 (85%)	13 (15%)	3	4
44	2m	88/101 (87%)	77 (88%)	11 (12%)	4	6
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	18
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	18
46	1o	78/80 (98%)	68 (87%)	10 (13%)	4	6
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12	20
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	8
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	5
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	12
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26	44
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21	37
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	16
50	1s	69/80 (86%)	61 (88%)	8 (12%)	5	8
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	7
51	1t	70/82 (85%)	69 (99%)	1 (1%)	59	79
51	2t	70/82 (85%)	67 (96%)	3 (4%)	26	44
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	1w	203/298 (68%)	184 (91%)	19 (9%)	8	13
54	2w	203/298 (68%)	180 (89%)	23 (11%)	5	8
56	1z	2/3 (67%)	2 (100%)	0	100	100
56	2z	2/3 (67%)	2 (100%)	0	100	100
All	All	9697/10666 (91%)	8887 (92%)	810 (8%)	10	17

All (810) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	38	LYS
3	1D	71	ASP
3	1D	82	ILE
3	1D	99	ASP
3	1D	106	ILE
3	1D	113	VAL
3	1D	173	VAL
3	1D	183	ARG
3	1D	200	ASP
3	1D	229	VAL
3	1D	259	THR
4	1E	7	VAL
4	1E	64	LYS
4	1E	72	VAL
4	1E	75	VAL
4	1E	90	THR
4	1E	116	VAL
4	1E	163	GLU
4	1E	170	LEU
4	1E	178	GLU
4	1E	181	LEU
4	1E	188	VAL
4	1E	195	LEU
5	1F	24	LEU
5	1F	28	ILE
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	72	ARG
5	1F	137	LYS
5	1F	162	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	183	VAL
5	1F	191	ARG
5	1F	192	LEU
5	1F	205	ARG
6	1G	3	LEU
6	1G	22	ARG
6	1G	31	VAL
6	1G	70	VAL
6	1G	77	ILE
6	1G	78	SER
6	1G	79	ASN
6	1G	109	VAL
6	1G	140	ILE
6	1G	148	MET
6	1G	159	VAL
6	1G	174	GLU
7	1H	44	VAL
7	1H	45	VAL
7	1H	49	VAL
7	1H	71	LEU
7	1H	84	SER
7	1H	90	LYS
7	1H	92	ILE
7	1H	97	ARG
7	1H	114	VAL
7	1H	127	GLU
7	1H	160	LYS
8	1I	9	LEU
8	1I	12	LEU
8	1I	38	LEU
8	1I	41	GLU
8	1I	42	SER
8	1I	57	ARG
8	1I	92	VAL
8	1I	101	LEU
8	1I	102	SER
8	1I	109	ILE
8	1I	116	LEU
8	1I	127	VAL
8	1I	140	LEU
9	1N	2	LYS
9	1N	5	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	1N	8	GLN
9	1N	14	VAL
9	1N	28	THR
9	1N	89	LYS
9	1N	137	LYS
9	1N	140	VAL
10	1O	52	VAL
11	1P	55	ARG
11	1P	75	ILE
11	1P	77	ARG
11	1P	98	GLU
11	1P	123	LEU
11	1P	147	LEU
11	1P	148	LEU
12	1Q	7	MET
12	1Q	35	VAL
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	111	GLU
12	1Q	139	GLU
13	1R	8	ARG
13	1R	24	GLN
13	1R	67	LEU
13	1R	83	ILE
13	1R	91	GLN
13	1R	104	ARG
13	1R	114	VAL
14	1S	3	ARG
14	1S	13	ARG
14	1S	36	TYR
14	1S	46	VAL
14	1S	52	SER
14	1S	69	VAL
14	1S	73	LEU
14	1S	83	LYS
14	1S	110	LEU
15	1T	6	LEU
15	1T	28	VAL
15	1T	36	GLU
15	1T	51	ARG
15	1T	74	ARG
15	1T	93	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	1T	96	ARG
15	1T	128	GLU
16	1U	27	LEU
16	1U	31	SER
16	1U	59	ARG
16	1U	74	LEU
17	1V	79	VAL
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	24	ILE
18	1W	92	ARG
18	1W	96	ILE
19	1X	57	LEU
20	1Y	8	LYS
20	1Y	40	GLU
20	1Y	43	ASN
20	1Y	44	ILE
20	1Y	64	GLU
20	1Y	70	SER
20	1Y	72	VAL
20	1Y	86	ARG
20	1Y	91	GLU
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	42	VAL
21	1Z	49	ARG
21	1Z	50	GLN
21	1Z	56	VAL
21	1Z	60	GLU
21	1Z	61	LEU
21	1Z	66	SER
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	126	VAL
21	1Z	129	SER
21	1Z	140	ASP
21	1Z	149	SER
21	1Z	155	LEU
21	1Z	161	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	10	82	ARG
23	11	21	ARG
23	11	37	ILE
23	11	40	ARG
23	11	46	LEU
23	11	95	LEU
24	12	19	VAL
24	12	65	ASN
25	13	3	ARG
25	13	23	LEU
25	13	54	VAL
25	13	58	VAL
26	14	14	ILE
26	14	44	THR
26	14	46	GLN
26	14	49	PHE
26	14	50	VAL
26	14	58	ARG
26	14	61	ARG
27	15	6	VAL
27	15	16	ARG
27	15	40	LYS
27	15	59	GLU
27	15	60	VAL
28	16	9	LEU
28	16	14	THR
28	16	19	ARG
28	16	48	VAL
28	16	52	VAL
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	58	ILE
31	19	8	LYS
33	1b	7	VAL
33	1b	10	LEU
33	1b	11	LEU
33	1b	12	GLU
33	1b	17	PHE
33	1b	19	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	23	ARG
33	1b	35	GLU
33	1b	47	THR
33	1b	61	LEU
33	1b	67	THR
33	1b	74	LYS
33	1b	75	LYS
33	1b	80	ILE
33	1b	107	THR
33	1b	108	ILE
33	1b	111	ARG
33	1b	112	VAL
33	1b	126	GLU
33	1b	165	VAL
33	1b	185	ILE
33	1b	187	LEU
33	1b	189	ASP
33	1b	191	ASP
33	1b	200	ILE
33	1b	208	ILE
33	1b	213	LEU
33	1b	215	LEU
33	1b	223	ILE
33	1b	231	GLU
33	1b	235	SER
34	1c	3	ASN
34	1c	15	THR
34	1c	28	GLN
34	1c	36	ASP
34	1c	64	VAL
34	1c	68	VAL
34	1c	104	GLN
34	1c	120	VAL
34	1c	162	GLN
34	1c	164	ARG
34	1c	190	ARG
34	1c	192	THR
34	1c	195	VAL
35	1d	8	VAL
35	1d	19	LEU
35	1d	31	CYS
35	1d	34	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	85	LYS
35	1d	108	LEU
35	1d	126	ILE
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	162	LEU
35	1d	184	LYS
35	1d	186	LEU
35	1d	194	LEU
35	1d	201	GLN
36	1e	41	VAL
36	1e	55	VAL
36	1e	79	GLU
36	1e	82	VAL
36	1e	100	VAL
36	1e	120	THR
36	1e	151	LEU
37	1f	10	LEU
37	1f	55	ASP
37	1f	72	VAL
37	1f	78	GLU
37	1f	81	ILE
38	1g	12	LEU
38	1g	13	GLN
38	1g	16	LEU
38	1g	21	VAL
38	1g	27	ILE
38	1g	50	ILE
38	1g	53	LYS
38	1g	59	LEU
38	1g	61	VAL
38	1g	66	VAL
38	1g	91	VAL
38	1g	98	SER
38	1g	124	LEU
38	1g	140	ASP
39	1h	2	LEU
39	1h	19	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	1h	39	LEU
39	1h	49	GLU
39	1h	52	ASP
39	1h	63	LEU
39	1h	95	VAL
39	1h	122	ARG
39	1h	127	LEU
39	1h	133	LEU
40	1i	17	VAL
40	1i	23	ASN
40	1i	42	ARG
40	1i	51	ARG
40	1i	54	ASP
40	1i	64	THR
40	1i	65	VAL
40	1i	74	ILE
40	1i	83	ARG
40	1i	89	ASN
40	1i	96	LEU
40	1i	99	LEU
40	1i	104	ARG
40	1i	105	ASP
40	1i	108	VAL
40	1i	124	GLN
40	1i	128	ARG
41	1j	8	LEU
41	1j	34	VAL
41	1j	38	ILE
41	1j	43	ARG
41	1j	49	VAL
41	1j	81	THR
41	1j	96	ILE
42	1k	24	SER
42	1k	51	LYS
42	1k	82	VAL
42	1k	93	GLN
42	1k	114	VAL
42	1k	117	ASN
43	1l	18	VAL
43	1l	33	ARG
43	1l	62	SER
43	1l	67	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	1l	106	ASP
44	1m	9	ILE
44	1m	11	ARG
44	1m	12	ASN
44	1m	19	LEU
44	1m	43	THR
44	1m	48	LEU
44	1m	49	THR
44	1m	78	ILE
44	1m	81	LEU
44	1m	98	VAL
44	1m	103	THR
44	1m	109	THR
44	1m	117	VAL
45	1n	7	ILE
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
46	1o	3	ILE
46	1o	11	VAL
46	1o	24	SER
46	1o	26	GLU
46	1o	27	VAL
46	1o	39	LEU
46	1o	56	LEU
46	1o	66	LEU
46	1o	87	ILE
46	1o	88	ARG
47	1p	1	MET
47	1p	8	ARG
47	1p	20	VAL
47	1p	21	VAL
47	1p	27	LYS
47	1p	45	THR
47	1p	54	GLU
47	1p	67	THR
48	1q	9	VAL
48	1q	14	LYS
48	1q	36	ILE
48	1q	37	LYS
48	1q	43	LEU
48	1q	60	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	1q	73	VAL
48	1q	86	GLU
48	1q	87	LYS
49	1r	25	THR
49	1r	37	VAL
49	1r	63	GLN
50	1s	9	VAL
50	1s	19	VAL
50	1s	28	LYS
50	1s	30	LEU
50	1s	32	LYS
50	1s	62	ILE
50	1s	66	MET
50	1s	77	THR
51	1t	84	LEU
54	1w	108	ILE
54	1w	115	THR
54	1w	136	GLU
54	1w	151	ASP
54	1w	152	LEU
54	1w	158	VAL
54	1w	181	GLN
54	1w	185	VAL
54	1w	196	THR
54	1w	198	THR
54	1w	208	GLU
54	1w	274	LEU
54	1w	293	ILE
54	1w	295	THR
54	1w	299	SER
54	1w	315	HIS
54	1w	320	THR
54	1w	321	THR
54	1w	333	THR
3	2D	3	VAL
3	2D	38	LYS
3	2D	99	ASP
3	2D	113	VAL
3	2D	173	VAL
3	2D	183	ARG
3	2D	200	ASP
3	2D	229	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2D	259	THR
4	2E	7	VAL
4	2E	14	ILE
4	2E	73	GLU
4	2E	75	VAL
4	2E	77	ILE
4	2E	89	ASP
4	2E	90	THR
4	2E	116	VAL
4	2E	145	LYS
4	2E	178	GLU
4	2E	181	LEU
4	2E	183	LEU
5	2F	20	LEU
5	2F	57	VAL
5	2F	70	THR
5	2F	112	MET
5	2F	114	VAL
5	2F	119	ARG
5	2F	124	LEU
5	2F	132	VAL
5	2F	133	ASN
5	2F	135	LYS
5	2F	153	SER
5	2F	158	THR
5	2F	162	LEU
5	2F	183	VAL
5	2F	186	ILE
5	2F	201	VAL
6	2G	4	ASP
6	2G	5	VAL
6	2G	15	VAL
6	2G	21	ARG
6	2G	26	GLN
6	2G	31	VAL
6	2G	43	LEU
6	2G	58	GLN
6	2G	67	LYS
6	2G	70	VAL
6	2G	71	THR
6	2G	91	ARG
6	2G	115	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	130	ASN
6	2G	140	ILE
6	2G	152	LEU
6	2G	161	THR
6	2G	165	THR
7	2H	23	ARG
7	2H	24	VAL
7	2H	25	LYS
7	2H	32	GLU
7	2H	37	VAL
7	2H	41	MET
7	2H	62	LYS
7	2H	63	SER
7	2H	72	ILE
7	2H	92	ILE
7	2H	114	VAL
7	2H	119	GLU
7	2H	122	THR
7	2H	127	GLU
7	2H	129	THR
7	2H	136	ILE
8	2I	4	ILE
8	2I	9	LEU
8	2I	20	ASP
8	2I	38	LEU
8	2I	40	THR
8	2I	41	GLU
8	2I	58	LEU
8	2I	61	ARG
8	2I	77	LEU
8	2I	79	ILE
8	2I	87	LYS
8	2I	114	LEU
8	2I	122	GLU
8	2I	127	VAL
8	2I	144	VAL
9	2N	8	GLN
9	2N	9	VAL
9	2N	10	GLU
9	2N	14	VAL
9	2N	28	THR
9	2N	38	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	2N	48	MET
9	2N	54	VAL
9	2N	62	VAL
9	2N	127	ASP
9	2N	137	LYS
9	2N	140	VAL
10	2O	28	SER
10	2O	52	VAL
10	2O	63	VAL
10	2O	69	ILE
10	2O	78	ARG
10	2O	108	GLU
10	2O	113	LYS
11	2P	55	ARG
11	2P	77	ARG
11	2P	123	LEU
11	2P	133	SER
11	2P	144	GLU
12	2Q	31	ASP
12	2Q	35	VAL
12	2Q	66	ILE
12	2Q	75	THR
12	2Q	109	VAL
13	2R	24	GLN
13	2R	67	LEU
13	2R	114	VAL
14	2S	21	THR
14	2S	36	TYR
14	2S	50	SER
14	2S	69	VAL
14	2S	85	VAL
14	2S	98	VAL
14	2S	110	LEU
15	2T	6	LEU
15	2T	17	THR
15	2T	28	VAL
15	2T	39	ARG
15	2T	40	THR
15	2T	74	ARG
15	2T	89	VAL
15	2T	115	ARG
15	2T	118	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	2U	5	LYS
16	2U	16	LYS
16	2U	59	ARG
16	2U	74	LEU
16	2U	85	LYS
17	2V	46	VAL
17	2V	51	VAL
17	2V	61	VAL
17	2V	79	VAL
18	2W	1	MET
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	28	SER
19	2X	1	MET
19	2X	48	LYS
19	2X	72	LYS
19	2X	81	VAL
19	2X	90	GLU
20	2Y	11	ASP
20	2Y	23	ARG
20	2Y	49	VAL
20	2Y	72	VAL
20	2Y	97	ARG
20	2Y	99	CYS
21	2Z	5	LEU
21	2Z	27	VAL
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	46	LYS
21	2Z	47	VAL
21	2Z	50	GLN
21	2Z	52	SER
21	2Z	66	SER
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	73	GLN
21	2Z	74	VAL
21	2Z	76	LEU
21	2Z	81	ARG
21	2Z	84	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	2Z	93	ASP
21	2Z	126	VAL
21	2Z	128	VAL
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	170	THR
23	21	35	THR
23	21	38	SER
23	21	40	ARG
23	21	46	LEU
23	21	59	THR
23	21	95	LEU
23	21	98	LEU
24	22	19	VAL
24	22	28	LYS
24	22	35	LEU
24	22	52	ASP
24	22	53	LEU
24	22	65	ASN
25	23	31	LEU
25	23	54	VAL
25	23	59	VAL
26	24	3	GLU
26	24	35	VAL
26	24	49	PHE
26	24	53	GLU
26	24	62	ARG
26	24	63	TYR
27	25	6	VAL
27	25	16	ARG
27	25	33	CYS
27	25	55	ARG
27	25	56	LYS
28	26	7	ILE
28	26	32	ASN
28	26	48	VAL
28	26	52	VAL
29	27	23	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	28	46	ARG
31	29	7	VAL
33	2b	7	VAL
33	2b	12	GLU
33	2b	19	HIS
33	2b	37	ASN
33	2b	41	ILE
33	2b	44	LEU
33	2b	47	THR
33	2b	67	THR
33	2b	71	VAL
33	2b	79	ASP
33	2b	81	VAL
33	2b	112	VAL
33	2b	118	LEU
33	2b	122	PHE
33	2b	126	GLU
33	2b	127	ILE
33	2b	135	GLN
33	2b	143	GLU
33	2b	150	SER
33	2b	154	LEU
33	2b	164	VAL
33	2b	168	THR
33	2b	172	ILE
33	2b	180	LEU
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP
33	2b	191	ASP
33	2b	196	LEU
33	2b	208	ILE
33	2b	229	VAL
33	2b	230	VAL
34	2c	14	ILE
34	2c	17	ASP
34	2c	36	ASP
34	2c	59	ARG
34	2c	85	ARG
34	2c	138	VAL
34	2c	192	THR
34	2c	207	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	17	VAL
35	2d	19	LEU
35	2d	28	SER
35	2d	31	CYS
35	2d	34	GLU
35	2d	70	ILE
35	2d	96	LEU
35	2d	115	ARG
35	2d	135	LEU
35	2d	162	LEU
35	2d	170	VAL
35	2d	175	SER
35	2d	178	VAL
35	2d	179	GLU
35	2d	188	LEU
35	2d	201	GLN
35	2d	203	VAL
36	2e	6	PHE
36	2e	20	GLN
36	2e	47	LYS
36	2e	51	VAL
36	2e	53	LEU
36	2e	83	GLU
36	2e	111	GLU
36	2e	117	ASP
36	2e	120	THR
36	2e	152	ARG
37	2f	43	LEU
37	2f	69	GLU
37	2f	72	VAL
37	2f	94	GLN
38	2g	21	VAL
38	2g	32	ARG
38	2g	79	ARG
38	2g	86	GLN
38	2g	135	VAL
39	2h	19	VAL
39	2h	25	ASP
39	2h	39	LEU
39	2h	63	LEU
39	2h	107	LEU
39	2h	114	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	2h	127	LEU
39	2h	133	LEU
40	2i	23	ASN
40	2i	53	VAL
40	2i	56	LEU
40	2i	58	HIS
40	2i	64	THR
40	2i	83	ARG
40	2i	96	LEU
40	2i	108	VAL
40	2i	113	LYS
40	2i	124	GLN
41	2j	13	HIS
41	2j	21	GLN
41	2j	38	ILE
41	2j	47	PHE
41	2j	49	VAL
41	2j	65	LEU
41	2j	72	VAL
41	2j	94	VAL
42	2k	33	THR
42	2k	80	VAL
42	2k	84	VAL
42	2k	105	VAL
42	2k	107	SER
43	2l	6	THR
43	2l	36	VAL
43	2l	39	VAL
43	2l	58	VAL
43	2l	97	ARG
43	2l	117	ARG
44	2m	4	ILE
44	2m	32	GLU
44	2m	47	ASP
44	2m	48	LEU
44	2m	55	ARG
44	2m	67	GLU
44	2m	78	ILE
44	2m	98	VAL
44	2m	105	THR
44	2m	106	ASN
44	2m	117	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	2n	7	ILE
45	2n	13	THR
45	2n	18	VAL
45	2n	33	VAL
46	2o	10	LYS
46	2o	11	VAL
46	2o	24	SER
46	2o	26	GLU
46	2o	27	VAL
46	2o	66	LEU
47	2p	1	MET
47	2p	2	VAL
47	2p	16	HIS
47	2p	20	VAL
47	2p	21	VAL
47	2p	28	ARG
47	2p	45	THR
47	2p	60	LEU
47	2p	72	ARG
48	2q	43	LEU
48	2q	57	VAL
48	2q	60	ILE
48	2q	65	ILE
49	2r	25	THR
49	2r	28	GLU
49	2r	37	VAL
49	2r	45	SER
49	2r	82	THR
50	2s	11	VAL
50	2s	27	GLU
50	2s	40	ILE
50	2s	49	ILE
50	2s	64	GLU
50	2s	69	HIS
50	2s	71	LEU
50	2s	77	THR
51	2t	9	ASN
51	2t	19	SER
51	2t	41	ILE
52	2u	7	ARG
52	2u	9	ARG
54	2w	103	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2w	129	ASN
54	2w	138	MET
54	2w	143	GLU
54	2w	145	LEU
54	2w	151	ASP
54	2w	158	VAL
54	2w	175	SER
54	2w	196	THR
54	2w	206	GLU
54	2w	215	ASP
54	2w	222	MET
54	2w	258	GLN
54	2w	267	MET
54	2w	268	ILE
54	2w	271	SER
54	2w	302	ILE
54	2w	312	VAL
54	2w	320	THR
54	2w	333	THR
54	2w	336	LEU
54	2w	343	ASP
54	2w	353	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	143	ASN
5	1F	69	HIS
5	1F	203	GLN
5	1F	204	ASN
6	1G	26	GLN
6	1G	108	ASN
8	1I	54	GLN
8	1I	74	ASN
9	1N	8	GLN
9	1N	131	GLN
12	1Q	12	GLN
12	1Q	89	ASN
12	1Q	113	GLN
13	1R	91	GLN
14	1S	61	ASN
15	1T	58	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1U	94	ASN
18	1W	34	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	55	HIS
21	1Z	73	GLN
21	1Z	121	HIS
21	1Z	151	HIS
22	10	35	ASN
24	12	46	GLN
26	14	46	GLN
28	16	20	ASN
30	18	35	GLN
33	1b	40	HIS
33	1b	78	GLN
33	1b	135	GLN
34	1c	6	HIS
34	1c	104	GLN
34	1c	162	GLN
34	1c	181	ASN
35	1d	123	HIS
35	1d	125	HIS
36	1e	78	HIS
38	1g	28	ASN
40	1i	23	ASN
40	1i	31	GLN
40	1i	73	GLN
40	1i	89	ASN
40	1i	117	HIS
40	1i	124	GLN
41	1j	56	HIS
41	1j	62	HIS
41	1j	68	HIS
41	1j	69	ASN
42	1k	93	GLN
43	1l	80	HIS
43	1l	99	HIS
44	1m	77	ASN
44	1m	106	ASN
46	1o	9	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	1o	13	GLN
47	1p	13	HIS
48	1q	26	GLN
49	1r	63	GLN
50	1s	83	HIS
54	1w	181	GLN
54	1w	189	GLN
54	1w	309	GLN
54	1w	344	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	75	HIS
6	2G	26	GLN
6	2G	79	ASN
6	2G	108	ASN
6	2G	132	ASN
10	2O	89	ASN
12	2Q	113	GLN
13	2R	71	GLN
15	2T	58	ASN
16	2U	72	HIS
19	2X	31	HIS
20	2Y	6	HIS
20	2Y	43	ASN
21	2Z	65	GLN
21	2Z	73	GLN
21	2Z	132	ASN
21	2Z	151	HIS
26	24	40	HIS
30	28	35	GLN
33	2b	16	HIS
33	2b	78	GLN
33	2b	95	GLN
33	2b	224	GLN
34	2c	37	GLN
34	2c	118	GLN
34	2c	139	GLN
34	2c	176	HIS
34	2c	181	ASN
35	2d	74	GLN
35	2d	77	ASN
35	2d	116	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	123	HIS
35	2d	125	HIS
36	2e	65	ASN
37	2f	7	ASN
37	2f	13	ASN
37	2f	32	ASN
38	2g	28	ASN
38	2g	68	ASN
38	2g	97	GLN
38	2g	106	GLN
40	2i	58	HIS
40	2i	89	ASN
41	2j	56	HIS
42	2k	78	GLN
42	2k	99	GLN
44	2m	12	ASN
44	2m	77	ASN
46	2o	13	GLN
46	2o	50	HIS
46	2o	62	GLN
47	2p	13	HIS
49	2r	63	GLN
50	2s	47	HIS
50	2s	83	HIS
51	2t	42	GLN
51	2t	75	ASN
51	2t	90	GLN
54	2w	258	GLN
54	2w	315	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	437 (15%)	33 (1%)
1	2A	2791/2915 (95%)	450 (16%)	24 (0%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	118/121 (97%)	17 (14%)	0
32	1a	1497/1521 (98%)	288 (19%)	0
32	2a	1501/1521 (98%)	295 (19%)	0
53	1v	8/24 (33%)	1 (12%)	0
53	2v	8/24 (33%)	1 (12%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	1x	72/74 (97%)	11 (15%)	0
55	2x	72/74 (97%)	7 (9%)	0
All	All	9050/9310 (97%)	1519 (16%)	57 (0%)

All (1519) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	119	A
1	1A	120	U
1	1A	182	A
1	1A	196	A
1	1A	197	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	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	261	G
1	1A	265	A
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(S)	G
1	1A	272(A)	U
1	1A	272(B)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	317	G
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	362	U
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	428	A
1	1A	442	G
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	529	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	652(F)	G
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	774	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	811	U
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	878	A
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	899	A
1	1A	907	U
1	1A	910	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	931	G
1	1A	932	G
1	1A	938	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	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1040	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1060	U
1	1A	1063	G
1	1A	1064	C
1	1A	1066	U
1	1A	1067	A
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1083	U
1	1A	1086	A
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1092	C
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1098	A
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1195	G
1	1A	1211	U
1	1A	1218	C
1	1A	1220	A
1	1A	1241	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1308	A
1	1A	1319	G
1	1A	1352	U
1	1A	1359	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1437	C
1	1A	1445	A
1	1A	1450	G
1	1A	1453	U
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1485	G
1	1A	1493	C
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1541	G
1	1A	1543	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1648	C
1	1A	1654	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1756	G
1	1A	1762	A
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	1812	A
1	1A	1816	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1848	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2102	U
1	1A	2104	G
1	1A	2105	C
1	1A	2107	C
1	1A	2112	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2117	A
1	1A	2119	A
1	1A	2120	G
1	1A	2122	U
1	1A	2123	G
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	2138	C
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2150	U
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2163	C
1	1A	2164	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2168	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2170	A
1	1A	2171	A
1	1A	2172	U
1	1A	2175	C
1	1A	2176	A
1	1A	2178	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2185	C
1	1A	2189	U
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2280	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2307	G
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	2354	G
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2407	G
1	1A	2410	G
1	1A	2422	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2506	U
1	1A	2518	A
1	1A	2525	G
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2578	G
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2663	G
1	1A	2673	G
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2714	G
1	1A	2721	A
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2761	G
1	1A	2765	A
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A
1	1A	2791	C
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2873	A
1	1A	2876	G
1	1A	2880	C
1	1A	2894	G
2	1B	13	A
2	1B	25	A
2	1B	33	G
2	1B	42	C
2	1B	45	A
2	1B	52	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
2	1B	120	A
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	40	C
32	1a	44	G
32	1a	47	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	76	C
32	1a	78	G
32	1a	91	C
32	1a	98	G
32	1a	99	U
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	137	C
32	1a	143	A
32	1a	144	G
32	1a	146	G
32	1a	150	C
32	1a	157	G
32	1a	159	G
32	1a	160	A
32	1a	163	C
32	1a	165	C
32	1a	170	U
32	1a	174	C
32	1a	182	U
32	1a	189(F)	U
32	1a	189(J)	G
32	1a	195	A
32	1a	196	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	223	U
32	1a	231	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	330	C
32	1a	332	G
32	1a	340	U
32	1a	341	C
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	346	G
32	1a	349	A
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	374	A
32	1a	384	G
32	1a	389	A
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	421	U
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	444	C
32	1a	452	A
32	1a	457	C
32	1a	460	G
32	1a	461	A
32	1a	470	C
32	1a	474	G
32	1a	475	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	485	G
32	1a	492	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	527	G7M
32	1a	528	C
32	1a	532	A
32	1a	545	C
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	564	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	618	C
32	1a	630	G
32	1a	650	G
32	1a	653	A
32	1a	657	G
32	1a	662	G
32	1a	665	A
32	1a	666	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	702	A
32	1a	703	G
32	1a	723	U
32	1a	735	C
32	1a	749	C
32	1a	755	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	853	G
32	1a	859	A
32	1a	876	G
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	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
32	1a	978	A
32	1a	983	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1009	G
32	1a	1013	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1035	A
32	1a	1036	G
32	1a	1040	U
32	1a	1043	C
32	1a	1044	A
32	1a	1045	C
32	1a	1049	U
32	1a	1053	G
32	1a	1054	C
32	1a	1056	U
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1092	A
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1103	C
32	1a	1108	G
32	1a	1122	U
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1135	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1159	U
32	1a	1160	G
32	1a	1161	C
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1217	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
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	1288	A
32	1a	1297	C
32	1a	1298	C
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1319	A
32	1a	1320	C
32	1a	1322	C
32	1a	1323	G
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1347	G
32	1a	1353	G
32	1a	1356	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1369	C
32	1a	1370	G
32	1a	1378	C
32	1a	1398	A
32	1a	1400	5MC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1452	C
32	1a	1460	A
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
53	1v	22	U
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	20	H2U
55	1x	21	H2U
55	1x	22	A
55	1x	37	MIA
55	1x	45	U
55	1x	51	C
55	1x	54	5MU
55	1x	56	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	76	C
1	2A	78	A
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	139(A)	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	197	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	248	G
1	2A	249	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	311	A
1	2A	312	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	389	G
1	2A	396	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	435	C
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	504	U
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	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(A)	A
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
1	2A	874	G
1	2A	878	A
1	2A	881	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1040	C
1	2A	1043	C
1	2A	1114	G
1	2A	1115	G
1	2A	1116	C
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1144	G
1	2A	1155	A
1	2A	1205	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
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	1276	A
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	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	1420	U
1	2A	1421	G
1	2A	1428	C
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	1465	G
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1543	C
1	2A	1547	C
1	2A	1554	A
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1587	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1743	C
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1836	C
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1981	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2099	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2103	C
1	2A	2106	G
1	2A	2108	C
1	2A	2111	C
1	2A	2114	A
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2142	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2153	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2162	G
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2170	A
1	2A	2172	U
1	2A	2174	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2178	C
1	2A	2185	C
1	2A	2186	G
1	2A	2188	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	2219	G
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2304	G
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2366	A
1	2A	2372	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2406	U
1	2A	2410	G
1	2A	2422	A
1	2A	2423	U
1	2A	2424	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2465	C
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2480	C
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	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2638	G
1	2A	2654	A
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2804	C
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2875	C
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	17	C
2	2B	35	U
2	2B	41	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	73	A
2	2B	85	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	116	G
2	2B	120	A
32	2a	9	G
32	2a	13	U
32	2a	22	G
32	2a	27	G
32	2a	30	U
32	2a	31	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	54	C
32	2a	65	U
32	2a	66	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	143	A
32	2a	144	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(A)	C
32	2a	189(E)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	220	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	274	A
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	329	A
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	422	C
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	438	G
32	2a	439	A
32	2a	442	C
32	2a	446	G
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	482	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	485	G
32	2a	495	A
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	513	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	536	C
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	595	G
32	2a	596	C
32	2a	618	C
32	2a	630	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	666	G
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	755	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	859	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	945	G
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	1000	U
32	2a	1001	A
32	2a	1003	G
32	2a	1004	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1012	U
32	2a	1013	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(D)	A
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1035	A
32	2a	1037	C
32	2a	1038	C
32	2a	1040	U
32	2a	1043	C
32	2a	1045	C
32	2a	1046	A
32	2a	1056	U
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1105	A
32	2a	1113	C
32	2a	1122	U
32	2a	1124	G
32	2a	1129	C
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1140	C
32	2a	1142	G
32	2a	1146	A
32	2a	1151	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1171	G
32	2a	1174	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1210	C
32	2a	1211	U
32	2a	1212	U
32	2a	1214	C
32	2a	1218	C
32	2a	1220	G
32	2a	1225	A
32	2a	1227	A
32	2a	1228	C
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1262	C
32	2a	1263	C
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	1281	U
32	2a	1282	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1287	A
32	2a	1292	U
32	2a	1297	C
32	2a	1299	A
32	2a	1300	G
32	2a	1301	U
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1313	U
32	2a	1317	C
32	2a	1320	C
32	2a	1322	C
32	2a	1323	G
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	1370	G
32	2a	1377	A
32	2a	1379	G
32	2a	1381	U
32	2a	1384	C
32	2a	1397	C
32	2a	1398	A
32	2a	1399	C
32	2a	1402	4OC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1493	A
32	2a	1494	G
32	2a	1497	G
32	2a	1499	A
32	2a	1504	G
32	2a	1506	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	22	U
55	2x	16	C
55	2x	18	G
55	2x	20	H2U
55	2x	21	H2U
55	2x	22	A
55	2x	37	MIA
55	2x	48	G

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	974	G
1	1A	1065	U
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1210	A
1	1A	1379	A
1	1A	1420	U
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1653	G
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2158	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2601	C
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	764	A
1	2A	827	U
1	2A	856	C
1	2A	896	A
1	2A	900	A
1	2A	1210	A
1	2A	1275	A
1	2A	1379	A
1	2A	1420	U
1	2A	1530	C
1	2A	1653	G
1	2A	1992	G
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 ⓘ

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
55	5MU	1x	54	55,57	19,22,23	1.37	4 (21%)	27,32,35	1.87	6 (22%)
55	4SU	1x	8	55	18,21,22	1.87	5 (27%)	25,30,33	2.03	4 (16%)
32	MA6	1a	1519	32	23,26,27	0.42	0	33,38,41	1.92	9 (27%)
32	5MC	2a	967	32	19,22,23	1.73	3 (15%)	26,32,35	1.10	2 (7%)
32	5MC	1a	1404	32	19,22,23	1.75	3 (15%)	26,32,35	1.15	2 (7%)
32	G7M	1a	527	32,57	23,26,27	1.53	3 (13%)	34,39,42	1.74	5 (14%)
32	UR3	1a	1498	32	19,22,23	0.98	0	26,32,35	1.71	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.69	3 (15%)	26,32,35	1.17	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
55	PSU	1x	32	55,57	18,21,22	1.33	2 (11%)	21,30,33	2.04	3 (14%)
55	PSU	1x	39	55	18,21,22	1.42	3 (16%)	21,30,33	1.90	3 (14%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.17	4 (19%)
1	5MU	1A	1939	57,1	19,22,23	1.49	5 (26%)	27,32,35	2.10	6 (22%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	1.96	8 (24%)
1	5MC	1A	1962	57,1	19,22,23	1.68	3 (15%)	26,32,35	1.09	3 (11%)
54	MEQ	1w	230	54	8,9,10	0.96	0	5,10,12	0.32	0
1	PSU	1A	2605	57,1	18,21,22	1.35	2 (11%)	21,30,33	2.22	4 (19%)
1	2MA	2A	2503	57,1	22,25,26	1.45	4 (18%)	32,37,40	2.41	8 (25%)
32	5MC	2a	1407	32,57	19,22,23	1.64	3 (15%)	26,32,35	1.23	3 (11%)
1	PSU	1A	1917	1	18,21,22	1.49	3 (16%)	21,30,33	2.00	5 (23%)
55	PSU	1x	55	55	18,21,22	1.31	2 (11%)	21,30,33	2.10	4 (19%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	2.00	5 (23%)
32	4OC	1a	1402	32,57	20,23,24	0.76	0	25,32,35	1.08	2 (8%)
55	PSU	2x	39	55	18,21,22	1.41	3 (16%)	21,30,33	1.74	4 (19%)
1	2MA	1A	2503	57,1	22,25,26	1.42	5 (22%)	32,37,40	2.36	8 (25%)
32	5MC	2a	1404	32	19,22,23	1.61	3 (15%)	26,32,35	1.14	2 (7%)
1	PSU	2A	2605	1	18,21,22	1.33	2 (11%)	21,30,33	1.96	5 (23%)
55	5MU	2x	54	55	19,22,23	1.42	4 (21%)	27,32,35	2.18	8 (29%)
1	5MU	2A	1939	57,1	19,22,23	1.46	5 (26%)	27,32,35	2.17	8 (29%)
43	0TD	1l	92	43	8,9,10	4.56	2 (25%)	6,11,13	8.74	3 (50%)
32	PSU	1a	516	32,57	18,21,22	1.40	2 (11%)	21,30,33	2.10	4 (19%)
1	OMG	1A	2251	57,55,1	23,26,27	1.23	2 (8%)	32,38,41	1.97	6 (18%)
1	OMC	2A	1920	57,1	19,22,23	0.82	0	25,31,34	0.93	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	2A	2552	57,1	19,22,23	1.17	2 (10%)	25,31,34	1.76	5 (20%)
32	5MC	2a	1400	32	19,22,23	1.72	3 (15%)	26,32,35	1.15	2 (7%)
54	MEQ	2w	230	54	8,9,10	0.84	0	5,10,12	0.83	0
32	G7M	2a	527	32,57	23,26,27	1.53	3 (13%)	34,39,42	1.72	5 (14%)
55	PSU	2x	32	55	18,21,22	1.35	2 (11%)	21,30,33	2.02	4 (19%)
32	M2G	1a	966	32	24,27,28	1.35	4 (16%)	33,40,43	1.88	5 (15%)
55	8AN	1x	76	55,57,56	21,24,25	1.40	3 (14%)	26,35,38	2.20	10 (38%)
1	5MC	2A	1942	1	19,22,23	1.70	2 (10%)	26,32,35	1.15	3 (11%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.13	9 (27%)
55	H2U	2x	20	55	18,21,22	0.99	2 (11%)	19,30,33	1.12	1 (5%)
32	M2G	2a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.88	6 (18%)
55	H2U	1x	20	55	18,21,22	0.88	2 (11%)	19,30,33	1.08	1 (5%)
55	MIA	2x	37	55	21,24,32	1.57	4 (19%)	30,35,47	2.06	9 (30%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.04	2 (8%)
55	MIA	1x	37	55	21,24,32	1.58	4 (19%)	30,35,47	2.04	7 (23%)
1	OMU	1A	2552	57,1	19,22,23	1.23	3 (15%)	25,31,34	1.68	5 (20%)
1	OMG	2A	2251	57,55,1	23,26,27	1.18	3 (13%)	32,38,41	1.99	7 (21%)
1	PSU	1A	1911	1	18,21,22	1.40	3 (16%)	21,30,33	1.98	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.19	4 (19%)
32	2MG	2a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.09	5 (15%)
55	H2U	1x	21	55	18,21,22	0.99	1 (5%)	19,30,33	1.60	2 (10%)
32	4OC	2a	1402	32,57	20,23,24	0.78	0	25,32,35	0.97	1 (4%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.10	9 (27%)
1	5MU	2A	1915	57,1	19,22,23	1.49	6 (31%)	27,32,35	2.22	7 (25%)
32	5MC	1a	967	32	19,22,23	1.48	3 (15%)	26,32,35	1.10	3 (11%)
55	4SU	2x	8	55	18,21,22	1.83	4 (22%)	25,30,33	1.88	5 (20%)
32	UR3	2a	1498	32	19,22,23	0.94	1 (5%)	26,32,35	1.72	3 (11%)
43	0TD	2l	92	43	8,9,10	4.64	1 (12%)	6,11,13	6.71	3 (50%)
55	H2U	2x	21	55	18,21,22	1.02	2 (11%)	19,30,33	1.28	3 (15%)
1	5MC	1A	1942	57,1	19,22,23	1.59	3 (15%)	26,32,35	1.26	4 (15%)
55	8AN	2x	76	55,57,56	21,24,25	1.39	3 (14%)	26,35,38	2.16	10 (38%)
32	2MG	1a	1207	32	23,26,27	1.26	3 (13%)	33,38,41	2.14	5 (15%)
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	27,32,35	2.31	6 (22%)
32	5MC	1a	1407	32	19,22,23	1.80	3 (15%)	26,32,35	1.15	4 (15%)
1	5MC	2A	1962	57,1	19,22,23	1.78	3 (15%)	26,32,35	1.16	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	1x	54	55,57	-	2/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,57	-	2/7/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	PSU	1x	32	55,57	-	0/7/25/26	0/2/2/2
55	PSU	1x	39	55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
54	MEQ	1w	230	54	-	4/8/9/11	-
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	1/7/25/26	0/3/3/3
32	5MC	2a	1407	32,57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	2/7/25/26	0/2/2/2
32	4OC	1a	1402	32,57	-	2/9/29/30	0/2/2/2
55	PSU	2x	39	55	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	1/7/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
32	PSU	1a	516	32,57	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,55,1	-	0/9/27/28	0/3/3/3
1	OMC	2A	1920	57,1	-	0/9/27/28	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	MEQ	2w	230	54	-	2/8/9/11	-
32	G7M	2a	527	32,57	-	3/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	2x	32	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
55	8AN	1x	76	55,57,56	-	1/7/25/26	0/3/3/3
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
55	H2U	2x	20	55	-	4/7/38/39	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
55	H2U	1x	20	55	-	2/7/38/39	0/2/2/2
55	MIA	2x	37	55	-	2/7/25/34	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
55	MIA	1x	37	55	-	2/7/25/34	0/3/3/3
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
1	OMG	2A	2251	57,55,1	-	0/9/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
55	H2U	1x	21	55	-	4/7/38/39	0/2/2/2
32	4OC	2a	1402	32,57	-	4/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	5MU	2A	1915	57,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
55	H2U	2x	21	55	-	5/7/38/39	0/2/2/2
1	5MC	1A	1942	57,1	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	55,57,56	-	1/7/25/26	0/3/3/3
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.77	1.69	1.82
43	1l	92	0TD	CB-SB	-12.31	1.69	1.82
32	1a	1407	5MC	C5-C4	6.64	1.49	1.44
1	2A	1962	5MC	C5-C4	6.63	1.49	1.44
32	1a	1404	5MC	C5-C4	6.45	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	967	5MC	C5-C4	6.45	1.49	1.44
32	2a	1400	5MC	C5-C4	6.43	1.49	1.44
1	1A	1962	5MC	C5-C4	6.08	1.48	1.44
1	2A	1942	5MC	C5-C4	5.97	1.48	1.44
32	2a	1407	5MC	C5-C4	5.92	1.48	1.44
32	1a	1400	5MC	C5-C4	5.87	1.48	1.44
32	2a	1404	5MC	C5-C4	5.71	1.48	1.44
1	1A	1942	5MC	C5-C4	5.68	1.48	1.44
32	1a	967	5MC	C5-C4	5.12	1.48	1.44
55	1x	8	4SU	C4-S4	-4.90	1.60	1.68
55	2x	8	4SU	C4-S4	-4.85	1.60	1.68
32	1a	527	G7M	C5-N7	-4.81	1.33	1.39
32	2a	527	G7M	C5-N7	-4.75	1.33	1.39
55	1x	37	MIA	C5-C4	4.75	1.47	1.39
55	2x	37	MIA	C5-C4	4.65	1.47	1.39
1	2A	2503	2MA	C5-C4	4.46	1.47	1.39
1	1A	2503	2MA	C5-C4	4.02	1.46	1.39
55	2x	76	8AN	C5-N7	-3.86	1.32	1.39
55	1x	76	8AN	C5-N7	-3.85	1.32	1.39
1	1A	1917	PSU	C6-C5	3.79	1.39	1.35
55	2x	55	PSU	C6-C5	3.72	1.39	1.35
1	1A	1911	PSU	C6-C5	3.64	1.39	1.35
1	2A	1911	PSU	C6-C5	3.63	1.39	1.35
55	2x	39	PSU	C6-C5	3.61	1.39	1.35
32	1a	516	PSU	C6-C5	3.61	1.39	1.35
55	1x	8	4SU	C4-N3	-3.56	1.33	1.37
1	2A	2605	PSU	C6-C5	3.51	1.39	1.35
55	1x	39	PSU	C6-C5	3.48	1.39	1.35
1	2A	1917	PSU	C6-C5	3.47	1.39	1.35
55	1x	55	PSU	C6-C5	3.45	1.39	1.35
55	2x	32	PSU	C6-C5	3.41	1.39	1.35
32	1a	527	G7M	C5-C4	3.38	1.46	1.38
32	2a	516	PSU	C6-C5	3.37	1.39	1.35
32	1a	1400	5MC	C6-C5	3.30	1.40	1.34
1	2A	1942	5MC	C6-C5	3.30	1.40	1.34
55	2x	76	8AN	C5-C4	-3.30	1.33	1.39
32	2a	966	M2G	C5-C4	3.29	1.47	1.38
55	2x	8	4SU	C4-N3	-3.27	1.34	1.37
32	1a	966	M2G	C5-C4	3.25	1.47	1.38
32	1a	1207	2MG	C5-C4	3.25	1.47	1.38
55	1x	76	8AN	C5-C4	-3.22	1.33	1.39
1	1A	2251	OMG	C5-C4	3.21	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	32	PSU	C6-C5	3.20	1.38	1.35
32	2a	1207	2MG	C5-C4	3.17	1.47	1.38
32	2a	527	G7M	C5-C4	3.11	1.46	1.38
32	1a	966	M2G	C2-N2	3.09	1.40	1.35
1	2A	1915	5MU	C6-C5	2.98	1.39	1.34
1	2A	2251	OMG	C5-C4	2.97	1.46	1.38
55	1x	54	5MU	C6-C5	2.93	1.39	1.34
1	1A	1917	PSU	C4-N3	-2.92	1.33	1.38
32	2a	1404	5MC	C6-C5	2.92	1.39	1.34
1	1A	1915	5MU	C4-N3	-2.90	1.33	1.38
55	1x	39	PSU	C4-N3	-2.88	1.33	1.38
1	2A	1915	5MU	C2-N1	2.85	1.42	1.38
55	2x	37	MIA	C5-C6	2.85	1.48	1.41
1	1A	1939	5MU	C4-N3	-2.83	1.33	1.38
55	2x	54	5MU	C6-C5	2.83	1.39	1.34
1	2A	1939	5MU	C6-C5	2.80	1.39	1.34
55	1x	8	4SU	C5-C4	-2.79	1.39	1.42
32	1a	516	PSU	C4-N3	-2.79	1.33	1.38
32	1a	967	5MC	C6-C5	2.77	1.39	1.34
55	2x	21	H2U	C2-N3	-2.76	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.75	1.33	1.38
55	1x	76	8AN	C5-C6	-2.75	1.33	1.41
1	1A	2251	OMG	C6-N1	-2.75	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.74	1.33	1.38
1	1A	1939	5MU	C6-C5	2.74	1.39	1.34
55	2x	8	4SU	C5-C4	-2.73	1.39	1.42
1	1A	1939	5MU	C2-N3	-2.73	1.33	1.38
55	2x	20	H2U	C4-N3	-2.72	1.33	1.37
1	1A	2605	PSU	C4-N3	-2.72	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.71	1.33	1.38
55	2x	54	5MU	C2-N1	2.70	1.42	1.38
32	2a	1407	5MC	C6-C5	2.69	1.39	1.34
32	2a	966	M2G	C2-N2	2.69	1.40	1.35
1	1A	1942	5MC	C6-C5	2.67	1.39	1.34
32	2a	967	5MC	C6-C5	2.67	1.39	1.34
1	1A	2605	PSU	C6-C5	2.65	1.38	1.35
55	2x	39	PSU	C4-N3	-2.65	1.33	1.38
55	2x	76	8AN	C5-C6	-2.64	1.33	1.41
1	1A	1939	5MU	C6-N1	-2.63	1.33	1.38
32	2a	1400	5MC	C6-C5	2.63	1.38	1.34
32	1a	1407	5MC	C6-C5	2.61	1.38	1.34
55	1x	37	MIA	C5-C6	2.60	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	54	5MU	C4-C5	2.60	1.49	1.44
1	2A	1911	PSU	C4-N3	-2.60	1.34	1.38
1	1A	1962	5MC	C6-C5	2.59	1.38	1.34
55	1x	32	PSU	C4-N3	-2.58	1.34	1.38
1	2A	1939	5MU	C4-C5	2.56	1.49	1.44
32	1a	1404	5MC	C6-C5	2.55	1.38	1.34
32	1a	1404	5MC	C6-N1	-2.53	1.33	1.38
32	1a	966	M2G	C6-N1	-2.53	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.52	1.34	1.38
1	1A	1915	5MU	C6-C5	2.52	1.38	1.34
1	2A	1962	5MC	C6-C5	2.52	1.38	1.34
32	1a	527	G7M	C6-N1	-2.51	1.34	1.38
55	2x	37	MIA	C8-N7	2.51	1.36	1.31
55	1x	54	5MU	C4-N3	-2.50	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.50	1.34	1.38
32	2a	527	G7M	C6-N1	-2.50	1.34	1.38
55	2x	20	H2U	C2-N3	-2.50	1.33	1.38
55	1x	37	MIA	C5-N7	-2.49	1.34	1.39
55	2x	55	PSU	C4-N3	-2.48	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.48	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.48	1.33	1.38
55	1x	21	H2U	C2-N3	-2.46	1.33	1.38
1	1A	2552	OMU	C4-N3	-2.46	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.46	1.34	1.39
32	2a	516	PSU	C4-N3	-2.45	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.45	1.34	1.38
55	2x	32	PSU	C4-N3	-2.43	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.42	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.41	1.33	1.38
1	2A	1915	5MU	C4-C5	2.40	1.48	1.44
1	2A	1939	5MU	C2-N3	-2.40	1.33	1.38
55	1x	20	H2U	C2-N3	-2.38	1.33	1.38
1	2A	2503	2MA	C5-N7	-2.35	1.34	1.39
55	1x	8	4SU	C2-N3	-2.34	1.33	1.38
55	2x	54	5MU	C4-N3	-2.33	1.34	1.38
55	2x	8	4SU	C2-N1	2.32	1.42	1.38
1	2A	2605	PSU	C4-N3	-2.32	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.32	1.34	1.38
1	1A	1915	5MU	C2-N1	2.31	1.42	1.38
1	1A	1915	5MU	C2-N3	-2.29	1.34	1.38
55	1x	37	MIA	C8-N7	2.29	1.36	1.31
1	1A	2552	OMU	C5-C4	-2.29	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2503	2MA	C5-C6	2.28	1.47	1.41
1	1A	1962	5MC	C6-N1	-2.28	1.34	1.38
1	1A	1939	5MU	C4-C5	2.27	1.48	1.44
55	2x	21	H2U	C4-N3	-2.27	1.33	1.37
32	2a	1400	5MC	C6-N1	-2.27	1.34	1.38
32	2a	967	5MC	C6-N1	-2.26	1.34	1.38
1	1A	1917	PSU	C2-N3	-2.26	1.33	1.37
1	1A	1942	5MC	C6-N1	-2.25	1.34	1.38
1	1A	2503	2MA	C5-C6	2.24	1.47	1.41
1	1A	1915	5MU	C6-N1	-2.21	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.21	1.34	1.38
55	1x	54	5MU	C4-C5	2.21	1.48	1.44
1	1A	2552	OMU	C2-N3	-2.20	1.34	1.38
43	1l	92	0TD	CB-CA	-2.18	1.54	1.54
32	1a	1407	5MC	C6-N1	-2.18	1.34	1.38
1	1A	2503	2MA	C8-N7	2.17	1.35	1.31
32	2a	1407	5MC	C6-N1	-2.15	1.34	1.38
55	1x	8	4SU	C2-N1	2.13	1.41	1.38
1	2A	2552	OMU	C2-N3	-2.12	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.12	1.34	1.39
32	1a	1207	2MG	C2-N3	2.12	1.36	1.32
55	1x	55	PSU	C4-N3	-2.11	1.34	1.38
32	2a	966	M2G	C6-N1	-2.09	1.34	1.38
32	2a	1498	UR3	C6-C5	2.09	1.39	1.35
55	2x	37	MIA	C5-N7	-2.09	1.35	1.39
32	1a	966	M2G	C5-N7	-2.09	1.34	1.39
1	2A	1915	5MU	C2-N3	-2.06	1.34	1.38
1	1A	1911	PSU	C2-N3	-2.06	1.34	1.37
55	1x	54	5MU	C2-N1	2.06	1.41	1.38
55	1x	39	PSU	C2-N3	-2.05	1.34	1.37
1	2A	1915	5MU	C6-N1	-2.03	1.34	1.38
32	1a	967	5MC	C6-N1	-2.02	1.34	1.38
55	1x	20	H2U	C4-N3	-2.02	1.34	1.37
55	2x	39	PSU	C2-N3	-2.02	1.34	1.37
1	2A	2503	2MA	C8-N7	2.02	1.35	1.31
1	1A	2503	2MA	C4-N9	-2.00	1.33	1.37

All (306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-20.98	64.66	102.36
43	2l	92	0TD	CSB-SB-CB	-15.79	73.98	102.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C5-C4-N3	-8.30	118.44	127.18
1	1A	2503	2MA	C5-C4-N3	-7.77	119.00	127.18
1	2A	2503	2MA	N3-C4-N9	7.17	136.09	126.99
32	2a	1498	UR3	C4-N3-C2	-7.10	118.86	124.58
1	1A	2605	PSU	N1-C2-N3	6.84	122.39	115.17
32	2a	1207	2MG	C2-N3-C4	6.81	120.52	112.00
32	1a	1207	2MG	C2-N3-C4	6.80	120.50	112.00
32	1a	1498	UR3	C4-N3-C2	-6.79	119.11	124.58
1	2A	1917	PSU	N1-C2-N3	6.79	122.33	115.17
55	2x	55	PSU	N1-C2-N3	6.77	122.31	115.17
1	1A	2503	2MA	N3-C4-N9	6.69	135.48	126.99
32	1a	516	PSU	N1-C2-N3	6.66	122.19	115.17
1	1A	1917	PSU	N1-C2-N3	6.47	121.99	115.17
32	1a	966	M2G	C5-C4-N3	-6.30	118.36	128.39
55	1x	55	PSU	N1-C2-N3	6.29	121.80	115.17
1	1A	1911	PSU	N1-C2-N3	6.26	121.77	115.17
32	2a	966	M2G	C5-C4-N3	-6.22	118.49	128.39
55	1x	32	PSU	N1-C2-N3	6.21	121.72	115.17
55	1x	39	PSU	N1-C2-N3	6.10	121.60	115.17
55	2x	32	PSU	N1-C2-N3	6.01	121.51	115.17
1	2A	1911	PSU	N1-C2-N3	5.99	121.48	115.17
32	2a	516	PSU	N1-C2-N3	5.98	121.48	115.17
1	1A	2251	OMG	C5-C4-N3	-5.98	118.87	128.39
32	1a	1207	2MG	C5-C4-N3	-5.98	118.88	128.39
32	2a	1207	2MG	C5-C4-N3	-5.94	118.93	128.39
1	2A	2251	OMG	C5-C4-N3	-5.89	119.02	128.39
55	1x	8	4SU	C4-N3-C2	-5.83	121.73	127.31
55	1x	37	MIA	C5-C4-N3	-5.81	118.72	126.72
1	2A	2605	PSU	N1-C2-N3	5.79	121.28	115.17
1	1A	1915	5MU	N3-C2-N1	5.77	122.41	114.89
55	1x	8	4SU	C5-C4-N3	5.75	120.10	114.75
1	1A	1915	5MU	C4-N3-C2	-5.69	119.88	127.34
1	2A	1915	5MU	N3-C2-N1	5.68	122.28	114.89
32	1a	527	G7M	N9-C4-N3	5.63	137.20	125.95
55	2x	76	8AN	N1-C2-N3	-5.52	120.22	128.58
55	2x	54	5MU	N3-C2-N1	5.50	122.05	114.89
55	1x	76	8AN	N1-C2-N3	-5.49	120.27	128.58
1	2A	1915	5MU	C4-N3-C2	-5.49	120.15	127.34
55	2x	37	MIA	C5-C4-N3	-5.45	119.22	126.72
1	2A	1939	5MU	C4-N3-C2	-5.44	120.20	127.34
55	2x	54	5MU	C4-N3-C2	-5.37	120.29	127.34
55	1x	21	H2U	N3-C2-N1	-5.36	111.26	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1939	5MU	N3-C2-N1	5.36	121.86	114.89
55	2x	8	4SU	C5-C4-N3	5.36	119.73	114.75
32	2a	527	G7M	C5-C4-N3	-5.28	118.18	128.15
55	2x	39	PSU	N1-C2-N3	5.24	120.69	115.17
1	1A	1939	5MU	C4-N3-C2	-5.19	120.54	127.34
32	1a	527	G7M	C5-C4-N3	-5.14	118.44	128.15
32	2a	527	G7M	N9-C4-N3	5.10	136.15	125.95
32	2a	1518	MA6	C5-C4-N3	-5.08	119.72	126.72
55	2x	8	4SU	C4-N3-C2	-4.97	122.55	127.31
1	1A	2251	OMG	C2-N3-C4	4.94	120.81	112.30
32	2a	527	G7M	C2-N3-C4	4.92	120.77	112.30
1	2A	2251	OMG	C2-N3-C4	4.89	120.73	112.30
55	1x	76	8AN	C5-C4-N3	-4.85	120.04	126.72
1	1A	1915	5MU	C5-C4-N3	4.83	119.53	115.32
32	1a	1518	MA6	N1-C2-N3	-4.83	121.27	128.58
1	1A	2251	OMG	N9-C4-N3	4.82	135.60	125.95
1	1A	1939	5MU	C5-C4-N3	4.82	119.51	115.32
55	2x	76	8AN	C5-C4-N3	-4.80	120.10	126.72
1	1A	1939	5MU	N3-C2-N1	4.78	121.11	114.89
1	2A	2251	OMG	N9-C4-N3	4.78	135.50	125.95
32	1a	966	M2G	N9-C4-N3	4.76	135.47	125.95
1	2A	2552	OMU	C4-N3-C2	-4.74	120.73	126.61
32	2a	1518	MA6	N1-C2-N3	-4.72	121.44	128.58
55	1x	37	MIA	N3-C4-N9	4.71	135.19	127.17
32	2a	1519	MA6	N1-C2-N3	-4.69	121.48	128.58
1	1A	2605	PSU	C4-N3-C2	-4.64	119.98	126.37
32	1a	966	M2G	C2-N3-C4	4.58	120.98	112.51
32	2a	966	M2G	C2-N3-C4	4.54	120.91	112.51
32	2a	966	M2G	N9-C4-N3	4.51	134.96	125.95
1	1A	1915	5MU	O4-C4-C5	-4.50	119.77	124.92
55	2x	55	PSU	C4-N3-C2	-4.50	120.17	126.37
1	2A	1915	5MU	C5-C4-N3	4.49	119.23	115.32
32	1a	1519	MA6	N1-C2-N3	-4.48	121.80	128.58
32	2a	1519	MA6	C5-C4-N3	-4.47	120.56	126.72
1	2A	1939	5MU	C5-C4-N3	4.43	119.18	115.32
55	1x	55	PSU	O2-C2-N1	-4.43	118.22	122.79
1	2A	1917	PSU	C4-N3-C2	-4.39	120.33	126.37
1	2A	1917	PSU	O2-C2-N1	-4.36	118.29	122.79
32	1a	527	G7M	C2-N3-C4	4.36	119.81	112.30
55	1x	54	5MU	N3-C2-N1	4.35	120.55	114.89
55	1x	54	5MU	O4-C4-C5	-4.34	119.95	124.92
32	1a	516	PSU	C4-N3-C2	-4.34	120.39	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2552	OMU	N3-C2-N1	4.32	120.51	114.89
1	1A	2552	OMU	C4-N3-C2	-4.31	121.26	126.61
55	1x	54	5MU	C4-N3-C2	-4.26	121.76	127.34
1	1A	1939	5MU	C5-C6-N1	-4.21	118.74	123.31
55	1x	32	PSU	C4-N3-C2	-4.20	120.58	126.37
32	2a	1207	2MG	N9-C4-N3	4.20	134.35	125.95
1	2A	2605	PSU	C4-N3-C2	-4.18	120.61	126.37
32	1a	1207	2MG	N9-C4-N3	4.17	134.29	125.95
32	2a	1519	MA6	C4-C5-N7	-4.17	105.81	110.58
55	2x	54	5MU	C5-C4-N3	4.15	118.93	115.32
55	2x	37	MIA	N3-C4-N9	4.13	134.20	127.17
1	2A	1939	5MU	C5-C6-N1	-4.11	118.85	123.31
32	2a	516	PSU	C4-N3-C2	-4.11	120.71	126.37
32	2a	1519	MA6	C5-N7-C8	4.09	109.88	103.45
32	1a	1519	MA6	C2-N1-C6	4.09	121.81	111.83
55	1x	55	PSU	C4-N3-C2	-4.07	120.77	126.37
32	1a	1518	MA6	C2-N1-C6	4.05	121.72	111.83
55	2x	32	PSU	O2-C2-N1	-4.01	118.65	122.79
1	2A	1911	PSU	C4-N3-C2	-4.01	120.84	126.37
55	2x	32	PSU	C4-N3-C2	-4.01	120.84	126.37
1	2A	1915	5MU	O4-C4-C5	-4.00	120.34	124.92
1	1A	1911	PSU	C4-N3-C2	-4.00	120.86	126.37
1	1A	1917	PSU	C4-N3-C2	-3.98	120.88	126.37
32	2a	1518	MA6	C4-C5-N7	-3.96	106.05	110.58
32	2a	1400	5MC	C5-C6-N1	-3.96	119.02	123.31
1	1A	2503	2MA	N6-C6-N1	3.92	122.32	117.03
32	1a	1519	MA6	C5-C4-N3	-3.92	121.32	126.72
32	1a	1518	MA6	C5-C4-N3	-3.89	121.36	126.72
55	2x	54	5MU	O4-C4-C5	-3.89	120.47	124.92
32	2a	1518	MA6	C2-N1-C6	3.88	121.32	111.83
32	2a	1519	MA6	C2-N1-C6	3.88	121.30	111.83
1	1A	2552	OMU	C5-C4-N3	3.87	120.22	114.80
32	2a	1518	MA6	C5-N7-C8	3.87	109.53	103.45
55	1x	54	5MU	C5-C4-N3	3.83	118.66	115.32
55	2x	37	MIA	C4-C5-N7	-3.82	106.22	110.58
1	1A	2552	OMU	N3-C2-N1	3.81	119.85	114.89
1	1A	1939	5MU	O4-C4-C5	-3.77	120.60	124.92
55	1x	32	PSU	O2-C2-N1	-3.76	118.92	122.79
1	2A	2552	OMU	C5-C4-N3	3.73	120.03	114.80
1	2A	1915	5MU	C5-C6-N1	-3.71	119.28	123.31
32	1a	1518	MA6	C5-N7-C8	3.71	109.28	103.45
32	2a	1404	5MC	C5-C6-N1	-3.69	119.30	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1519	MA6	C4-C5-N7	-3.67	106.39	110.58
55	1x	37	MIA	C2-N3-C4	3.67	120.79	111.83
32	1a	1400	5MC	C5-C6-N1	-3.66	119.34	123.31
1	1A	1942	5MC	C5-C6-N1	-3.65	119.35	123.31
55	2x	37	MIA	C2-N3-C4	3.63	120.70	111.83
1	1A	2605	PSU	O2-C2-N1	-3.63	119.04	122.79
32	1a	1519	MA6	C5-N7-C8	3.63	109.15	103.45
1	2A	2503	2MA	N6-C6-N1	3.59	121.87	117.03
32	1a	1518	MA6	C4-C5-N7	-3.59	106.48	110.58
55	1x	37	MIA	N3-C2-N1	-3.58	123.16	128.58
32	2a	1518	MA6	C2-N3-C4	3.57	120.55	111.83
55	2x	37	MIA	N3-C2-N1	-3.55	123.21	128.58
32	2a	1519	MA6	N9-C8-N7	-3.53	108.93	113.94
32	1a	1207	2MG	C6-C5-N7	3.52	136.70	130.29
1	1A	2503	2MA	C4-N9-C8	3.51	109.42	105.74
55	1x	39	PSU	C4-N3-C2	-3.49	121.56	126.37
55	2x	55	PSU	O2-C2-N1	-3.49	119.19	122.79
55	1x	8	4SU	N3-C2-N1	3.48	119.42	114.89
32	1a	1404	5MC	C5-C6-N1	-3.48	119.53	123.31
43	2l	92	0TD	OD2-CG-CB	3.42	120.54	113.15
1	1A	1915	5MU	C5-C6-N1	-3.41	119.61	123.31
1	2A	1942	5MC	C5-C6-N1	-3.40	119.62	123.31
55	1x	76	8AN	N9-C8-N7	-3.39	109.13	113.94
32	2a	1519	MA6	C2-N3-C4	3.38	120.08	111.83
55	2x	8	4SU	C5-C4-S4	-3.37	120.46	124.31
55	1x	37	MIA	C4-C5-N7	-3.36	106.74	110.58
55	2x	76	8AN	N9-C8-N7	-3.36	109.17	113.94
32	1a	967	5MC	C5-C6-N1	-3.35	119.67	123.31
43	1l	92	0TD	OD2-CG-CB	3.35	120.39	113.15
32	1a	1518	MA6	N9-C8-N7	-3.35	109.19	113.94
1	2A	1962	5MC	C5-C6-N1	-3.33	119.69	123.31
55	2x	54	5MU	C5-C6-N1	-3.29	119.74	123.31
32	1a	516	PSU	O2-C2-N1	-3.27	119.41	122.79
32	2a	1518	MA6	N9-C8-N7	-3.27	109.30	113.94
55	2x	21	H2U	N3-C2-N1	-3.27	113.36	116.65
32	2a	516	PSU	O2-C2-N1	-3.27	119.42	122.79
32	2a	1207	2MG	C6-C5-N7	3.26	136.23	130.29
55	1x	20	H2U	C5-C6-N1	-3.22	101.78	111.52
32	1a	1518	MA6	C2-N3-C4	3.22	119.69	111.83
55	2x	39	PSU	C4-N3-C2	-3.20	121.96	126.37
55	1x	8	4SU	C5-C4-S4	-3.20	120.65	124.31
55	2x	76	8AN	C2-N3-C4	3.20	119.64	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1498	UR3	C5-C4-N3	3.20	119.25	115.04
1	2A	2503	2MA	C4-N9-C8	3.19	109.09	105.74
55	1x	76	8AN	C2-N3-C4	3.18	119.60	111.83
55	1x	76	8AN	C4'-O4'-C1'	-3.18	102.45	109.47
32	2a	967	5MC	C5-C6-N1	-3.16	119.88	123.31
32	2a	966	M2G	C6-C5-N7	3.15	136.02	130.29
32	2a	1518	MA6	C4-C5-C6	3.15	119.16	115.91
55	1x	76	8AN	C5-N7-C8	3.12	108.36	103.45
32	2a	1498	UR3	C5-C4-N3	3.11	119.14	115.04
32	1a	1519	MA6	N9-C8-N7	-3.10	109.54	113.94
55	2x	76	8AN	C5-N7-C8	3.09	108.31	103.45
1	1A	2552	OMU	O4-C4-C5	-3.09	119.84	125.16
55	1x	54	5MU	C5-C6-N1	-3.08	119.97	123.31
32	2a	1407	5MC	C5-C6-N1	-3.08	119.97	123.31
1	2A	1911	PSU	O2-C2-N1	-3.07	119.62	122.79
32	1a	966	M2G	C6-C5-N7	3.07	135.87	130.29
32	2a	1518	MA6	N3-C4-N9	3.06	132.37	127.17
55	2x	8	4SU	N3-C2-N1	3.05	118.86	114.89
1	2A	1939	5MU	O4-C4-C5	-3.03	121.45	124.92
32	1a	1407	5MC	C5-C6-N1	-3.03	120.02	123.31
1	2A	2251	OMG	C6-C5-N7	3.02	135.79	130.29
55	1x	76	8AN	C5-C4-N9	3.01	109.10	105.81
55	1x	21	H2U	C5-C6-N1	-3.01	102.42	111.52
32	1a	1519	MA6	C2-N3-C4	2.98	119.12	111.83
1	2A	2503	2MA	C4-C5-N7	-2.98	107.17	110.58
1	1A	1911	PSU	O2-C2-N1	-2.95	119.75	122.79
55	1x	39	PSU	O2-C2-N1	-2.94	119.75	122.79
1	2A	1939	5MU	O2-C2-N1	-2.94	118.97	122.80
32	1a	1407	5MC	C5-C4-N3	-2.93	118.75	121.75
32	2a	1407	5MC	C5-C4-N3	-2.93	118.75	121.75
55	2x	76	8AN	C5-C4-N9	2.92	108.99	105.81
1	1A	2251	OMG	C6-C5-N7	2.90	135.58	130.29
32	1a	1207	2MG	C4-C5-N7	-2.89	106.09	110.67
1	2A	1942	5MC	C5-C4-N3	-2.89	118.79	121.75
32	1a	1404	5MC	C5-C4-N3	-2.88	118.81	121.75
1	1A	1962	5MC	C5-C6-N1	-2.86	120.20	123.31
1	1A	2503	2MA	C4-C5-N7	-2.85	107.32	110.58
32	2a	1407	5MC	O2-C2-N3	-2.84	117.85	122.33
55	2x	76	8AN	C4'-O4'-C1'	-2.80	103.27	109.47
55	2x	37	MIA	C4-N9-C8	2.80	108.67	105.74
1	1A	1942	5MC	C5-C4-N3	-2.77	118.92	121.75
32	1a	527	G7M	O6-C6-C5	-2.75	121.86	128.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1917	PSU	O2-C2-N1	-2.75	119.95	122.79
55	2x	37	MIA	C5-N7-C8	2.75	107.77	103.45
55	2x	20	H2U	N3-C2-N1	2.75	119.41	116.65
55	2x	54	5MU	O2-C2-N1	-2.73	119.24	122.80
32	2a	966	M2G	C4-C5-N7	-2.72	106.36	110.67
1	2A	2552	OMU	O2-C2-N1	-2.71	119.27	122.80
1	1A	1962	5MC	C5-C4-N3	-2.70	118.99	121.75
55	2x	21	H2U	O2-C2-N1	2.69	126.34	123.10
1	1A	1915	5MU	O2-C2-N1	-2.67	119.32	122.80
55	2x	39	PSU	O2-C2-N1	-2.67	120.04	122.79
1	1A	1920	OMC	O2-C2-N3	-2.66	118.13	122.33
55	1x	37	MIA	C4-N9-C8	2.65	108.52	105.74
1	2A	2552	OMU	O4-C4-C5	-2.65	120.59	125.16
32	1a	1400	5MC	C5-C4-N3	-2.65	119.04	121.75
32	2a	1207	2MG	C4-C5-N7	-2.65	106.48	110.67
1	2A	2251	OMG	O6-C6-C5	-2.65	119.55	126.53
1	1A	2251	OMG	O6-C6-C5	-2.57	119.75	126.53
32	2a	1404	5MC	C5-C4-N3	-2.57	119.12	121.75
55	1x	37	MIA	C5-N7-C8	2.57	107.49	103.45
55	1x	54	5MU	O2-C2-N1	-2.56	119.47	122.80
1	2A	1962	5MC	C5-C4-N3	-2.56	119.13	121.75
32	2a	1519	MA6	N3-C4-N9	2.55	131.50	127.17
32	1a	1402	4OC	C6-C5-C4	2.55	120.07	117.00
55	2x	55	PSU	C5-C6-N1	-2.54	118.61	122.14
1	2A	2605	PSU	O2-C2-N1	-2.52	120.19	122.79
1	1A	2605	PSU	C5-C6-N1	-2.50	118.67	122.14
32	1a	966	M2G	C4-C5-N7	-2.49	106.72	110.67
1	2A	2503	2MA	C2-N1-C6	2.49	121.93	118.10
1	1A	2503	2MA	C2-N1-C6	2.48	121.91	118.10
1	1A	2503	2MA	N9-C8-N7	-2.46	110.45	113.94
1	2A	2503	2MA	C5-N7-C8	2.46	107.31	103.45
1	1A	2503	2MA	C5-N7-C8	2.45	107.30	103.45
43	2l	92	0TD	OD1-CG-CB	-2.44	117.34	122.44
1	1A	1939	5MU	O2-C2-N1	-2.43	119.64	122.80
32	2a	516	PSU	O4'-C1'-C2'	2.41	108.48	105.15
32	1a	1519	MA6	C4-C5-C6	2.40	118.39	115.91
1	2A	1911	PSU	C6-C5-C4	-2.40	116.56	118.17
32	2a	967	5MC	C5-C4-N3	-2.38	119.32	121.75
32	2a	1519	MA6	C4-C5-C6	2.37	118.36	115.91
32	1a	967	5MC	C5-C4-N3	-2.37	119.32	121.75
32	1a	1518	MA6	N3-C4-N9	2.36	131.18	127.17
55	1x	76	8AN	C4-C5-N7	-2.36	107.89	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1400	5MC	C5-C4-N3	-2.34	119.35	121.75
55	2x	37	MIA	C6-C5-N7	2.34	136.60	132.09
32	1a	1407	5MC	CM5-C5-C6	-2.32	119.70	122.85
1	1A	2251	OMG	C5-C6-N1	2.32	119.16	113.25
55	2x	76	8AN	C4-C5-N7	-2.29	107.96	110.58
32	2a	1498	UR3	C3U-N3-C4	2.28	121.03	117.87
1	1A	1917	PSU	C5-C6-N1	-2.28	118.97	122.14
32	1a	1402	4OC	O2-C2-N3	-2.28	118.73	122.33
1	1A	1920	OMC	C1'-N1-C2	2.26	123.44	118.44
32	2a	527	G7M	C5-C6-N1	2.26	116.52	111.84
1	2A	1917	PSU	C5-C6-N1	-2.26	119.00	122.14
1	2A	1962	5MC	CM5-C5-C6	-2.25	119.81	122.85
55	2x	8	4SU	C1'-N1-C2	2.25	121.63	117.59
55	2x	37	MIA	N9-C8-N7	-2.24	110.75	113.94
32	2a	527	G7M	O6-C6-C5	-2.23	123.03	128.01
55	2x	21	H2U	C5-C6-N1	-2.23	104.78	111.52
32	1a	1519	MA6	N3-C4-N9	2.21	130.93	127.17
1	1A	1911	PSU	C5-C6-N1	-2.21	119.08	122.14
55	2x	76	8AN	N3-C4-N9	2.20	130.90	127.17
55	1x	76	8AN	N3-C4-N9	2.17	130.86	127.17
32	2a	1402	4OC	C6-C5-C4	2.17	119.62	117.00
32	1a	527	G7M	C5-C6-N1	2.17	116.32	111.84
55	2x	39	PSU	C6-C5-C4	-2.16	116.71	118.17
1	1A	1942	5MC	O2-C2-N3	-2.16	118.92	122.33
1	2A	1939	5MU	C5M-C5-C4	2.15	121.08	118.78
1	2A	1915	5MU	O2-C2-N1	-2.15	120.00	122.80
32	1a	516	PSU	C5-C6-N1	-2.14	119.17	122.14
1	1A	1917	PSU	O2-C2-N3	-2.14	118.06	121.86
55	1x	76	8AN	C6-C5-C4	2.14	120.10	117.18
55	2x	76	8AN	C6-C5-C4	2.12	120.07	117.18
1	2A	2503	2MA	N9-C8-N7	-2.11	110.94	113.94
1	1A	1942	5MC	N1-C2-N3	2.10	122.45	118.80
1	2A	2251	OMG	C5-C6-N1	2.09	118.57	113.25
1	2A	2251	OMG	C4-C5-N7	-2.08	107.37	110.67
32	2a	516	PSU	C5-C6-N1	-2.08	119.25	122.14
55	2x	32	PSU	C6-C5-C4	-2.07	116.78	118.17
55	2x	54	5MU	C5M-C5-C6	-2.06	120.06	122.85
32	1a	1407	5MC	O2-C2-N3	-2.06	119.08	122.33
1	2A	2605	PSU	O4-C4-C5	-2.05	118.91	124.01
1	2A	2605	PSU	C5-C6-N1	-2.05	119.29	122.14
1	2A	1915	5MU	O2-C2-N3	-2.05	117.71	121.49
32	1a	1498	UR3	C3U-N3-C4	2.04	120.70	117.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	O2-C2-N1	-2.03	120.15	122.80
55	2x	54	5MU	C5M-C5-C4	2.03	120.95	118.78
43	1l	92	0TD	OD1-CG-CB	-2.03	118.20	122.44
1	2A	1942	5MC	O2-C2-N3	-2.02	119.15	122.33
1	1A	1962	5MC	CM5-C5-C6	-2.01	120.13	122.85
1	2A	1920	OMC	O2-C2-N3	-2.00	119.17	122.33
55	1x	55	PSU	C5-C6-N1	-2.00	119.36	122.14
32	1a	967	5MC	O2-C2-N3	-2.00	119.17	122.33
1	2A	1939	5MU	C5M-C5-C6	-2.00	120.14	122.85
32	2a	966	M2G	O6-C6-C5	-2.00	121.25	126.53

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	O-C-CA-CB
54	1w	230	MEQ	C-CA-CB-CG
54	1w	230	MEQ	O-C-CA-CB
32	2a	1402	4OC	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB
55	2x	20	H2U	O4'-C1'-N1-C6
55	2x	21	H2U	O4'-C4'-C5'-O5'
55	1x	37	MIA	O4'-C4'-C5'-O5'
55	1x	37	MIA	C3'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
55	2x	21	H2U	C3'-C4'-C5'-O5'
55	2x	37	MIA	O4'-C4'-C5'-O5'
55	1x	76	8AN	C4'-C5'-O5'-P
54	2w	230	MEQ	CA-CB-CG-CD
55	1x	21	H2U	C2'-C1'-N1-C2
55	1x	21	H2U	C2'-C1'-N1-C6
55	2x	21	H2U	C2'-C1'-N1-C6
55	2x	21	H2U	C2'-C1'-N1-C2
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
55	1x	20	H2U	O4'-C4'-C5'-O5'
55	2x	20	H2U	O4'-C4'-C5'-O5'
55	2x	37	MIA	C3'-C4'-C5'-O5'
55	1x	20	H2U	C3'-C4'-C5'-O5'
55	1x	21	H2U	C4'-C5'-O5'-P
55	2x	20	H2U	C3'-C4'-C5'-O5'
55	1x	54	5MU	C3'-C4'-C5'-O5'
55	1x	54	5MU	O4'-C4'-C5'-O5'
55	2x	20	H2U	O4'-C1'-N1-C2
54	1w	230	MEQ	OE1-CD-CG-CB
32	2a	1402	4OC	C3'-C2'-O2'-CM2
32	2a	516	PSU	O4'-C1'-C5-C4
32	2a	1519	MA6	C4'-C5'-O5'-P
1	2A	2503	2MA	C4'-C5'-O5'-P
32	2a	527	G7M	C4'-C5'-O5'-P
55	2x	21	H2U	C4'-C5'-O5'-P
54	1w	230	MEQ	NE2-CD-CG-CB
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
32	2a	516	PSU	O4'-C1'-C5-C6
55	1x	21	H2U	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1402	4OC	C2'-C1'-N1-C2
1	1A	1915	5MU	C3'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
54	2w	230	MEQ	N-CA-CB-CG

There are no ring outliers.

34 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1x	8	4SU	1	0
32	1a	1519	MA6	2	0
32	1a	1400	5MC	2	0
1	1A	1939	5MU	1	0
32	1a	1518	MA6	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1w	230	MEQ	2	0
1	1A	1917	PSU	1	0
32	1a	1402	4OC	2	0
32	2a	1404	5MC	2	0
1	2A	1939	5MU	1	0
43	1l	92	0TD	1	0
32	1a	516	PSU	1	0
1	1A	2251	OMG	1	0
32	2a	1400	5MC	1	0
32	2a	527	G7M	1	0
32	1a	966	M2G	2	0
55	1x	76	8AN	2	0
1	2A	1942	5MC	1	0
32	2a	1518	MA6	1	0
55	2x	20	H2U	1	0
32	2a	966	M2G	1	0
55	1x	20	H2U	1	0
1	1A	1920	OMC	1	0
1	1A	2552	OMU	1	0
32	2a	1207	2MG	1	0
55	1x	21	H2U	1	0
32	2a	1402	4OC	1	0
32	2a	1519	MA6	3	0
1	2A	1915	5MU	2	0
32	1a	967	5MC	1	0
55	2x	8	4SU	1	0
43	2l	92	0TD	1	0
55	2x	76	8AN	1	0
1	1A	1915	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2691 ligands modelled in this entry, 2689 are monoatomic - leaving 2 for Mogul analysis.

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

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

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.34	169 (5%) 28 24	22, 38, 91, 104	0
1	2A	2789/2915 (95%)	0.08	129 (4%) 37 33	33, 57, 88, 101	0
2	1B	120/121 (99%)	-0.17	0 100 100	32, 53, 65, 80	0
2	2B	120/121 (99%)	0.71	0 100 100	58, 75, 82, 91	0
3	1D	275/276 (99%)	-0.10	2 (0%) 84 81	23, 39, 53, 77	0
3	2D	275/276 (99%)	0.35	6 (2%) 62 58	30, 50, 62, 76	0
4	1E	204/206 (99%)	0.01	0 100 100	21, 41, 61, 72	0
4	2E	204/206 (99%)	0.51	6 (2%) 53 50	34, 57, 70, 77	0
5	1F	203/210 (96%)	0.03	3 (1%) 72 68	19, 42, 67, 80	0
5	2F	203/210 (96%)	0.82	10 (4%) 35 31	36, 65, 77, 84	0
6	1G	181/182 (99%)	1.01	19 (10%) 11 8	51, 66, 76, 84	0
6	2G	181/182 (99%)	1.43	33 (18%) 3 3	69, 77, 82, 87	0
7	1H	174/180 (96%)	0.42	5 (2%) 53 50	39, 55, 65, 76	0
7	2H	174/180 (96%)	1.67	53 (30%) 1 1	68, 78, 85, 88	0
8	1I	146/148 (98%)	1.01	11 (7%) 20 17	48, 70, 77, 81	0
8	2I	146/148 (98%)	1.47	28 (19%) 3 2	58, 73, 79, 84	0
9	1N	140/140 (100%)	-0.05	0 100 100	28, 40, 59, 76	0
9	2N	140/140 (100%)	0.85	8 (5%) 29 25	45, 63, 74, 78	0
10	1O	122/122 (100%)	0.10	0 100 100	32, 43, 59, 64	0
10	2O	122/122 (100%)	0.35	0 100 100	45, 54, 66, 71	0
11	1P	149/150 (99%)	0.12	1 (0%) 84 81	22, 44, 64, 72	0
11	2P	149/150 (99%)	0.85	7 (4%) 36 32	38, 66, 79, 84	0
12	1Q	141/141 (100%)	0.12	4 (2%) 55 51	28, 42, 53, 67	0
12	2Q	141/141 (100%)	0.93	14 (9%) 13 9	49, 62, 72, 78	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.14	0 100 100	26, 37, 50, 62	0
13	2R	118/118 (100%)	0.39	1 (0%) 82 80	41, 52, 61, 70	0
14	1S	110/112 (98%)	0.36	1 (0%) 81 78	40, 53, 65, 70	0
14	2S	110/112 (98%)	1.55	28 (25%) 1 1	62, 70, 78, 84	0
15	1T	131/146 (89%)	0.19	2 (1%) 72 68	34, 46, 67, 74	0
15	2T	131/146 (89%)	0.58	4 (3%) 51 47	49, 58, 72, 79	0
16	1U	116/118 (98%)	-0.30	0 100 100	23, 33, 46, 58	0
16	2U	116/118 (98%)	0.66	2 (1%) 69 65	43, 58, 70, 76	0
17	1V	101/101 (100%)	-0.04	2 (1%) 65 60	22, 42, 58, 77	0
17	2V	101/101 (100%)	0.81	3 (2%) 52 48	45, 66, 75, 79	0
18	1W	112/113 (99%)	-0.20	1 (0%) 81 78	25, 33, 53, 74	0
18	2W	112/113 (99%)	0.37	1 (0%) 81 78	41, 51, 66, 78	0
19	1X	95/96 (98%)	0.18	2 (2%) 63 59	32, 40, 62, 75	0
19	2X	95/96 (98%)	0.58	5 (5%) 32 28	48, 61, 71, 77	0
20	1Y	107/110 (97%)	0.57	4 (3%) 45 41	39, 50, 64, 77	0
20	2Y	107/110 (97%)	1.26	19 (17%) 4 3	59, 69, 77, 82	0
21	1Z	154/206 (74%)	0.78	8 (5%) 33 29	42, 59, 72, 81	0
21	2Z	160/206 (77%)	1.30	20 (12%) 8 6	62, 73, 80, 85	0
22	10	76/85 (89%)	0.09	3 (3%) 43 39	30, 40, 57, 65	0
22	20	76/85 (89%)	0.92	6 (7%) 18 15	48, 62, 71, 76	0
23	11	97/98 (98%)	0.19	2 (2%) 63 59	32, 44, 68, 75	0
23	21	97/98 (98%)	0.55	3 (3%) 51 47	43, 57, 72, 78	0
24	12	70/72 (97%)	0.27	3 (4%) 40 36	35, 50, 62, 72	0
24	22	70/72 (97%)	0.96	2 (2%) 53 50	61, 69, 75, 76	0
25	13	59/60 (98%)	-0.12	1 (1%) 69 65	29, 36, 58, 71	0
25	23	59/60 (98%)	0.59	2 (3%) 48 44	53, 59, 72, 75	0
26	14	69/71 (97%)	1.61	22 (31%) 1 1	61, 78, 86, 90	0
26	24	69/71 (97%)	1.80	22 (31%) 1 1	72, 82, 88, 90	0
27	15	59/60 (98%)	-0.12	2 (3%) 48 44	22, 36, 56, 70	0
27	25	59/60 (98%)	0.38	1 (1%) 69 65	37, 54, 65, 78	0
28	16	53/54 (98%)	-0.00	0 100 100	36, 43, 56, 62	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%)	0.70	3 (5%) 29 25	50, 60, 67, 71	0
29	17	48/49 (97%)	0.07	4 (8%) 17 14	22, 29, 64, 69	0
29	27	48/49 (97%)	0.34	4 (8%) 17 14	34, 45, 67, 74	0
30	18	64/65 (98%)	-0.19	0 100 100	28, 35, 43, 54	0
30	28	64/65 (98%)	0.58	1 (1%) 70 66	44, 54, 61, 64	0
31	19	37/37 (100%)	0.05	0 100 100	31, 41, 52, 58	0
31	29	37/37 (100%)	0.97	5 (13%) 7 5	54, 64, 72, 73	0
32	1a	1488/1521 (97%)	0.71	98 (6%) 24 20	39, 73, 91, 100	0
32	2a	1491/1521 (98%)	0.71	113 (7%) 20 16	48, 74, 90, 100	0
33	1b	231/256 (90%)	1.51	59 (25%) 1 1	68, 77, 84, 87	0
33	2b	231/256 (90%)	1.76	88 (38%) 1 0	68, 79, 85, 88	0
34	1c	206/239 (86%)	1.82	88 (42%) 0 0	68, 77, 84, 89	0
34	2c	206/239 (86%)	1.75	71 (34%) 1 1	69, 79, 84, 87	0
35	1d	208/209 (99%)	1.47	53 (25%) 1 1	60, 73, 80, 85	0
35	2d	208/209 (99%)	1.32	29 (13%) 6 5	61, 70, 77, 83	0
36	1e	148/162 (91%)	0.93	8 (5%) 31 28	50, 67, 75, 82	0
36	2e	148/162 (91%)	1.20	16 (10%) 11 8	58, 71, 77, 80	0
37	1f	100/101 (99%)	1.06	8 (8%) 18 15	60, 70, 76, 78	0
37	2f	100/101 (99%)	1.09	10 (10%) 12 9	63, 71, 77, 80	0
38	1g	155/156 (99%)	1.32	30 (19%) 3 2	66, 74, 82, 87	0
38	2g	155/156 (99%)	1.50	30 (19%) 3 2	70, 77, 86, 89	0
39	1h	137/138 (99%)	0.98	8 (5%) 29 25	58, 69, 76, 80	0
39	2h	137/138 (99%)	1.04	12 (8%) 15 12	65, 72, 76, 79	0
40	1i	127/128 (99%)	1.83	46 (36%) 1 1	64, 78, 82, 83	0
40	2i	127/128 (99%)	2.33	68 (53%) 0 0	71, 81, 86, 88	0
41	1j	97/105 (92%)	2.19	52 (53%) 0 0	66, 80, 85, 87	0
41	2j	96/105 (91%)	2.34	58 (60%) 0 0	72, 82, 88, 90	0
42	1k	114/129 (88%)	1.07	13 (11%) 10 7	48, 68, 77, 80	0
42	2k	114/129 (88%)	1.17	16 (14%) 6 5	56, 72, 81, 85	0
43	1l	121/132 (91%)	1.15	14 (11%) 9 7	50, 62, 70, 72	0
43	2l	121/132 (91%)	1.01	9 (7%) 20 17	56, 63, 71, 76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	118/126 (93%)	1.73	40 (33%) 1 1	68, 78, 81, 85	0
44	2m	116/126 (92%)	2.16	62 (53%) 0 0	72, 80, 84, 85	0
45	1n	60/61 (98%)	1.98	24 (40%) 1 0	70, 76, 82, 85	0
45	2n	60/61 (98%)	2.13	33 (55%) 0 0	74, 80, 83, 84	0
46	1o	88/89 (98%)	1.07	9 (10%) 12 9	51, 67, 75, 77	0
46	2o	88/89 (98%)	1.13	8 (9%) 15 12	60, 70, 77, 79	0
47	1p	82/88 (93%)	1.69	26 (31%) 1 1	64, 73, 80, 83	0
47	2p	82/88 (93%)	1.51	19 (23%) 2 1	63, 70, 75, 78	0
48	1q	99/105 (94%)	1.15	11 (11%) 10 7	58, 68, 75, 79	0
48	2q	99/105 (94%)	0.95	8 (8%) 18 14	60, 68, 75, 81	0
49	1r	68/88 (77%)	0.94	7 (10%) 12 9	59, 68, 76, 80	0
49	2r	68/88 (77%)	1.10	7 (10%) 12 9	62, 71, 78, 82	0
50	1s	83/93 (89%)	2.06	39 (46%) 0 0	72, 80, 85, 85	0
50	2s	83/93 (89%)	2.14	45 (54%) 0 0	71, 83, 86, 91	0
51	1t	96/106 (90%)	1.30	13 (13%) 7 5	61, 70, 78, 82	0
51	2t	96/106 (90%)	1.20	15 (15%) 5 4	59, 69, 77, 80	0
52	1u	23/27 (85%)	2.08	10 (43%) 0 0	71, 77, 80, 82	0
52	2u	23/27 (85%)	2.05	11 (47%) 0 0	74, 78, 80, 81	0
53	1v	9/24 (37%)	0.91	3 (33%) 1 1	55, 58, 82, 87	0
53	2v	9/24 (37%)	1.21	3 (33%) 1 1	64, 66, 86, 86	0
54	1w	248/354 (70%)	0.68	12 (4%) 35 32	35, 64, 78, 84	0
54	2w	252/354 (71%)	0.96	23 (9%) 15 12	52, 71, 83, 91	0
55	1x	65/74 (87%)	0.21	0 100 100	36, 66, 80, 83	0
55	2x	65/74 (87%)	0.49	1 (1%) 72 68	53, 76, 83, 86	0
56	1z	5/7 (71%)	1.85	2 (40%) 1 0	42, 46, 55, 68	0
56	2z	4/7 (57%)	2.78	2 (50%) 0 0	59, 64, 65, 66	0
All	All	21072/22160 (95%)	0.60	2127 (10%) 12 9	19, 64, 84, 104	0

All (2127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	2147	G	9.0
1	1A	2114	A	8.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2113	U	7.9
1	1A	2178	C	7.6
45	1n	2	ALA	7.6
1	2A	2105	C	7.5
1	2A	2117	A	7.2
1	2A	2146	C	7.1
1	2A	2145	C	7.0
1	1A	2115	G	7.0
40	2i	11	LYS	6.9
1	1A	2117	A	6.8
1	1A	2121	G	6.8
1	2A	2111	C	6.7
1	2A	2177	C	6.6
21	2Z	174	VAL	6.6
1	1A	1072	C	6.6
50	1s	84	GLY	6.5
1	1A	2116	G	6.4
1	2A	2158	A	6.4
38	2g	80	VAL	6.4
1	2A	2138	C	6.4
1	1A	2179	C	6.3
1	1A	1093	G	6.3
1	2A	2120	G	6.3
1	2A	2104	G	6.2
26	24	49	PHE	6.2
1	1A	1058	G	6.2
1	2A	2159	G	6.1
1	1A	1088	A	6.1
1	1A	2141	G	6.0
1	1A	2159	G	6.0
1	1A	2112	G	6.0
1	1A	2169	A	5.8
1	1A	1068	G	5.8
1	1A	2167	U	5.7
1	2A	2110	G	5.7
1	1A	1087	G	5.7
1	1A	2122	U	5.7
20	2Y	1	MET	5.7
1	2A	2123	G	5.6
45	2n	2	ALA	5.6
1	2A	2178	C	5.6
7	1H	2	SER	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1069	A	5.5
50	2s	52	TYR	5.5
1	2A	2122	U	5.4
6	2G	52	ILE	5.4
1	1A	2145	C	5.4
1	1A	1097	U	5.4
44	2m	7	VAL	5.4
50	1s	71	LEU	5.4
33	2b	165	VAL	5.3
1	1A	2120	G	5.3
1	2A	2121	G	5.3
1	2A	2144	U	5.3
1	1A	1070	A	5.3
44	2m	102	ARG	5.3
41	2j	75	ILE	5.3
1	1A	1098	A	5.3
1	1A	1071	G	5.3
40	1i	15	ALA	5.3
38	1g	85	TYR	5.2
1	1A	1094	U	5.2
1	1A	2110	G	5.2
56	1z	3	ALA	5.2
1	1A	2170	A	5.1
14	2S	60	GLY	5.1
21	1Z	51	ALA	5.1
50	1s	20	LEU	5.1
1	1A	1063	G	5.1
1	1A	2111	C	5.0
44	2m	118	ALA	5.0
1	1A	2147	G	5.0
42	2k	14	VAL	5.0
34	1c	2	GLY	5.0
1	2A	2119	A	4.9
1	1A	1064	C	4.9
1	1A	1099	G	4.9
1	2A	2148	G	4.9
33	1b	17	PHE	4.9
21	2Z	146	ILE	4.9
1	2A	2134	A	4.9
17	2V	42	GLY	4.9
1	2A	2108	C	4.9
29	17	45	ALA	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2168	G	4.9
29	27	45	ALA	4.8
40	2i	14	VAL	4.8
1	2A	2109	U	4.8
26	14	59	PHE	4.8
40	2i	9	ARG	4.8
1	1A	2119	A	4.8
5	2F	208	GLY	4.8
51	1t	103	GLY	4.8
34	1c	65	ALA	4.8
44	1m	119	GLY	4.8
32	1a	1036	G	4.7
1	1A	1081	U	4.7
1	1A	2180	U	4.7
38	2g	83	ALA	4.7
1	1A	1057	A	4.7
1	2A	2179	C	4.7
1	1A	1073	A	4.7
1	1A	2174	C	4.7
1	1A	2175	C	4.7
32	2a	1034	G	4.7
34	2c	2	GLY	4.6
41	2j	76	ASN	4.6
43	1l	126	LYS	4.6
1	1A	1059	G	4.6
16	2U	90	VAL	4.6
1	2A	2182	G	4.6
1	1A	2146	C	4.6
38	2g	81	GLY	4.6
1	1A	2129	C	4.5
38	2g	82	GLY	4.5
50	2s	2	PRO	4.5
32	1a	1035	A	4.5
33	1b	230	VAL	4.5
23	2l	2	SER	4.5
32	1a	1025	U	4.5
44	2m	30	ALA	4.5
40	2i	10	ARG	4.5
38	2g	84	ASN	4.5
1	1A	1092	C	4.5
1	1A	2118	U	4.5
1	1A	1086	A	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2106	G	4.4
1	2A	2115	G	4.4
1	2A	2133	G	4.4
35	1d	69	GLY	4.4
26	24	50	VAL	4.4
26	24	56	VAL	4.4
1	2A	2113	U	4.4
1	2A	2112	G	4.4
1	2A	2170	A	4.4
32	2a	1035	A	4.4
1	2A	2118	U	4.4
1	2A	2116	G	4.4
32	1a	1003	G	4.4
54	2w	190	GLY	4.4
1	1A	2177	C	4.3
1	2A	2137	C	4.3
40	2i	5	TYR	4.3
3	1D	276	LYS	4.3
33	1b	10	LEU	4.3
56	2z	4	ALA	4.3
32	2a	1219	U	4.3
1	1A	1100	C	4.3
1	1A	2166	G	4.3
32	1a	1024	G	4.3
52	1u	23	PRO	4.3
44	2m	98	VAL	4.3
41	2j	47	PHE	4.3
21	2Z	166	SER	4.3
1	1A	1060	U	4.3
1	1A	2108	C	4.3
6	2G	53	LEU	4.3
32	1a	1286	A	4.3
34	1c	100	ALA	4.3
44	1m	2	ALA	4.3
1	1A	2104	G	4.2
1	1A	2125	G	4.2
29	17	46	VAL	4.2
40	2i	18	PHE	4.2
38	2g	2	ALA	4.2
14	2S	3	ARG	4.2
38	2g	85	TYR	4.2
1	2A	2114	A	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	156	TRP	4.2
38	1g	80	VAL	4.2
40	2i	102	LEU	4.2
44	1m	118	ALA	4.2
1	1A	1067	A	4.2
26	14	54	GLY	4.2
1	1A	2148	G	4.2
32	2a	1030(A)	G	4.2
32	2a	1036	G	4.2
50	1s	9	VAL	4.2
7	1H	175	LYS	4.2
33	1b	132	LYS	4.2
7	2H	2	SER	4.2
1	2A	2183	C	4.2
40	2i	2	GLU	4.2
1	1A	1101	U	4.2
32	2a	1033	G	4.2
32	2a	1119	C	4.1
53	2v	22	U	4.1
40	2i	105	ASP	4.1
38	2g	5	ARG	4.1
1	2A	2128	C	4.1
32	2a	1038	C	4.1
1	1A	2109	U	4.1
40	2i	13	ALA	4.1
1	2A	2181	G	4.1
45	2n	21	TYR	4.1
44	2m	54	VAL	4.1
1	2A	1536	C	4.1
44	2m	5	ALA	4.1
56	2z	5	ALA	4.1
32	2a	1003	G	4.1
42	2k	126	ARG	4.0
41	1j	8	LEU	4.0
1	1A	1062	G	4.0
32	1a	1005	A	4.0
33	2b	237	ALA	4.0
27	15	59	GLU	4.0
23	11	2	SER	4.0
41	1j	4	ILE	4.0
33	1b	7	VAL	4.0
40	2i	15	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2158	A	4.0
32	1a	1039	C	4.0
1	1A	2102	U	4.0
1	1A	2130	U	4.0
41	1j	74	ILE	4.0
40	2i	7	THR	4.0
15	1T	131	ALA	4.0
29	27	48	LYS	4.0
1	2A	2157	G	4.0
1	1A	1077	A	4.0
41	2j	93	GLY	4.0
26	14	52	THR	4.0
40	1i	14	VAL	4.0
42	2k	13	GLN	4.0
3	2D	2	ALA	3.9
15	2T	130	ALA	3.9
41	2j	27	ALA	3.9
1	2A	2154	G	3.9
20	1Y	1	MET	3.9
22	20	10	THR	3.9
42	2k	31	THR	3.9
33	2b	36	ARG	3.9
34	2c	168	ALA	3.9
1	1A	2160	G	3.9
32	2a	1026	G	3.9
33	1b	11	LEU	3.9
1	2A	2130	U	3.9
1	1A	2128	C	3.9
33	1b	229	VAL	3.9
21	1Z	146	ILE	3.9
33	1b	19	HIS	3.9
40	2i	66	ARG	3.9
32	2a	1004	A	3.9
33	1b	129	GLU	3.9
47	1p	82	GLN	3.9
1	1A	2124	G	3.9
1	2A	2165	G	3.9
32	1a	1034	G	3.9
32	2a	1024	G	3.9
44	2m	17	VAL	3.9
44	2m	117	VAL	3.9
40	2i	6	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
51	2t	103	GLY	3.9
47	2p	82	GLN	3.9
1	2A	2176	A	3.9
1	1A	2181	G	3.8
1	2A	2139	C	3.8
32	2a	1029	C	3.8
34	1c	48	TYR	3.8
40	2i	62	TYR	3.8
45	2n	30	ALA	3.8
40	2i	91	ASP	3.8
40	1i	56	LEU	3.8
1	2A	2129	C	3.8
33	2b	10	LEU	3.8
40	2i	96	LEU	3.8
41	2j	41	PRO	3.8
41	2j	77	PRO	3.8
1	2A	2126	A	3.8
1	2A	2135	A	3.8
1	2A	2169	A	3.8
26	24	54	GLY	3.8
34	2c	8	ILE	3.8
41	2j	74	ILE	3.8
32	2a	1032	G	3.8
7	2H	44	VAL	3.8
50	1s	24	ALA	3.8
54	2w	351	LEU	3.8
1	2A	2142	C	3.8
40	2i	104	ARG	3.7
6	2G	50	ALA	3.7
15	1T	130	ALA	3.7
36	2e	23	GLY	3.7
6	1G	146	TYR	3.7
33	2b	236	TYR	3.7
20	2Y	57	GLN	3.7
1	2A	2107	C	3.7
1	1A	2149	G	3.7
1	2A	2149	G	3.7
34	2c	207	VAL	3.7
41	1j	34	VAL	3.7
50	2s	29	ARG	3.7
33	2b	38	GLY	3.7
41	1j	93	GLY	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	236	TYR	3.7
1	2A	2185	C	3.7
7	2H	45	VAL	3.7
26	14	56	VAL	3.7
45	2n	18	VAL	3.7
1	1A	1089	G	3.7
1	2A	2131	G	3.7
12	2Q	61	GLY	3.7
42	1k	98	LEU	3.7
1	2A	2167	U	3.7
26	24	51	ASP	3.7
38	2g	112	PRO	3.7
37	2f	6	VAL	3.7
40	2i	126	SER	3.7
41	1j	35	SER	3.7
32	2a	1030(B)	C	3.7
1	1A	1074	G	3.7
6	2G	139	LEU	3.7
14	2S	32	LEU	3.7
33	1b	97	TRP	3.6
52	2u	14	TRP	3.6
1	1A	2105	C	3.6
54	1w	350	ALA	3.6
35	2d	23	GLY	3.6
11	2P	15	ARG	3.6
41	2j	37	PRO	3.6
47	1p	42	ARG	3.6
1	1A	2131	G	3.6
1	1A	2165	G	3.6
1	1A	2135	A	3.6
34	2c	135	LYS	3.6
19	1X	95	LEU	3.6
1	2A	2124	G	3.6
8	1I	90	GLY	3.6
40	2i	19	LEU	3.6
33	2b	200	ILE	3.6
50	2s	76	PRO	3.6
1	1A	2142	C	3.6
32	1a	1038	C	3.6
44	1m	87	TYR	3.6
44	2m	87	TYR	3.6
32	1a	1001(A)	G	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	109	VAL	3.6
44	2m	53	VAL	3.6
40	1i	8	GLY	3.6
40	1i	13	ALA	3.6
41	1j	50	ILE	3.6
51	1t	9	ASN	3.6
33	1b	9	GLU	3.5
1	1A	2106	G	3.5
1	2A	2166	G	3.5
33	1b	38	GLY	3.5
32	1a	1447	A	3.5
8	2I	133	HIS	3.5
33	2b	71	VAL	3.5
37	1f	21	LEU	3.5
19	1X	94	GLY	3.5
1	1A	2123	G	3.5
33	2b	140	HIS	3.5
1	1A	1075	C	3.5
32	1a	1019	C	3.5
41	1j	36	GLY	3.5
50	2s	84	GLY	3.5
14	2S	35	ILE	3.5
32	1a	374	A	3.5
1	2A	2160	G	3.5
27	25	60	VAL	3.5
1	1A	1079	C	3.5
32	1a	1028	C	3.5
32	1a	1000	U	3.5
32	1a	1020	U	3.5
38	2g	16	LEU	3.5
45	1n	7	ILE	3.5
44	2m	58	GLU	3.4
38	1g	5	ARG	3.4
1	1A	2133	G	3.4
32	1a	1002	G	3.4
32	1a	1026	G	3.4
41	2j	100	THR	3.4
1	1A	1080	C	3.4
32	1a	1029	C	3.4
40	2i	8	GLY	3.4
32	1a	1040	U	3.4
43	1l	91	LYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	63	ILE	3.4
36	2e	20	GLN	3.4
7	2H	43	VAL	3.4
32	1a	1023	G	3.4
32	2a	630	G	3.4
32	2a	1031	G	3.4
40	2i	103	THR	3.4
43	2l	94	PRO	3.4
47	1p	41	PRO	3.4
44	2m	18	ALA	3.4
36	2e	109	ILE	3.4
1	1A	1509	C	3.4
1	1A	2164	C	3.4
1	2A	2180	U	3.4
32	1a	1027	C	3.4
12	2Q	60	ARG	3.4
26	14	55	ARG	3.4
41	1j	46	ARG	3.4
1	1A	2173	A	3.4
38	1g	118	VAL	3.4
40	1i	102	LEU	3.4
41	2j	67	THR	3.4
1	2A	2100	G	3.4
41	2j	50	ILE	3.4
41	2j	30	SER	3.4
1	1A	1082	U	3.4
1	1A	2144	U	3.4
52	1u	18	TYR	3.4
38	1g	156	TRP	3.4
41	1j	99	LYS	3.4
7	2H	50	VAL	3.4
8	2I	3	VAL	3.4
35	1d	101	LEU	3.4
41	2j	40	LEU	3.4
41	2j	81	THR	3.4
44	2m	60	VAL	3.4
6	1G	151	ALA	3.4
33	1b	201	ILE	3.4
34	1c	163	ALA	3.4
34	2c	182	ILE	3.4
40	2i	43	ALA	3.4
45	2n	7	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	134	GLU	3.4
1	2A	2184	G	3.3
32	2a	1002	G	3.3
1	1A	2107	C	3.3
32	1a	1037	C	3.3
33	1b	37	ASN	3.3
7	2H	114	VAL	3.3
39	2h	2	LEU	3.3
41	2j	65	LEU	3.3
32	2a	1016	A	3.3
45	2n	31	ARG	3.3
33	1b	237	ALA	3.3
41	1j	47	PHE	3.3
1	1A	2127	G	3.3
34	2c	4	LYS	3.3
1	2A	2140	C	3.3
1	2A	2143	C	3.3
1	2A	2174	C	3.3
35	1d	96	LEU	3.3
50	2s	16	LEU	3.3
26	24	52	THR	3.3
41	1j	10	GLY	3.3
50	2s	68	GLY	3.3
1	1A	1046	A	3.3
6	1G	50	ALA	3.3
35	2d	54	TYR	3.3
6	2G	152	LEU	3.3
33	2b	125	PRO	3.3
34	1c	115	LEU	3.3
41	1j	40	LEU	3.3
7	2H	79	VAL	3.3
52	1u	4	GLY	3.3
1	1A	1045	A	3.3
14	2S	61	ASN	3.3
52	1u	21	TYR	3.3
1	1A	2132	U	3.3
43	1l	89	ARG	3.3
44	1m	97	PRO	3.3
1	2A	2793	G	3.3
42	1k	14	VAL	3.3
43	2l	18	VAL	3.3
1	2A	2163	C	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	2r	20	ALA	3.3
1	1A	887	A	3.2
1	1A	1095	A	3.2
1	1A	1096	A	3.2
41	2j	63	PHE	3.2
45	1n	16	PHE	3.2
42	2k	75	TYR	3.2
43	1l	64	TYR	3.2
32	2a	1257	U	3.2
35	1d	162	LEU	3.2
51	2t	98	PRO	3.2
25	23	60	GLU	3.2
50	2s	14	HIS	3.2
34	1c	142	MET	3.2
40	2i	86	VAL	3.2
34	1c	192	THR	3.2
42	1k	118	GLY	3.2
8	1I	79	ILE	3.2
1	1A	2162	G	3.2
1	1A	2190	G	3.2
1	2A	2168	G	3.2
32	1a	1021	G	3.2
32	2a	1037	C	3.2
41	2j	32	ALA	3.2
20	2Y	89	PHE	3.2
41	1j	5	ARG	3.2
34	2c	48	TYR	3.2
39	1h	2	LEU	3.2
48	1q	28	PRO	3.2
1	1A	2150	U	3.2
34	1c	99	VAL	3.2
39	1h	93	VAL	3.2
50	2s	79	THR	3.2
1	2A	1533	G	3.2
38	2g	155	ARG	3.2
52	2u	15	ARG	3.2
50	1s	13	ASP	3.2
1	1A	2176	A	3.2
32	1a	1531	A	3.2
44	2m	106	ASN	3.2
34	1c	184	TYR	3.2
39	1h	94	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	1k	25	TYR	3.2
42	1k	75	TYR	3.2
8	2I	81	VAL	3.2
34	2c	13	GLY	3.2
40	2i	44	VAL	3.2
6	2G	20	ILE	3.2
41	1j	98	ILE	3.2
33	1b	225	ALA	3.2
32	2a	1118	C	3.2
34	1c	62	ASP	3.2
35	2d	157	LEU	3.2
44	2m	19	LEU	3.2
51	2t	99	LEU	3.2
32	1a	1001	A	3.2
26	14	17	GLY	3.2
45	1n	33	VAL	3.2
1	1A	1065	U	3.2
44	2m	78	ILE	3.2
50	2s	49	ILE	3.2
7	2H	165	ALA	3.1
33	2b	135	GLN	3.1
47	1p	48	TRP	3.1
29	17	48	LYS	3.1
32	2a	1030	C	3.1
8	2I	38	LEU	3.1
40	2i	99	LEU	3.1
45	2n	6	LEU	3.1
35	2d	154	ASN	3.1
1	1A	2157	G	3.1
1	2A	2162	G	3.1
32	2a	1221	G	3.1
32	2a	1222	G	3.1
7	2H	14	GLY	3.1
7	2H	169	VAL	3.1
21	1Z	141	VAL	3.1
34	2c	74	GLY	3.1
38	2g	154	TYR	3.1
32	1a	1257	U	3.1
32	2a	1532	U	3.1
21	2Z	164	ALA	3.1
41	2j	43	ARG	3.1
41	2j	99	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	163	PHE	3.1
50	1s	16	LEU	3.1
32	2a	1363	C	3.1
20	2Y	59	GLY	3.1
1	2A	2101	G	3.1
1	2A	2155	G	3.1
4	2E	25	VAL	3.1
6	2G	28	VAL	3.1
35	2d	2	GLY	3.1
44	1m	112	GLY	3.1
44	2m	100	GLY	3.1
52	2u	11	GLY	3.1
32	2a	1220	G	3.1
1	1A	548	A	3.1
32	2a	1001	A	3.1
40	1i	5	TYR	3.1
40	1i	10	ARG	3.1
41	1j	87	THR	3.1
1	1A	1078	U	3.1
40	2i	12	GLU	3.1
40	2i	79	LEU	3.1
41	2j	78	ASN	3.1
1	1A	889	C	3.1
1	2A	2136	C	3.1
20	2Y	58	GLY	3.1
34	1c	68	VAL	3.1
34	1c	120	VAL	3.1
35	1d	132	ARG	3.1
41	1j	49	VAL	3.1
45	1n	25	VAL	3.1
6	2G	146	TYR	3.1
7	2H	94	TYR	3.1
33	2b	107	THR	3.1
38	2g	27	ILE	3.1
34	2c	37	GLN	3.1
46	2o	9	GLN	3.1
1	2A	2127	G	3.1
6	2G	151	ALA	3.1
20	2Y	54	LYS	3.1
40	2i	94	ALA	3.1
51	2t	97	ALA	3.1
41	2j	68	HIS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	4	LEU	3.1
26	24	59	PHE	3.1
33	2b	44	LEU	3.1
51	2t	84	LEU	3.1
33	2b	37	ASN	3.1
7	2H	170	ARG	3.1
38	2g	79	ARG	3.1
41	1j	66	ARG	3.1
11	2P	26	GLY	3.1
33	1b	18	GLY	3.1
34	1c	57	ILE	3.1
34	2c	77	ILE	3.1
50	1s	45	VAL	3.1
50	1s	32	LYS	3.0
50	1s	33	THR	3.0
50	1s	77	THR	3.0
41	1j	64	GLU	3.0
1	2A	2125	G	3.0
32	1a	630	G	3.0
35	2d	39	PRO	3.0
38	1g	12	LEU	3.0
50	1s	5	LEU	3.0
50	2s	35	SER	3.0
12	1Q	60	ARG	3.0
40	2i	42	ARG	3.0
21	2Z	106	GLY	3.0
40	2i	67	GLY	3.0
50	2s	34	TRP	3.0
33	2b	7	VAL	3.0
41	2j	44	VAL	3.0
38	1g	154	TYR	3.0
41	1j	86	MET	3.0
43	2l	64	TYR	3.0
1	1A	2134	A	3.0
1	1A	2172	U	3.0
6	2G	142	PRO	3.0
32	2a	1025	U	3.0
33	1b	202	PRO	3.0
53	2v	14	A	3.0
33	2b	11	LEU	3.0
34	1c	34	LEU	3.0
51	2t	10	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1056	G	3.0
1	2A	2151	G	3.0
1	2A	2186	G	3.0
14	2S	20	ARG	3.0
32	2a	1131	G	3.0
40	1i	9	ARG	3.0
34	2c	3	ASN	3.0
11	2P	116	GLY	3.0
34	1c	78	GLY	3.0
6	2G	15	VAL	3.0
7	2H	11	VAL	3.0
34	2c	5	ILE	3.0
34	2c	195	VAL	3.0
46	1o	3	ILE	3.0
1	1A	2136	C	3.0
1	1A	2143	C	3.0
32	1a	1018	C	3.0
44	1m	102	ARG	3.0
1	1A	883	G	3.0
32	1a	1030(A)	G	3.0
8	1I	136	VAL	3.0
33	1b	41	ILE	3.0
34	1c	70	VAL	3.0
44	2m	15	VAL	3.0
51	1t	100	ILE	3.0
21	1Z	2	GLU	3.0
33	2b	34	ALA	3.0
44	2m	23	TYR	3.0
1	2A	2175	C	3.0
32	2a	1018	C	3.0
32	2a	1028	C	3.0
45	1n	39	LEU	3.0
50	2s	15	LEU	3.0
21	2Z	93	ASP	3.0
37	2f	54	LYS	3.0
32	2a	1020	U	3.0
33	2b	57	PHE	3.0
45	1n	32	SER	3.0
50	2s	53	ASN	3.0
33	2b	136	VAL	2.9
50	1s	19	VAL	2.9
41	2j	42	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	97	TRP	2.9
34	2c	71	ALA	2.9
33	1b	131	PRO	2.9
8	1I	141	LYS	2.9
33	2b	121	LEU	2.9
34	1c	4	LYS	2.9
34	2c	184	TYR	2.9
38	1g	16	LEU	2.9
40	2i	4	TYR	2.9
45	1n	34	TYR	2.9
1	1A	1102	C	2.9
33	1b	42	ILE	2.9
40	2i	81	ILE	2.9
33	1b	136	VAL	2.9
35	1d	121	VAL	2.9
40	2i	108	VAL	2.9
1	2A	1171	G	2.9
1	2A	2153	G	2.9
26	24	55	ARG	2.9
35	2d	48	ALA	2.9
36	2e	21	ALA	2.9
41	2j	18	ALA	2.9
32	2a	1030(C)	G	2.9
48	1q	87	LYS	2.9
51	1t	74	LYS	2.9
21	2Z	125	LEU	2.9
40	2i	125	TYR	2.9
1	2A	277	C	2.9
1	2A	2132	U	2.9
40	1i	67	GLY	2.9
20	1Y	91	GLU	2.9
6	1G	114	ILE	2.9
32	1a	1004	A	2.9
32	2a	1030(D)	A	2.9
33	2b	39	ILE	2.9
41	2j	49	VAL	2.9
40	1i	7	THR	2.9
6	1G	139	LEU	2.9
32	2a	1001(A)	G	2.9
6	2G	147	ASP	2.9
45	1n	21	TYR	2.9
26	24	66	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	90	GLU	2.9
35	2d	16	GLY	2.9
40	2i	39	GLY	2.9
1	1A	1090	U	2.9
1	2A	2102	U	2.9
41	1j	78	ASN	2.9
1	1A	2139	C	2.9
1	1A	2140	C	2.9
6	1G	51	ARG	2.9
23	2l	26	ARG	2.9
38	2g	118	VAL	2.9
41	2j	79	ARG	2.9
44	2m	92	HIS	2.9
52	1u	24	ARG	2.9
26	14	69	LYS	2.9
47	2p	12	LYS	2.9
34	2c	15	THR	2.9
36	2e	86	ALA	2.9
52	2u	23	PRO	2.9
54	2w	205	ALA	2.9
33	2b	196	LEU	2.9
50	2s	71	LEU	2.9
1	1A	1091	G	2.9
1	2A	2141	G	2.9
20	2Y	60	PHE	2.9
32	2a	1023	G	2.9
36	2e	10	MET	2.9
44	2m	21	TYR	2.9
4	2E	29	GLY	2.9
7	2H	82	GLY	2.9
38	1g	81	GLY	2.9
44	1m	100	GLY	2.9
33	2b	127	ILE	2.8
35	2d	159	ARG	2.8
36	2e	25	ARG	2.8
38	2g	115	ARG	2.8
40	2i	83	ARG	2.8
9	2N	9	VAL	2.8
34	1c	207	VAL	2.8
49	1r	86	VAL	2.8
50	1s	41	VAL	2.8
1	1A	886	C	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1006	C	2.8
32	1a	1041	A	2.8
32	1a	1503	A	2.8
45	1n	20	ALA	2.8
28	26	11	LEU	2.8
44	2m	70	LEU	2.8
33	1b	134	GLU	2.8
40	1i	18	PHE	2.8
32	2a	1124	G	2.8
41	1j	75	ILE	2.8
41	1j	96	ILE	2.8
48	2q	97	SER	2.8
7	2H	49	VAL	2.8
32	2a	204	U	2.8
41	2j	34	VAL	2.8
47	1p	2	VAL	2.8
53	1v	22	U	2.8
6	1G	2	PRO	2.8
32	2a	1397	C	2.8
40	1i	76	ALA	2.8
44	2m	51	ALA	2.8
45	1n	10	ALA	2.8
1	2A	652(B)	A	2.8
32	2a	1130	A	2.8
33	1b	61	LEU	2.8
34	2c	101	LEU	2.8
40	1i	19	LEU	2.8
51	2t	13	LEU	2.8
41	1j	83	GLU	2.8
47	1p	68	ASP	2.8
33	1b	133	LYS	2.8
33	2b	152	PHE	2.8
40	2i	20	ARG	2.8
41	2j	66	ARG	2.8
45	1n	3	ARG	2.8
45	1n	31	ARG	2.8
20	2Y	55	TYR	2.8
33	2b	66	GLY	2.8
47	1p	17	TYR	2.8
8	2I	71	ILE	2.8
33	1b	39	ILE	2.8
33	1b	172	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	39	ILE	2.8
44	2m	4	ILE	2.8
5	2F	89	VAL	2.8
34	1c	55	VAL	2.8
50	2s	9	VAL	2.8
1	1A	2182	G	2.8
32	1a	78	G	2.8
33	1b	62	ALA	2.8
33	1b	98	LEU	2.8
45	1n	30	ALA	2.8
1	1A	2185	C	2.8
32	1a	999	C	2.8
1	2A	2173	A	2.8
32	2a	1014	A	2.8
20	2Y	94	LYS	2.8
41	2j	55	LYS	2.8
41	1j	63	PHE	2.8
34	2c	159	GLY	2.8
38	1g	82	GLY	2.8
26	14	67	TYR	2.8
26	24	32	TYR	2.8
50	2s	80	TYR	2.8
6	1G	76	SER	2.8
22	10	9	SER	2.8
35	2d	140	VAL	2.8
38	1g	9	VAL	2.8
44	1m	98	VAL	2.8
1	1A	1026	U	2.8
34	1c	169	ALA	2.8
39	2h	112	LEU	2.8
41	2j	20	ALA	2.8
48	1q	98	LEU	2.8
32	2a	1009	G	2.8
3	2D	38	LYS	2.8
22	20	11	ARG	2.8
40	2i	118	LYS	2.8
1	1A	653	A	2.8
1	1A	2126	A	2.8
1	2A	645	C	2.8
32	1a	1016	A	2.8
14	2S	34	HIS	2.8
41	1j	54	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	54	PHE	2.8
7	2H	92	ILE	2.7
34	1c	182	ILE	2.7
47	2p	48	TRP	2.7
26	24	67	TYR	2.7
33	2b	148	TYR	2.7
35	1d	37	PRO	2.7
35	1d	207	TYR	2.7
6	2G	149	VAL	2.7
50	2s	60	VAL	2.7
34	2c	52	LEU	2.7
40	1i	106	ALA	2.7
40	2i	27	THR	2.7
40	2i	82	ALA	2.7
1	2A	271(K)	U	2.7
12	2Q	22	LYS	2.7
32	2a	1122	U	2.7
44	1m	99	ARG	2.7
50	2s	3	ARG	2.7
33	2b	95	GLN	2.7
1	2A	1537	G	2.7
1	2A	2751	G	2.7
32	2a	1202	G	2.7
1	1A	1177	A	2.7
1	1A	2103	C	2.7
32	2a	1005	A	2.7
32	2a	1149	C	2.7
32	2a	1286	A	2.7
44	1m	16	ASP	2.7
8	2I	90	GLY	2.7
36	1e	23	GLY	2.7
38	2g	34	GLY	2.7
40	1i	6	GLY	2.7
44	2m	95	GLY	2.7
5	2F	6	VAL	2.7
40	1i	17	VAL	2.7
34	1c	188	LEU	2.7
22	10	10	THR	2.7
40	2i	61	ALA	2.7
44	1m	49	THR	2.7
50	2s	77	THR	2.7
54	1w	102	MET	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	1i	12	GLU	2.7
1	1A	1066	U	2.7
1	1A	2189	U	2.7
42	1k	13	GLN	2.7
54	1w	189	GLN	2.7
1	1A	2186	G	2.7
1	2A	11	G	2.7
32	1a	1032	G	2.7
46	2o	20	GLY	2.7
46	2o	89	GLY	2.7
52	2u	16	GLY	2.7
1	2A	1178	C	2.7
32	1a	1007	C	2.7
32	2a	1006	C	2.7
53	2v	15	A	2.7
33	2b	172	ILE	2.7
38	1g	84	ASN	2.7
6	2G	70	VAL	2.7
26	14	50	VAL	2.7
20	2Y	90	LEU	2.7
33	2b	133	LYS	2.7
33	2b	230	VAL	2.7
40	2i	28	VAL	2.7
21	1Z	1	MET	2.7
34	1c	61	ALA	2.7
35	1d	195	ALA	2.7
40	1i	42	ARG	2.7
44	2m	33	ALA	2.7
46	2o	88	ARG	2.7
50	1s	39	THR	2.7
1	2A	2150	U	2.7
7	1H	174	GLY	2.7
7	2H	9	ILE	2.7
7	2H	123	PHE	2.7
12	2Q	69	PHE	2.7
40	2i	101	PHE	2.7
26	24	29	PRO	2.7
45	1n	42	ILE	2.7
1	1A	2156	G	2.7
1	1A	2138	C	2.7
32	2a	1147	C	2.7
14	2S	28	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	154	LEU	2.7
40	1i	65	VAL	2.7
40	1i	108	VAL	2.7
44	1m	53	VAL	2.7
44	2m	88	ARG	2.7
47	2p	28	ARG	2.7
51	1t	10	LEU	2.7
33	1b	33	TYR	2.7
47	1p	39	TYR	2.7
54	2w	350	ALA	2.7
34	1c	118	GLN	2.7
5	2F	131	GLY	2.6
34	2c	171	GLY	2.6
38	1g	34	GLY	2.6
40	1i	80	GLY	2.6
46	1o	89	GLY	2.6
6	1G	80	PHE	2.6
7	2H	21	PRO	2.6
33	1b	200	ILE	2.6
33	2b	70	PHE	2.6
34	2c	39	ILE	2.6
36	1e	6	PHE	2.6
50	1s	40	ILE	2.6
7	2H	41	MET	2.6
8	2I	27	ARG	2.6
19	2X	65	ARG	2.6
24	12	69	ARG	2.6
45	1n	29	ARG	2.6
24	22	35	LEU	2.6
33	1b	44	LEU	2.6
1	1A	2805	G	2.6
1	2A	888	C	2.6
1	2A	2188	C	2.6
1	2A	2804	C	2.6
8	2I	127	VAL	2.6
35	1d	194	LEU	2.6
41	1j	65	LEU	2.6
44	1m	66	LEU	2.6
32	1a	76	C	2.6
6	2G	54	GLU	2.6
32	1a	1017	G	2.6
32	1a	1033	G	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1119	C	2.6
32	2a	1019	C	2.6
40	2i	36	TYR	2.6
40	2i	92	TYR	2.6
41	1j	18	ALA	2.6
47	2p	38	TYR	2.6
47	2p	76	GLN	2.6
54	2w	150	THR	2.6
5	1F	16	GLY	2.6
40	1i	75	ASP	2.6
34	1c	135	LYS	2.6
41	2j	31	GLY	2.6
45	2n	4	LYS	2.6
45	2n	55	GLY	2.6
51	2t	74	LYS	2.6
14	2S	87	PHE	2.6
40	2i	37	PHE	2.6
45	2n	16	PHE	2.6
46	1o	19	PRO	2.6
47	1p	46	PRO	2.6
33	2b	83	MET	2.6
44	1m	94	ARG	2.6
54	2w	102	MET	2.6
35	1d	135	LEU	2.6
41	2j	85	LEU	2.6
50	1s	30	LEU	2.6
26	14	21	VAL	2.6
33	2b	174	VAL	2.6
34	2c	68	VAL	2.6
40	1i	2	GLU	2.6
40	1i	86	VAL	2.6
43	1l	18	VAL	2.6
1	1A	2137	C	2.6
21	2Z	7	ALA	2.6
32	1a	1030	C	2.6
51	1t	59	ALA	2.6
1	1A	2207	G	2.6
35	2d	20	TYR	2.6
40	1i	36	TYR	2.6
8	2I	118	LYS	2.6
41	2j	14	LYS	2.6
33	2b	72	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	2h	90	GLY	2.6
44	2m	6	GLY	2.6
47	1p	10	GLY	2.6
47	1p	47	ASP	2.6
52	2u	4	GLY	2.6
54	1w	330	GLY	2.6
6	1G	113	ARG	2.6
33	1b	36	ARG	2.6
35	1d	29	PRO	2.6
37	2f	47	ARG	2.6
41	1j	77	PRO	2.6
44	2m	55	ARG	2.6
45	2n	14	PRO	2.6
47	2p	19	ILE	2.6
45	1n	37	PHE	2.6
8	1I	58	LEU	2.6
9	2N	116	LEU	2.6
34	2c	12	LEU	2.6
34	2c	90	GLU	2.6
38	1g	8	GLU	2.6
44	1m	96	LEU	2.6
20	2Y	72	VAL	2.6
35	1d	140	VAL	2.6
38	1g	37	ASN	2.6
42	2k	16	SER	2.6
8	2I	146	ALA	2.6
15	2T	131	ALA	2.6
34	1c	113	ALA	2.6
34	2c	69	HIS	2.6
35	1d	123	HIS	2.6
41	1j	100	THR	2.6
44	1m	42	ALA	2.6
1	1A	529	A	2.6
32	2a	959	A	2.6
32	2a	1256	A	2.6
53	1v	15	A	2.6
26	14	63	TYR	2.6
41	1j	7	LYS	2.6
45	2n	15	LYS	2.6
1	1A	1176	G	2.6
1	2A	2207	G	2.6
32	2a	1373	G	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	1k	42	TRP	2.6
33	1b	14	GLY	2.6
35	2d	50	ARG	2.6
40	1i	39	GLY	2.6
40	2i	21	PRO	2.6
41	1j	52	GLY	2.6
44	2m	24	GLY	2.6
50	1s	59	PRO	2.6
33	1b	127	ILE	2.6
32	2a	950	U	2.6
7	2H	124	GLU	2.6
14	2S	48	LEU	2.6
40	1i	40	LEU	2.6
44	2m	90	LEU	2.6
54	2w	325	GLU	2.6
33	2b	93	VAL	2.6
34	1c	106	VAL	2.6
35	1d	105	VAL	2.6
34	2c	180	ALA	2.6
40	2i	55	ALA	2.6
45	2n	59	ALA	2.6
49	1r	20	ALA	2.6
50	1s	4	SER	2.6
50	2s	24	ALA	2.6
44	2m	46	LYS	2.6
1	1A	1460	A	2.6
32	2a	1225	A	2.6
50	1s	52	TYR	2.6
1	1A	888	C	2.5
1	2A	2164	C	2.5
32	2a	1027	C	2.5
44	2m	64	TRP	2.5
7	2H	39	PRO	2.5
8	2I	8	PRO	2.5
12	1Q	61	GLY	2.5
39	2h	72	PRO	2.5
41	2j	17	ASP	2.5
43	2l	63	GLY	2.5
52	1u	16	GLY	2.5
8	2I	109	ILE	2.5
32	2a	1017	G	2.5
36	2e	13	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	2Q	104	PHE	2.5
25	13	60	GLU	2.5
26	14	49	PHE	2.5
1	1A	1083	U	2.5
1	2A	1113	U	2.5
6	1G	3	LEU	2.5
32	1a	1532	U	2.5
33	2b	69	LEU	2.5
34	1c	43	LEU	2.5
41	1j	90	LEU	2.5
7	2H	35	VAL	2.5
7	2H	52	VAL	2.5
34	2c	76	VAL	2.5
36	2e	51	VAL	2.5
34	2c	187	ALA	2.5
35	2d	149	ALA	2.5
39	1h	28	ALA	2.5
42	2k	69	ALA	2.5
45	2n	10	ALA	2.5
47	2p	45	THR	2.5
7	1H	3	ARG	2.5
29	27	41	ARG	2.5
41	2j	5	ARG	2.5
41	2j	28	ARG	2.5
52	2u	10	ARG	2.5
1	1A	2171	A	2.5
4	2E	151	TYR	2.5
26	24	63	TYR	2.5
32	2a	1503	A	2.5
7	2H	55	PRO	2.5
32	1a	989	C	2.5
7	2H	136	ILE	2.5
33	2b	58	ILE	2.5
34	1c	77	ILE	2.5
34	2c	57	ILE	2.5
34	2c	167	TRP	2.5
41	2j	6	ILE	2.5
21	2Z	168	GLU	2.5
1	1A	2101	G	2.5
1	1A	2151	G	2.5
6	2G	43	LEU	2.5
12	2Q	2	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	29	PHE	2.5
32	1a	377	G	2.5
32	1a	988	G	2.5
32	2a	1022	G	2.5
33	2b	158	LEU	2.5
35	2d	21	LEU	2.5
44	1m	48	LEU	2.5
9	2N	131	GLN	2.5
7	2H	13	LYS	2.5
7	2H	85	LYS	2.5
33	1b	22	LYS	2.5
34	1c	151	VAL	2.5
34	2c	153	VAL	2.5
34	2c	181	ASN	2.5
40	1i	41	VAL	2.5
43	2l	124	LYS	2.5
44	1m	27	LYS	2.5
44	2m	40	ASN	2.5
45	2n	25	VAL	2.5
47	2p	16	HIS	2.5
8	2I	115	ALA	2.5
33	1b	34	ALA	2.5
33	1b	188	ALA	2.5
33	2b	161	ALA	2.5
34	2c	53	ALA	2.5
38	2g	152	ALA	2.5
7	2H	38	SER	2.5
34	2c	192	THR	2.5
41	2j	35	SER	2.5
50	1s	29	ARG	2.5
7	2H	12	PRO	2.5
7	2H	36	PRO	2.5
8	2I	89	TYR	2.5
33	1b	232	PRO	2.5
33	2b	91	PRO	2.5
33	2b	199	TYR	2.5
38	1g	151	TYR	2.5
41	2j	91	PRO	2.5
34	2c	78	GLY	2.5
34	2c	155	GLY	2.5
43	1l	14	GLY	2.5
8	1I	10	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	231	GLU	2.5
40	1i	105	ASP	2.5
44	2m	16	ASP	2.5
32	2a	995	C	2.5
8	2I	68	LEU	2.5
34	2c	188	LEU	2.5
35	2d	155	LEU	2.5
44	2m	34	LEU	2.5
41	1j	33	GLN	2.5
27	15	60	VAL	2.5
32	2a	1150	U	2.5
34	1c	64	VAL	2.5
34	1c	198	VAL	2.5
38	1g	28	ASN	2.5
1	2A	2156	G	2.5
32	2a	1011	G	2.5
34	1c	127	ARG	2.5
35	1d	153	ARG	2.5
40	1i	126	SER	2.5
41	2j	59	SER	2.5
49	2r	69	THR	2.5
20	2Y	5	MET	2.5
36	1e	10	MET	2.5
44	1m	86	CYS	2.5
45	2n	38	GLY	2.5
54	2w	208	GLU	2.5
43	2l	7	ILE	2.5
46	1o	87	ILE	2.5
1	1A	2790	A	2.5
33	2b	61	LEU	2.5
44	2m	31	LYS	2.5
47	2p	50	LYS	2.5
1	1A	2161	C	2.5
1	2A	2803	C	2.5
32	2a	1217	C	2.5
33	2b	19	HIS	2.5
50	1s	83	HIS	2.5
5	2F	183	VAL	2.5
7	2H	17	VAL	2.5
44	1m	40	ASN	2.5
50	2s	11	VAL	2.5
41	1j	45	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	1p	72	ARG	2.5
49	1r	87	ARG	2.5
34	2c	129	ALA	2.5
35	1d	149	ALA	2.5
44	2m	37	THR	2.5
1	2A	2318	G	2.5
7	2H	128	PRO	2.4
33	2b	131	PRO	2.4
7	2H	48	GLY	2.4
44	2m	69	GLU	2.4
51	2t	47	GLY	2.4
44	2m	9	ILE	2.4
47	1p	40	ASP	2.4
19	2X	95	LEU	2.4
34	1c	87	LEU	2.4
12	2Q	65	PHE	2.4
21	2Z	136	PHE	2.4
34	1c	79	ARG	2.4
41	1j	28	ARG	2.4
41	2j	70	ARG	2.4
1	2A	2103	C	2.4
6	1G	149	VAL	2.4
8	1I	142	VAL	2.4
34	2c	66	VAL	2.4
39	2h	129	VAL	2.4
40	2i	29	ASN	2.4
42	1k	117	ASN	2.4
50	2s	45	VAL	2.4
8	2I	53	ALA	2.4
32	2a	1148	U	2.4
34	1c	117	ALA	2.4
35	1d	113	SER	2.4
48	2q	79	SER	2.4
6	1G	137	GLU	2.4
1	1A	2154	G	2.4
1	2A	100	G	2.4
5	2F	135	LYS	2.4
31	29	31	LYS	2.4
32	1a	378	G	2.4
33	1b	227	GLY	2.4
34	2c	185	GLY	2.4
50	2s	8	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	134	ILE	2.4
42	1k	36	ASP	2.4
44	2m	39	ILE	2.4
48	2q	90	ILE	2.4
49	2r	50	ILE	2.4
39	2h	107	LEU	2.4
40	1i	4	TYR	2.4
41	1j	84	GLN	2.4
42	2k	103	LEU	2.4
45	2n	44	LEU	2.4
49	1r	31	LEU	2.4
50	1s	22	LEU	2.4
50	2s	61	TYR	2.4
35	1d	118	ARG	2.4
38	2g	32	ARG	2.4
40	1i	33	PHE	2.4
41	1j	43	ARG	2.4
41	2j	11	PHE	2.4
45	1n	23	ARG	2.4
45	2n	36	PHE	2.4
50	2s	10	PHE	2.4
50	2s	36	ARG	2.4
32	2a	1447	A	2.4
34	1c	66	VAL	2.4
34	1c	167	TRP	2.4
36	1e	100	VAL	2.4
41	1j	44	VAL	2.4
54	2w	185	VAL	2.4
1	1A	34	C	2.4
1	2A	1509	C	2.4
33	1b	13	ALA	2.4
34	2c	160	ALA	2.4
41	1j	32	ALA	2.4
44	2m	42	ALA	2.4
1	2A	271(L)	U	2.4
32	2a	1121	U	2.4
6	2G	76	SER	2.4
7	2H	175	LYS	2.4
8	2I	70	GLU	2.4
26	24	57	GLU	2.4
38	2g	98	SER	2.4
42	1k	24	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	1m	58	GLU	2.4
34	1c	74	GLY	2.4
39	1h	96	GLY	2.4
46	2o	86	GLY	2.4
50	1s	26	GLY	2.4
34	2c	152	ILE	2.4
50	1s	12	ASP	2.4
1	1A	2184	G	2.4
1	2A	2319	G	2.4
11	2P	68	GLN	2.4
32	1a	1353	G	2.4
32	2a	1190	G	2.4
34	1c	47	LEU	2.4
44	2m	48	LEU	2.4
45	2n	53	LEU	2.4
47	1p	76	GLN	2.4
12	2Q	59	ARG	2.4
33	2b	53	ARG	2.4
34	2c	79	ARG	2.4
38	1g	153	HIS	2.4
40	2i	16	ARG	2.4
40	2i	128	ARG	2.4
50	1s	47	HIS	2.4
14	2S	92	TYR	2.4
35	1d	20	TYR	2.4
35	1d	38	TYR	2.4
40	2i	33	PHE	2.4
7	2H	37	VAL	2.4
9	2N	5	VAL	2.4
12	2Q	102	VAL	2.4
33	1b	71	VAL	2.4
35	2d	92	VAL	2.4
1	1A	229	A	2.4
18	2W	60	ASN	2.4
44	2m	72	ALA	2.4
54	1w	349	ALA	2.4
54	2w	349	ALA	2.4
3	1D	38	LYS	2.4
3	2D	276	LYS	2.4
6	2G	182	LYS	2.4
20	2Y	91	GLU	2.4
1	1A	1076	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	990	C	2.4
33	1b	234	PRO	2.4
33	2b	232	PRO	2.4
35	1d	136	PRO	2.4
41	2j	53	PRO	2.4
43	2l	5	PRO	2.4
50	2s	59	PRO	2.4
32	1a	991	U	2.4
47	2p	63	GLY	2.4
6	1G	52	ILE	2.4
26	14	14	ILE	2.4
33	2b	108	ILE	2.4
41	2j	82	ILE	2.4
6	2G	138	GLN	2.4
7	2H	51	ARG	2.4
33	1b	221	LEU	2.4
34	1c	33	LEU	2.4
34	1c	196	LEU	2.4
34	2c	62	ASP	2.4
34	2c	6	HIS	2.4
37	2f	45	LEU	2.4
45	2n	3	ARG	2.4
47	1p	73	LEU	2.4
52	1u	22	ARG	2.4
52	2u	6	ARG	2.4
33	2b	92	TYR	2.4
34	1c	193	TYR	2.4
35	1d	4	TYR	2.4
35	2d	206	PHE	2.4
37	2f	63	TYR	2.4
45	2n	34	TYR	2.4
6	2G	160	VAL	2.4
34	1c	86	VAL	2.4
35	2d	112	VAL	2.4
43	1l	39	VAL	2.4
20	2Y	34	LYS	2.4
1	1A	1103	A	2.4
1	2A	1847	A	2.4
21	2Z	51	ALA	2.4
33	2b	132	LYS	2.4
35	1d	30	LYS	2.4
32	2a	964	A	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	1j	26	ALA	2.4
35	1d	192	GLU	2.4
47	2p	54	GLU	2.4
34	1c	95	THR	2.3
35	1d	51	PRO	2.3
44	1m	43	THR	2.3
44	2m	113	PRO	2.3
47	1p	22	THR	2.3
47	2p	59	TRP	2.4
1	1A	1175	U	2.3
23	2l	84	GLY	2.3
45	1n	38	GLY	2.3
7	2H	71	LEU	2.3
33	2b	41	ILE	2.3
38	1g	41	ARG	2.3
41	2j	96	ILE	2.3
44	2m	110	ARG	2.3
41	2j	33	GLN	2.3
50	2s	30	LEU	2.3
51	1t	55	ILE	2.3
52	1u	13	ILE	2.3
54	2w	151	ASP	2.3
54	2w	215	ASP	2.3
35	1d	33	MET	2.3
38	1g	18	TYR	2.3
44	2m	59	TYR	2.3
47	1p	80	PHE	2.3
7	2H	15	VAL	2.3
17	2V	61	VAL	2.3
34	1c	130	VAL	2.3
37	1f	88	VAL	2.3
40	1i	26	VAL	2.3
50	2s	67	VAL	2.3
32	1a	998	G	2.3
32	1a	1139	G	2.3
32	2a	973	G	2.3
41	1j	76	ASN	2.3
42	2k	117	ASN	2.3
20	1Y	78	ALA	2.3
33	1b	20	GLU	2.3
34	2c	146	ALA	2.3
35	1d	150	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	1i	94	ALA	2.3
44	1m	28	ALA	2.3
45	2n	5	ALA	2.3
50	1s	50	ALA	2.3
51	1t	67	ALA	2.3
51	2t	95	ALA	2.3
33	2b	234	PRO	2.3
34	1c	174	PRO	2.3
35	2d	40	PRO	2.3
32	1a	1030(D)	A	2.3
7	2H	22	GLY	2.3
8	2I	106	GLY	2.3
12	1Q	15	GLY	2.3
14	1S	60	GLY	2.3
23	1l	26	ARG	2.3
33	2b	130	ARG	2.3
33	2b	151	GLY	2.3
36	2e	18	ARG	2.3
40	2i	72	GLY	2.3
44	2m	112	GLY	2.3
50	2s	78	ARG	2.3
8	2I	104	GLN	2.3
32	1a	1135	U	2.3
32	2a	421	U	2.3
5	2F	181	LEU	2.3
12	2Q	120	ILE	2.3
14	2S	54	LEU	2.3
33	1b	223	ILE	2.3
33	2b	211	ILE	2.3
34	1c	28	GLN	2.3
35	1d	5	ILE	2.3
40	1i	99	LEU	2.3
42	1k	48	ILE	2.3
45	2n	39	LEU	2.3
50	1s	31	ILE	2.3
1	1A	2188	C	2.3
1	2A	1043	C	2.3
32	1a	1054	C	2.3
32	1a	1137	C	2.3
32	1a	1158	C	2.3
32	2a	1218	C	2.3
33	2b	48	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	11	LYS	2.3
20	2Y	81	LYS	2.3
8	2I	144	VAL	2.3
33	1b	165	VAL	2.3
33	2b	184	VAL	2.3
38	2g	44	TYR	2.3
39	2h	19	VAL	2.3
39	2h	51	VAL	2.3
50	2s	51	VAL	2.3
17	1V	43	GLU	2.3
50	2s	17	GLU	2.3
41	2j	69	ASN	2.3
47	1p	14	ASN	2.3
7	2H	10	PRO	2.3
38	1g	39	ALA	2.3
43	1l	5	PRO	2.3
47	2p	7	ALA	2.3
8	2I	86	THR	2.3
29	17	47	ARG	2.3
32	1a	1274	G	2.3
32	2a	1117	G	2.3
35	1d	89	THR	2.3
35	2d	132	ARG	2.3
5	2F	16	GLY	2.3
7	2H	78	GLY	2.3
14	2S	96	GLY	2.3
32	2a	977	A	2.3
32	2a	1289	A	2.3
33	2b	18	GLY	2.3
34	2c	205	GLY	2.3
47	1p	13	HIS	2.3
50	1s	14	HIS	2.3
50	2s	69	HIS	2.3
19	2X	70	LEU	2.3
34	2c	84	ILE	2.3
41	1j	38	ILE	2.3
45	1n	6	LEU	2.3
32	1a	841	U	2.3
32	1a	1012	U	2.3
32	2a	1000	U	2.3
34	1c	36	ASP	2.3
1	2A	652(T)	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	22	LYS	2.3
40	2i	97	LYS	2.3
20	1Y	60	PHE	2.3
33	2b	122	PHE	2.3
34	2c	186	PHE	2.3
36	2e	45	PHE	2.3
38	1g	43	PHE	2.3
26	24	35	VAL	2.3
34	1c	76	VAL	2.3
34	1c	195	VAL	2.3
34	2c	70	VAL	2.3
38	2g	75	VAL	2.3
47	2p	20	VAL	2.3
20	2Y	56	PRO	2.3
33	1b	123	ALA	2.3
33	1b	125	PRO	2.3
34	1c	108	ASN	2.3
35	1d	32	ALA	2.3
40	1i	43	ALA	2.3
14	2S	97	ARG	2.3
19	2X	68	ARG	2.3
26	24	58	ARG	2.3
33	1b	130	ARG	2.3
44	2m	29	ARG	2.3
44	1m	37	THR	2.3
44	2m	49	THR	2.3
49	1r	25	THR	2.3
26	14	46	GLN	2.3
1	1A	1173	G	2.3
1	2A	883	G	2.3
1	2A	2152	G	2.3
22	20	9	SER	2.3
32	1a	350	G	2.3
32	2a	951	G	2.3
50	1s	35	SER	2.3
54	2w	299	SER	2.3
38	2g	38	LEU	2.3
47	1p	60	LEU	2.3
32	2a	1015	A	2.3
32	2a	1180	A	2.3
32	2a	1183	A	2.3
32	2a	1248	A	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	2u	13	ILE	2.3
41	1j	80	LYS	2.3
32	1a	1148	U	2.3
22	20	68	GLU	2.3
32	2a	1116	C	2.3
45	2n	37	PHE	2.3
46	2o	6	GLU	2.3
35	1d	170	VAL	2.3
45	2n	33	VAL	2.3
50	2s	19	VAL	2.3
6	2G	17	PRO	2.3
34	2c	7	PRO	2.3
6	2G	123	ASN	2.2
7	2H	20	ALA	2.2
33	2b	62	ALA	2.2
24	12	70	GLN	2.2
26	24	4	GLY	2.2
33	2b	65	GLY	2.2
34	1c	37	GLN	2.2
36	1e	38	GLN	2.2
39	2h	96	GLY	2.2
51	2t	96	GLY	2.2
4	2E	195	LEU	2.2
6	1G	152	LEU	2.2
16	2U	62	ILE	2.2
21	2Z	157	LEU	2.2
36	2e	119	LEU	2.2
44	2m	22	ILE	2.2
45	2n	17	LYS	2.2
50	1s	38	SER	2.2
51	1t	68	LYS	2.2
1	1A	1174	A	2.2
6	2G	150	ASP	2.2
1	1A	2152	G	2.2
32	1a	79	G	2.2
32	2a	1370	G	2.2
1	1A	271(K)	U	2.2
32	1a	202	U	2.2
32	2a	1446	U	2.2
7	2H	53	GLU	2.2
34	1c	44	GLU	2.2
34	1c	186	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2794	C	2.2
5	1F	6	VAL	2.2
14	2S	13	ARG	2.2
14	2S	17	ARG	2.2
14	2S	98	VAL	2.2
21	2Z	141	VAL	2.2
25	23	2	PRO	2.2
33	1b	15	VAL	2.2
37	1f	6	VAL	2.2
41	1j	51	ARG	2.2
41	2j	46	ARG	2.2
44	1m	117	VAL	2.2
44	2m	99	ARG	2.2
45	1n	35	ARG	2.2
50	1s	11	VAL	2.2
51	1t	98	PRO	2.2
33	2b	29	ALA	2.2
34	1c	92	ALA	2.2
42	1k	68	ALA	2.2
33	2b	33	TYR	2.2
44	1m	59	TYR	2.2
47	1p	38	TYR	2.2
50	1s	80	TYR	2.2
41	1j	56	HIS	2.2
41	2j	56	HIS	2.2
45	2n	49	HIS	2.2
54	2w	331	HIS	2.2
17	1V	101	GLY	2.2
35	2d	167	GLY	2.2
44	1m	68	GLY	2.2
45	1n	28	GLY	2.2
45	2n	58	LYS	2.2
7	2H	171	LEU	2.2
14	2S	58	LEU	2.2
34	1c	52	LEU	2.2
35	1d	157	LEU	2.2
38	1g	38	LEU	2.2
49	1r	85	LEU	2.2
28	26	54	ILE	2.2
48	1q	62	SER	2.2
42	2k	36	ASP	2.2
6	2G	100	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	26	42	TRP	2.2
33	2b	24	TRP	2.2
1	1A	890	A	2.2
32	2a	975	A	2.2
32	2a	1123	A	2.2
32	2a	1146	A	2.2
33	2b	20	GLU	2.2
40	1i	35	GLU	2.2
1	2A	2206	G	2.2
32	2a	1010	G	2.2
38	2g	149	ARG	2.2
40	1i	104	ARG	2.2
48	2q	68	ARG	2.2
54	1w	319	PHE	2.2
54	2w	307	PHE	2.2
29	27	46	VAL	2.2
34	1c	75	VAL	2.2
34	2c	103	VAL	2.2
35	1d	198	VAL	2.2
36	1e	115	VAL	2.2
44	1m	60	VAL	2.2
54	2w	158	VAL	2.2
32	1a	221	C	2.2
32	1a	1030(B)	C	2.2
32	2a	1137	C	2.2
7	1H	13	LYS	2.2
14	2S	59	LYS	2.2
33	1b	107	THR	2.2
34	1c	107	GLN	2.2
37	1f	63	TYR	2.2
40	1i	88	TYR	2.2
43	1l	98	TYR	2.2
44	1m	105	THR	2.2
48	2q	95	TYR	2.2
8	1I	9	LEU	2.2
14	2S	45	GLY	2.2
36	1e	85	GLY	2.2
42	2k	86	GLY	2.2
44	1m	90	LEU	2.2
48	2q	80	GLY	2.2
26	14	31	ILE	2.2
44	2m	25	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	1s	62	ILE	2.2
35	2d	53	ASP	2.2
50	2s	13	ASP	2.2
6	1G	48	GLU	2.2
35	2d	156	GLU	2.2
54	2w	297	GLU	2.2
7	2H	6	ARG	2.2
21	1Z	4	ARG	2.2
26	14	58	ARG	2.2
38	2g	76	ARG	2.2
44	2m	57	ARG	2.2
45	2n	61	TRP	2.2
32	1a	1285	A	2.2
32	1a	1287	A	2.2
32	2a	1159	U	2.2
53	1v	14	A	2.2
33	1b	70	PHE	2.2
34	2c	203	PHE	2.2
36	2e	26	PHE	2.2
40	1i	49	PRO	2.2
8	2I	37	VAL	2.2
38	1g	21	VAL	2.2
40	2i	53	VAL	2.2
48	2q	9	VAL	2.2
1	1A	2187	G	2.2
1	2A	1042	G	2.2
32	1a	1031	G	2.2
34	1c	160	ALA	2.2
35	1d	22	LYS	2.2
47	1p	43	LYS	2.2
55	2x	70	G	2.2
5	2F	166	ALA	2.2
34	2c	176	HIS	2.2
50	2s	23	ASN	2.2
51	1t	66	ALA	2.2
56	1z	4	ALA	2.2
3	2D	166	GLN	2.2
35	1d	42	GLN	2.2
1	2A	2896	C	2.2
9	2N	73	THR	2.2
33	2b	73	THR	2.2
34	1c	165	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	101	LEU	2.2
34	1c	178	LEU	2.2
34	2c	42	LEU	2.2
35	1d	54	TYR	2.2
45	2n	13	THR	2.2
48	1q	95	TYR	2.2
52	2u	17	THR	2.2
8	1I	72	LEU	2.2
8	2I	34	GLY	2.2
15	2T	99	LEU	2.2
42	2k	66	LEU	2.2
44	2m	89	GLY	2.2
45	2n	27	CYS	2.2
46	2o	31	LEU	2.2
47	2p	6	LEU	2.2
48	2q	98	LEU	2.2
50	1s	68	GLY	2.2
26	14	15	ILE	2.2
38	1g	49	ILE	2.2
38	1g	120	ILE	2.2
44	2m	84	ILE	2.2
54	2w	192	ILE	2.2
33	2b	124	SER	2.2
35	1d	208	SER	2.2
54	1w	310	SER	2.2
33	2b	79	ASP	2.2
35	1d	156	GLU	2.2
35	2d	179	GLU	2.2
41	2j	73	ASP	2.2
44	2m	73	GLU	2.2
22	10	11	ARG	2.2
52	1u	14	TRP	2.2
9	2N	140	VAL	2.1
21	2Z	90	VAL	2.1
33	2b	229	VAL	2.1
34	1c	103	VAL	2.1
34	2c	106	VAL	2.1
34	2c	141	VAL	2.1
36	2e	41	VAL	2.1
40	2i	17	VAL	2.1
40	2i	26	VAL	2.1
14	2S	37	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	6	HIS	2.1
34	1c	71	ALA	2.1
34	1c	98	ASN	2.1
34	2c	60	ALA	2.1
34	2c	65	ALA	2.1
40	1i	84	ALA	2.1
40	2i	38	GLN	2.1
42	2k	15	ALA	2.1
44	1m	51	ALA	2.1
54	2w	347	GLN	2.1
1	1A	2206	G	2.1
4	2E	10	GLY	2.1
6	2G	175	LEU	2.1
7	2H	88	LEU	2.1
32	1a	1202	G	2.1
32	1a	1371	G	2.1
32	2a	1253	G	2.1
35	1d	19	LEU	2.1
35	1d	171	GLY	2.1
40	2i	80	GLY	2.1
50	2s	48	THR	2.1
54	1w	320	THR	2.1
33	2b	42	ILE	2.1
34	2c	202	ILE	2.1
48	1q	59	ILE	2.1
1	2A	34	C	2.1
32	1a	1066	C	2.1
32	2a	1223	C	2.1
6	2G	83	ARG	2.1
12	1Q	5	ARG	2.1
33	2b	129	GLU	2.1
33	2b	143	GLU	2.1
33	2b	150	SER	2.1
46	1o	88	ARG	2.1
52	1u	9	ARG	2.1
52	2u	24	ARG	2.1
3	2D	68	LYS	2.1
33	2b	139	LYS	2.1
34	1c	73	PRO	2.1
43	1l	17	LYS	2.1
44	2m	41	PRO	2.1
44	2m	97	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	2r	23	LYS	2.1
24	12	37	PHE	2.1
34	2c	128	PHE	2.1
54	2w	160	PHE	2.1
34	2c	75	VAL	2.1
35	1d	104	VAL	2.1
37	1f	90	VAL	2.1
44	1m	17	VAL	2.1
47	2p	51	VAL	2.1
32	1a	960	U	2.1
32	1a	1446	U	2.1
33	1b	63	MET	2.1
1	1A	1847	A	2.1
1	2A	6	A	2.1
8	1I	146	ALA	2.1
36	2e	48	ALA	2.1
40	2i	84	ALA	2.1
35	1d	154	ASN	2.1
6	1G	133	LEU	2.1
8	2I	101	LEU	2.1
39	1h	119	LEU	2.1
40	2i	47	LEU	2.1
41	1j	85	LEU	2.1
41	2j	10	GLY	2.1
45	1n	53	LEU	2.1
46	1o	66	LEU	2.1
50	2s	20	LEU	2.1
54	1w	321	THR	2.1
54	2w	348	LEU	2.1
3	2D	106	ILE	2.1
6	2G	39	ILE	2.1
8	2I	88	ILE	2.1
26	24	31	ILE	2.1
35	2d	5	ILE	2.1
44	1m	84	ILE	2.1
47	2p	33	ILE	2.1
6	2G	181	ARG	2.1
17	2V	12	TYR	2.1
35	1d	191	ARG	2.1
37	2f	59	TYR	2.1
40	2i	93	ARG	2.1
43	1l	19	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	50	GLU	2.1
46	1o	78	TYR	2.1
50	1s	61	TYR	2.1
1	2A	271(M)	G	2.1
32	1a	1009	G	2.1
32	2a	1182	G	2.1
1	1A	154(A)	C	2.1
11	1P	133	SER	2.1
32	1a	369	C	2.1
32	1a	1043	C	2.1
32	1a	1147	C	2.1
32	1a	1363	C	2.1
32	2a	1039	C	2.1
32	2a	1054	C	2.1
37	1f	55	ASP	2.1
38	2g	77	SER	2.1
31	29	15	LYS	2.1
37	1f	54	LYS	2.1
40	2i	95	LYS	2.1
43	2l	123	LYS	2.1
51	2t	48	LYS	2.1
40	1i	21	PRO	2.1
41	2j	39	PRO	2.1
21	2Z	32	HIS	2.1
34	1c	128	PHE	2.1
35	1d	79	PHE	2.1
38	1g	26	PHE	2.1
40	1i	37	PHE	2.1
47	1p	16	HIS	2.1
50	2s	74	PHE	2.1
26	14	33	VAL	2.1
26	14	60	GLN	2.1
34	2c	198	VAL	2.1
54	2w	183	VAL	2.1
1	2A	2172	U	2.1
30	28	51	ALA	2.1
33	1b	24	TRP	2.1
32	2a	1125	U	2.1
33	2b	123	ALA	2.1
34	1c	129	ALA	2.1
35	2d	164	ALA	2.1
37	2f	35	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	2	ALA	2.1
42	1k	100	ALA	2.1
1	2A	528	A	2.1
6	1G	82	LEU	2.1
7	2H	174	GLY	2.1
19	2X	92	LEU	2.1
21	2Z	155	LEU	2.1
32	2a	974	A	2.1
33	2b	145	LEU	2.1
34	1c	175	LEU	2.1
34	2c	32	LEU	2.1
35	1d	23	GLY	2.1
35	1d	120	LEU	2.1
35	1d	124	GLY	2.1
47	2p	74	LEU	2.1
50	2s	22	LEU	2.1
41	1j	92	THR	2.1
45	2n	22	THR	2.1
54	1w	114	GLY	2.1
5	1F	17	ARG	2.1
21	1Z	103	ARG	2.1
44	1m	3	ARG	2.1
44	1m	93	ARG	2.1
54	1w	311	ARG	2.1
12	2Q	64	ILE	2.1
21	1Z	120	ILE	2.1
34	1c	202	ILE	2.1
14	2S	36	TYR	2.1
21	2Z	99	TYR	2.1
26	24	25	TYR	2.1
40	1i	62	TYR	2.1
40	2i	88	TYR	2.1
49	1r	34	TYR	2.1
34	1c	147	LYS	2.1
37	2f	55	ASP	2.1
40	1i	91	ASP	2.1
50	1s	18	LYS	2.1
51	2t	11	SER	2.1
51	2t	37	SER	2.1
32	1a	70	G	2.1
32	1a	73	G	2.1
32	1a	181	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1117	G	2.1
1	1A	885	C	2.1
1	1A	2163	C	2.1
32	1a	456	C	2.1
32	1a	1262	C	2.1
32	2a	1129	C	2.1
32	2a	1321	C	2.1
34	1c	109	PRO	2.1
43	1l	125	PRO	2.1
6	2G	23	PHE	2.1
9	2N	8	GLN	2.1
34	1c	162	GLN	2.1
38	1g	7	ALA	2.1
4	2E	5	LEU	2.1
8	2I	67	ARG	2.1
11	2P	85	LEU	2.1
32	1a	1159	U	2.1
33	2b	187	LEU	2.1
34	1c	18	TRP	2.1
34	2c	204	LEU	2.1
35	1d	21	LEU	2.1
35	1d	36	ARG	2.1
35	1d	155	LEU	2.1
36	2e	151	LEU	2.1
37	2f	13	ASN	2.1
39	2h	18	ARG	2.1
41	2j	8	LEU	2.1
36	1e	22	GLY	2.1
43	1l	63	GLY	2.1
47	1p	81	ARG	2.1
50	2s	72	GLY	2.1
7	2H	106	THR	2.1
26	14	53	GLU	2.1
35	2d	192	GLU	2.1
42	2k	57	THR	2.1
1	2A	887	A	2.1
26	24	15	ILE	2.1
31	29	17	ILE	2.1
32	2a	986	A	2.1
32	2a	1151	A	2.1
50	2s	40	ILE	2.1
20	2Y	95	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	65	LYS	2.1
33	2b	189	ASP	2.1
34	1c	201	TYR	2.1
39	2h	94	TYR	2.1
42	2k	25	TYR	2.1
46	1o	69	TYR	2.1
39	1h	87	SER	2.1
41	1j	30	SER	2.1
43	1l	22	SER	2.1
38	1g	47	CYS	2.1
1	1A	545	G	2.0
1	1A	614(B)	G	2.0
1	1A	2183	C	2.1
1	2A	1179	C	2.1
1	2A	2805	G	2.0
1	2A	2893	G	2.0
32	1a	201	C	2.1
32	1a	357	G	2.0
32	1a	1246	C	2.1
32	2a	1042	G	2.0
32	2a	1132	C	2.1
33	2b	78	GLN	2.0
14	2S	14	VAL	2.0
34	2c	99	VAL	2.0
37	2f	91	VAL	2.0
38	2g	66	VAL	2.0
49	2r	43	PHE	2.0
7	2H	145	ALA	2.0
12	2Q	56	ARG	2.0
12	2Q	136	ALA	2.0
21	2Z	131	ARG	2.0
26	14	62	ARG	2.0
34	1c	50	ALA	2.0
34	1c	137	ALA	2.0
35	1d	115	ARG	2.0
41	2j	60	ARG	2.0
49	2r	67	ALA	2.0
51	2t	52	ALA	2.0
6	2G	62	LEU	2.0
33	2b	118	LEU	2.0
34	1c	32	LEU	2.0
39	1h	112	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	2I	41	GLU	2.0
33	1b	228	GLY	2.0
34	1c	25	GLY	2.0
34	2c	80	GLY	2.0
44	1m	95	GLY	2.0
48	1q	80	GLY	2.0
1	1A	12	U	2.0
6	2G	145	THR	2.0
7	2H	68	THR	2.0
26	24	5	ILE	2.0
31	29	10	ILE	2.0
33	2b	185	ILE	2.0
40	2i	64	THR	2.0
41	2j	80	LYS	2.0
44	1m	9	ILE	2.0
44	1m	109	THR	2.0
50	2s	63	THR	2.0
54	1w	295	THR	2.0
32	2a	1531	A	2.0
12	2Q	74	TYR	2.0
34	2c	23	TYR	2.0
47	1p	23	ASP	2.0
8	1I	91	SER	2.0
41	1j	41	PRO	2.0
41	1j	59	SER	2.0
43	2l	116	SER	2.0
50	1s	42	PRO	2.0
54	2w	267	MET	2.0
1	1A	1532	C	2.0
1	2A	1118	C	2.0
6	1G	115	ARG	2.0
7	2H	113	VAL	2.0
9	2N	134	ARG	2.0
11	2P	83	VAL	2.0
14	2S	46	VAL	2.0
20	2Y	42	VAL	2.0
22	20	74	ARG	2.0
26	24	62	ARG	2.0
32	1a	1008	C	2.0
32	1a	1218	C	2.0
32	2a	979	C	2.0
32	2a	999	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1007	C	2.0
32	2a	1109	C	2.0
33	2b	144	ARG	2.0
34	2c	116	VAL	2.0
35	1d	209	ARG	2.0
38	2g	9	VAL	2.0
38	2g	17	VAL	2.0
42	2k	54	ARG	2.0
46	2o	18	PHE	2.0
47	1p	62	VAL	2.0
48	1q	23	VAL	2.0
48	1q	27	PHE	2.0
50	2s	41	VAL	2.0
1	1A	1047	G	2.0
1	2A	1112	G	2.0
5	2F	113	ALA	2.0
32	1a	1010	G	2.0
32	2a	1021	G	2.0
7	2H	64	LEU	2.0
11	2P	105	LEU	2.0
13	2R	41	ALA	2.0
18	1W	65	LEU	2.0
21	2Z	5	LEU	2.0
22	20	84	LEU	2.0
24	22	44	LEU	2.0
34	1c	187	ALA	2.0
35	2d	162	LEU	2.0
35	2d	176	LEU	2.0
39	2h	36	LEU	2.0
41	1j	71	LEU	2.0
44	1m	30	ALA	2.0
45	1n	5	ALA	2.0
33	2b	86	GLU	2.0
46	1o	57	LEU	2.0
48	1q	74	LEU	2.0
49	2r	66	LEU	2.0
31	29	37	GLY	2.0
33	2b	89	GLY	2.0
34	1c	45	LYS	2.0
51	1t	14	LYS	2.0
26	14	22	ILE	2.0
45	2n	42	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
51	1t	63	ILE	2.0
1	1A	1963	U	2.0
1	2A	272(A)	U	2.0
1	2A	614(A)	U	2.0
1	2A	2897	U	2.0
32	2a	1211	U	2.0
1	2A	2171	A	2.0
6	2G	2	PRO	2.0
8	2I	96	ASP	2.0
15	2T	1	MET	2.0
20	2Y	107	ASP	2.0
32	1a	393	A	2.0
32	1a	1183	A	2.0
32	1a	1261	A	2.0
32	2a	978	A	2.0
32	2a	1324	A	2.0
21	2Z	1	MET	2.0
6	2G	12	TYR	2.0
14	2S	31	SER	2.0
33	1b	16	HIS	2.0
34	1c	23	TYR	2.0
37	1f	33	TYR	2.0
41	2j	62	HIS	2.0
48	1q	66	SER	2.0
50	1s	69	HIS	2.0

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

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
55	H2U	2x	20	20/21	0.66	0.17	81,91,97,105	0
55	H2U	2x	21	20/21	0.71	0.17	82,92,100,106	0
55	H2U	1x	21	20/21	0.76	0.15	79,87,97,116	0
55	5MU	2x	54	21/22	0.81	0.14	78,82,88,99	0
55	PSU	2x	55	20/21	0.81	0.12	74,78,89,91	0
32	2MG	2a	1207	24/25	0.87	0.12	76,82,85,91	0
32	2MG	1a	1207	24/25	0.87	0.14	72,81,87,92	0
43	0TD	1l	92	10/11	0.88	0.14	56,59,63,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	PSU	1x	55	20/21	0.89	0.12	69,74,83,84	0
55	H2U	1x	20	20/21	0.89	0.10	72,79,85,90	0
55	5MU	1x	54	21/22	0.90	0.12	65,74,80,87	0
32	PSU	2a	516	20/21	0.90	0.13	59,69,78,79	0
55	PSU	2x	32	20/21	0.90	0.12	68,73,78,82	0
55	MIA	2x	37	22/30	0.90	0.12	62,70,72,75	0
1	5MU	2A	1915	21/22	0.91	0.11	66,70,77,78	0
43	0TD	2l	92	10/11	0.91	0.14	58,63,68,87	0
32	G7M	2a	527	24/25	0.91	0.14	61,65,71,73	0
32	PSU	1a	516	20/21	0.92	0.13	64,72,77,78	0
32	M2G	2a	966	25/26	0.92	0.15	54,68,75,82	0
55	PSU	1x	32	20/21	0.92	0.11	60,66,73,74	0
32	5MC	2a	1404	21/22	0.93	0.11	46,54,59,61	0
32	G7M	1a	527	24/25	0.93	0.13	51,60,66,68	0
55	MIA	1x	37	22/30	0.93	0.10	55,64,68,72	0
55	4SU	2x	8	20/21	0.93	0.10	74,80,83,84	0
32	M2G	1a	966	25/26	0.93	0.12	56,59,72,76	0
32	5MC	1a	967	21/22	0.93	0.12	58,63,72,75	0
32	5MC	2a	967	21/22	0.93	0.13	60,67,73,80	0
1	PSU	2A	1917	20/21	0.93	0.08	57,63,68,74	0
55	PSU	2x	39	20/21	0.94	0.09	59,71,75,77	0
32	4OC	2a	1402	22/23	0.94	0.11	50,62,63,71	0
1	PSU	2A	1911	20/21	0.94	0.09	54,62,65,68	0
1	5MU	1A	1915	21/22	0.94	0.10	49,57,60,66	0
32	5MC	2a	1400	21/22	0.94	0.12	61,68,73,75	0
55	8AN	2x	76	22/23	0.94	0.10	45,56,63,66	0
1	PSU	1A	1911	20/21	0.95	0.09	46,54,61,62	0
54	MEQ	2w	230	10/11	0.95	0.13	52,55,57,64	0
55	4SU	1x	8	20/21	0.95	0.08	55,62,67,77	0
32	MA6	2a	1518	24/25	0.96	0.11	49,58,64,65	0
32	MA6	2a	1519	24/25	0.96	0.10	51,60,64,65	0
32	5MC	1a	1400	21/22	0.96	0.11	49,58,62,64	0
32	5MC	1a	1404	21/22	0.96	0.10	42,46,51,52	0
55	PSU	1x	39	20/21	0.96	0.09	56,59,62,63	0
32	MA6	1a	1519	24/25	0.96	0.10	43,47,51,52	0
1	OMC	2A	1920	21/22	0.96	0.08	50,60,63,64	0
1	5MC	2A	1942	21/22	0.96	0.09	46,51,53,55	0
1	OMG	2A	2251	24/25	0.96	0.09	33,45,48,49	0
1	PSU	1A	1917	20/21	0.96	0.08	49,54,59,59	0
55	8AN	1x	76	22/23	0.96	0.08	31,40,46,47	0
32	UR3	2a	1498	21/22	0.96	0.10	52,57,64,65	0
1	PSU	2A	2605	20/21	0.97	0.08	31,38,41,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	4OC	1a	1402	22/23	0.97	0.09	45,50,53,56	0
1	5MC	1A	1942	21/22	0.97	0.08	31,37,44,49	0
32	5MC	1a	1407	21/22	0.97	0.08	35,44,49,51	0
1	5MC	1A	1962	21/22	0.97	0.08	33,38,45,55	0
1	5MU	2A	1939	21/22	0.97	0.08	33,40,43,45	0
1	PSU	1A	2605	20/21	0.97	0.08	24,29,33,37	0
1	5MC	2A	1962	21/22	0.97	0.08	37,45,50,59	0
54	MEQ	1w	230	10/11	0.97	0.09	32,39,43,44	0
32	5MC	2a	1407	21/22	0.97	0.09	46,51,57,63	0
1	2MA	2A	2503	23/24	0.97	0.08	31,39,44,45	0
32	MA6	1a	1518	24/25	0.98	0.10	38,45,51,52	0
1	OMC	1A	1920	21/22	0.98	0.07	40,47,52,55	0
1	5MU	1A	1939	21/22	0.98	0.07	24,29,34,34	0
1	OMG	1A	2251	24/25	0.98	0.06	27,30,35,37	0
1	2MA	1A	2503	23/24	0.98	0.05	20,24,26,27	0
1	OMU	1A	2552	21/22	0.98	0.06	26,31,35,35	0
1	OMU	2A	2552	21/22	0.98	0.06	38,43,44,46	0
32	UR3	1a	1498	21/22	0.98	0.08	41,48,53,56	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
57	MG	1A	3952	1/1	0.39	0.27	83,83,83,83	0
57	MG	1A	4056	1/1	0.57	0.20	63,63,63,63	0
57	MG	1A	4059	1/1	0.57	0.18	62,62,62,62	0
57	MG	1A	4000	1/1	0.59	0.17	89,89,89,89	0
57	MG	2A	3714	1/1	0.61	0.20	43,43,43,43	0
57	MG	2A	3425	1/1	0.62	0.39	82,82,82,82	0
57	MG	1a	1762	1/1	0.62	0.23	81,81,81,81	0
57	MG	2A	3586	1/1	0.63	0.21	50,50,50,50	0
57	MG	1A	3592	1/1	0.65	0.23	61,61,61,61	0
57	MG	1A	3921	1/1	0.65	0.19	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1O	204	1/1	0.66	0.30	67,67,67,67	0
57	MG	1a	1771	1/1	0.67	0.18	82,82,82,82	0
57	MG	1A	3629	1/1	0.67	0.25	60,60,60,60	0
57	MG	2a	1771	1/1	0.67	0.18	79,79,79,79	0
57	MG	1A	3922	1/1	0.68	0.24	66,66,66,66	0
57	MG	2A	3838	1/1	0.69	0.27	80,80,80,80	0
57	MG	1a	1675	1/1	0.70	0.21	87,87,87,87	0
57	MG	1E	310	1/1	0.70	0.23	72,72,72,72	0
57	MG	2A	3624	1/1	0.70	0.22	68,68,68,68	0
57	MG	1a	1768	1/1	0.70	0.17	73,73,73,73	0
57	MG	1A	3512	1/1	0.70	0.24	74,74,74,74	0
57	MG	2A	3190	1/1	0.70	0.30	77,77,77,77	0
57	MG	1U	211	1/1	0.71	0.51	74,74,74,74	0
57	MG	1A	3404	1/1	0.71	0.21	61,61,61,61	0
57	MG	1A	3500	1/1	0.72	0.35	70,70,70,70	0
57	MG	1l	202	1/1	0.72	0.11	80,80,80,80	0
57	MG	2a	1724	1/1	0.72	0.26	68,68,68,68	0
57	MG	2A	3651	1/1	0.72	0.23	76,76,76,76	0
57	MG	2a	1777	1/1	0.72	0.23	73,73,73,73	0
57	MG	2r	101	1/1	0.72	0.29	82,82,82,82	0
57	MG	2A	3258	1/1	0.73	0.14	90,90,90,90	0
57	MG	2a	1741	1/1	0.73	0.25	78,78,78,78	0
57	MG	2A	3380	1/1	0.73	0.21	63,63,63,63	0
57	MG	1A	3613	1/1	0.73	0.21	65,65,65,65	0
57	MG	15	109	1/1	0.73	0.17	61,61,61,61	0
57	MG	28	103	1/1	0.74	0.18	69,69,69,69	0
57	MG	2A	3437	1/1	0.74	0.27	77,77,77,77	0
57	MG	1A	4026	1/1	0.74	0.20	57,57,57,57	0
57	MG	2a	1762	1/1	0.74	0.28	69,69,69,69	0
57	MG	2A	3755	1/1	0.74	0.14	84,84,84,84	0
57	MG	2A	3834	1/1	0.74	0.20	79,79,79,79	0
57	MG	1A	3851	1/1	0.74	0.19	72,72,72,72	0
57	MG	2A	3824	1/1	0.75	0.16	39,39,39,39	0
57	MG	2A	3578	1/1	0.75	0.24	67,67,67,67	0
57	MG	1a	1714	1/1	0.75	0.24	82,82,82,82	0
57	MG	1A	4102	1/1	0.75	0.28	105,105,105,105	0
57	MG	1x	110	1/1	0.75	0.33	79,79,79,79	0
57	MG	1A	3773	1/1	0.75	0.13	53,53,53,53	0
57	MG	2A	3472	1/1	0.75	0.24	75,75,75,75	0
57	MG	2A	3808	1/1	0.75	0.14	54,54,54,54	0
57	MG	2a	1772	1/1	0.75	0.21	74,74,74,74	0
57	MG	2A	3813	1/1	0.75	0.17	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3820	1/1	0.75	0.21	53,53,53,53	0
57	MG	2x	101	1/1	0.75	0.14	81,81,81,81	0
57	MG	2a	1757	1/1	0.76	0.28	68,68,68,68	0
57	MG	1B	230	1/1	0.76	0.24	83,83,83,83	0
57	MG	1a	1640	1/1	0.76	0.42	74,74,74,74	0
57	MG	2B	202	1/1	0.76	0.20	76,76,76,76	0
57	MG	1A	3873	1/1	0.76	0.22	63,63,63,63	0
57	MG	1A	4003	1/1	0.76	0.27	71,71,71,71	0
57	MG	1A	3348	1/1	0.76	0.21	65,65,65,65	0
57	MG	2A	3788	1/1	0.77	0.21	70,70,70,70	0
57	MG	2A	3085	1/1	0.77	0.23	69,69,69,69	0
57	MG	2A	3189	1/1	0.77	0.21	60,60,60,60	0
57	MG	1a	1661	1/1	0.77	0.21	73,73,73,73	0
57	MG	1A	3955	1/1	0.77	0.16	68,68,68,68	0
57	MG	2A	3277	1/1	0.77	0.18	78,78,78,78	0
57	MG	1A	3683	1/1	0.77	0.18	61,61,61,61	0
57	MG	1a	1716	1/1	0.77	0.45	75,75,75,75	0
57	MG	1a	1750	1/1	0.77	0.26	73,73,73,73	0
57	MG	2a	1651	1/1	0.77	0.33	71,71,71,71	0
57	MG	2a	1675	1/1	0.77	0.31	70,70,70,70	0
57	MG	2a	1684	1/1	0.77	0.30	71,71,71,71	0
57	MG	2A	3451	1/1	0.77	0.35	75,75,75,75	0
57	MG	2a	1731	1/1	0.77	0.21	71,71,71,71	0
57	MG	1A	3900	1/1	0.77	0.21	74,74,74,74	0
57	MG	1A	3332	1/1	0.77	0.24	68,68,68,68	0
57	MG	1A	3817	1/1	0.77	0.19	65,65,65,65	0
57	MG	2A	3611	1/1	0.77	0.19	48,48,48,48	0
57	MG	1a	1812	1/1	0.77	0.37	71,71,71,71	0
57	MG	1A	3681	1/1	0.77	0.16	49,49,49,49	0
57	MG	2a	1780	1/1	0.77	0.22	73,73,73,73	0
57	MG	1A	4093	1/1	0.77	0.19	74,74,74,74	0
57	MG	2A	3003	1/1	0.77	0.21	69,69,69,69	0
57	MG	2A	3757	1/1	0.78	0.14	49,49,49,49	0
57	MG	2A	3759	1/1	0.78	0.17	74,74,74,74	0
57	MG	2a	1694	1/1	0.78	0.36	75,75,75,75	0
57	MG	1A	3893	1/1	0.78	0.23	47,47,47,47	0
57	MG	2A	3293	1/1	0.78	0.28	70,70,70,70	0
57	MG	2A	3059	1/1	0.78	0.24	71,71,71,71	0
57	MG	1a	1781	1/1	0.78	0.18	71,71,71,71	0
57	MG	2A	3639	1/1	0.78	0.18	69,69,69,69	0
57	MG	2A	3642	1/1	0.78	0.27	62,62,62,62	0
57	MG	1A	3782	1/1	0.78	0.22	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3660	1/1	0.78	0.15	60,60,60,60	0
57	MG	1A	3818	1/1	0.78	0.15	55,55,55,55	0
57	MG	2a	1605	1/1	0.78	0.22	75,75,75,75	0
57	MG	1A	3982	1/1	0.78	0.23	46,46,46,46	0
57	MG	1A	3023	1/1	0.79	0.17	56,56,56,56	0
57	MG	1A	3763	1/1	0.79	0.28	77,77,77,77	0
57	MG	1B	222	1/1	0.79	0.24	61,61,61,61	0
57	MG	1B	223	1/1	0.79	0.15	65,65,65,65	0
57	MG	1a	1740	1/1	0.79	0.27	70,70,70,70	0
57	MG	2a	1756	1/1	0.79	0.25	78,78,78,78	0
57	MG	2A	3471	1/1	0.79	0.18	72,72,72,72	0
57	MG	1a	1744	1/1	0.79	0.21	82,82,82,82	0
57	MG	2E	301	1/1	0.79	0.29	73,73,73,73	0
57	MG	2A	3511	1/1	0.79	0.13	67,67,67,67	0
57	MG	2A	3532	1/1	0.79	0.17	52,52,52,52	0
57	MG	2a	1644	1/1	0.79	0.39	74,74,74,74	0
57	MG	2A	3263	1/1	0.79	0.60	78,78,78,78	0
57	MG	1A	3974	1/1	0.79	0.21	73,73,73,73	0
57	MG	1A	3866	1/1	0.80	0.20	39,39,39,39	0
57	MG	2A	3590	1/1	0.80	0.26	70,70,70,70	0
57	MG	1a	1660	1/1	0.80	0.26	77,77,77,77	0
57	MG	2P	201	1/1	0.80	0.15	70,70,70,70	0
57	MG	1A	3801	1/1	0.80	0.23	59,59,59,59	0
57	MG	2A	3626	1/1	0.80	0.22	64,64,64,64	0
57	MG	2a	1606	1/1	0.80	0.23	77,77,77,77	0
57	MG	2a	1634	1/1	0.80	0.23	70,70,70,70	0
57	MG	1A	4009	1/1	0.80	0.17	61,61,61,61	0
57	MG	2A	3321	1/1	0.80	0.25	68,68,68,68	0
57	MG	2a	1660	1/1	0.80	0.20	81,81,81,81	0
57	MG	2A	3323	1/1	0.80	0.15	57,57,57,57	0
57	MG	1a	1676	1/1	0.80	0.37	74,74,74,74	0
57	MG	2A	3685	1/1	0.80	0.18	64,64,64,64	0
57	MG	2a	1717	1/1	0.80	0.27	66,66,66,66	0
57	MG	1a	1683	1/1	0.80	0.20	83,83,83,83	0
57	MG	2A	3715	1/1	0.80	0.20	76,76,76,76	0
57	MG	2A	3728	1/1	0.80	0.24	74,74,74,74	0
57	MG	1a	1700	1/1	0.80	0.16	81,81,81,81	0
57	MG	2A	3440	1/1	0.80	0.15	69,69,69,69	0
57	MG	1A	4025	1/1	0.80	0.17	69,69,69,69	0
57	MG	1A	3091	1/1	0.80	0.19	56,56,56,56	0
57	MG	1A	3715	1/1	0.80	0.10	25,25,25,25	0
57	MG	2A	3509	1/1	0.80	0.20	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3164	1/1	0.80	0.19	77,77,77,77	0
57	MG	1A	3977	1/1	0.80	0.24	76,76,76,76	0
57	MG	1A	3719	1/1	0.80	0.21	73,73,73,73	0
57	MG	2A	3260	1/1	0.81	0.25	68,68,68,68	0
57	MG	1a	1794	1/1	0.81	0.17	74,74,74,74	0
57	MG	1A	3950	1/1	0.81	0.15	71,71,71,71	0
57	MG	2A	3722	1/1	0.81	0.13	66,66,66,66	0
57	MG	2A	3534	1/1	0.81	0.14	57,57,57,57	0
57	MG	1a	1659	1/1	0.81	0.20	80,80,80,80	0
57	MG	1a	1725	1/1	0.81	0.30	75,75,75,75	0
57	MG	2a	1682	1/1	0.81	0.42	73,73,73,73	0
57	MG	1E	308	1/1	0.81	0.11	24,24,24,24	0
57	MG	1A	3867	1/1	0.81	0.13	70,70,70,70	0
57	MG	1a	1662	1/1	0.81	0.24	71,71,71,71	0
57	MG	2A	3094	1/1	0.81	0.28	73,73,73,73	0
57	MG	2A	3632	1/1	0.81	0.17	66,66,66,66	0
57	MG	2A	3633	1/1	0.81	0.24	70,70,70,70	0
57	MG	1A	3854	1/1	0.81	0.20	59,59,59,59	0
57	MG	1A	4037	1/1	0.81	0.11	45,45,45,45	0
57	MG	2A	3851	1/1	0.81	0.13	64,64,64,64	0
57	MG	1A	3811	1/1	0.81	0.20	54,54,54,54	0
57	MG	2B	205	1/1	0.81	0.20	77,77,77,77	0
57	MG	2B	217	1/1	0.81	0.17	75,75,75,75	0
57	MG	2a	1779	1/1	0.81	0.33	78,78,78,78	0
57	MG	18	104	1/1	0.81	0.12	68,68,68,68	0
57	MG	2a	1782	1/1	0.81	0.26	68,68,68,68	0
57	MG	2a	1784	1/1	0.81	0.18	86,86,86,86	0
57	MG	2A	3672	1/1	0.81	0.21	70,70,70,70	0
57	MG	2A	3676	1/1	0.81	0.21	75,75,75,75	0
57	MG	1A	3019	1/1	0.82	0.15	48,48,48,48	0
57	MG	1A	4084	1/1	0.82	0.14	70,70,70,70	0
57	MG	1A	4013	1/1	0.82	0.25	63,63,63,63	0
57	MG	1A	3582	1/1	0.82	0.13	34,34,34,34	0
57	MG	2A	3716	1/1	0.82	0.17	67,67,67,67	0
57	MG	2A	3504	1/1	0.82	0.21	71,71,71,71	0
57	MG	1B	217	1/1	0.82	0.17	55,55,55,55	0
57	MG	2a	1671	1/1	0.82	0.28	80,80,80,80	0
57	MG	2A	3733	1/1	0.82	0.15	49,49,49,49	0
57	MG	1A	3821	1/1	0.82	0.16	67,67,67,67	0
57	MG	1a	1774	1/1	0.82	0.21	72,72,72,72	0
57	MG	1a	1698	1/1	0.82	0.19	74,74,74,74	0
57	MG	1a	1612	1/1	0.82	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
57	MG	2A	3791	1/1	0.82	0.14	54,54,54,54	0
57	MG	1a	1623	1/1	0.82	0.30	74,74,74,74	0
57	MG	2A	3285	1/1	0.82	0.13	64,64,64,64	0
57	MG	1b	302	1/1	0.82	0.15	80,80,80,80	0
57	MG	2A	3306	1/1	0.82	0.45	76,76,76,76	0
57	MG	2A	3320	1/1	0.82	0.26	80,80,80,80	0
57	MG	1A	3830	1/1	0.82	0.14	54,54,54,54	0
57	MG	1v	102	1/1	0.82	0.23	77,77,77,77	0
57	MG	2A	3346	1/1	0.82	0.21	69,69,69,69	0
57	MG	2B	203	1/1	0.82	0.12	64,64,64,64	0
57	MG	2A	3361	1/1	0.82	0.29	67,67,67,67	0
57	MG	1A	3956	1/1	0.82	0.20	67,67,67,67	0
57	MG	1a	1730	1/1	0.82	0.25	74,74,74,74	0
57	MG	2i	201	1/1	0.82	0.17	78,78,78,78	0
57	MG	2G	201	1/1	0.82	0.22	79,79,79,79	0
57	MG	2A	3020	1/1	0.82	0.33	69,69,69,69	0
57	MG	2x	105	1/1	0.82	0.12	71,71,71,71	0
57	MG	1A	3810	1/1	0.83	0.20	57,57,57,57	0
57	MG	1A	4043	1/1	0.83	0.28	85,85,85,85	0
57	MG	1a	1728	1/1	0.83	0.21	59,59,59,59	0
57	MG	2A	3234	1/1	0.83	0.42	76,76,76,76	0
57	MG	2A	3701	1/1	0.83	0.21	68,68,68,68	0
57	MG	2A	3709	1/1	0.83	0.18	73,73,73,73	0
57	MG	2A	3710	1/1	0.83	0.12	71,71,71,71	0
57	MG	1a	1803	1/1	0.83	0.14	72,72,72,72	0
57	MG	1A	3603	1/1	0.83	0.09	35,35,35,35	0
57	MG	1A	3781	1/1	0.83	0.23	68,68,68,68	0
57	MG	1a	1622	1/1	0.83	0.12	62,62,62,62	0
57	MG	2A	3278	1/1	0.83	0.45	75,75,75,75	0
57	MG	1a	1747	1/1	0.83	0.25	67,67,67,67	0
57	MG	2A	3746	1/1	0.83	0.12	72,72,72,72	0
57	MG	2A	3560	1/1	0.83	0.23	73,73,73,73	0
57	MG	2A	3563	1/1	0.83	0.30	68,68,68,68	0
57	MG	1A	3895	1/1	0.83	0.12	75,75,75,75	0
57	MG	2A	3784	1/1	0.83	0.11	47,47,47,47	0
57	MG	2A	3582	1/1	0.83	0.13	68,68,68,68	0
57	MG	1A	4028	1/1	0.83	0.14	48,48,48,48	0
57	MG	2A	3310	1/1	0.83	0.26	64,64,64,64	0
57	MG	2A	3599	1/1	0.83	0.22	47,47,47,47	0
57	MG	2A	3814	1/1	0.83	0.14	68,68,68,68	0
57	MG	2A	3816	1/1	0.83	0.12	60,60,60,60	0
57	MG	2A	3818	1/1	0.83	0.23	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3017	1/1	0.83	0.17	61,61,61,61	0
57	MG	1a	1649	1/1	0.83	0.21	81,81,81,81	0
57	MG	1A	4035	1/1	0.83	0.29	56,56,56,56	0
57	MG	2A	3060	1/1	0.83	0.24	68,68,68,68	0
57	MG	1a	1772	1/1	0.83	0.17	74,74,74,74	0
57	MG	2A	3366	1/1	0.83	0.28	70,70,70,70	0
57	MG	1a	1773	1/1	0.83	0.27	79,79,79,79	0
57	MG	2A	3102	1/1	0.83	0.42	68,68,68,68	0
57	MG	2B	210	1/1	0.83	0.14	75,75,75,75	0
57	MG	1A	3918	1/1	0.84	0.11	58,58,58,58	0
57	MG	2A	3470	1/1	0.84	0.22	70,70,70,70	0
57	MG	1A	3447	1/1	0.84	0.20	61,61,61,61	0
57	MG	2T	202	1/1	0.84	0.17	66,66,66,66	0
57	MG	1A	4042	1/1	0.84	0.28	61,61,61,61	0
57	MG	2A	3484	1/1	0.84	0.21	54,54,54,54	0
57	MG	2A	3253	1/1	0.84	0.25	61,61,61,61	0
57	MG	2a	1610	1/1	0.84	0.24	69,69,69,69	0
57	MG	1A	3988	1/1	0.84	0.15	66,66,66,66	0
57	MG	1A	4049	1/1	0.84	0.14	57,57,57,57	0
57	MG	1a	1805	1/1	0.84	0.23	71,71,71,71	0
57	MG	1a	1807	1/1	0.84	0.23	73,73,73,73	0
57	MG	2a	1664	1/1	0.84	0.25	71,71,71,71	0
57	MG	1a	1708	1/1	0.84	0.15	69,69,69,69	0
57	MG	1A	3997	1/1	0.84	0.10	41,41,41,41	0
57	MG	1A	3690	1/1	0.84	0.10	53,53,53,53	0
57	MG	2A	3296	1/1	0.84	0.25	61,61,61,61	0
57	MG	2a	1691	1/1	0.84	0.29	75,75,75,75	0
57	MG	1n	102	1/1	0.84	0.20	68,68,68,68	0
57	MG	1a	1613	1/1	0.84	0.10	83,83,83,83	0
57	MG	2A	3795	1/1	0.84	0.12	56,56,56,56	0
57	MG	1A	4073	1/1	0.84	0.16	73,73,73,73	0
57	MG	1A	3218	1/1	0.84	0.25	61,61,61,61	0
57	MG	1A	3883	1/1	0.84	0.17	64,64,64,64	0
57	MG	1A	3506	1/1	0.84	0.12	72,72,72,72	0
57	MG	1A	4014	1/1	0.84	0.18	68,68,68,68	0
57	MG	2A	3365	1/1	0.84	0.23	68,68,68,68	0
57	MG	1A	3597	1/1	0.84	0.16	56,56,56,56	0
57	MG	2A	3378	1/1	0.84	0.37	73,73,73,73	0
57	MG	2A	3650	1/1	0.84	0.28	80,80,80,80	0
57	MG	2A	3847	1/1	0.84	0.19	73,73,73,73	0
57	MG	1A	3965	1/1	0.84	0.13	39,39,39,39	0
57	MG	2A	3390	1/1	0.84	0.19	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3670	1/1	0.84	0.16	77,77,77,77	0
57	MG	1A	3770	1/1	0.84	0.11	27,27,27,27	0
57	MG	1a	1666	1/1	0.84	0.15	72,72,72,72	0
57	MG	1a	1668	1/1	0.84	0.10	76,76,76,76	0
57	MG	1l	201	1/1	0.85	0.22	72,72,72,72	0
57	MG	1A	3574	1/1	0.85	0.32	50,50,50,50	0
57	MG	1A	3738	1/1	0.85	0.10	28,28,28,28	0
57	MG	1A	3576	1/1	0.85	0.10	36,36,36,36	0
57	MG	2A	3752	1/1	0.85	0.13	64,64,64,64	0
57	MG	2A	3379	1/1	0.85	0.11	68,68,68,68	0
57	MG	1a	1688	1/1	0.85	0.26	60,60,60,60	0
57	MG	1B	231	1/1	0.85	0.25	67,67,67,67	0
57	MG	2A	3767	1/1	0.85	0.15	53,53,53,53	0
57	MG	2A	3412	1/1	0.85	0.25	67,67,67,67	0
57	MG	1A	3877	1/1	0.85	0.25	29,29,29,29	0
57	MG	1A	3630	1/1	0.85	0.13	42,42,42,42	0
57	MG	2A	3036	1/1	0.85	0.37	74,74,74,74	0
57	MG	2A	3042	1/1	0.85	0.29	73,73,73,73	0
57	MG	1A	4030	1/1	0.85	0.11	51,51,51,51	0
57	MG	1S	203	1/1	0.85	0.13	73,73,73,73	0
57	MG	1a	1723	1/1	0.85	0.32	71,71,71,71	0
57	MG	1A	3966	1/1	0.85	0.11	42,42,42,42	0
57	MG	2A	3501	1/1	0.85	0.12	49,49,49,49	0
57	MG	2A	3097	1/1	0.85	0.27	71,71,71,71	0
57	MG	1A	3969	1/1	0.85	0.12	32,32,32,32	0
57	MG	2A	3837	1/1	0.85	0.15	40,40,40,40	0
57	MG	2A	3119	1/1	0.85	0.12	72,72,72,72	0
57	MG	2A	3124	1/1	0.85	0.15	66,66,66,66	0
57	MG	2A	3141	1/1	0.85	0.28	61,61,61,61	0
57	MG	2A	3546	1/1	0.85	0.15	58,58,58,58	0
57	MG	2A	3555	1/1	0.85	0.28	61,61,61,61	0
57	MG	1A	3888	1/1	0.85	0.14	31,31,31,31	0
57	MG	2A	3166	1/1	0.85	0.21	74,74,74,74	0
57	MG	2A	3572	1/1	0.85	0.10	45,45,45,45	0
57	MG	1a	1739	1/1	0.85	0.15	64,64,64,64	0
57	MG	2E	302	1/1	0.85	0.29	63,63,63,63	0
57	MG	1A	3349	1/1	0.85	0.22	53,53,53,53	0
57	MG	1A	4045	1/1	0.85	0.25	66,66,66,66	0
57	MG	2R	201	1/1	0.85	0.15	54,54,54,54	0
57	MG	2T	201	1/1	0.85	0.15	59,59,59,59	0
57	MG	2A	3589	1/1	0.85	0.18	59,59,59,59	0
57	MG	2I	101	1/1	0.85	0.37	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3235	1/1	0.85	0.31	59,59,59,59	0
57	MG	2A	3598	1/1	0.85	0.19	71,71,71,71	0
57	MG	2A	3247	1/1	0.85	0.26	64,64,64,64	0
57	MG	1a	1614	1/1	0.85	0.31	67,67,67,67	0
57	MG	2a	1616	1/1	0.85	0.14	73,73,73,73	0
57	MG	2A	3612	1/1	0.85	0.22	62,62,62,62	0
57	MG	2A	3257	1/1	0.85	0.27	69,69,69,69	0
57	MG	2a	1646	1/1	0.85	0.32	75,75,75,75	0
57	MG	1a	1621	1/1	0.85	0.34	73,73,73,73	0
57	MG	2A	3259	1/1	0.85	0.11	73,73,73,73	0
57	MG	1A	3894	1/1	0.85	0.08	81,81,81,81	0
57	MG	2A	3637	1/1	0.85	0.22	71,71,71,71	0
57	MG	1A	3826	1/1	0.85	0.12	66,66,66,66	0
57	MG	1a	1627	1/1	0.85	0.18	58,58,58,58	0
57	MG	2A	3646	1/1	0.85	0.14	54,54,54,54	0
57	MG	1A	3994	1/1	0.85	0.13	30,30,30,30	0
57	MG	2A	3282	1/1	0.85	0.16	62,62,62,62	0
57	MG	1a	1646	1/1	0.85	0.29	61,61,61,61	0
57	MG	2A	3662	1/1	0.85	0.21	61,61,61,61	0
57	MG	2A	3663	1/1	0.85	0.10	79,79,79,79	0
57	MG	2a	1732	1/1	0.85	0.20	77,77,77,77	0
57	MG	2A	3666	1/1	0.85	0.18	56,56,56,56	0
57	MG	2a	1742	1/1	0.85	0.28	68,68,68,68	0
57	MG	2a	1744	1/1	0.85	0.17	74,74,74,74	0
57	MG	2a	1754	1/1	0.85	0.15	77,77,77,77	0
57	MG	1A	4069	1/1	0.85	0.12	47,47,47,47	0
57	MG	1a	1655	1/1	0.85	0.21	77,77,77,77	0
57	MG	1A	3504	1/1	0.85	0.31	80,80,80,80	0
57	MG	1A	4077	1/1	0.85	0.16	66,66,66,66	0
57	MG	2A	3687	1/1	0.85	0.18	62,62,62,62	0
57	MG	2A	3700	1/1	0.85	0.14	58,58,58,58	0
57	MG	1A	3191	1/1	0.85	0.17	57,57,57,57	0
57	MG	2A	3708	1/1	0.85	0.13	65,65,65,65	0
57	MG	1A	3085	1/1	0.85	0.15	43,43,43,43	0
57	MG	1A	3864	1/1	0.85	0.12	30,30,30,30	0
57	MG	2A	3711	1/1	0.85	0.12	69,69,69,69	0
57	MG	2A	3341	1/1	0.85	0.26	73,73,73,73	0
57	MG	1A	4012	1/1	0.85	0.24	69,69,69,69	0
57	MG	2A	3355	1/1	0.85	0.16	67,67,67,67	0
57	MG	1A	4086	1/1	0.86	0.19	71,71,71,71	0
57	MG	2A	3554	1/1	0.86	0.15	68,68,68,68	0
57	MG	1A	3707	1/1	0.86	0.15	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
57	MG	1A	4095	1/1	0.86	0.15	59,59,59,59	0
57	MG	1A	3896	1/1	0.86	0.12	51,51,51,51	0
57	MG	1A	3711	1/1	0.86	0.14	62,62,62,62	0
57	MG	2A	3835	1/1	0.86	0.15	43,43,43,43	0
57	MG	2A	3262	1/1	0.86	0.15	68,68,68,68	0
57	MG	1A	3910	1/1	0.86	0.10	70,70,70,70	0
57	MG	2A	3840	1/1	0.86	0.23	70,70,70,70	0
57	MG	2A	3265	1/1	0.86	0.14	71,71,71,71	0
57	MG	2A	3267	1/1	0.86	0.21	64,64,64,64	0
57	MG	2A	3274	1/1	0.86	0.14	72,72,72,72	0
57	MG	1a	1667	1/1	0.86	0.28	70,70,70,70	0
57	MG	1A	3397	1/1	0.86	0.16	63,63,63,63	0
57	MG	2A	3279	1/1	0.86	0.15	77,77,77,77	0
57	MG	2B	212	1/1	0.86	0.18	85,85,85,85	0
57	MG	2A	3281	1/1	0.86	0.20	68,68,68,68	0
57	MG	1A	3356	1/1	0.86	0.26	63,63,63,63	0
57	MG	1A	3416	1/1	0.86	0.32	64,64,64,64	0
57	MG	2A	3631	1/1	0.86	0.36	81,81,81,81	0
57	MG	1A	3940	1/1	0.86	0.16	63,63,63,63	0
57	MG	1A	3836	1/1	0.86	0.14	54,54,54,54	0
57	MG	1a	1696	1/1	0.86	0.24	72,72,72,72	0
57	MG	1A	3739	1/1	0.86	0.12	33,33,33,33	0
57	MG	2A	3319	1/1	0.86	0.20	74,74,74,74	0
57	MG	1x	101	1/1	0.86	0.20	69,69,69,69	0
57	MG	1A	4031	1/1	0.86	0.14	51,51,51,51	0
57	MG	1A	3743	1/1	0.86	0.11	25,25,25,25	0
57	MG	2A	3333	1/1	0.86	0.20	75,75,75,75	0
57	MG	2a	1614	1/1	0.86	0.13	69,69,69,69	0
57	MG	2A	3661	1/1	0.86	0.11	46,46,46,46	0
57	MG	2a	1629	1/1	0.86	0.18	58,58,58,58	0
57	MG	2a	1632	1/1	0.86	0.23	64,64,64,64	0
57	MG	2A	3336	1/1	0.86	0.31	74,74,74,74	0
57	MG	1Y	202	1/1	0.86	0.14	62,62,62,62	0
57	MG	1A	3750	1/1	0.86	0.10	39,39,39,39	0
57	MG	1a	1718	1/1	0.86	0.22	73,73,73,73	0
57	MG	1A	3530	1/1	0.86	0.19	60,60,60,60	0
57	MG	2A	3058	1/1	0.86	0.12	64,64,64,64	0
57	MG	1a	1724	1/1	0.86	0.34	72,72,72,72	0
57	MG	2a	1672	1/1	0.86	0.25	58,58,58,58	0
57	MG	2A	3370	1/1	0.86	0.13	72,72,72,72	0
57	MG	2a	1678	1/1	0.86	0.25	73,73,73,73	0
57	MG	2A	3697	1/1	0.86	0.19	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
57	MG	2a	1683	1/1	0.86	0.20	71,71,71,71	0
57	MG	1A	3379	1/1	0.86	0.20	57,57,57,57	0
57	MG	1A	3634	1/1	0.86	0.07	29,29,29,29	0
57	MG	1a	1729	1/1	0.86	0.22	63,63,63,63	0
57	MG	2a	1709	1/1	0.86	0.15	55,55,55,55	0
57	MG	2a	1713	1/1	0.86	0.17	65,65,65,65	0
57	MG	2a	1715	1/1	0.86	0.22	50,50,50,50	0
57	MG	1A	3876	1/1	0.86	0.18	49,49,49,49	0
57	MG	2a	1721	1/1	0.86	0.18	61,61,61,61	0
57	MG	2a	1722	1/1	0.86	0.24	80,80,80,80	0
57	MG	1a	1731	1/1	0.86	0.09	64,64,64,64	0
57	MG	2A	3413	1/1	0.86	0.36	62,62,62,62	0
57	MG	2A	3420	1/1	0.86	0.37	69,69,69,69	0
57	MG	2a	1733	1/1	0.86	0.18	49,49,49,49	0
57	MG	2a	1739	1/1	0.86	0.10	66,66,66,66	0
57	MG	2A	3111	1/1	0.86	0.30	80,80,80,80	0
57	MG	1A	3467	1/1	0.86	0.19	54,54,54,54	0
57	MG	1A	3979	1/1	0.86	0.11	44,44,44,44	0
57	MG	1A	4065	1/1	0.86	0.14	39,39,39,39	0
57	MG	2A	3143	1/1	0.86	0.13	77,77,77,77	0
57	MG	1a	1746	1/1	0.86	0.22	66,66,66,66	0
57	MG	1A	3482	1/1	0.86	0.24	71,71,71,71	0
57	MG	2A	3483	1/1	0.86	0.12	42,42,42,42	0
57	MG	1a	1748	1/1	0.86	0.25	68,68,68,68	0
57	MG	1A	3686	1/1	0.86	0.24	62,62,62,62	0
57	MG	2A	3760	1/1	0.86	0.21	71,71,71,71	0
57	MG	2A	3503	1/1	0.86	0.23	64,64,64,64	0
57	MG	2A	3193	1/1	0.86	0.27	71,71,71,71	0
57	MG	2A	3507	1/1	0.86	0.18	56,56,56,56	0
57	MG	2g	201	1/1	0.86	0.12	75,75,75,75	0
57	MG	2A	3212	1/1	0.86	0.17	62,62,62,62	0
57	MG	1A	3380	1/1	0.86	0.14	63,63,63,63	0
57	MG	1a	1648	1/1	0.86	0.18	68,68,68,68	0
57	MG	1A	3706	1/1	0.86	0.17	61,61,61,61	0
57	MG	2A	3852	1/1	0.87	0.16	73,73,73,73	0
57	MG	1A	3487	1/1	0.87	0.12	54,54,54,54	0
57	MG	1A	3748	1/1	0.87	0.10	58,58,58,58	0
57	MG	2B	204	1/1	0.87	0.13	67,67,67,67	0
57	MG	2A	3362	1/1	0.87	0.29	74,74,74,74	0
57	MG	2A	3140	1/1	0.87	0.20	68,68,68,68	0
57	MG	1A	3442	1/1	0.87	0.20	71,71,71,71	0
57	MG	1F	305	1/1	0.87	0.17	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2D	307	1/1	0.87	0.14	59,59,59,59	0
57	MG	2A	3373	1/1	0.87	0.15	59,59,59,59	0
57	MG	2A	3374	1/1	0.87	0.12	58,58,58,58	0
57	MG	2E	308	1/1	0.87	0.23	72,72,72,72	0
57	MG	2A	3160	1/1	0.87	0.17	70,70,70,70	0
57	MG	2A	3658	1/1	0.87	0.19	58,58,58,58	0
57	MG	1a	1665	1/1	0.87	0.12	64,64,64,64	0
57	MG	1A	3620	1/1	0.87	0.14	60,60,60,60	0
57	MG	1A	3246	1/1	0.87	0.22	76,76,76,76	0
57	MG	1A	3183	1/1	0.87	0.13	45,45,45,45	0
57	MG	1A	3417	1/1	0.87	0.15	56,56,56,56	0
57	MG	10	104	1/1	0.87	0.25	66,66,66,66	0
57	MG	10	105	1/1	0.87	0.13	64,64,64,64	0
57	MG	2A	3675	1/1	0.87	0.13	40,40,40,40	0
57	MG	2A	3432	1/1	0.87	0.31	69,69,69,69	0
57	MG	1A	4015	1/1	0.87	0.10	36,36,36,36	0
57	MG	1a	1692	1/1	0.87	0.20	58,58,58,58	0
57	MG	1A	3656	1/1	0.87	0.18	48,48,48,48	0
57	MG	2A	3467	1/1	0.87	0.29	71,71,71,71	0
57	MG	2a	1643	1/1	0.87	0.19	65,65,65,65	0
57	MG	1a	1605	1/1	0.87	0.13	72,72,72,72	0
57	MG	1A	3972	1/1	0.87	0.15	51,51,51,51	0
57	MG	1a	1701	1/1	0.87	0.10	62,62,62,62	0
57	MG	1A	4091	1/1	0.87	0.24	63,63,63,63	0
57	MG	1A	4092	1/1	0.87	0.17	53,53,53,53	0
57	MG	2A	3489	1/1	0.87	0.16	48,48,48,48	0
57	MG	1a	1620	1/1	0.87	0.36	79,79,79,79	0
57	MG	1x	106	1/1	0.87	0.18	83,83,83,83	0
57	MG	2a	1677	1/1	0.87	0.14	77,77,77,77	0
57	MG	1A	3904	1/1	0.87	0.11	43,43,43,43	0
57	MG	2A	3727	1/1	0.87	0.12	69,69,69,69	0
57	MG	1a	1721	1/1	0.87	0.24	69,69,69,69	0
57	MG	2A	3013	1/1	0.87	0.38	78,78,78,78	0
57	MG	2A	3739	1/1	0.87	0.32	70,70,70,70	0
57	MG	1A	3662	1/1	0.87	0.11	26,26,26,26	0
57	MG	2a	1695	1/1	0.87	0.28	70,70,70,70	0
57	MG	2A	3529	1/1	0.87	0.21	46,46,46,46	0
57	MG	1A	3978	1/1	0.87	0.15	44,44,44,44	0
57	MG	2A	3533	1/1	0.87	0.16	79,79,79,79	0
57	MG	2A	3021	1/1	0.87	0.12	58,58,58,58	0
57	MG	2A	3029	1/1	0.87	0.12	53,53,53,53	0
57	MG	1a	1626	1/1	0.87	0.12	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	210	1/1	0.87	0.25	49,49,49,49	0
57	MG	2A	3786	1/1	0.87	0.16	52,52,52,52	0
57	MG	2A	3556	1/1	0.87	0.16	61,61,61,61	0
57	MG	1a	1635	1/1	0.87	0.20	74,74,74,74	0
57	MG	1a	1637	1/1	0.87	0.26	73,73,73,73	0
57	MG	2A	3804	1/1	0.87	0.15	42,42,42,42	0
57	MG	2A	3805	1/1	0.87	0.11	50,50,50,50	0
57	MG	1B	213	1/1	0.87	0.18	55,55,55,55	0
57	MG	2a	1751	1/1	0.87	0.42	74,74,74,74	0
57	MG	2a	1752	1/1	0.87	0.24	71,71,71,71	0
57	MG	2A	3810	1/1	0.87	0.18	74,74,74,74	0
57	MG	2A	3812	1/1	0.87	0.14	70,70,70,70	0
57	MG	2A	3076	1/1	0.87	0.32	65,65,65,65	0
57	MG	2A	3580	1/1	0.87	0.09	51,51,51,51	0
57	MG	2a	1770	1/1	0.87	0.15	77,77,77,77	0
57	MG	2A	3083	1/1	0.87	0.15	66,66,66,66	0
57	MG	2A	3084	1/1	0.87	0.15	75,75,75,75	0
57	MG	1A	3734	1/1	0.87	0.12	27,27,27,27	0
57	MG	2A	3331	1/1	0.87	0.18	61,61,61,61	0
57	MG	2A	3825	1/1	0.87	0.15	68,68,68,68	0
57	MG	1A	3920	1/1	0.87	0.18	38,38,38,38	0
57	MG	1A	3678	1/1	0.87	0.12	38,38,38,38	0
57	MG	1A	3523	1/1	0.87	0.24	62,62,62,62	0
57	MG	1a	1657	1/1	0.87	0.17	73,73,73,73	0
57	MG	2q	202	1/1	0.87	0.21	72,72,72,72	0
57	MG	2A	3622	1/1	0.87	0.36	66,66,66,66	0
57	MG	2A	3348	1/1	0.87	0.10	71,71,71,71	0
57	MG	2A	3350	1/1	0.87	0.18	71,71,71,71	0
57	MG	2A	3091	1/1	0.88	0.21	69,69,69,69	0
57	MG	1A	3971	1/1	0.88	0.10	56,56,56,56	0
57	MG	1A	3891	1/1	0.88	0.10	52,52,52,52	0
57	MG	1A	3343	1/1	0.88	0.21	75,75,75,75	0
57	MG	2A	3107	1/1	0.88	0.39	72,72,72,72	0
57	MG	2A	3638	1/1	0.88	0.14	70,70,70,70	0
57	MG	1a	1765	1/1	0.88	0.15	68,68,68,68	0
57	MG	2B	209	1/1	0.88	0.27	73,73,73,73	0
57	MG	1A	3976	1/1	0.88	0.12	56,56,56,56	0
57	MG	2A	3643	1/1	0.88	0.15	65,65,65,65	0
57	MG	2A	3644	1/1	0.88	0.17	69,69,69,69	0
57	MG	2B	219	1/1	0.88	0.23	73,73,73,73	0
57	MG	2A	3120	1/1	0.88	0.14	60,60,60,60	0
57	MG	1a	1672	1/1	0.88	0.10	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
57	MG	1A	3345	1/1	0.88	0.24	65,65,65,65	0
57	MG	2A	3654	1/1	0.88	0.14	69,69,69,69	0
57	MG	2A	3655	1/1	0.88	0.11	42,42,42,42	0
57	MG	1A	3455	1/1	0.88	0.11	53,53,53,53	0
57	MG	1a	1678	1/1	0.88	0.22	60,60,60,60	0
57	MG	2A	3377	1/1	0.88	0.16	64,64,64,64	0
57	MG	1a	1776	1/1	0.88	0.24	57,57,57,57	0
57	MG	2Z	301	1/1	0.88	0.12	74,74,74,74	0
57	MG	1a	1779	1/1	0.88	0.14	50,50,50,50	0
57	MG	23	102	1/1	0.88	0.23	61,61,61,61	0
57	MG	1A	3204	1/1	0.88	0.12	73,73,73,73	0
57	MG	2A	3170	1/1	0.88	0.18	74,74,74,74	0
57	MG	1a	1790	1/1	0.88	0.20	79,79,79,79	0
57	MG	1a	1684	1/1	0.88	0.14	69,69,69,69	0
57	MG	2A	3418	1/1	0.88	0.20	67,67,67,67	0
57	MG	1a	1801	1/1	0.88	0.13	63,63,63,63	0
57	MG	1a	1686	1/1	0.88	0.17	79,79,79,79	0
57	MG	2A	3217	1/1	0.88	0.22	66,66,66,66	0
57	MG	2A	3233	1/1	0.88	0.14	73,73,73,73	0
57	MG	2a	1641	1/1	0.88	0.24	70,70,70,70	0
57	MG	1A	3025	1/1	0.88	0.14	59,59,59,59	0
57	MG	2A	3446	1/1	0.88	0.14	52,52,52,52	0
57	MG	1a	1806	1/1	0.88	0.12	62,62,62,62	0
57	MG	2A	3237	1/1	0.88	0.13	74,74,74,74	0
57	MG	2A	3468	1/1	0.88	0.14	54,54,54,54	0
57	MG	2A	3469	1/1	0.88	0.18	57,57,57,57	0
57	MG	2A	3245	1/1	0.88	0.19	63,63,63,63	0
57	MG	2A	3246	1/1	0.88	0.14	60,60,60,60	0
57	MG	2a	1673	1/1	0.88	0.37	73,73,73,73	0
57	MG	1A	3732	1/1	0.88	0.14	54,54,54,54	0
57	MG	2A	3725	1/1	0.88	0.21	72,72,72,72	0
57	MG	2A	3726	1/1	0.88	0.17	65,65,65,65	0
57	MG	2A	3249	1/1	0.88	0.17	70,70,70,70	0
57	MG	1a	1808	1/1	0.88	0.16	66,66,66,66	0
57	MG	1A	3827	1/1	0.88	0.14	31,31,31,31	0
57	MG	2A	3736	1/1	0.88	0.13	66,66,66,66	0
57	MG	1A	3097	1/1	0.88	0.27	67,67,67,67	0
57	MG	2A	3741	1/1	0.88	0.14	48,48,48,48	0
57	MG	2a	1698	1/1	0.88	0.23	69,69,69,69	0
57	MG	2a	1708	1/1	0.88	0.17	63,63,63,63	0
57	MG	1A	3376	1/1	0.88	0.19	41,41,41,41	0
57	MG	1A	3290	1/1	0.88	0.27	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
57	MG	1a	1707	1/1	0.88	0.15	64,64,64,64	0
57	MG	1A	3638	1/1	0.88	0.08	33,33,33,33	0
57	MG	1A	3929	1/1	0.88	0.11	48,48,48,48	0
57	MG	1A	3939	1/1	0.88	0.14	74,74,74,74	0
57	MG	1B	203	1/1	0.88	0.18	64,64,64,64	0
57	MG	2A	3769	1/1	0.88	0.12	74,74,74,74	0
57	MG	2A	3771	1/1	0.88	0.20	77,77,77,77	0
57	MG	2A	3275	1/1	0.88	0.10	66,66,66,66	0
57	MG	1A	3298	1/1	0.88	0.23	61,61,61,61	0
57	MG	1a	1722	1/1	0.88	0.14	68,68,68,68	0
57	MG	1A	3947	1/1	0.88	0.22	65,65,65,65	0
57	MG	2A	3792	1/1	0.88	0.21	40,40,40,40	0
57	MG	2a	1746	1/1	0.88	0.14	61,61,61,61	0
57	MG	2a	1747	1/1	0.88	0.25	62,62,62,62	0
57	MG	2A	3793	1/1	0.88	0.12	42,42,42,42	0
57	MG	1A	3323	1/1	0.88	0.26	58,58,58,58	0
57	MG	1a	1642	1/1	0.88	0.10	80,80,80,80	0
57	MG	1A	3326	1/1	0.88	0.15	56,56,56,56	0
57	MG	2A	3286	1/1	0.88	0.24	74,74,74,74	0
57	MG	2a	1760	1/1	0.88	0.19	68,68,68,68	0
57	MG	1A	3954	1/1	0.88	0.11	65,65,65,65	0
57	MG	2A	3576	1/1	0.88	0.22	71,71,71,71	0
57	MG	1A	3412	1/1	0.88	0.23	63,63,63,63	0
57	MG	2A	3051	1/1	0.88	0.10	64,64,64,64	0
57	MG	2A	3308	1/1	0.88	0.21	54,54,54,54	0
57	MG	1A	3331	1/1	0.88	0.30	72,72,72,72	0
57	MG	1a	1733	1/1	0.88	0.15	54,54,54,54	0
57	MG	2A	3822	1/1	0.88	0.11	75,75,75,75	0
57	MG	1E	306	1/1	0.88	0.19	58,58,58,58	0
57	MG	2f	201	1/1	0.88	0.16	59,59,59,59	0
57	MG	2A	3061	1/1	0.88	0.21	57,57,57,57	0
57	MG	1A	4033	1/1	0.88	0.12	38,38,38,38	0
57	MG	2A	3324	1/1	0.88	0.11	69,69,69,69	0
57	MG	1A	3198	1/1	0.88	0.10	43,43,43,43	0
57	MG	1A	3439	1/1	0.88	0.48	46,46,46,46	0
57	MG	1A	3698	1/1	0.88	0.15	62,62,62,62	0
57	MG	1a	1759	1/1	0.89	0.10	60,60,60,60	0
57	MG	2A	3581	1/1	0.89	0.17	62,62,62,62	0
57	MG	1A	3444	1/1	0.89	0.25	49,49,49,49	0
57	MG	2A	3096	1/1	0.89	0.23	74,74,74,74	0
57	MG	2A	3828	1/1	0.89	0.10	56,56,56,56	0
57	MG	1A	3852	1/1	0.89	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
57	MG	1A	3948	1/1	0.89	0.18	61,61,61,61	0
57	MG	2A	3595	1/1	0.89	0.15	71,71,71,71	0
57	MG	2A	3104	1/1	0.89	0.21	62,62,62,62	0
57	MG	2A	3329	1/1	0.89	0.17	71,71,71,71	0
57	MG	2A	3842	1/1	0.89	0.18	58,58,58,58	0
57	MG	2A	3844	1/1	0.89	0.21	73,73,73,73	0
57	MG	2A	3846	1/1	0.89	0.14	57,57,57,57	0
57	MG	2A	3610	1/1	0.89	0.16	54,54,54,54	0
57	MG	2A	3849	1/1	0.89	0.16	50,50,50,50	0
57	MG	2A	3330	1/1	0.89	0.14	63,63,63,63	0
57	MG	1a	1769	1/1	0.89	0.18	64,64,64,64	0
57	MG	2A	3110	1/1	0.89	0.16	50,50,50,50	0
57	MG	1A	3136	1/1	0.89	0.12	42,42,42,42	0
57	MG	1A	3855	1/1	0.89	0.11	28,28,28,28	0
57	MG	2A	3628	1/1	0.89	0.13	70,70,70,70	0
57	MG	2A	3342	1/1	0.89	0.15	60,60,60,60	0
57	MG	2A	3343	1/1	0.89	0.22	66,66,66,66	0
57	MG	1A	3953	1/1	0.89	0.14	52,52,52,52	0
57	MG	1G	202	1/1	0.89	0.17	66,66,66,66	0
57	MG	1O	203	1/1	0.89	0.10	59,59,59,59	0
57	MG	2D	303	1/1	0.89	0.17	65,65,65,65	0
57	MG	2A	3352	1/1	0.89	0.13	76,76,76,76	0
57	MG	2A	3641	1/1	0.89	0.19	73,73,73,73	0
57	MG	2A	3354	1/1	0.89	0.33	73,73,73,73	0
57	MG	1A	3367	1/1	0.89	0.18	53,53,53,53	0
57	MG	1A	3765	1/1	0.89	0.14	57,57,57,57	0
57	MG	2A	3156	1/1	0.89	0.31	76,76,76,76	0
57	MG	2A	3648	1/1	0.89	0.17	84,84,84,84	0
57	MG	1a	1785	1/1	0.89	0.17	70,70,70,70	0
57	MG	1A	3611	1/1	0.89	0.09	22,22,22,22	0
57	MG	2W	201	1/1	0.89	0.15	58,58,58,58	0
57	MG	2A	3653	1/1	0.89	0.09	61,61,61,61	0
57	MG	1A	3958	1/1	0.89	0.11	74,74,74,74	0
57	MG	1a	1800	1/1	0.89	0.19	57,57,57,57	0
57	MG	2A	3180	1/1	0.89	0.13	73,73,73,73	0
57	MG	1A	3514	1/1	0.89	0.25	58,58,58,58	0
57	MG	1A	3462	1/1	0.89	0.13	63,63,63,63	0
57	MG	1A	3524	1/1	0.89	0.30	59,59,59,59	0
57	MG	2a	1611	1/1	0.89	0.23	67,67,67,67	0
57	MG	2A	3201	1/1	0.89	0.15	61,61,61,61	0
57	MG	2A	3202	1/1	0.89	0.11	68,68,68,68	0
57	MG	2a	1624	1/1	0.89	0.28	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
57	MG	2a	1626	1/1	0.89	0.32	67,67,67,67	0
57	MG	2A	3391	1/1	0.89	0.21	59,59,59,59	0
57	MG	2A	3392	1/1	0.89	0.49	65,65,65,65	0
57	MG	2A	3402	1/1	0.89	0.27	60,60,60,60	0
57	MG	2a	1636	1/1	0.89	0.22	67,67,67,67	0
57	MG	2a	1638	1/1	0.89	0.23	69,69,69,69	0
57	MG	2A	3203	1/1	0.89	0.26	71,71,71,71	0
57	MG	1A	3793	1/1	0.89	0.10	32,32,32,32	0
57	MG	1a	1601	1/1	0.89	0.17	63,63,63,63	0
57	MG	2A	3689	1/1	0.89	0.10	60,60,60,60	0
57	MG	2A	3693	1/1	0.89	0.15	67,67,67,67	0
57	MG	2A	3695	1/1	0.89	0.10	47,47,47,47	0
57	MG	2A	3696	1/1	0.89	0.19	65,65,65,65	0
57	MG	1A	3800	1/1	0.89	0.19	55,55,55,55	0
57	MG	2A	3698	1/1	0.89	0.12	56,56,56,56	0
57	MG	2A	3421	1/1	0.89	0.26	59,59,59,59	0
57	MG	1A	4064	1/1	0.89	0.10	58,58,58,58	0
57	MG	2A	3428	1/1	0.89	0.22	59,59,59,59	0
57	MG	1A	3071	1/1	0.89	0.23	66,66,66,66	0
57	MG	2a	1679	1/1	0.89	0.20	60,60,60,60	0
57	MG	2a	1681	1/1	0.89	0.36	66,66,66,66	0
57	MG	2A	3435	1/1	0.89	0.13	69,69,69,69	0
57	MG	1A	3975	1/1	0.89	0.14	42,42,42,42	0
57	MG	2A	3239	1/1	0.89	0.20	62,62,62,62	0
57	MG	1A	3803	1/1	0.89	0.39	64,64,64,64	0
57	MG	1a	1717	1/1	0.89	0.16	53,53,53,53	0
57	MG	2A	3717	1/1	0.89	0.11	38,38,38,38	0
57	MG	1A	3572	1/1	0.89	0.28	62,62,62,62	0
57	MG	1A	4079	1/1	0.89	0.12	66,66,66,66	0
57	MG	1x	105	1/1	0.89	0.22	74,74,74,74	0
57	MG	1A	3721	1/1	0.89	0.16	50,50,50,50	0
57	MG	1x	109	1/1	0.89	0.13	55,55,55,55	0
57	MG	1A	3027	1/1	0.89	0.13	41,41,41,41	0
57	MG	2A	3734	1/1	0.89	0.13	63,63,63,63	0
57	MG	2A	3477	1/1	0.89	0.15	54,54,54,54	0
57	MG	2A	3480	1/1	0.89	0.16	61,61,61,61	0
57	MG	2a	1726	1/1	0.89	0.14	58,58,58,58	0
57	MG	2A	3740	1/1	0.89	0.14	78,78,78,78	0
57	MG	1A	4089	1/1	0.89	0.13	58,58,58,58	0
57	MG	2A	3261	1/1	0.89	0.14	76,76,76,76	0
57	MG	1A	3317	1/1	0.89	0.20	53,53,53,53	0
57	MG	2A	3493	1/1	0.89	0.18	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
57	MG	2A	3756	1/1	0.89	0.14	70,70,70,70	0
57	MG	1A	3736	1/1	0.89	0.07	26,26,26,26	0
57	MG	1A	3822	1/1	0.89	0.12	58,58,58,58	0
57	MG	1A	3353	1/1	0.89	0.13	45,45,45,45	0
57	MG	2a	1750	1/1	0.89	0.14	73,73,73,73	0
57	MG	1A	3587	1/1	0.89	0.12	31,31,31,31	0
57	MG	2A	3768	1/1	0.89	0.10	59,59,59,59	0
57	MG	1A	4001	1/1	0.89	0.17	50,50,50,50	0
57	MG	1a	1738	1/1	0.89	0.15	66,66,66,66	0
57	MG	2A	3780	1/1	0.89	0.14	63,63,63,63	0
57	MG	2A	3047	1/1	0.89	0.24	69,69,69,69	0
57	MG	1A	3588	1/1	0.89	0.08	38,38,38,38	0
57	MG	2a	1768	1/1	0.89	0.33	70,70,70,70	0
57	MG	1a	1653	1/1	0.89	0.17	66,66,66,66	0
57	MG	1A	3745	1/1	0.89	0.12	26,26,26,26	0
57	MG	2A	3539	1/1	0.89	0.15	39,39,39,39	0
57	MG	2a	1775	1/1	0.89	0.25	59,59,59,59	0
57	MG	1B	214	1/1	0.89	0.07	59,59,59,59	0
57	MG	1A	3837	1/1	0.89	0.15	56,56,56,56	0
57	MG	2A	3800	1/1	0.89	0.12	66,66,66,66	0
57	MG	1A	3938	1/1	0.89	0.08	26,26,26,26	0
57	MG	2A	3295	1/1	0.89	0.22	58,58,58,58	0
57	MG	1A	3841	1/1	0.89	0.12	58,58,58,58	0
57	MG	2A	3297	1/1	0.89	0.12	64,64,64,64	0
57	MG	2A	3571	1/1	0.89	0.21	61,61,61,61	0
57	MG	2n	101	1/1	0.89	0.19	77,77,77,77	0
57	MG	2A	3301	1/1	0.89	0.14	60,60,60,60	0
57	MG	2A	3573	1/1	0.89	0.18	61,61,61,61	0
57	MG	1a	1756	1/1	0.89	0.19	75,75,75,75	0
57	MG	2x	102	1/1	0.89	0.19	65,65,65,65	0
57	MG	1a	1758	1/1	0.89	0.10	69,69,69,69	0
57	MG	2A	3634	1/1	0.90	0.16	69,69,69,69	0
57	MG	2A	3376	1/1	0.90	0.10	66,66,66,66	0
57	MG	1a	1796	1/1	0.90	0.14	71,71,71,71	0
57	MG	1B	235	1/1	0.90	0.17	81,81,81,81	0
57	MG	1D	312	1/1	0.90	0.25	63,63,63,63	0
57	MG	1A	3934	1/1	0.90	0.14	61,61,61,61	0
57	MG	2A	3382	1/1	0.90	0.13	69,69,69,69	0
57	MG	2A	3386	1/1	0.90	0.23	49,49,49,49	0
57	MG	1A	4022	1/1	0.90	0.16	65,65,65,65	0
57	MG	2A	3230	1/1	0.90	0.15	65,65,65,65	0
57	MG	2B	216	1/1	0.90	0.11	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3315	1/1	0.90	0.22	52,52,52,52	0
57	MG	2A	3396	1/1	0.90	0.23	72,72,72,72	0
57	MG	2D	302	1/1	0.90	0.22	56,56,56,56	0
57	MG	2A	3652	1/1	0.90	0.16	48,48,48,48	0
57	MG	2A	3400	1/1	0.90	0.15	56,56,56,56	0
57	MG	1A	3120	1/1	0.90	0.19	56,56,56,56	0
57	MG	2A	3406	1/1	0.90	0.29	58,58,58,58	0
57	MG	2A	3408	1/1	0.90	0.38	64,64,64,64	0
57	MG	1F	312	1/1	0.90	0.13	58,58,58,58	0
57	MG	2N	201	1/1	0.90	0.14	63,63,63,63	0
57	MG	1a	1687	1/1	0.90	0.14	69,69,69,69	0
57	MG	2A	3414	1/1	0.90	0.13	71,71,71,71	0
57	MG	2A	3415	1/1	0.90	0.32	64,64,64,64	0
57	MG	1F	315	1/1	0.90	0.14	58,58,58,58	0
57	MG	2A	3241	1/1	0.90	0.21	68,68,68,68	0
57	MG	1a	1689	1/1	0.90	0.25	59,59,59,59	0
57	MG	1A	3541	1/1	0.90	0.33	59,59,59,59	0
57	MG	1G	205	1/1	0.90	0.22	65,65,65,65	0
57	MG	2A	3682	1/1	0.90	0.11	59,59,59,59	0
57	MG	2A	3683	1/1	0.90	0.12	57,57,57,57	0
57	MG	1A	3560	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3433	1/1	0.90	0.18	60,60,60,60	0
57	MG	2A	3250	1/1	0.90	0.17	59,59,59,59	0
57	MG	2A	3691	1/1	0.90	0.17	75,75,75,75	0
57	MG	2a	1615	1/1	0.90	0.13	66,66,66,66	0
57	MG	1A	3669	1/1	0.90	0.13	40,40,40,40	0
57	MG	2a	1619	1/1	0.90	0.15	62,62,62,62	0
57	MG	2A	3439	1/1	0.90	0.15	58,58,58,58	0
57	MG	2a	1625	1/1	0.90	0.24	70,70,70,70	0
57	MG	1Q	206	1/1	0.90	0.13	58,58,58,58	0
57	MG	2a	1628	1/1	0.90	0.13	57,57,57,57	0
57	MG	2A	3445	1/1	0.90	0.11	68,68,68,68	0
57	MG	2a	1630	1/1	0.90	0.18	59,59,59,59	0
57	MG	1A	3843	1/1	0.90	0.09	41,41,41,41	0
57	MG	1T	203	1/1	0.90	0.20	64,64,64,64	0
57	MG	1a	1711	1/1	0.90	0.19	63,63,63,63	0
57	MG	2a	1637	1/1	0.90	0.34	67,67,67,67	0
57	MG	2A	3002	1/1	0.90	0.34	71,71,71,71	0
57	MG	1A	3844	1/1	0.90	0.21	40,40,40,40	0
57	MG	1A	3322	1/1	0.90	0.12	47,47,47,47	0
57	MG	10	102	1/1	0.90	0.12	54,54,54,54	0
57	MG	1A	3755	1/1	0.90	0.09	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1648	1/1	0.90	0.23	69,69,69,69	0
57	MG	2A	3473	1/1	0.90	0.26	69,69,69,69	0
57	MG	1A	3369	1/1	0.90	0.14	56,56,56,56	0
57	MG	1l	102	1/1	0.90	0.11	62,62,62,62	0
57	MG	2a	1666	1/1	0.90	0.21	66,66,66,66	0
57	MG	2a	1667	1/1	0.90	0.17	60,60,60,60	0
57	MG	1A	4044	1/1	0.90	0.07	23,23,23,23	0
57	MG	2A	3723	1/1	0.90	0.12	70,70,70,70	0
57	MG	1A	3243	1/1	0.90	0.19	54,54,54,54	0
57	MG	1A	3038	1/1	0.90	0.15	58,58,58,58	0
57	MG	1a	1726	1/1	0.90	0.20	58,58,58,58	0
57	MG	2A	3500	1/1	0.90	0.12	39,39,39,39	0
57	MG	1a	1602	1/1	0.90	0.26	78,78,78,78	0
57	MG	1A	3961	1/1	0.90	0.13	52,52,52,52	0
57	MG	1A	3276	1/1	0.90	0.14	59,59,59,59	0
57	MG	1A	3468	1/1	0.90	0.15	59,59,59,59	0
57	MG	1A	3967	1/1	0.90	0.13	25,25,25,25	0
57	MG	2a	1688	1/1	0.90	0.24	73,73,73,73	0
57	MG	1A	3394	1/1	0.90	0.13	58,58,58,58	0
57	MG	2a	1692	1/1	0.90	0.14	71,71,71,71	0
57	MG	2A	3513	1/1	0.90	0.16	64,64,64,64	0
57	MG	2A	3751	1/1	0.90	0.13	41,41,41,41	0
57	MG	2a	1697	1/1	0.90	0.09	70,70,70,70	0
57	MG	2A	3515	1/1	0.90	0.09	64,64,64,64	0
57	MG	2A	3517	1/1	0.90	0.12	46,46,46,46	0
57	MG	2A	3526	1/1	0.90	0.12	71,71,71,71	0
57	MG	1A	3594	1/1	0.90	0.08	26,26,26,26	0
57	MG	1A	3795	1/1	0.90	0.13	38,38,38,38	0
57	MG	2A	3303	1/1	0.90	0.18	64,64,64,64	0
57	MG	2A	3761	1/1	0.90	0.16	48,48,48,48	0
57	MG	2A	3089	1/1	0.90	0.12	47,47,47,47	0
57	MG	1A	3796	1/1	0.90	0.18	43,43,43,43	0
57	MG	1A	3885	1/1	0.90	0.28	42,42,42,42	0
57	MG	2A	3313	1/1	0.90	0.39	70,70,70,70	0
57	MG	1A	3799	1/1	0.90	0.10	42,42,42,42	0
57	MG	1a	1629	1/1	0.90	0.43	77,77,77,77	0
57	MG	2A	3557	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	3889	1/1	0.90	0.13	35,35,35,35	0
57	MG	1a	1753	1/1	0.90	0.11	81,81,81,81	0
57	MG	2A	3567	1/1	0.90	0.23	55,55,55,55	0
57	MG	1A	3710	1/1	0.90	0.10	53,53,53,53	0
57	MG	2A	3794	1/1	0.90	0.09	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3278	1/1	0.90	0.13	50,50,50,50	0
57	MG	1A	3287	1/1	0.90	0.10	53,53,53,53	0
57	MG	2A	3803	1/1	0.90	0.15	59,59,59,59	0
57	MG	2A	3114	1/1	0.90	0.15	73,73,73,73	0
57	MG	1A	3809	1/1	0.90	0.12	54,54,54,54	0
57	MG	1A	3289	1/1	0.90	0.31	60,60,60,60	0
57	MG	2a	1759	1/1	0.90	0.22	80,80,80,80	0
57	MG	1A	3165	1/1	0.90	0.23	63,63,63,63	0
57	MG	1B	209	1/1	0.90	0.36	67,67,67,67	0
57	MG	2a	1767	1/1	0.90	0.34	71,71,71,71	0
57	MG	1A	3724	1/1	0.90	0.12	46,46,46,46	0
57	MG	2a	1769	1/1	0.90	0.20	59,59,59,59	0
57	MG	1A	3175	1/1	0.90	0.14	40,40,40,40	0
57	MG	1A	3819	1/1	0.90	0.14	53,53,53,53	0
57	MG	1A	4006	1/1	0.90	0.09	61,61,61,61	0
57	MG	1A	3429	1/1	0.90	0.12	65,65,65,65	0
57	MG	1a	1778	1/1	0.90	0.15	75,75,75,75	0
57	MG	2A	3609	1/1	0.90	0.14	37,37,37,37	0
57	MG	1A	3430	1/1	0.90	0.21	59,59,59,59	0
57	MG	2a	1781	1/1	0.90	0.20	82,82,82,82	0
57	MG	2A	3176	1/1	0.90	0.23	58,58,58,58	0
57	MG	2A	3830	1/1	0.90	0.14	54,54,54,54	0
57	MG	1B	225	1/1	0.90	0.09	66,66,66,66	0
57	MG	2A	3617	1/1	0.90	0.11	57,57,57,57	0
57	MG	1B	229	1/1	0.90	0.09	61,61,61,61	0
57	MG	2l	201	1/1	0.90	0.14	65,65,65,65	0
57	MG	1A	3825	1/1	0.90	0.10	66,66,66,66	0
57	MG	2A	3369	1/1	0.90	0.23	50,50,50,50	0
57	MG	2A	3192	1/1	0.90	0.23	71,71,71,71	0
57	MG	1A	3737	1/1	0.90	0.11	43,43,43,43	0
57	MG	2A	3200	1/1	0.90	0.27	66,66,66,66	0
57	MG	2x	103	1/1	0.90	0.12	68,68,68,68	0
57	MG	2x	104	1/1	0.90	0.15	69,69,69,69	0
57	MG	2A	3375	1/1	0.90	0.12	73,73,73,73	0
58	K	1A	3543	1/1	0.90	0.12	81,81,81,81	0
57	MG	1A	3557	1/1	0.91	0.11	40,40,40,40	0
57	MG	1A	3831	1/1	0.91	0.20	35,35,35,35	0
57	MG	2A	3831	1/1	0.91	0.12	39,39,39,39	0
57	MG	2A	3832	1/1	0.91	0.21	56,56,56,56	0
57	MG	1a	1673	1/1	0.91	0.19	64,64,64,64	0
57	MG	1a	1674	1/1	0.91	0.16	77,77,77,77	0
57	MG	1A	3284	1/1	0.91	0.15	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3712	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3284	1/1	0.91	0.26	66,66,66,66	0
57	MG	1a	1677	1/1	0.91	0.22	64,64,64,64	0
57	MG	1A	3567	1/1	0.91	0.20	77,77,77,77	0
57	MG	1A	3973	1/1	0.91	0.14	59,59,59,59	0
57	MG	2A	3005	1/1	0.91	0.24	60,60,60,60	0
57	MG	1A	3432	1/1	0.91	0.13	65,65,65,65	0
57	MG	2A	3850	1/1	0.91	0.10	72,72,72,72	0
57	MG	1A	3285	1/1	0.91	0.33	66,66,66,66	0
57	MG	2A	3300	1/1	0.91	0.26	65,65,65,65	0
57	MG	1A	3440	1/1	0.91	0.21	59,59,59,59	0
57	MG	2A	3302	1/1	0.91	0.36	70,70,70,70	0
57	MG	1A	3725	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3026	1/1	0.91	0.14	64,64,64,64	0
57	MG	2B	206	1/1	0.91	0.24	75,75,75,75	0
57	MG	2B	208	1/1	0.91	0.20	63,63,63,63	0
57	MG	2A	3027	1/1	0.91	0.20	56,56,56,56	0
57	MG	2A	3028	1/1	0.91	0.10	58,58,58,58	0
57	MG	2B	211	1/1	0.91	0.22	68,68,68,68	0
57	MG	1A	3728	1/1	0.91	0.17	61,61,61,61	0
57	MG	2A	3317	1/1	0.91	0.11	69,69,69,69	0
57	MG	1a	1690	1/1	0.91	0.31	57,57,57,57	0
57	MG	1A	3731	1/1	0.91	0.09	17,17,17,17	0
57	MG	2A	3043	1/1	0.91	0.08	60,60,60,60	0
57	MG	2A	3615	1/1	0.91	0.09	66,66,66,66	0
57	MG	2A	3044	1/1	0.91	0.35	62,62,62,62	0
57	MG	1A	3580	1/1	0.91	0.07	30,30,30,30	0
57	MG	2A	3048	1/1	0.91	0.10	54,54,54,54	0
57	MG	2E	305	1/1	0.91	0.10	36,36,36,36	0
57	MG	1A	3054	1/1	0.91	0.08	32,32,32,32	0
57	MG	2F	302	1/1	0.91	0.20	44,44,44,44	0
57	MG	2A	3055	1/1	0.91	0.14	53,53,53,53	0
57	MG	2A	3629	1/1	0.91	0.12	76,76,76,76	0
57	MG	2A	3056	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3057	1/1	0.91	0.47	59,59,59,59	0
57	MG	1A	3872	1/1	0.91	0.11	68,68,68,68	0
57	MG	1A	3354	1/1	0.91	0.18	53,53,53,53	0
57	MG	2U	201	1/1	0.91	0.16	59,59,59,59	0
57	MG	1A	3589	1/1	0.91	0.14	18,18,18,18	0
57	MG	1a	1709	1/1	0.91	0.14	69,69,69,69	0
57	MG	2A	3078	1/1	0.91	0.17	62,62,62,62	0
57	MG	1A	3452	1/1	0.91	0.27	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3351	1/1	0.91	0.24	68,68,68,68	0
57	MG	2a	1602	1/1	0.91	0.22	64,64,64,64	0
57	MG	1a	1712	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3879	1/1	0.91	0.08	43,43,43,43	0
57	MG	1F	316	1/1	0.91	0.15	47,47,47,47	0
57	MG	1A	3151	1/1	0.91	0.30	44,44,44,44	0
57	MG	2A	3649	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3160	1/1	0.91	0.13	61,61,61,61	0
57	MG	2A	3363	1/1	0.91	0.10	63,63,63,63	0
57	MG	2a	1618	1/1	0.91	0.30	65,65,65,65	0
57	MG	1I	201	1/1	0.91	0.12	68,68,68,68	0
57	MG	1A	3299	1/1	0.91	0.22	54,54,54,54	0
57	MG	2A	3368	1/1	0.91	0.12	64,64,64,64	0
57	MG	1A	3314	1/1	0.91	0.12	57,57,57,57	0
57	MG	1Q	204	1/1	0.91	0.08	52,52,52,52	0
57	MG	2A	3106	1/1	0.91	0.29	60,60,60,60	0
57	MG	1A	3890	1/1	0.91	0.29	37,37,37,37	0
57	MG	2A	3108	1/1	0.91	0.32	66,66,66,66	0
57	MG	1A	4017	1/1	0.91	0.15	54,54,54,54	0
57	MG	1A	3469	1/1	0.91	0.33	67,67,67,67	0
57	MG	1A	3614	1/1	0.91	0.15	64,64,64,64	0
57	MG	2A	3671	1/1	0.91	0.11	57,57,57,57	0
57	MG	2a	1640	1/1	0.91	0.32	70,70,70,70	0
57	MG	2A	3116	1/1	0.91	0.32	69,69,69,69	0
57	MG	1A	3474	1/1	0.91	0.10	63,63,63,63	0
57	MG	1Z	301	1/1	0.91	0.09	62,62,62,62	0
57	MG	2A	3385	1/1	0.91	0.33	61,61,61,61	0
57	MG	1A	4027	1/1	0.91	0.09	47,47,47,47	0
57	MG	2a	1649	1/1	0.91	0.16	59,59,59,59	0
57	MG	1A	3623	1/1	0.91	0.18	49,49,49,49	0
57	MG	2a	1656	1/1	0.91	0.26	58,58,58,58	0
57	MG	1A	3220	1/1	0.91	0.20	61,61,61,61	0
57	MG	2A	3142	1/1	0.91	0.25	65,65,65,65	0
57	MG	2A	3394	1/1	0.91	0.23	42,42,42,42	0
57	MG	1A	3240	1/1	0.91	0.33	40,40,40,40	0
57	MG	2a	1669	1/1	0.91	0.29	60,60,60,60	0
57	MG	2A	3144	1/1	0.91	0.15	66,66,66,66	0
57	MG	1A	3491	1/1	0.91	0.12	68,68,68,68	0
57	MG	1A	3784	1/1	0.91	0.13	47,47,47,47	0
57	MG	19	101	1/1	0.91	0.14	54,54,54,54	0
57	MG	2A	3410	1/1	0.91	0.20	64,64,64,64	0
57	MG	1A	4036	1/1	0.91	0.09	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3791	1/1	0.91	0.08	33,33,33,33	0
57	MG	1a	1603	1/1	0.91	0.16	71,71,71,71	0
57	MG	1A	3392	1/1	0.91	0.20	65,65,65,65	0
57	MG	2A	3185	1/1	0.91	0.12	71,71,71,71	0
57	MG	2A	3188	1/1	0.91	0.18	62,62,62,62	0
57	MG	2a	1687	1/1	0.91	0.26	67,67,67,67	0
57	MG	1A	3642	1/1	0.91	0.09	52,52,52,52	0
57	MG	1A	3651	1/1	0.91	0.15	57,57,57,57	0
57	MG	1A	3503	1/1	0.91	0.11	71,71,71,71	0
57	MG	1A	3931	1/1	0.91	0.10	55,55,55,55	0
57	MG	2A	3194	1/1	0.91	0.23	60,60,60,60	0
57	MG	1A	4053	1/1	0.91	0.10	42,42,42,42	0
57	MG	1A	3319	1/1	0.91	0.15	50,50,50,50	0
57	MG	2a	1700	1/1	0.91	0.21	63,63,63,63	0
57	MG	2a	1701	1/1	0.91	0.32	71,71,71,71	0
57	MG	1a	1770	1/1	0.91	0.15	73,73,73,73	0
57	MG	1A	3161	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3204	1/1	0.91	0.15	69,69,69,69	0
57	MG	2A	3209	1/1	0.91	0.08	65,65,65,65	0
57	MG	2a	1716	1/1	0.91	0.21	52,52,52,52	0
57	MG	2A	3735	1/1	0.91	0.17	59,59,59,59	0
57	MG	2a	1719	1/1	0.91	0.14	49,49,49,49	0
57	MG	1A	3245	1/1	0.91	0.12	58,58,58,58	0
57	MG	2A	3463	1/1	0.91	0.14	45,45,45,45	0
57	MG	2A	3216	1/1	0.91	0.17	57,57,57,57	0
57	MG	1A	3411	1/1	0.91	0.12	58,58,58,58	0
57	MG	2a	1727	1/1	0.91	0.21	65,65,65,65	0
57	MG	2a	1730	1/1	0.91	0.23	61,61,61,61	0
57	MG	1A	4066	1/1	0.91	0.12	56,56,56,56	0
57	MG	2A	3747	1/1	0.91	0.12	54,54,54,54	0
57	MG	2A	3750	1/1	0.91	0.13	75,75,75,75	0
57	MG	2a	1735	1/1	0.91	0.23	80,80,80,80	0
57	MG	2a	1736	1/1	0.91	0.20	56,56,56,56	0
57	MG	1a	1631	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3945	1/1	0.91	0.16	59,59,59,59	0
57	MG	2A	3754	1/1	0.91	0.19	71,71,71,71	0
57	MG	1A	4072	1/1	0.91	0.10	47,47,47,47	0
57	MG	1A	3682	1/1	0.91	0.14	60,60,60,60	0
57	MG	1a	1641	1/1	0.91	0.19	70,70,70,70	0
57	MG	1A	3053	1/1	0.91	0.11	52,52,52,52	0
57	MG	2A	3243	1/1	0.91	0.16	63,63,63,63	0
57	MG	1a	1791	1/1	0.91	0.09	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
57	MG	2a	1753	1/1	0.91	0.18	68,68,68,68	0
57	MG	2A	3763	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3485	1/1	0.91	0.09	33,33,33,33	0
57	MG	1A	3812	1/1	0.91	0.07	46,46,46,46	0
57	MG	2A	3492	1/1	0.91	0.15	57,57,57,57	0
57	MG	1A	4080	1/1	0.91	0.17	58,58,58,58	0
57	MG	2a	1761	1/1	0.91	0.26	67,67,67,67	0
57	MG	2A	3774	1/1	0.91	0.09	66,66,66,66	0
57	MG	2a	1765	1/1	0.91	0.28	68,68,68,68	0
57	MG	2a	1766	1/1	0.91	0.25	66,66,66,66	0
57	MG	2A	3495	1/1	0.91	0.13	54,54,54,54	0
57	MG	2A	3248	1/1	0.91	0.12	64,64,64,64	0
57	MG	1A	4081	1/1	0.91	0.17	50,50,50,50	0
57	MG	1A	3685	1/1	0.91	0.09	63,63,63,63	0
57	MG	1A	3254	1/1	0.91	0.27	57,57,57,57	0
57	MG	1A	3688	1/1	0.91	0.18	74,74,74,74	0
57	MG	1A	3528	1/1	0.91	0.09	56,56,56,56	0
57	MG	1A	3098	1/1	0.91	0.12	55,55,55,55	0
57	MG	2a	1778	1/1	0.91	0.24	62,62,62,62	0
57	MG	1A	3705	1/1	0.91	0.20	82,82,82,82	0
57	MG	1a	1809	1/1	0.91	0.16	76,76,76,76	0
57	MG	1A	3099	1/1	0.91	0.21	72,72,72,72	0
57	MG	2A	3525	1/1	0.91	0.19	52,52,52,52	0
57	MG	1a	1813	1/1	0.91	0.12	77,77,77,77	0
57	MG	2A	3527	1/1	0.91	0.11	51,51,51,51	0
57	MG	2A	3528	1/1	0.91	0.16	43,43,43,43	0
57	MG	1A	4100	1/1	0.91	0.18	71,71,71,71	0
57	MG	2j	201	1/1	0.91	0.13	75,75,75,75	0
57	MG	2A	3530	1/1	0.91	0.10	41,41,41,41	0
57	MG	1A	3549	1/1	0.91	0.16	62,62,62,62	0
57	MG	2A	3268	1/1	0.91	0.33	72,72,72,72	0
57	MG	2A	3269	1/1	0.91	0.34	57,57,57,57	0
57	MG	2A	3819	1/1	0.91	0.09	62,62,62,62	0
57	MG	2A	3536	1/1	0.91	0.21	67,67,67,67	0
57	MG	2A	3821	1/1	0.91	0.25	65,65,65,65	0
57	MG	2A	3271	1/1	0.91	0.24	61,61,61,61	0
57	MG	1B	202	1/1	0.91	0.19	58,58,58,58	0
57	MG	2A	3553	1/1	0.91	0.13	70,70,70,70	0
57	MG	2A	3427	1/1	0.92	0.11	73,73,73,73	0
57	MG	1a	1702	1/1	0.92	0.18	63,63,63,63	0
57	MG	2A	3776	1/1	0.92	0.11	74,74,74,74	0
57	MG	2A	3778	1/1	0.92	0.08	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3429	1/1	0.92	0.15	60,60,60,60	0
57	MG	2A	3783	1/1	0.92	0.11	65,65,65,65	0
57	MG	1A	3464	1/1	0.92	0.16	43,43,43,43	0
57	MG	1A	3942	1/1	0.92	0.13	30,30,30,30	0
57	MG	1A	3612	1/1	0.92	0.08	17,17,17,17	0
57	MG	2A	3436	1/1	0.92	0.13	62,62,62,62	0
57	MG	1B	220	1/1	0.92	0.12	60,60,60,60	0
57	MG	2A	3150	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3151	1/1	0.92	0.15	67,67,67,67	0
57	MG	2A	3442	1/1	0.92	0.16	62,62,62,62	0
57	MG	1A	3775	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3802	1/1	0.92	0.18	66,66,66,66	0
57	MG	1A	3237	1/1	0.92	0.18	60,60,60,60	0
57	MG	2A	3448	1/1	0.92	0.25	66,66,66,66	0
57	MG	2A	3161	1/1	0.92	0.16	71,71,71,71	0
57	MG	2A	3807	1/1	0.92	0.24	57,57,57,57	0
57	MG	2A	3454	1/1	0.92	0.18	66,66,66,66	0
57	MG	2A	3163	1/1	0.92	0.19	60,60,60,60	0
57	MG	2A	3811	1/1	0.92	0.11	67,67,67,67	0
57	MG	2A	3466	1/1	0.92	0.10	44,44,44,44	0
57	MG	1a	1715	1/1	0.92	0.09	54,54,54,54	0
57	MG	1A	3358	1/1	0.92	0.18	48,48,48,48	0
57	MG	1A	3129	1/1	0.92	0.26	40,40,40,40	0
57	MG	1A	3786	1/1	0.92	0.20	52,52,52,52	0
57	MG	1a	1719	1/1	0.92	0.44	73,73,73,73	0
57	MG	2A	3182	1/1	0.92	0.11	59,59,59,59	0
57	MG	1A	3788	1/1	0.92	0.15	32,32,32,32	0
57	MG	1B	233	1/1	0.92	0.16	72,72,72,72	0
57	MG	2A	3823	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3472	1/1	0.92	0.15	63,63,63,63	0
57	MG	1A	3627	1/1	0.92	0.13	50,50,50,50	0
57	MG	2A	3191	1/1	0.92	0.17	55,55,55,55	0
57	MG	1A	3311	1/1	0.92	0.13	66,66,66,66	0
57	MG	1A	3480	1/1	0.92	0.09	66,66,66,66	0
57	MG	2A	3491	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	3798	1/1	0.92	0.11	36,36,36,36	0
57	MG	2A	3196	1/1	0.92	0.09	57,57,57,57	0
57	MG	1A	3631	1/1	0.92	0.07	31,31,31,31	0
57	MG	2A	3497	1/1	0.92	0.10	62,62,62,62	0
57	MG	1F	306	1/1	0.92	0.17	63,63,63,63	0
57	MG	1F	307	1/1	0.92	0.13	63,63,63,63	0
57	MG	1a	1732	1/1	0.92	0.13	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
57	MG	1A	3374	1/1	0.92	0.08	45,45,45,45	0
57	MG	2A	3506	1/1	0.92	0.16	57,57,57,57	0
57	MG	2A	3207	1/1	0.92	0.15	62,62,62,62	0
57	MG	2A	3508	1/1	0.92	0.17	52,52,52,52	0
57	MG	2A	3208	1/1	0.92	0.13	63,63,63,63	0
57	MG	1A	3635	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3211	1/1	0.92	0.28	64,64,64,64	0
57	MG	1A	3970	1/1	0.92	0.23	75,75,75,75	0
57	MG	1A	3486	1/1	0.92	0.10	52,52,52,52	0
57	MG	1G	203	1/1	0.92	0.09	70,70,70,70	0
57	MG	2A	3227	1/1	0.92	0.26	68,68,68,68	0
57	MG	2B	207	1/1	0.92	0.11	64,64,64,64	0
57	MG	1G	204	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	3241	1/1	0.92	0.20	55,55,55,55	0
57	MG	1A	3490	1/1	0.92	0.23	61,61,61,61	0
57	MG	1O	202	1/1	0.92	0.23	72,72,72,72	0
57	MG	1A	3377	1/1	0.92	0.12	54,54,54,54	0
57	MG	2B	213	1/1	0.92	0.15	62,62,62,62	0
57	MG	1A	3658	1/1	0.92	0.14	59,59,59,59	0
57	MG	1P	203	1/1	0.92	0.22	39,39,39,39	0
57	MG	1Q	201	1/1	0.92	0.36	43,43,43,43	0
57	MG	1a	1760	1/1	0.92	0.15	68,68,68,68	0
57	MG	2A	3540	1/1	0.92	0.17	59,59,59,59	0
57	MG	2A	3544	1/1	0.92	0.09	48,48,48,48	0
57	MG	1A	3166	1/1	0.92	0.24	40,40,40,40	0
57	MG	2A	3552	1/1	0.92	0.24	61,61,61,61	0
57	MG	1A	3663	1/1	0.92	0.10	28,28,28,28	0
57	MG	1A	3316	1/1	0.92	0.20	61,61,61,61	0
57	MG	1T	201	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	3820	1/1	0.92	0.13	51,51,51,51	0
57	MG	2A	3252	1/1	0.92	0.12	51,51,51,51	0
57	MG	2O	201	1/1	0.92	0.12	68,68,68,68	0
57	MG	1A	3981	1/1	0.92	0.10	36,36,36,36	0
57	MG	2P	202	1/1	0.92	0.14	58,58,58,58	0
57	MG	1V	204	1/1	0.92	0.18	55,55,55,55	0
57	MG	1V	207	1/1	0.92	0.08	70,70,70,70	0
57	MG	2A	3570	1/1	0.92	0.16	56,56,56,56	0
57	MG	1A	3060	1/1	0.92	0.12	45,45,45,45	0
57	MG	2U	202	1/1	0.92	0.20	61,61,61,61	0
57	MG	1A	3318	1/1	0.92	0.16	47,47,47,47	0
57	MG	1A	3177	1/1	0.92	0.18	50,50,50,50	0
57	MG	1A	3398	1/1	0.92	0.20	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
57	MG	23	101	1/1	0.92	0.14	61,61,61,61	0
57	MG	2A	3577	1/1	0.92	0.17	64,64,64,64	0
57	MG	25	107	1/1	0.92	0.10	58,58,58,58	0
57	MG	28	102	1/1	0.92	0.20	60,60,60,60	0
57	MG	1A	3684	1/1	0.92	0.11	53,53,53,53	0
57	MG	29	101	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3264	1/1	0.92	0.11	58,58,58,58	0
57	MG	1A	3516	1/1	0.92	0.12	70,70,70,70	0
57	MG	15	103	1/1	0.92	0.14	40,40,40,40	0
57	MG	2A	3584	1/1	0.92	0.08	40,40,40,40	0
57	MG	15	108	1/1	0.92	0.15	51,51,51,51	0
57	MG	2a	1612	1/1	0.92	0.15	61,61,61,61	0
57	MG	1a	1792	1/1	0.92	0.07	65,65,65,65	0
57	MG	1A	3522	1/1	0.92	0.07	56,56,56,56	0
57	MG	2A	3273	1/1	0.92	0.10	68,68,68,68	0
57	MG	2A	3597	1/1	0.92	0.09	39,39,39,39	0
57	MG	1a	1795	1/1	0.92	0.07	62,62,62,62	0
57	MG	2a	1620	1/1	0.92	0.20	53,53,53,53	0
57	MG	2a	1622	1/1	0.92	0.15	70,70,70,70	0
57	MG	17	103	1/1	0.92	0.17	43,43,43,43	0
57	MG	2A	3602	1/1	0.92	0.13	56,56,56,56	0
57	MG	2A	3605	1/1	0.92	0.19	46,46,46,46	0
57	MG	2A	3276	1/1	0.92	0.13	72,72,72,72	0
57	MG	1A	3832	1/1	0.92	0.14	55,55,55,55	0
57	MG	1A	3833	1/1	0.92	0.09	50,50,50,50	0
57	MG	2a	1631	1/1	0.92	0.26	72,72,72,72	0
57	MG	1A	4010	1/1	0.92	0.09	63,63,63,63	0
57	MG	2A	3614	1/1	0.92	0.12	51,51,51,51	0
57	MG	1A	3320	1/1	0.92	0.28	65,65,65,65	0
57	MG	1A	3407	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3618	1/1	0.92	0.19	70,70,70,70	0
57	MG	1a	1604	1/1	0.92	0.09	60,60,60,60	0
57	MG	1A	3693	1/1	0.92	0.10	42,42,42,42	0
57	MG	1A	3695	1/1	0.92	0.14	65,65,65,65	0
57	MG	1A	3140	1/1	0.92	0.12	55,55,55,55	0
57	MG	1A	3702	1/1	0.92	0.11	43,43,43,43	0
57	MG	2A	3630	1/1	0.92	0.21	55,55,55,55	0
57	MG	1A	3529	1/1	0.92	0.18	60,60,60,60	0
57	MG	2a	1650	1/1	0.92	0.24	61,61,61,61	0
57	MG	1e	202	1/1	0.92	0.11	73,73,73,73	0
57	MG	2A	3299	1/1	0.92	0.13	64,64,64,64	0
57	MG	1f	201	1/1	0.92	0.23	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
57	MG	1A	3853	1/1	0.92	0.09	47,47,47,47	0
57	MG	1A	3256	1/1	0.92	0.15	52,52,52,52	0
57	MG	1A	3537	1/1	0.92	0.24	50,50,50,50	0
57	MG	1A	3858	1/1	0.92	0.11	32,32,32,32	0
57	MG	1v	104	1/1	0.92	0.14	60,60,60,60	0
57	MG	1A	3324	1/1	0.92	0.30	55,55,55,55	0
57	MG	1A	3190	1/1	0.92	0.20	37,37,37,37	0
57	MG	1a	1630	1/1	0.92	0.29	69,69,69,69	0
57	MG	1A	3553	1/1	0.92	0.32	39,39,39,39	0
57	MG	1A	3330	1/1	0.92	0.13	45,45,45,45	0
57	MG	1A	3146	1/1	0.92	0.10	37,37,37,37	0
57	MG	1a	1639	1/1	0.92	0.27	72,72,72,72	0
57	MG	2A	3004	1/1	0.92	0.16	54,54,54,54	0
57	MG	2A	3326	1/1	0.92	0.17	69,69,69,69	0
57	MG	1A	3564	1/1	0.92	0.13	48,48,48,48	0
57	MG	2A	3007	1/1	0.92	0.20	53,53,53,53	0
57	MG	1A	3723	1/1	0.92	0.07	38,38,38,38	0
57	MG	2a	1690	1/1	0.92	0.16	70,70,70,70	0
57	MG	1A	3565	1/1	0.92	0.13	38,38,38,38	0
57	MG	2A	3335	1/1	0.92	0.20	59,59,59,59	0
57	MG	2a	1693	1/1	0.92	0.50	72,72,72,72	0
57	MG	1a	1643	1/1	0.92	0.30	79,79,79,79	0
57	MG	1a	1645	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3150	1/1	0.92	0.08	42,42,42,42	0
57	MG	2A	3669	1/1	0.92	0.13	60,60,60,60	0
57	MG	1A	3436	1/1	0.92	0.24	60,60,60,60	0
57	MG	1A	3336	1/1	0.92	0.25	67,67,67,67	0
57	MG	2a	1704	1/1	0.92	0.16	60,60,60,60	0
57	MG	1a	1651	1/1	0.92	0.20	59,59,59,59	0
57	MG	2A	3674	1/1	0.92	0.09	68,68,68,68	0
57	MG	2A	3349	1/1	0.92	0.15	49,49,49,49	0
57	MG	1A	4054	1/1	0.92	0.11	51,51,51,51	0
57	MG	1A	3201	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3578	1/1	0.92	0.10	34,34,34,34	0
57	MG	2A	3684	1/1	0.92	0.19	56,56,56,56	0
57	MG	2A	3353	1/1	0.92	0.14	61,61,61,61	0
57	MG	1A	3735	1/1	0.92	0.11	37,37,37,37	0
57	MG	2a	1723	1/1	0.92	0.15	63,63,63,63	0
57	MG	1A	3286	1/1	0.92	0.15	54,54,54,54	0
57	MG	2A	3690	1/1	0.92	0.14	43,43,43,43	0
57	MG	2A	3359	1/1	0.92	0.19	55,55,55,55	0
57	MG	1A	3581	1/1	0.92	0.12	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3112	1/1	0.92	0.20	50,50,50,50	0
57	MG	2A	3053	1/1	0.92	0.14	66,66,66,66	0
57	MG	1A	4070	1/1	0.92	0.12	34,34,34,34	0
57	MG	1A	3446	1/1	0.92	0.19	59,59,59,59	0
57	MG	1A	3114	1/1	0.92	0.25	37,37,37,37	0
57	MG	1A	3902	1/1	0.92	0.11	58,58,58,58	0
57	MG	2a	1740	1/1	0.92	0.12	64,64,64,64	0
57	MG	2A	3705	1/1	0.92	0.10	52,52,52,52	0
57	MG	2A	3706	1/1	0.92	0.08	75,75,75,75	0
57	MG	2a	1743	1/1	0.92	0.20	60,60,60,60	0
57	MG	1a	1669	1/1	0.92	0.13	79,79,79,79	0
57	MG	2A	3371	1/1	0.92	0.20	55,55,55,55	0
57	MG	1a	1671	1/1	0.92	0.25	66,66,66,66	0
57	MG	2A	3062	1/1	0.92	0.15	57,57,57,57	0
57	MG	2A	3712	1/1	0.92	0.09	68,68,68,68	0
57	MG	1A	3903	1/1	0.92	0.11	29,29,29,29	0
57	MG	1A	3450	1/1	0.92	0.26	65,65,65,65	0
57	MG	1A	3907	1/1	0.92	0.09	48,48,48,48	0
57	MG	1A	3351	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3093	1/1	0.92	0.16	42,42,42,42	0
57	MG	1A	3752	1/1	0.92	0.11	47,47,47,47	0
57	MG	2A	3381	1/1	0.92	0.17	63,63,63,63	0
57	MG	2A	3090	1/1	0.92	0.16	65,65,65,65	0
57	MG	1A	3456	1/1	0.92	0.19	53,53,53,53	0
57	MG	2a	1763	1/1	0.92	0.23	59,59,59,59	0
57	MG	2a	1764	1/1	0.92	0.23	64,64,64,64	0
57	MG	1A	3758	1/1	0.92	0.07	34,34,34,34	0
57	MG	2A	3730	1/1	0.92	0.16	59,59,59,59	0
57	MG	2A	3731	1/1	0.92	0.09	49,49,49,49	0
57	MG	2A	3387	1/1	0.92	0.22	53,53,53,53	0
57	MG	1A	3928	1/1	0.92	0.10	66,66,66,66	0
57	MG	1A	3759	1/1	0.92	0.08	52,52,52,52	0
57	MG	2A	3098	1/1	0.92	0.08	54,54,54,54	0
57	MG	2A	3737	1/1	0.92	0.17	67,67,67,67	0
57	MG	2A	3101	1/1	0.92	0.21	68,68,68,68	0
57	MG	1A	4096	1/1	0.92	0.17	46,46,46,46	0
57	MG	2A	3397	1/1	0.92	0.52	64,64,64,64	0
57	MG	2A	3743	1/1	0.92	0.09	51,51,51,51	0
57	MG	2A	3398	1/1	0.92	0.27	64,64,64,64	0
57	MG	1A	3761	1/1	0.92	0.06	36,36,36,36	0
57	MG	1A	3932	1/1	0.92	0.11	53,53,53,53	0
57	MG	2A	3403	1/1	0.92	0.23	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
57	MG	1B	201	1/1	0.92	0.12	54,54,54,54	0
57	MG	1a	1691	1/1	0.92	0.11	53,53,53,53	0
57	MG	1A	3601	1/1	0.92	0.07	38,38,38,38	0
57	MG	1A	3936	1/1	0.92	0.07	42,42,42,42	0
57	MG	1a	1697	1/1	0.92	0.16	58,58,58,58	0
57	MG	1A	3291	1/1	0.92	0.23	41,41,41,41	0
57	MG	2q	201	1/1	0.92	0.09	71,71,71,71	0
57	MG	1a	1699	1/1	0.92	0.23	61,61,61,61	0
57	MG	1A	3769	1/1	0.92	0.13	25,25,25,25	0
57	MG	2A	3762	1/1	0.92	0.14	72,72,72,72	0
57	MG	1B	212	1/1	0.92	0.18	50,50,50,50	0
57	MG	2A	3134	1/1	0.92	0.17	48,48,48,48	0
57	MG	2A	3138	1/1	0.92	0.20	48,48,48,48	0
57	MG	2A	3426	1/1	0.92	0.32	54,54,54,54	0
57	MG	2A	3770	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3863	1/1	0.93	0.07	34,34,34,34	0
57	MG	2A	3088	1/1	0.93	0.11	48,48,48,48	0
57	MG	1A	3163	1/1	0.93	0.08	34,34,34,34	0
57	MG	2A	3340	1/1	0.93	0.13	60,60,60,60	0
57	MG	1A	3617	1/1	0.93	0.10	31,31,31,31	0
57	MG	1A	3618	1/1	0.93	0.06	30,30,30,30	0
57	MG	1A	3325	1/1	0.93	0.25	71,71,71,71	0
57	MG	2A	3345	1/1	0.93	0.16	55,55,55,55	0
57	MG	1A	3280	1/1	0.93	0.12	49,49,49,49	0
57	MG	2A	3613	1/1	0.93	0.09	41,41,41,41	0
57	MG	1A	3624	1/1	0.93	0.20	52,52,52,52	0
57	MG	1A	3746	1/1	0.93	0.09	29,29,29,29	0
57	MG	1A	3747	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	4023	1/1	0.93	0.14	65,65,65,65	0
57	MG	1R	204	1/1	0.93	0.18	40,40,40,40	0
57	MG	2B	214	1/1	0.93	0.23	59,59,59,59	0
57	MG	2B	215	1/1	0.93	0.14	74,74,74,74	0
57	MG	1A	4024	1/1	0.93	0.10	68,68,68,68	0
57	MG	2A	3625	1/1	0.93	0.18	66,66,66,66	0
57	MG	1A	3881	1/1	0.93	0.11	55,55,55,55	0
57	MG	1A	3502	1/1	0.93	0.08	54,54,54,54	0
57	MG	1A	3283	1/1	0.93	0.06	36,36,36,36	0
57	MG	2A	3360	1/1	0.93	0.24	66,66,66,66	0
57	MG	1A	3413	1/1	0.93	0.13	46,46,46,46	0
57	MG	1A	3415	1/1	0.93	0.10	53,53,53,53	0
57	MG	1Y	201	1/1	0.93	0.19	58,58,58,58	0
57	MG	2E	307	1/1	0.93	0.18	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3633	1/1	0.93	0.06	22,22,22,22	0
57	MG	2A	3635	1/1	0.93	0.09	41,41,41,41	0
57	MG	1A	3202	1/1	0.93	0.20	38,38,38,38	0
57	MG	1A	3059	1/1	0.93	0.17	45,45,45,45	0
57	MG	2A	3125	1/1	0.93	0.13	54,54,54,54	0
57	MG	2A	3131	1/1	0.93	0.18	68,68,68,68	0
57	MG	1A	3636	1/1	0.93	0.09	42,42,42,42	0
57	MG	2Q	203	1/1	0.93	0.09	62,62,62,62	0
57	MG	2A	3136	1/1	0.93	0.16	66,66,66,66	0
57	MG	1A	3764	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3515	1/1	0.93	0.13	41,41,41,41	0
57	MG	2T	203	1/1	0.93	0.21	56,56,56,56	0
57	MG	1A	3897	1/1	0.93	0.14	64,64,64,64	0
57	MG	1A	3418	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3649	1/1	0.93	0.10	30,30,30,30	0
57	MG	1A	4048	1/1	0.93	0.07	63,63,63,63	0
57	MG	1A	3771	1/1	0.93	0.07	41,41,41,41	0
57	MG	2I	102	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3419	1/1	0.93	0.10	68,68,68,68	0
57	MG	2A	3153	1/1	0.93	0.16	56,56,56,56	0
57	MG	25	101	1/1	0.93	0.32	62,62,62,62	0
57	MG	25	105	1/1	0.93	0.14	55,55,55,55	0
57	MG	25	106	1/1	0.93	0.13	55,55,55,55	0
57	MG	1a	1757	1/1	0.93	0.15	69,69,69,69	0
57	MG	28	101	1/1	0.93	0.19	55,55,55,55	0
57	MG	1A	3654	1/1	0.93	0.11	70,70,70,70	0
57	MG	1A	3776	1/1	0.93	0.06	26,26,26,26	0
57	MG	2A	3389	1/1	0.93	0.29	46,46,46,46	0
57	MG	2A	3162	1/1	0.93	0.13	67,67,67,67	0
57	MG	2a	1603	1/1	0.93	0.09	67,67,67,67	0
57	MG	2a	1604	1/1	0.93	0.35	63,63,63,63	0
57	MG	1A	3915	1/1	0.93	0.10	61,61,61,61	0
57	MG	1A	3917	1/1	0.93	0.14	58,58,58,58	0
57	MG	2a	1608	1/1	0.93	0.08	61,61,61,61	0
57	MG	2A	3667	1/1	0.93	0.13	61,61,61,61	0
57	MG	2A	3165	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3422	1/1	0.93	0.13	47,47,47,47	0
57	MG	2A	3167	1/1	0.93	0.11	61,61,61,61	0
57	MG	1a	1606	1/1	0.93	0.37	76,76,76,76	0
57	MG	1a	1608	1/1	0.93	0.28	67,67,67,67	0
57	MG	2A	3177	1/1	0.93	0.15	61,61,61,61	0
57	MG	1A	3048	1/1	0.93	0.22	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
57	MG	2A	3677	1/1	0.93	0.18	55,55,55,55	0
57	MG	2a	1621	1/1	0.93	0.29	62,62,62,62	0
57	MG	2A	3681	1/1	0.93	0.12	44,44,44,44	0
57	MG	2A	3181	1/1	0.93	0.20	67,67,67,67	0
57	MG	1A	3219	1/1	0.93	0.20	44,44,44,44	0
57	MG	2A	3409	1/1	0.93	0.12	53,53,53,53	0
57	MG	1A	3026	1/1	0.93	0.16	71,71,71,71	0
57	MG	1a	1618	1/1	0.93	0.16	58,58,58,58	0
57	MG	2A	3688	1/1	0.93	0.07	64,64,64,64	0
57	MG	1A	3666	1/1	0.93	0.10	25,25,25,25	0
57	MG	1A	3433	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	4074	1/1	0.93	0.19	57,57,57,57	0
57	MG	1A	4076	1/1	0.93	0.10	47,47,47,47	0
57	MG	1a	1780	1/1	0.93	0.11	66,66,66,66	0
57	MG	1A	3675	1/1	0.93	0.06	16,16,16,16	0
57	MG	2a	1639	1/1	0.93	0.37	69,69,69,69	0
57	MG	2A	3422	1/1	0.93	0.31	59,59,59,59	0
57	MG	1a	1782	1/1	0.93	0.14	50,50,50,50	0
57	MG	2A	3699	1/1	0.93	0.14	64,64,64,64	0
57	MG	2A	3197	1/1	0.93	0.10	58,58,58,58	0
57	MG	2A	3198	1/1	0.93	0.19	64,64,64,64	0
57	MG	2a	1647	1/1	0.93	0.29	65,65,65,65	0
57	MG	2A	3703	1/1	0.93	0.12	54,54,54,54	0
57	MG	1a	1783	1/1	0.93	0.12	52,52,52,52	0
57	MG	1a	1784	1/1	0.93	0.12	76,76,76,76	0
57	MG	1A	4078	1/1	0.93	0.12	64,64,64,64	0
57	MG	2a	1655	1/1	0.93	0.32	64,64,64,64	0
57	MG	1A	3677	1/1	0.93	0.07	35,35,35,35	0
57	MG	2a	1657	1/1	0.93	0.19	75,75,75,75	0
57	MG	1A	3227	1/1	0.93	0.10	61,61,61,61	0
57	MG	1A	3935	1/1	0.93	0.06	43,43,43,43	0
57	MG	1a	1634	1/1	0.93	0.25	82,82,82,82	0
57	MG	1A	3176	1/1	0.93	0.26	57,57,57,57	0
57	MG	1A	3542	1/1	0.93	0.22	54,54,54,54	0
57	MG	1a	1798	1/1	0.93	0.16	66,66,66,66	0
57	MG	1a	1638	1/1	0.93	0.27	62,62,62,62	0
57	MG	2A	3719	1/1	0.93	0.21	47,47,47,47	0
57	MG	1A	3292	1/1	0.93	0.23	48,48,48,48	0
57	MG	2a	1676	1/1	0.93	0.16	68,68,68,68	0
57	MG	2A	3447	1/1	0.93	0.17	63,63,63,63	0
57	MG	2A	3224	1/1	0.93	0.19	41,41,41,41	0
57	MG	1A	3296	1/1	0.93	0.16	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1680	1/1	0.93	0.27	57,57,57,57	0
57	MG	1A	3802	1/1	0.93	0.18	52,52,52,52	0
57	MG	2A	3461	1/1	0.93	0.23	65,65,65,65	0
57	MG	2A	3232	1/1	0.93	0.21	61,61,61,61	0
57	MG	1A	3016	1/1	0.93	0.30	51,51,51,51	0
57	MG	2a	1685	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3805	1/1	0.93	0.09	55,55,55,55	0
57	MG	1a	1644	1/1	0.93	0.25	61,61,61,61	0
57	MG	2A	3236	1/1	0.93	0.10	63,63,63,63	0
57	MG	1A	3445	1/1	0.93	0.12	39,39,39,39	0
57	MG	2A	3238	1/1	0.93	0.07	75,75,75,75	0
57	MG	1a	1811	1/1	0.93	0.18	65,65,65,65	0
57	MG	1A	4097	1/1	0.93	0.15	57,57,57,57	0
57	MG	1A	3178	1/1	0.93	0.08	62,62,62,62	0
57	MG	2A	3478	1/1	0.93	0.13	52,52,52,52	0
57	MG	1a	1814	1/1	0.93	0.10	88,88,88,88	0
57	MG	1b	301	1/1	0.93	0.08	76,76,76,76	0
57	MG	2A	3748	1/1	0.93	0.09	68,68,68,68	0
57	MG	1A	4101	1/1	0.93	0.11	55,55,55,55	0
57	MG	2a	1705	1/1	0.93	0.17	61,61,61,61	0
57	MG	2a	1707	1/1	0.93	0.16	71,71,71,71	0
57	MG	1e	201	1/1	0.93	0.15	53,53,53,53	0
57	MG	2A	3486	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3689	1/1	0.93	0.09	29,29,29,29	0
57	MG	1A	3300	1/1	0.93	0.11	56,56,56,56	0
57	MG	1A	3692	1/1	0.93	0.14	55,55,55,55	0
57	MG	1A	3361	1/1	0.93	0.10	47,47,47,47	0
57	MG	1B	205	1/1	0.93	0.21	71,71,71,71	0
57	MG	1v	101	1/1	0.93	0.23	64,64,64,64	0
57	MG	1B	206	1/1	0.93	0.07	44,44,44,44	0
57	MG	1B	208	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	3363	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3764	1/1	0.93	0.17	57,57,57,57	0
57	MG	1x	102	1/1	0.93	0.09	58,58,58,58	0
57	MG	1x	103	1/1	0.93	0.09	64,64,64,64	0
57	MG	1A	3696	1/1	0.93	0.07	47,47,47,47	0
57	MG	1B	211	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3310	1/1	0.93	0.19	35,35,35,35	0
57	MG	2A	3773	1/1	0.93	0.09	66,66,66,66	0
57	MG	1A	3963	1/1	0.93	0.08	52,52,52,52	0
57	MG	1A	3179	1/1	0.93	0.16	65,65,65,65	0
57	MG	1A	3088	1/1	0.93	0.11	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3516	1/1	0.93	0.09	49,49,49,49	0
57	MG	1A	3463	1/1	0.93	0.16	63,63,63,63	0
57	MG	2A	3519	1/1	0.93	0.11	42,42,42,42	0
57	MG	1A	3154	1/1	0.93	0.14	50,50,50,50	0
57	MG	2a	1745	1/1	0.93	0.10	53,53,53,53	0
57	MG	1A	3829	1/1	0.93	0.10	33,33,33,33	0
57	MG	1A	3465	1/1	0.93	0.21	47,47,47,47	0
57	MG	2a	1749	1/1	0.93	0.12	75,75,75,75	0
57	MG	2A	3015	1/1	0.93	0.22	60,60,60,60	0
57	MG	1B	226	1/1	0.93	0.11	55,55,55,55	0
57	MG	1A	3583	1/1	0.93	0.12	53,53,53,53	0
57	MG	2A	3280	1/1	0.93	0.25	64,64,64,64	0
57	MG	1A	3252	1/1	0.93	0.22	70,70,70,70	0
57	MG	1a	1682	1/1	0.93	0.41	68,68,68,68	0
57	MG	1A	3253	1/1	0.93	0.12	59,59,59,59	0
57	MG	1A	3716	1/1	0.93	0.07	31,31,31,31	0
57	MG	1A	3055	1/1	0.93	0.15	51,51,51,51	0
57	MG	1A	3390	1/1	0.93	0.28	43,43,43,43	0
57	MG	2A	3039	1/1	0.93	0.29	62,62,62,62	0
57	MG	2A	3040	1/1	0.93	0.09	61,61,61,61	0
57	MG	1E	302	1/1	0.93	0.21	56,56,56,56	0
57	MG	1A	3593	1/1	0.93	0.09	37,37,37,37	0
57	MG	1A	3193	1/1	0.93	0.24	45,45,45,45	0
57	MG	1A	3848	1/1	0.93	0.22	44,44,44,44	0
57	MG	1E	313	1/1	0.93	0.08	50,50,50,50	0
57	MG	1a	1694	1/1	0.93	0.32	59,59,59,59	0
57	MG	1A	3259	1/1	0.93	0.11	52,52,52,52	0
57	MG	1A	3983	1/1	0.93	0.08	17,17,17,17	0
57	MG	1A	3268	1/1	0.93	0.19	38,38,38,38	0
57	MG	2A	3311	1/1	0.93	0.25	62,62,62,62	0
57	MG	2a	1776	1/1	0.93	0.21	70,70,70,70	0
57	MG	1F	308	1/1	0.93	0.12	44,44,44,44	0
57	MG	1A	3484	1/1	0.93	0.13	60,60,60,60	0
57	MG	2A	3575	1/1	0.93	0.07	54,54,54,54	0
57	MG	2A	3827	1/1	0.93	0.07	37,37,37,37	0
57	MG	1F	313	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3485	1/1	0.93	0.30	61,61,61,61	0
57	MG	1a	1704	1/1	0.93	0.09	62,62,62,62	0
57	MG	2a	1785	1/1	0.93	0.09	66,66,66,66	0
57	MG	2e	202	1/1	0.93	0.22	69,69,69,69	0
57	MG	2A	3322	1/1	0.93	0.06	62,62,62,62	0
57	MG	2A	3833	1/1	0.93	0.12	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
57	MG	2A	3065	1/1	0.93	0.13	52,52,52,52	0
57	MG	1a	1706	1/1	0.93	0.29	74,74,74,74	0
57	MG	2A	3836	1/1	0.93	0.07	77,77,77,77	0
57	MG	2A	3325	1/1	0.93	0.19	52,52,52,52	0
57	MG	2A	3585	1/1	0.93	0.13	42,42,42,42	0
57	MG	1A	3006	1/1	0.93	0.12	53,53,53,53	0
57	MG	2A	3841	1/1	0.93	0.14	53,53,53,53	0
57	MG	2A	3081	1/1	0.93	0.16	61,61,61,61	0
57	MG	1A	3856	1/1	0.93	0.07	34,34,34,34	0
57	MG	2A	3845	1/1	0.93	0.13	57,57,57,57	0
57	MG	2A	3592	1/1	0.93	0.19	59,59,59,59	0
57	MG	1A	3401	1/1	0.93	0.11	52,52,52,52	0
57	MG	2A	3596	1/1	0.93	0.14	59,59,59,59	0
57	MG	2A	3569	1/1	0.94	0.10	55,55,55,55	0
57	MG	2A	3298	1/1	0.94	0.09	62,62,62,62	0
57	MG	2A	3054	1/1	0.94	0.17	64,64,64,64	0
57	MG	1A	3118	1/1	0.94	0.15	46,46,46,46	0
57	MG	1A	3668	1/1	0.94	0.08	38,38,38,38	0
57	MG	1N	202	1/1	0.94	0.08	45,45,45,45	0
57	MG	1O	201	1/1	0.94	0.13	57,57,57,57	0
57	MG	2A	3304	1/1	0.94	0.26	69,69,69,69	0
57	MG	1A	3391	1/1	0.94	0.23	53,53,53,53	0
57	MG	2A	3579	1/1	0.94	0.06	69,69,69,69	0
57	MG	1A	3078	1/1	0.94	0.10	44,44,44,44	0
57	MG	1A	3393	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3063	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3783	1/1	0.94	0.08	35,35,35,35	0
57	MG	2A	3316	1/1	0.94	0.12	60,60,60,60	0
57	MG	2A	3067	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3587	1/1	0.94	0.10	44,44,44,44	0
57	MG	2A	3069	1/1	0.94	0.08	61,61,61,61	0
57	MG	2A	3074	1/1	0.94	0.22	55,55,55,55	0
57	MG	2A	3591	1/1	0.94	0.14	59,59,59,59	0
57	MG	1P	206	1/1	0.94	0.06	39,39,39,39	0
57	MG	1A	3260	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3079	1/1	0.94	0.16	51,51,51,51	0
57	MG	1A	3263	1/1	0.94	0.07	47,47,47,47	0
57	MG	1A	4034	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3787	1/1	0.94	0.21	57,57,57,57	0
57	MG	2A	3327	1/1	0.94	0.24	53,53,53,53	0
57	MG	2A	3328	1/1	0.94	0.10	74,74,74,74	0
57	MG	1A	3571	1/1	0.94	0.18	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3338	1/1	0.94	0.10	60,60,60,60	0
57	MG	1A	3302	1/1	0.94	0.23	53,53,53,53	0
57	MG	1A	3344	1/1	0.94	0.14	39,39,39,39	0
57	MG	2F	301	1/1	0.94	0.18	49,49,49,49	0
57	MG	2A	3334	1/1	0.94	0.14	56,56,56,56	0
57	MG	2F	307	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3916	1/1	0.94	0.11	39,39,39,39	0
57	MG	1A	3406	1/1	0.94	0.09	45,45,45,45	0
57	MG	2A	3616	1/1	0.94	0.09	45,45,45,45	0
57	MG	2O	202	1/1	0.94	0.17	61,61,61,61	0
57	MG	2A	3337	1/1	0.94	0.11	66,66,66,66	0
57	MG	2A	3339	1/1	0.94	0.17	65,65,65,65	0
57	MG	2A	3621	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	4047	1/1	0.94	0.07	41,41,41,41	0
57	MG	2A	3623	1/1	0.94	0.19	55,55,55,55	0
57	MG	1A	3797	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3919	1/1	0.94	0.11	58,58,58,58	0
57	MG	1A	4050	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3344	1/1	0.94	0.09	56,56,56,56	0
57	MG	2V	201	1/1	0.94	0.11	53,53,53,53	0
57	MG	2V	202	1/1	0.94	0.21	67,67,67,67	0
57	MG	1A	3303	1/1	0.94	0.28	53,53,53,53	0
57	MG	1A	3476	1/1	0.94	0.14	32,32,32,32	0
57	MG	20	101	1/1	0.94	0.08	62,62,62,62	0
57	MG	2A	3105	1/1	0.94	0.20	65,65,65,65	0
57	MG	10	106	1/1	0.94	0.23	67,67,67,67	0
57	MG	1A	3479	1/1	0.94	0.23	43,43,43,43	0
57	MG	11	104	1/1	0.94	0.17	58,58,58,58	0
57	MG	23	103	1/1	0.94	0.10	62,62,62,62	0
57	MG	12	101	1/1	0.94	0.08	53,53,53,53	0
57	MG	13	103	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3923	1/1	0.94	0.10	62,62,62,62	0
57	MG	1A	3924	1/1	0.94	0.09	66,66,66,66	0
57	MG	26	101	1/1	0.94	0.11	61,61,61,61	0
57	MG	2A	3357	1/1	0.94	0.34	69,69,69,69	0
57	MG	2A	3118	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	3927	1/1	0.94	0.09	70,70,70,70	0
57	MG	17	101	1/1	0.94	0.09	34,34,34,34	0
57	MG	2A	3121	1/1	0.94	0.09	50,50,50,50	0
57	MG	2A	3647	1/1	0.94	0.08	62,62,62,62	0
57	MG	1a	1749	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3410	1/1	0.94	0.10	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
57	MG	2A	3126	1/1	0.94	0.14	47,47,47,47	0
57	MG	2a	1607	1/1	0.94	0.14	61,61,61,61	0
57	MG	1a	1752	1/1	0.94	0.25	68,68,68,68	0
57	MG	2A	3133	1/1	0.94	0.18	52,52,52,52	0
57	MG	18	103	1/1	0.94	0.10	54,54,54,54	0
57	MG	1a	1754	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3372	1/1	0.94	0.17	65,65,65,65	0
57	MG	1a	1755	1/1	0.94	0.10	61,61,61,61	0
57	MG	1A	4067	1/1	0.94	0.11	47,47,47,47	0
57	MG	2a	1617	1/1	0.94	0.21	67,67,67,67	0
57	MG	1A	3586	1/1	0.94	0.09	59,59,59,59	0
57	MG	1A	3304	1/1	0.94	0.24	57,57,57,57	0
57	MG	1A	3306	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3664	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3933	1/1	0.94	0.10	53,53,53,53	0
57	MG	2A	3149	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3806	1/1	0.94	0.20	63,63,63,63	0
57	MG	1a	1764	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	3234	1/1	0.94	0.17	42,42,42,42	0
57	MG	1a	1766	1/1	0.94	0.08	82,82,82,82	0
57	MG	1a	1767	1/1	0.94	0.14	84,84,84,84	0
57	MG	1A	3699	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3388	1/1	0.94	0.22	50,50,50,50	0
57	MG	1A	3236	1/1	0.94	0.07	42,42,42,42	0
57	MG	2A	3679	1/1	0.94	0.09	57,57,57,57	0
57	MG	1a	1611	1/1	0.94	0.08	69,69,69,69	0
57	MG	1A	3149	1/1	0.94	0.11	43,43,43,43	0
57	MG	1A	3355	1/1	0.94	0.11	49,49,49,49	0
57	MG	2A	3393	1/1	0.94	0.29	61,61,61,61	0
57	MG	1A	3595	1/1	0.94	0.11	45,45,45,45	0
57	MG	1a	1616	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	4083	1/1	0.94	0.08	45,45,45,45	0
57	MG	2A	3171	1/1	0.94	0.13	62,62,62,62	0
57	MG	2A	3173	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3401	1/1	0.94	0.14	57,57,57,57	0
57	MG	1a	1777	1/1	0.94	0.10	67,67,67,67	0
57	MG	1A	3944	1/1	0.94	0.12	53,53,53,53	0
57	MG	2A	3405	1/1	0.94	0.36	67,67,67,67	0
57	MG	2a	1653	1/1	0.94	0.26	60,60,60,60	0
57	MG	1A	3279	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	4087	1/1	0.94	0.15	53,53,53,53	0
57	MG	1A	3600	1/1	0.94	0.06	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1625	1/1	0.94	0.18	57,57,57,57	0
57	MG	2a	1662	1/1	0.94	0.14	60,60,60,60	0
57	MG	2A	3411	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3187	1/1	0.94	0.23	54,54,54,54	0
57	MG	2A	3704	1/1	0.94	0.18	55,55,55,55	0
57	MG	1A	3496	1/1	0.94	0.10	42,42,42,42	0
57	MG	1A	3498	1/1	0.94	0.15	54,54,54,54	0
57	MG	1a	1628	1/1	0.94	0.54	74,74,74,74	0
57	MG	2A	3416	1/1	0.94	0.11	55,55,55,55	0
57	MG	2a	1674	1/1	0.94	0.35	60,60,60,60	0
57	MG	1a	1787	1/1	0.94	0.12	66,66,66,66	0
57	MG	1a	1788	1/1	0.94	0.10	70,70,70,70	0
57	MG	1A	3824	1/1	0.94	0.18	50,50,50,50	0
57	MG	2A	3713	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3605	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3423	1/1	0.94	0.35	65,65,65,65	0
57	MG	1A	3610	1/1	0.94	0.18	50,50,50,50	0
57	MG	1A	3499	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	4099	1/1	0.94	0.13	55,55,55,55	0
57	MG	1A	3722	1/1	0.94	0.13	41,41,41,41	0
57	MG	1A	3125	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3959	1/1	0.94	0.13	62,62,62,62	0
57	MG	1A	3420	1/1	0.94	0.15	38,38,38,38	0
57	MG	1a	1802	1/1	0.94	0.17	63,63,63,63	0
57	MG	2A	3206	1/1	0.94	0.17	60,60,60,60	0
57	MG	1A	3359	1/1	0.94	0.10	43,43,43,43	0
57	MG	1A	3127	1/1	0.94	0.12	68,68,68,68	0
57	MG	2A	3732	1/1	0.94	0.14	40,40,40,40	0
57	MG	1A	3729	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3210	1/1	0.94	0.27	58,58,58,58	0
57	MG	2A	3444	1/1	0.94	0.14	52,52,52,52	0
57	MG	1A	3730	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3362	1/1	0.94	0.08	47,47,47,47	0
57	MG	2a	1702	1/1	0.94	0.18	64,64,64,64	0
57	MG	2A	3213	1/1	0.94	0.19	67,67,67,67	0
57	MG	2A	3215	1/1	0.94	0.12	59,59,59,59	0
57	MG	1A	3619	1/1	0.94	0.07	34,34,34,34	0
57	MG	1A	3508	1/1	0.94	0.25	52,52,52,52	0
57	MG	2A	3455	1/1	0.94	0.15	55,55,55,55	0
57	MG	2a	1710	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3220	1/1	0.94	0.35	48,48,48,48	0
57	MG	2a	1714	1/1	0.94	0.15	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3462	1/1	0.94	0.12	46,46,46,46	0
57	MG	2A	3749	1/1	0.94	0.09	77,77,77,77	0
57	MG	2A	3223	1/1	0.94	0.16	44,44,44,44	0
57	MG	1A	3845	1/1	0.94	0.14	39,39,39,39	0
57	MG	1A	3242	1/1	0.94	0.13	55,55,55,55	0
57	MG	1A	3365	1/1	0.94	0.21	51,51,51,51	0
57	MG	1a	1815	1/1	0.94	0.14	67,67,67,67	0
57	MG	1A	3366	1/1	0.94	0.07	68,68,68,68	0
57	MG	1a	1656	1/1	0.94	0.29	61,61,61,61	0
57	MG	1A	3113	1/1	0.94	0.21	47,47,47,47	0
57	MG	2a	1728	1/1	0.94	0.16	52,52,52,52	0
57	MG	1B	218	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3521	1/1	0.94	0.22	58,58,58,58	0
57	MG	1B	221	1/1	0.94	0.21	51,51,51,51	0
57	MG	1A	3159	1/1	0.94	0.25	35,35,35,35	0
57	MG	2A	3240	1/1	0.94	0.12	60,60,60,60	0
57	MG	1a	1663	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	3744	1/1	0.94	0.08	55,55,55,55	0
57	MG	2A	3244	1/1	0.94	0.17	56,56,56,56	0
57	MG	2A	3487	1/1	0.94	0.10	24,24,24,24	0
57	MG	2A	3488	1/1	0.94	0.16	61,61,61,61	0
57	MG	2A	3772	1/1	0.94	0.12	64,64,64,64	0
57	MG	1A	3980	1/1	0.94	0.09	58,58,58,58	0
57	MG	1v	103	1/1	0.94	0.07	52,52,52,52	0
57	MG	1A	3632	1/1	0.94	0.07	22,22,22,22	0
57	MG	1B	228	1/1	0.94	0.09	40,40,40,40	0
57	MG	2a	1748	1/1	0.94	0.15	57,57,57,57	0
57	MG	1A	3441	1/1	0.94	0.11	62,62,62,62	0
57	MG	2A	3781	1/1	0.94	0.06	52,52,52,52	0
57	MG	1a	1670	1/1	0.94	0.14	73,73,73,73	0
57	MG	1A	3209	1/1	0.94	0.18	53,53,53,53	0
57	MG	1A	3865	1/1	0.94	0.07	26,26,26,26	0
57	MG	2A	3254	1/1	0.94	0.21	54,54,54,54	0
57	MG	2a	1755	1/1	0.94	0.23	46,46,46,46	0
57	MG	1x	108	1/1	0.94	0.19	53,53,53,53	0
57	MG	1A	3250	1/1	0.94	0.10	47,47,47,47	0
57	MG	2a	1758	1/1	0.94	0.12	65,65,65,65	0
57	MG	1A	3212	1/1	0.94	0.20	43,43,43,43	0
57	MG	1x	112	1/1	0.94	0.15	63,63,63,63	0
57	MG	1B	236	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3798	1/1	0.94	0.11	58,58,58,58	0
57	MG	1D	310	1/1	0.94	0.09	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3133	1/1	0.94	0.12	35,35,35,35	0
57	MG	2A	3514	1/1	0.94	0.08	35,35,35,35	0
57	MG	1D	313	1/1	0.94	0.15	45,45,45,45	0
57	MG	1a	1679	1/1	0.94	0.07	47,47,47,47	0
57	MG	1a	1680	1/1	0.94	0.22	68,68,68,68	0
57	MG	1A	3110	1/1	0.94	0.13	43,43,43,43	0
57	MG	1A	3874	1/1	0.94	0.14	45,45,45,45	0
57	MG	2A	3270	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	4005	1/1	0.94	0.07	48,48,48,48	0
57	MG	2A	3272	1/1	0.94	0.11	53,53,53,53	0
57	MG	1a	1685	1/1	0.94	0.21	65,65,65,65	0
57	MG	2A	3023	1/1	0.94	0.21	45,45,45,45	0
57	MG	1A	3538	1/1	0.94	0.21	37,37,37,37	0
57	MG	1A	4008	1/1	0.94	0.12	76,76,76,76	0
57	MG	1A	3386	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3878	1/1	0.94	0.16	62,62,62,62	0
57	MG	2A	3030	1/1	0.94	0.07	48,48,48,48	0
57	MG	2a	1783	1/1	0.94	0.08	73,73,73,73	0
57	MG	1A	3652	1/1	0.94	0.07	59,59,59,59	0
57	MG	2A	3542	1/1	0.94	0.20	63,63,63,63	0
57	MG	2d	301	1/1	0.94	0.09	69,69,69,69	0
57	MG	2e	201	1/1	0.94	0.12	72,72,72,72	0
57	MG	1A	3451	1/1	0.94	0.14	62,62,62,62	0
57	MG	1A	3544	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3548	1/1	0.94	0.13	49,49,49,49	0
57	MG	2A	3550	1/1	0.94	0.17	54,54,54,54	0
57	MG	2A	3551	1/1	0.94	0.12	56,56,56,56	0
57	MG	1a	1693	1/1	0.94	0.26	53,53,53,53	0
57	MG	2l	202	1/1	0.94	0.11	56,56,56,56	0
57	MG	1A	3546	1/1	0.94	0.09	35,35,35,35	0
57	MG	1A	4016	1/1	0.94	0.08	50,50,50,50	0
57	MG	2A	3289	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3387	1/1	0.94	0.25	59,59,59,59	0
57	MG	2v	101	1/1	0.94	0.09	55,55,55,55	0
57	MG	2A	3294	1/1	0.94	0.12	61,61,61,61	0
57	MG	2A	3558	1/1	0.94	0.20	47,47,47,47	0
57	MG	1A	4021	1/1	0.94	0.11	53,53,53,53	0
57	MG	2A	3562	1/1	0.94	0.08	56,56,56,56	0
57	MG	1A	3550	1/1	0.94	0.15	46,46,46,46	0
57	MG	1A	3665	1/1	0.94	0.09	60,60,60,60	0
57	MG	1A	3670	1/1	0.95	0.12	41,41,41,41	0
57	MG	2A	3073	1/1	0.95	0.09	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1Q	205	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3307	1/1	0.95	0.27	58,58,58,58	0
57	MG	2A	3075	1/1	0.95	0.16	49,49,49,49	0
57	MG	2A	3309	1/1	0.95	0.17	66,66,66,66	0
57	MG	2A	3574	1/1	0.95	0.19	62,62,62,62	0
57	MG	1A	3673	1/1	0.95	0.11	31,31,31,31	0
57	MG	2A	3077	1/1	0.95	0.17	49,49,49,49	0
57	MG	2A	3312	1/1	0.95	0.10	51,51,51,51	0
57	MG	1A	3471	1/1	0.95	0.10	39,39,39,39	0
57	MG	1S	202	1/1	0.95	0.10	58,58,58,58	0
57	MG	1A	4038	1/1	0.95	0.09	48,48,48,48	0
57	MG	2A	3082	1/1	0.95	0.14	60,60,60,60	0
57	MG	1A	4041	1/1	0.95	0.09	28,28,28,28	0
57	MG	1T	202	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3912	1/1	0.95	0.14	36,36,36,36	0
57	MG	2A	3087	1/1	0.95	0.26	56,56,56,56	0
57	MG	1U	205	1/1	0.95	0.15	39,39,39,39	0
57	MG	1U	207	1/1	0.95	0.17	37,37,37,37	0
57	MG	1A	3568	1/1	0.95	0.20	42,42,42,42	0
57	MG	1A	3346	1/1	0.95	0.12	54,54,54,54	0
57	MG	2B	218	1/1	0.95	0.19	63,63,63,63	0
57	MG	1V	206	1/1	0.95	0.10	58,58,58,58	0
57	MG	2A	3593	1/1	0.95	0.14	43,43,43,43	0
57	MG	2A	3095	1/1	0.95	0.11	30,30,30,30	0
57	MG	2D	306	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3347	1/1	0.95	0.07	45,45,45,45	0
57	MG	1W	201	1/1	0.95	0.11	49,49,49,49	0
57	MG	2A	3332	1/1	0.95	0.08	64,64,64,64	0
57	MG	1W	205	1/1	0.95	0.09	30,30,30,30	0
57	MG	2E	306	1/1	0.95	0.07	53,53,53,53	0
57	MG	1X	102	1/1	0.95	0.09	50,50,50,50	0
57	MG	1X	104	1/1	0.95	0.16	41,41,41,41	0
57	MG	2A	3608	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3573	1/1	0.95	0.11	50,50,50,50	0
57	MG	2F	304	1/1	0.95	0.09	46,46,46,46	0
57	MG	2F	305	1/1	0.95	0.11	55,55,55,55	0
57	MG	2F	306	1/1	0.95	0.12	44,44,44,44	0
57	MG	1a	1736	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3338	1/1	0.95	0.07	65,65,65,65	0
57	MG	1a	1737	1/1	0.95	0.14	63,63,63,63	0
57	MG	1A	3475	1/1	0.95	0.25	53,53,53,53	0
57	MG	1A	3145	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
57	MG	1A	3577	1/1	0.95	0.11	57,57,57,57	0
57	MG	1a	1741	1/1	0.95	0.09	66,66,66,66	0
57	MG	2Q	202	1/1	0.95	0.23	57,57,57,57	0
57	MG	2A	3113	1/1	0.95	0.14	51,51,51,51	0
57	MG	2Q	204	1/1	0.95	0.13	50,50,50,50	0
57	MG	10	103	1/1	0.95	0.24	48,48,48,48	0
57	MG	2A	3619	1/1	0.95	0.18	47,47,47,47	0
57	MG	1A	4051	1/1	0.95	0.04	19,19,19,19	0
57	MG	2A	3347	1/1	0.95	0.07	70,70,70,70	0
57	MG	1A	4052	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3478	1/1	0.95	0.08	51,51,51,51	0
57	MG	11	101	1/1	0.95	0.38	47,47,47,47	0
57	MG	1A	3579	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3087	1/1	0.95	0.09	36,36,36,36	0
57	MG	2W	202	1/1	0.95	0.23	50,50,50,50	0
57	MG	1A	3305	1/1	0.95	0.18	50,50,50,50	0
57	MG	1A	3481	1/1	0.95	0.11	62,62,62,62	0
57	MG	2A	3128	1/1	0.95	0.13	51,51,51,51	0
57	MG	2A	3356	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3129	1/1	0.95	0.18	46,46,46,46	0
57	MG	2A	3358	1/1	0.95	0.11	56,56,56,56	0
57	MG	1A	3264	1/1	0.95	0.16	48,48,48,48	0
57	MG	23	104	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3132	1/1	0.95	0.24	64,64,64,64	0
57	MG	1A	3930	1/1	0.95	0.06	63,63,63,63	0
57	MG	1A	3483	1/1	0.95	0.08	63,63,63,63	0
57	MG	16	102	1/1	0.95	0.07	56,56,56,56	0
57	MG	2A	3364	1/1	0.95	0.13	64,64,64,64	0
57	MG	1A	3808	1/1	0.95	0.08	39,39,39,39	0
57	MG	1A	3307	1/1	0.95	0.12	54,54,54,54	0
57	MG	2A	3367	1/1	0.95	0.10	61,61,61,61	0
57	MG	1a	1761	1/1	0.95	0.18	70,70,70,70	0
57	MG	1A	3697	1/1	0.95	0.14	55,55,55,55	0
57	MG	1a	1763	1/1	0.95	0.12	59,59,59,59	0
57	MG	1A	3226	1/1	0.95	0.23	50,50,50,50	0
57	MG	2A	3145	1/1	0.95	0.11	36,36,36,36	0
57	MG	2A	3146	1/1	0.95	0.17	62,62,62,62	0
57	MG	1A	3061	1/1	0.95	0.20	51,51,51,51	0
57	MG	1A	3813	1/1	0.95	0.22	63,63,63,63	0
57	MG	1A	3815	1/1	0.95	0.11	62,62,62,62	0
57	MG	2A	3656	1/1	0.95	0.17	62,62,62,62	0
57	MG	2A	3657	1/1	0.95	0.25	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
57	MG	2a	1613	1/1	0.95	0.19	65,65,65,65	0
57	MG	1A	3357	1/1	0.95	0.13	62,62,62,62	0
57	MG	2A	3659	1/1	0.95	0.08	45,45,45,45	0
57	MG	2A	3154	1/1	0.95	0.14	48,48,48,48	0
57	MG	1A	3489	1/1	0.95	0.14	45,45,45,45	0
57	MG	2A	3158	1/1	0.95	0.15	43,43,43,43	0
57	MG	2A	3159	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3943	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3665	1/1	0.95	0.07	69,69,69,69	0
57	MG	2A	3383	1/1	0.95	0.07	47,47,47,47	0
57	MG	2a	1623	1/1	0.95	0.07	59,59,59,59	0
57	MG	1A	3228	1/1	0.95	0.22	36,36,36,36	0
57	MG	1a	1607	1/1	0.95	0.11	65,65,65,65	0
57	MG	1A	3116	1/1	0.95	0.16	49,49,49,49	0
57	MG	2a	1627	1/1	0.95	0.23	69,69,69,69	0
57	MG	1a	1610	1/1	0.95	0.08	72,72,72,72	0
57	MG	1a	1775	1/1	0.95	0.17	61,61,61,61	0
57	MG	2A	3673	1/1	0.95	0.06	59,59,59,59	0
57	MG	1A	3709	1/1	0.95	0.10	52,52,52,52	0
57	MG	1A	3235	1/1	0.95	0.12	45,45,45,45	0
57	MG	2a	1633	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3169	1/1	0.95	0.19	44,44,44,44	0
57	MG	1A	3281	1/1	0.95	0.11	62,62,62,62	0
57	MG	2A	3678	1/1	0.95	0.16	64,64,64,64	0
57	MG	1A	3951	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3282	1/1	0.95	0.17	40,40,40,40	0
57	MG	1a	1617	1/1	0.95	0.08	65,65,65,65	0
57	MG	1A	3714	1/1	0.95	0.17	49,49,49,49	0
57	MG	2A	3399	1/1	0.95	0.38	56,56,56,56	0
57	MG	2A	3179	1/1	0.95	0.06	51,51,51,51	0
57	MG	2a	1645	1/1	0.95	0.16	63,63,63,63	0
57	MG	1A	3426	1/1	0.95	0.26	39,39,39,39	0
57	MG	1A	3063	1/1	0.95	0.09	56,56,56,56	0
57	MG	1A	3717	1/1	0.95	0.07	43,43,43,43	0
57	MG	2A	3404	1/1	0.95	0.30	69,69,69,69	0
57	MG	1A	3718	1/1	0.95	0.05	16,16,16,16	0
57	MG	2A	3692	1/1	0.95	0.07	39,39,39,39	0
57	MG	2a	1652	1/1	0.95	0.18	60,60,60,60	0
57	MG	1a	1624	1/1	0.95	0.18	60,60,60,60	0
57	MG	2a	1654	1/1	0.95	0.16	48,48,48,48	0
57	MG	2A	3407	1/1	0.95	0.19	58,58,58,58	0
57	MG	1a	1789	1/1	0.95	0.07	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3609	1/1	0.95	0.06	36,36,36,36	0
57	MG	2a	1659	1/1	0.95	0.33	59,59,59,59	0
57	MG	1A	3185	1/1	0.95	0.12	37,37,37,37	0
57	MG	1A	3962	1/1	0.95	0.12	77,77,77,77	0
57	MG	1A	3835	1/1	0.95	0.21	65,65,65,65	0
57	MG	2a	1665	1/1	0.95	0.16	64,64,64,64	0
57	MG	1A	3964	1/1	0.95	0.12	32,32,32,32	0
57	MG	1A	3152	1/1	0.95	0.14	48,48,48,48	0
57	MG	2A	3195	1/1	0.95	0.19	58,58,58,58	0
57	MG	2a	1670	1/1	0.95	0.18	54,54,54,54	0
57	MG	1a	1797	1/1	0.95	0.09	70,70,70,70	0
57	MG	1A	3368	1/1	0.95	0.10	50,50,50,50	0
57	MG	1a	1632	1/1	0.95	0.10	31,31,31,31	0
57	MG	2A	3199	1/1	0.95	0.14	56,56,56,56	0
57	MG	1a	1633	1/1	0.95	0.14	59,59,59,59	0
57	MG	1A	3838	1/1	0.95	0.06	23,23,23,23	0
57	MG	2A	3424	1/1	0.95	0.13	59,59,59,59	0
57	MG	1A	3840	1/1	0.95	0.11	42,42,42,42	0
57	MG	1B	207	1/1	0.95	0.10	48,48,48,48	0
57	MG	1A	3507	1/1	0.95	0.33	57,57,57,57	0
57	MG	1A	3435	1/1	0.95	0.22	69,69,69,69	0
57	MG	1A	3616	1/1	0.95	0.07	36,36,36,36	0
57	MG	2A	3718	1/1	0.95	0.26	62,62,62,62	0
57	MG	1A	3510	1/1	0.95	0.30	35,35,35,35	0
57	MG	2A	3721	1/1	0.95	0.11	61,61,61,61	0
57	MG	1a	1810	1/1	0.95	0.20	59,59,59,59	0
57	MG	1A	3092	1/1	0.95	0.19	51,51,51,51	0
57	MG	1A	3513	1/1	0.95	0.27	48,48,48,48	0
57	MG	1A	3192	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3066	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3049	1/1	0.95	0.12	31,31,31,31	0
57	MG	2A	3729	1/1	0.95	0.11	63,63,63,63	0
57	MG	2A	3441	1/1	0.95	0.12	56,56,56,56	0
57	MG	2a	1696	1/1	0.95	0.14	61,61,61,61	0
57	MG	1a	1647	1/1	0.95	0.06	55,55,55,55	0
57	MG	1B	219	1/1	0.95	0.07	37,37,37,37	0
57	MG	2a	1699	1/1	0.95	0.19	62,62,62,62	0
57	MG	1A	3518	1/1	0.95	0.27	66,66,66,66	0
57	MG	1A	3378	1/1	0.95	0.08	57,57,57,57	0
57	MG	1e	203	1/1	0.95	0.13	62,62,62,62	0
57	MG	2a	1703	1/1	0.95	0.19	58,58,58,58	0
57	MG	2A	3225	1/1	0.95	0.17	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1652	1/1	0.95	0.09	75,75,75,75	0
57	MG	2A	3229	1/1	0.95	0.14	56,56,56,56	0
57	MG	1A	3329	1/1	0.95	0.09	60,60,60,60	0
57	MG	2A	3231	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3002	1/1	0.95	0.11	44,44,44,44	0
57	MG	1n	101	1/1	0.95	0.30	70,70,70,70	0
57	MG	1A	3740	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3984	1/1	0.95	0.16	32,32,32,32	0
57	MG	1a	1658	1/1	0.95	0.08	64,64,64,64	0
57	MG	1A	3987	1/1	0.95	0.07	63,63,63,63	0
57	MG	2a	1718	1/1	0.95	0.14	65,65,65,65	0
57	MG	1A	3381	1/1	0.95	0.17	27,27,27,27	0
57	MG	1A	3989	1/1	0.95	0.08	82,82,82,82	0
57	MG	1A	3991	1/1	0.95	0.10	35,35,35,35	0
57	MG	1B	232	1/1	0.95	0.09	66,66,66,66	0
57	MG	2A	3242	1/1	0.95	0.12	53,53,53,53	0
57	MG	1x	104	1/1	0.95	0.39	73,73,73,73	0
57	MG	1a	1664	1/1	0.95	0.09	61,61,61,61	0
57	MG	2A	3482	1/1	0.95	0.11	58,58,58,58	0
57	MG	1A	3992	1/1	0.95	0.08	26,26,26,26	0
57	MG	1A	3382	1/1	0.95	0.16	39,39,39,39	0
57	MG	1A	3995	1/1	0.95	0.08	29,29,29,29	0
57	MG	1B	238	1/1	0.95	0.06	41,41,41,41	0
57	MG	2A	3766	1/1	0.95	0.20	67,67,67,67	0
57	MG	1D	302	1/1	0.95	0.20	42,42,42,42	0
57	MG	2a	1738	1/1	0.95	0.11	64,64,64,64	0
57	MG	2A	3001	1/1	0.95	0.10	60,60,60,60	0
57	MG	2A	3251	1/1	0.95	0.17	61,61,61,61	0
57	MG	1D	309	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3449	1/1	0.95	0.12	73,73,73,73	0
57	MG	1A	3999	1/1	0.95	0.08	32,32,32,32	0
57	MG	2A	3256	1/1	0.95	0.09	67,67,67,67	0
57	MG	2A	3496	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3870	1/1	0.95	0.11	50,50,50,50	0
57	MG	2A	3777	1/1	0.95	0.10	50,50,50,50	0
57	MG	1D	314	1/1	0.95	0.09	34,34,34,34	0
57	MG	2A	3779	1/1	0.95	0.09	56,56,56,56	0
57	MG	1A	3871	1/1	0.95	0.09	32,32,32,32	0
57	MG	2A	3014	1/1	0.95	0.16	53,53,53,53	0
57	MG	2A	3782	1/1	0.95	0.09	59,59,59,59	0
57	MG	1E	305	1/1	0.95	0.20	33,33,33,33	0
57	MG	2A	3505	1/1	0.95	0.05	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3384	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3079	1/1	0.95	0.15	52,52,52,52	0
57	MG	2A	3790	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3082	1/1	0.95	0.15	32,32,32,32	0
57	MG	1E	311	1/1	0.95	0.20	41,41,41,41	0
57	MG	2A	3266	1/1	0.95	0.20	54,54,54,54	0
57	MG	2A	3512	1/1	0.95	0.11	52,52,52,52	0
57	MG	2A	3025	1/1	0.95	0.20	51,51,51,51	0
57	MG	2A	3796	1/1	0.95	0.09	39,39,39,39	0
57	MG	2A	3797	1/1	0.95	0.08	41,41,41,41	0
57	MG	1E	312	1/1	0.95	0.12	63,63,63,63	0
57	MG	1A	4007	1/1	0.95	0.07	71,71,71,71	0
57	MG	1A	3875	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3639	1/1	0.95	0.07	31,31,31,31	0
57	MG	1A	3641	1/1	0.95	0.12	36,36,36,36	0
57	MG	2A	3521	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3523	1/1	0.95	0.11	41,41,41,41	0
57	MG	2A	3032	1/1	0.95	0.11	47,47,47,47	0
57	MG	2a	1774	1/1	0.95	0.11	68,68,68,68	0
57	MG	1A	3753	1/1	0.95	0.09	57,57,57,57	0
57	MG	2A	3037	1/1	0.95	0.13	66,66,66,66	0
57	MG	1A	3389	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3646	1/1	0.95	0.05	21,21,21,21	0
57	MG	2A	3041	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3647	1/1	0.95	0.10	22,22,22,22	0
57	MG	1A	3056	1/1	0.95	0.09	49,49,49,49	0
57	MG	1G	201	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3457	1/1	0.95	0.19	44,44,44,44	0
57	MG	2A	3283	1/1	0.95	0.17	63,63,63,63	0
57	MG	1A	3337	1/1	0.95	0.09	54,54,54,54	0
57	MG	1a	1695	1/1	0.95	0.26	67,67,67,67	0
57	MG	2A	3543	1/1	0.95	0.20	68,68,68,68	0
57	MG	1A	3547	1/1	0.95	0.09	24,24,24,24	0
57	MG	2A	3826	1/1	0.95	0.12	56,56,56,56	0
57	MG	2A	3545	1/1	0.95	0.09	62,62,62,62	0
57	MG	2A	3287	1/1	0.95	0.13	60,60,60,60	0
57	MG	2A	3288	1/1	0.95	0.13	51,51,51,51	0
57	MG	2A	3549	1/1	0.95	0.12	33,33,33,33	0
57	MG	1A	3655	1/1	0.95	0.07	28,28,28,28	0
57	MG	2A	3291	1/1	0.95	0.11	63,63,63,63	0
57	MG	1A	3210	1/1	0.95	0.07	51,51,51,51	0
57	MG	1N	201	1/1	0.95	0.20	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3342	1/1	0.95	0.11	61,61,61,61	0
57	MG	1A	3174	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3466	1/1	0.95	0.08	54,54,54,54	0
57	MG	1A	3301	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3899	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3562	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3143	1/1	0.95	0.28	37,37,37,37	0
57	MG	1A	3399	1/1	0.95	0.12	43,43,43,43	0
57	MG	1A	3640	1/1	0.96	0.07	30,30,30,30	0
57	MG	1F	314	1/1	0.96	0.10	33,33,33,33	0
57	MG	1A	3090	1/1	0.96	0.13	29,29,29,29	0
57	MG	1A	3882	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	3754	1/1	0.96	0.16	73,73,73,73	0
57	MG	1A	3884	1/1	0.96	0.11	32,32,32,32	0
57	MG	2A	3668	1/1	0.96	0.10	66,66,66,66	0
57	MG	1A	3531	1/1	0.96	0.17	36,36,36,36	0
57	MG	1A	3644	1/1	0.96	0.08	20,20,20,20	0
57	MG	1A	3534	1/1	0.96	0.12	34,34,34,34	0
57	MG	1A	3536	1/1	0.96	0.25	33,33,33,33	0
57	MG	2A	3022	1/1	0.96	0.18	50,50,50,50	0
57	MG	1A	3312	1/1	0.96	0.14	49,49,49,49	0
57	MG	1A	3892	1/1	0.96	0.17	64,64,64,64	0
57	MG	1N	204	1/1	0.96	0.26	44,44,44,44	0
57	MG	1A	3372	1/1	0.96	0.25	32,32,32,32	0
57	MG	1A	3539	1/1	0.96	0.18	44,44,44,44	0
57	MG	1A	3767	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3653	1/1	0.96	0.09	33,33,33,33	0
57	MG	2A	3031	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3313	1/1	0.96	0.08	43,43,43,43	0
57	MG	25	102	1/1	0.96	0.08	64,64,64,64	0
57	MG	25	104	1/1	0.96	0.11	45,45,45,45	0
57	MG	2A	3033	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3041	1/1	0.96	0.24	36,36,36,36	0
57	MG	1A	4039	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	4040	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3449	1/1	0.96	0.19	65,65,65,65	0
57	MG	1A	3772	1/1	0.96	0.06	45,45,45,45	0
57	MG	1A	3901	1/1	0.96	0.07	63,63,63,63	0
57	MG	1R	202	1/1	0.96	0.23	44,44,44,44	0
57	MG	2A	3456	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3458	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3255	1/1	0.96	0.13	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1S	201	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	3199	1/1	0.96	0.11	24,24,24,24	0
57	MG	2A	3465	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3659	1/1	0.96	0.05	32,32,32,32	0
57	MG	2A	3050	1/1	0.96	0.10	65,65,65,65	0
57	MG	2A	3702	1/1	0.96	0.06	61,61,61,61	0
57	MG	1a	1703	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	4046	1/1	0.96	0.11	56,56,56,56	0
57	MG	1a	1705	1/1	0.96	0.06	59,59,59,59	0
57	MG	1A	3779	1/1	0.96	0.05	22,22,22,22	0
57	MG	1A	3780	1/1	0.96	0.30	33,33,33,33	0
57	MG	1U	204	1/1	0.96	0.14	50,50,50,50	0
57	MG	1A	3453	1/1	0.96	0.10	61,61,61,61	0
57	MG	1a	1710	1/1	0.96	0.10	60,60,60,60	0
57	MG	1A	3454	1/1	0.96	0.12	45,45,45,45	0
57	MG	2A	3481	1/1	0.96	0.13	54,54,54,54	0
57	MG	1U	209	1/1	0.96	0.31	44,44,44,44	0
57	MG	1A	3258	1/1	0.96	0.22	50,50,50,50	0
57	MG	2A	3064	1/1	0.96	0.06	37,37,37,37	0
57	MG	1V	202	1/1	0.96	0.35	35,35,35,35	0
57	MG	2A	3066	1/1	0.96	0.17	48,48,48,48	0
57	MG	1A	3044	1/1	0.96	0.05	23,23,23,23	0
57	MG	1A	3785	1/1	0.96	0.09	62,62,62,62	0
57	MG	1A	3147	1/1	0.96	0.16	38,38,38,38	0
57	MG	2A	3490	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3724	1/1	0.96	0.09	61,61,61,61	0
57	MG	1A	3460	1/1	0.96	0.14	38,38,38,38	0
57	MG	1W	202	1/1	0.96	0.07	48,48,48,48	0
57	MG	1W	204	1/1	0.96	0.18	39,39,39,39	0
57	MG	1A	3203	1/1	0.96	0.11	50,50,50,50	0
57	MG	1X	101	1/1	0.96	0.24	37,37,37,37	0
57	MG	1A	4061	1/1	0.96	0.12	61,61,61,61	0
57	MG	2A	3498	1/1	0.96	0.14	43,43,43,43	0
57	MG	1X	103	1/1	0.96	0.17	42,42,42,42	0
57	MG	1a	1727	1/1	0.96	0.13	70,70,70,70	0
57	MG	2a	1642	1/1	0.96	0.16	48,48,48,48	0
57	MG	1A	3789	1/1	0.96	0.05	48,48,48,48	0
57	MG	1X	105	1/1	0.96	0.12	57,57,57,57	0
57	MG	1A	3671	1/1	0.96	0.08	24,24,24,24	0
57	MG	1A	3792	1/1	0.96	0.08	33,33,33,33	0
57	MG	2A	3292	1/1	0.96	0.14	61,61,61,61	0
57	MG	1Y	203	1/1	0.96	0.21	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1Y	204	1/1	0.96	0.12	63,63,63,63	0
57	MG	2A	3742	1/1	0.96	0.13	64,64,64,64	0
57	MG	1a	1735	1/1	0.96	0.14	44,44,44,44	0
57	MG	1A	3672	1/1	0.96	0.09	64,64,64,64	0
57	MG	1Z	302	1/1	0.96	0.06	42,42,42,42	0
57	MG	1A	3321	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3385	1/1	0.96	0.11	49,49,49,49	0
57	MG	1A	3676	1/1	0.96	0.09	51,51,51,51	0
57	MG	1A	3046	1/1	0.96	0.07	37,37,37,37	0
57	MG	2A	3518	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3099	1/1	0.96	0.16	53,53,53,53	0
57	MG	1A	3267	1/1	0.96	0.19	28,28,28,28	0
57	MG	2a	1663	1/1	0.96	0.34	65,65,65,65	0
57	MG	2A	3522	1/1	0.96	0.11	54,54,54,54	0
57	MG	10	107	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3305	1/1	0.96	0.20	59,59,59,59	0
57	MG	2A	3103	1/1	0.96	0.17	50,50,50,50	0
57	MG	1A	3062	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3270	1/1	0.96	0.19	37,37,37,37	0
57	MG	11	103	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3271	1/1	0.96	0.21	30,30,30,30	0
57	MG	1A	3328	1/1	0.96	0.18	63,63,63,63	0
57	MG	12	102	1/1	0.96	0.16	54,54,54,54	0
57	MG	13	101	1/1	0.96	0.09	32,32,32,32	0
57	MG	2A	3535	1/1	0.96	0.09	36,36,36,36	0
57	MG	2A	3314	1/1	0.96	0.18	57,57,57,57	0
57	MG	1A	3272	1/1	0.96	0.18	33,33,33,33	0
57	MG	15	101	1/1	0.96	0.17	42,42,42,42	0
57	MG	2A	3541	1/1	0.96	0.07	36,36,36,36	0
57	MG	2A	3318	1/1	0.96	0.12	59,59,59,59	0
57	MG	2A	3775	1/1	0.96	0.07	70,70,70,70	0
57	MG	1A	3274	1/1	0.96	0.07	56,56,56,56	0
57	MG	2A	3117	1/1	0.96	0.11	54,54,54,54	0
57	MG	15	104	1/1	0.96	0.28	33,33,33,33	0
57	MG	2a	1686	1/1	0.96	0.23	68,68,68,68	0
57	MG	1A	3395	1/1	0.96	0.07	42,42,42,42	0
57	MG	2A	3547	1/1	0.96	0.08	43,43,43,43	0
57	MG	1A	3010	1/1	0.96	0.04	33,33,33,33	0
57	MG	1A	4085	1/1	0.96	0.11	49,49,49,49	0
57	MG	2A	3123	1/1	0.96	0.23	48,48,48,48	0
57	MG	1A	3477	1/1	0.96	0.16	36,36,36,36	0
57	MG	2A	3785	1/1	0.96	0.05	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3011	1/1	0.96	0.08	37,37,37,37	0
57	MG	17	105	1/1	0.96	0.13	43,43,43,43	0
57	MG	2A	3789	1/1	0.96	0.13	45,45,45,45	0
57	MG	1A	4088	1/1	0.96	0.17	50,50,50,50	0
57	MG	1A	3213	1/1	0.96	0.15	56,56,56,56	0
57	MG	2A	3130	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	4090	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3101	1/1	0.96	0.27	45,45,45,45	0
57	MG	1A	3402	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3816	1/1	0.96	0.05	59,59,59,59	0
57	MG	1A	3403	1/1	0.96	0.07	52,52,52,52	0
57	MG	2a	1706	1/1	0.96	0.18	55,55,55,55	0
57	MG	2A	3566	1/1	0.96	0.08	60,60,60,60	0
57	MG	2A	3137	1/1	0.96	0.13	50,50,50,50	0
57	MG	2A	3568	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3105	1/1	0.96	0.22	33,33,33,33	0
57	MG	2a	1712	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3341	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3700	1/1	0.96	0.07	53,53,53,53	0
57	MG	2A	3806	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3590	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3069	1/1	0.96	0.11	33,33,33,33	0
57	MG	1A	3957	1/1	0.96	0.07	65,65,65,65	0
57	MG	1A	3823	1/1	0.96	0.10	20,20,20,20	0
57	MG	1A	3408	1/1	0.96	0.14	57,57,57,57	0
57	MG	2A	3147	1/1	0.96	0.15	36,36,36,36	0
57	MG	2A	3148	1/1	0.96	0.12	60,60,60,60	0
57	MG	1A	3409	1/1	0.96	0.11	50,50,50,50	0
57	MG	1a	1615	1/1	0.96	0.09	65,65,65,65	0
57	MG	1A	3221	1/1	0.96	0.21	40,40,40,40	0
57	MG	1A	3225	1/1	0.96	0.07	57,57,57,57	0
57	MG	2a	1729	1/1	0.96	0.20	72,72,72,72	0
57	MG	1A	3598	1/1	0.96	0.08	25,25,25,25	0
57	MG	2A	3155	1/1	0.96	0.11	46,46,46,46	0
57	MG	1A	3070	1/1	0.96	0.10	15,15,15,15	0
57	MG	1A	3493	1/1	0.96	0.16	35,35,35,35	0
57	MG	1A	3051	1/1	0.96	0.14	45,45,45,45	0
57	MG	1A	3414	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	3074	1/1	0.96	0.30	50,50,50,50	0
57	MG	1A	3230	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3231	1/1	0.96	0.18	34,34,34,34	0
57	MG	1a	1793	1/1	0.96	0.10	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1B	215	1/1	0.96	0.07	51,51,51,51	0
57	MG	1B	216	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3232	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3168	1/1	0.96	0.11	43,43,43,43	0
57	MG	2A	3601	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3839	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3604	1/1	0.96	0.09	37,37,37,37	0
57	MG	1A	3352	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3607	1/1	0.96	0.07	31,31,31,31	0
57	MG	1A	3015	1/1	0.96	0.20	35,35,35,35	0
57	MG	2A	3172	1/1	0.96	0.17	53,53,53,53	0
57	MG	1A	3842	1/1	0.96	0.10	33,33,33,33	0
57	MG	1A	3615	1/1	0.96	0.10	22,22,22,22	0
57	MG	1A	3421	1/1	0.96	0.30	45,45,45,45	0
57	MG	2A	3848	1/1	0.96	0.07	57,57,57,57	0
57	MG	1B	224	1/1	0.96	0.11	50,50,50,50	0
57	MG	1A	3726	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3004	1/1	0.96	0.07	32,32,32,32	0
57	MG	1A	3850	1/1	0.96	0.08	35,35,35,35	0
57	MG	2B	201	1/1	0.96	0.08	58,58,58,58	0
57	MG	2A	3184	1/1	0.96	0.30	63,63,63,63	0
57	MG	1A	3032	1/1	0.96	0.18	36,36,36,36	0
57	MG	1A	3511	1/1	0.96	0.35	44,44,44,44	0
57	MG	1A	3084	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3621	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3126	1/1	0.96	0.09	33,33,33,33	0
57	MG	1B	234	1/1	0.96	0.12	56,56,56,56	0
57	MG	2A	3384	1/1	0.96	0.25	60,60,60,60	0
57	MG	1A	3001	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	3128	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3859	1/1	0.96	0.07	39,39,39,39	0
57	MG	2a	1773	1/1	0.96	0.18	62,62,62,62	0
57	MG	1a	1650	1/1	0.96	0.11	50,50,50,50	0
57	MG	1A	3860	1/1	0.96	0.10	54,54,54,54	0
57	MG	1D	304	1/1	0.96	0.12	41,41,41,41	0
57	MG	1D	306	1/1	0.96	0.06	39,39,39,39	0
57	MG	1a	1654	1/1	0.96	0.09	52,52,52,52	0
57	MG	1A	3861	1/1	0.96	0.06	50,50,50,50	0
57	MG	1A	3998	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3862	1/1	0.96	0.11	26,26,26,26	0
57	MG	1t	201	1/1	0.96	0.15	53,53,53,53	0
57	MG	1A	3628	1/1	0.96	0.06	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3434	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3360	1/1	0.96	0.17	40,40,40,40	0
57	MG	1E	304	1/1	0.96	0.20	36,36,36,36	0
57	MG	2E	304	1/1	0.96	0.24	68,68,68,68	0
57	MG	2A	3645	1/1	0.96	0.23	36,36,36,36	0
57	MG	1A	3086	1/1	0.96	0.20	46,46,46,46	0
57	MG	1A	3741	1/1	0.96	0.09	32,32,32,32	0
57	MG	1A	3742	1/1	0.96	0.07	29,29,29,29	0
57	MG	1A	3039	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3058	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3248	1/1	0.96	0.06	29,29,29,29	0
57	MG	1x	107	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	4011	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3525	1/1	0.96	0.14	52,52,52,52	0
57	MG	2A	3221	1/1	0.96	0.21	48,48,48,48	0
57	MG	2t	201	1/1	0.96	0.20	55,55,55,55	0
57	MG	2A	3222	1/1	0.96	0.07	53,53,53,53	0
57	MG	1A	3526	1/1	0.96	0.13	66,66,66,66	0
57	MG	1A	3089	1/1	0.96	0.16	60,60,60,60	0
57	MG	1A	3749	1/1	0.96	0.04	38,38,38,38	0
57	MG	1A	3141	1/1	0.96	0.06	35,35,35,35	0
57	MG	2Q	201	1/1	0.96	0.14	50,50,50,50	0
57	MG	2A	3228	1/1	0.96	0.07	56,56,56,56	0
59	ZN	1n	103	1/1	0.96	0.06	89,89,89,89	0
59	ZN	24	501	1/1	0.96	0.09	112,112,112,112	0
57	MG	2A	3178	1/1	0.97	0.13	54,54,54,54	0
57	MG	1B	227	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3075	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3517	1/1	0.97	0.19	48,48,48,48	0
57	MG	2F	303	1/1	0.97	0.07	68,68,68,68	0
57	MG	1A	3985	1/1	0.97	0.10	23,23,23,23	0
57	MG	2A	3183	1/1	0.97	0.07	56,56,56,56	0
57	MG	2A	3636	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3142	1/1	0.97	0.17	34,34,34,34	0
57	MG	1A	3622	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3519	1/1	0.97	0.18	51,51,51,51	0
57	MG	2A	3640	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3395	1/1	0.97	0.11	44,44,44,44	0
57	MG	1A	3040	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3275	1/1	0.97	0.14	36,36,36,36	0
57	MG	1A	3993	1/1	0.97	0.05	25,25,25,25	0
57	MG	1B	237	1/1	0.97	0.08	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1636	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3448	1/1	0.97	0.14	49,49,49,49	0
57	MG	1d	301	1/1	0.97	0.30	50,50,50,50	0
57	MG	1D	301	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	3115	1/1	0.97	0.12	40,40,40,40	0
57	MG	1D	303	1/1	0.97	0.08	46,46,46,46	0
57	MG	1A	3229	1/1	0.97	0.07	29,29,29,29	0
57	MG	1A	3327	1/1	0.97	0.11	55,55,55,55	0
57	MG	1D	307	1/1	0.97	0.09	33,33,33,33	0
57	MG	1m	3001	1/1	0.97	0.08	70,70,70,70	0
57	MG	1D	308	1/1	0.97	0.05	40,40,40,40	0
57	MG	1A	3527	1/1	0.97	0.13	62,62,62,62	0
57	MG	1A	3064	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3388	1/1	0.97	0.09	43,43,43,43	0
57	MG	1A	4002	1/1	0.97	0.05	52,52,52,52	0
57	MG	1A	3184	1/1	0.97	0.17	41,41,41,41	0
57	MG	1E	301	1/1	0.97	0.24	34,34,34,34	0
57	MG	1A	3033	1/1	0.97	0.06	42,42,42,42	0
57	MG	2A	3419	1/1	0.97	0.15	37,37,37,37	0
57	MG	1E	303	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3532	1/1	0.97	0.13	34,34,34,34	0
57	MG	1A	3533	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3187	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3148	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3458	1/1	0.97	0.05	40,40,40,40	0
57	MG	2A	3218	1/1	0.97	0.07	43,43,43,43	0
57	MG	2A	3219	1/1	0.97	0.15	49,49,49,49	0
57	MG	1A	3643	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3459	1/1	0.97	0.07	53,53,53,53	0
57	MG	2A	3430	1/1	0.97	0.06	41,41,41,41	0
57	MG	2A	3431	1/1	0.97	0.16	37,37,37,37	0
57	MG	2a	1601	1/1	0.97	0.19	56,56,56,56	0
57	MG	1A	3756	1/1	0.97	0.04	62,62,62,62	0
57	MG	1x	111	1/1	0.97	0.11	56,56,56,56	0
57	MG	1F	301	1/1	0.97	0.12	41,41,41,41	0
57	MG	1F	303	1/1	0.97	0.16	32,32,32,32	0
57	MG	2A	3226	1/1	0.97	0.17	54,54,54,54	0
57	MG	1A	3757	1/1	0.97	0.04	41,41,41,41	0
57	MG	1A	3083	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3461	1/1	0.97	0.12	49,49,49,49	0
57	MG	1A	3760	1/1	0.97	0.05	46,46,46,46	0
57	MG	2A	3443	1/1	0.97	0.14	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1F	311	1/1	0.97	0.10	34,34,34,34	0
57	MG	2A	3011	1/1	0.97	0.10	47,47,47,47	0
57	MG	2A	3012	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	4018	1/1	0.97	0.10	56,56,56,56	0
57	MG	1A	3648	1/1	0.97	0.04	28,28,28,28	0
57	MG	2A	3694	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3762	1/1	0.97	0.07	21,21,21,21	0
57	MG	2A	3450	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3037	1/1	0.97	0.22	32,32,32,32	0
57	MG	2A	3452	1/1	0.97	0.13	67,67,67,67	0
57	MG	2A	3453	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3019	1/1	0.97	0.23	36,36,36,36	0
57	MG	1A	3238	1/1	0.97	0.14	46,46,46,46	0
57	MG	1A	3396	1/1	0.97	0.13	44,44,44,44	0
57	MG	1A	3766	1/1	0.97	0.07	49,49,49,49	0
57	MG	2A	3459	1/1	0.97	0.17	51,51,51,51	0
57	MG	1A	3339	1/1	0.97	0.12	62,62,62,62	0
57	MG	2A	3024	1/1	0.97	0.10	43,43,43,43	0
57	MG	2A	3707	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3340	1/1	0.97	0.26	38,38,38,38	0
57	MG	2A	3464	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	4029	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3239	1/1	0.97	0.06	53,53,53,53	0
57	MG	1A	3400	1/1	0.97	0.29	55,55,55,55	0
57	MG	1A	3554	1/1	0.97	0.13	38,38,38,38	0
57	MG	1a	1681	1/1	0.97	0.17	63,63,63,63	0
57	MG	1A	3556	1/1	0.97	0.07	46,46,46,46	0
57	MG	1A	3774	1/1	0.97	0.06	60,60,60,60	0
57	MG	1A	3898	1/1	0.97	0.10	41,41,41,41	0
57	MG	2A	3034	1/1	0.97	0.08	42,42,42,42	0
57	MG	2A	3474	1/1	0.97	0.10	69,69,69,69	0
57	MG	2A	3476	1/1	0.97	0.08	62,62,62,62	0
57	MG	1A	3660	1/1	0.97	0.07	26,26,26,26	0
57	MG	2A	3255	1/1	0.97	0.08	60,60,60,60	0
57	MG	2A	3479	1/1	0.97	0.04	43,43,43,43	0
57	MG	1A	3661	1/1	0.97	0.08	34,34,34,34	0
57	MG	2A	3038	1/1	0.97	0.22	54,54,54,54	0
57	MG	1P	202	1/1	0.97	0.18	32,32,32,32	0
57	MG	1A	3288	1/1	0.97	0.07	41,41,41,41	0
57	MG	1P	204	1/1	0.97	0.17	33,33,33,33	0
57	MG	1P	205	1/1	0.97	0.24	32,32,32,32	0
57	MG	1A	3558	1/1	0.97	0.11	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1P	207	1/1	0.97	0.24	35,35,35,35	0
57	MG	2A	3046	1/1	0.97	0.04	31,31,31,31	0
57	MG	2a	1658	1/1	0.97	0.19	52,52,52,52	0
57	MG	1A	3664	1/1	0.97	0.06	27,27,27,27	0
57	MG	1Q	202	1/1	0.97	0.10	31,31,31,31	0
57	MG	2a	1661	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3559	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3905	1/1	0.97	0.11	38,38,38,38	0
57	MG	2A	3738	1/1	0.97	0.05	56,56,56,56	0
57	MG	1A	3906	1/1	0.97	0.05	49,49,49,49	0
57	MG	2A	3494	1/1	0.97	0.09	39,39,39,39	0
57	MG	1Q	207	1/1	0.97	0.06	41,41,41,41	0
57	MG	2a	1668	1/1	0.97	0.15	60,60,60,60	0
57	MG	1R	201	1/1	0.97	0.06	42,42,42,42	0
57	MG	1A	3470	1/1	0.97	0.19	38,38,38,38	0
57	MG	2A	3744	1/1	0.97	0.14	58,58,58,58	0
57	MG	2A	3745	1/1	0.97	0.06	70,70,70,70	0
57	MG	1R	203	1/1	0.97	0.13	29,29,29,29	0
57	MG	1A	3667	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3911	1/1	0.97	0.06	62,62,62,62	0
57	MG	1A	3029	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3913	1/1	0.97	0.04	35,35,35,35	0
57	MG	1A	3914	1/1	0.97	0.03	36,36,36,36	0
57	MG	1A	3563	1/1	0.97	0.12	44,44,44,44	0
57	MG	2A	3753	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3194	1/1	0.97	0.09	40,40,40,40	0
57	MG	1U	202	1/1	0.97	0.27	35,35,35,35	0
57	MG	1U	203	1/1	0.97	0.23	43,43,43,43	0
57	MG	2A	3510	1/1	0.97	0.18	58,58,58,58	0
57	MG	1A	3473	1/1	0.97	0.10	49,49,49,49	0
57	MG	2A	3070	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3197	1/1	0.97	0.12	35,35,35,35	0
57	MG	1U	206	1/1	0.97	0.17	47,47,47,47	0
57	MG	2a	1689	1/1	0.97	0.13	47,47,47,47	0
57	MG	1A	4055	1/1	0.97	0.08	42,42,42,42	0
57	MG	1A	3790	1/1	0.97	0.45	27,27,27,27	0
57	MG	1U	210	1/1	0.97	0.11	34,34,34,34	0
57	MG	2A	3290	1/1	0.97	0.13	53,53,53,53	0
57	MG	1A	4057	1/1	0.97	0.10	16,16,16,16	0
57	MG	1V	201	1/1	0.97	0.25	30,30,30,30	0
57	MG	2A	3080	1/1	0.97	0.08	56,56,56,56	0
57	MG	1a	1720	1/1	0.97	0.16	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3047	1/1	0.97	0.05	24,24,24,24	0
57	MG	1V	203	1/1	0.97	0.09	30,30,30,30	0
57	MG	1A	4060	1/1	0.97	0.05	22,22,22,22	0
57	MG	1V	205	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3674	1/1	0.97	0.08	29,29,29,29	0
57	MG	1A	4062	1/1	0.97	0.05	40,40,40,40	0
57	MG	2A	3531	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3293	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3295	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3102	1/1	0.97	0.10	33,33,33,33	0
57	MG	2A	3092	1/1	0.97	0.15	46,46,46,46	0
57	MG	2A	3093	1/1	0.97	0.09	58,58,58,58	0
57	MG	2A	3537	1/1	0.97	0.07	37,37,37,37	0
57	MG	2a	1711	1/1	0.97	0.11	60,60,60,60	0
57	MG	2A	3538	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3925	1/1	0.97	0.07	41,41,41,41	0
57	MG	2A	3787	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	4068	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3155	1/1	0.97	0.11	59,59,59,59	0
57	MG	1A	3072	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3249	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3130	1/1	0.97	0.06	41,41,41,41	0
57	MG	2a	1720	1/1	0.97	0.22	57,57,57,57	0
57	MG	2A	3100	1/1	0.97	0.04	52,52,52,52	0
57	MG	1A	3251	1/1	0.97	0.11	60,60,60,60	0
57	MG	1A	3132	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3208	1/1	0.97	0.06	38,38,38,38	0
57	MG	2a	1725	1/1	0.97	0.08	53,53,53,53	0
57	MG	1A	3687	1/1	0.97	0.03	15,15,15,15	0
57	MG	1A	3162	1/1	0.97	0.09	38,38,38,38	0
57	MG	1a	1742	1/1	0.97	0.05	49,49,49,49	0
57	MG	1a	1743	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3807	1/1	0.97	0.08	37,37,37,37	0
57	MG	2A	3109	1/1	0.97	0.14	51,51,51,51	0
57	MG	1A	3108	1/1	0.97	0.19	34,34,34,34	0
57	MG	1A	4082	1/1	0.97	0.11	45,45,45,45	0
57	MG	2a	1734	1/1	0.97	0.08	63,63,63,63	0
57	MG	1A	3584	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3691	1/1	0.97	0.13	48,48,48,48	0
57	MG	2a	1737	1/1	0.97	0.12	73,73,73,73	0
57	MG	1A	3941	1/1	0.97	0.09	42,42,42,42	0
57	MG	1a	1751	1/1	0.97	0.04	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
57	MG	1A	3488	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3211	1/1	0.97	0.21	37,37,37,37	0
57	MG	1A	3308	1/1	0.97	0.24	61,61,61,61	0
57	MG	2A	3815	1/1	0.97	0.10	65,65,65,65	0
57	MG	1A	3814	1/1	0.97	0.06	38,38,38,38	0
57	MG	2A	3122	1/1	0.97	0.07	57,57,57,57	0
57	MG	1A	3946	1/1	0.97	0.09	47,47,47,47	0
57	MG	1A	3309	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3492	1/1	0.97	0.22	32,32,32,32	0
57	MG	1A	3949	1/1	0.97	0.05	57,57,57,57	0
57	MG	2A	3127	1/1	0.97	0.08	49,49,49,49	0
57	MG	13	102	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	4094	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3257	1/1	0.97	0.16	41,41,41,41	0
57	MG	1A	3423	1/1	0.97	0.23	44,44,44,44	0
57	MG	1A	3135	1/1	0.97	0.17	45,45,45,45	0
57	MG	2A	3829	1/1	0.97	0.07	40,40,40,40	0
57	MG	15	107	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	4098	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3701	1/1	0.97	0.07	42,42,42,42	0
57	MG	2A	3583	1/1	0.97	0.14	54,54,54,54	0
57	MG	1A	3427	1/1	0.97	0.10	64,64,64,64	0
57	MG	1A	3704	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3596	1/1	0.97	0.06	45,45,45,45	0
57	MG	17	104	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3588	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3839	1/1	0.97	0.06	66,66,66,66	0
57	MG	1A	3073	1/1	0.97	0.04	27,27,27,27	0
57	MG	18	101	1/1	0.97	0.10	45,45,45,45	0
57	MG	18	102	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3501	1/1	0.97	0.07	51,51,51,51	0
57	MG	1A	3708	1/1	0.97	0.10	57,57,57,57	0
57	MG	2A	3594	1/1	0.97	0.05	37,37,37,37	0
57	MG	1B	204	1/1	0.97	0.12	51,51,51,51	0
57	MG	1A	3960	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3214	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3828	1/1	0.97	0.12	27,27,27,27	0
57	MG	1A	3431	1/1	0.97	0.16	40,40,40,40	0
57	MG	1A	3602	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3262	1/1	0.97	0.05	33,33,33,33	0
57	MG	2A	3603	1/1	0.97	0.18	63,63,63,63	0
57	MG	1A	3604	1/1	0.97	0.04	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3505	1/1	0.97	0.10	66,66,66,66	0
57	MG	2A	3606	1/1	0.97	0.14	52,52,52,52	0
57	MG	2A	3157	1/1	0.97	0.26	50,50,50,50	0
57	MG	1a	1786	1/1	0.97	0.08	52,52,52,52	0
57	MG	1a	1609	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3606	1/1	0.97	0.09	26,26,26,26	0
57	MG	1A	3607	1/1	0.97	0.07	27,27,27,27	0
57	MG	1A	3608	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3167	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3370	1/1	0.97	0.15	45,45,45,45	0
57	MG	1A	3173	1/1	0.97	0.10	24,24,24,24	0
57	MG	1A	3509	1/1	0.97	0.13	36,36,36,36	0
57	MG	1A	3265	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3375	1/1	0.97	0.36	47,47,47,47	0
57	MG	1a	1619	1/1	0.97	0.06	51,51,51,51	0
57	MG	2A	3620	1/1	0.97	0.12	54,54,54,54	0
57	MG	1A	3139	1/1	0.97	0.10	42,42,42,42	0
57	MG	1a	1799	1/1	0.97	0.07	58,58,58,58	0
57	MG	2D	305	1/1	0.97	0.13	42,42,42,42	0
57	MG	1A	3028	1/1	0.97	0.23	33,33,33,33	0
57	MG	1A	3846	1/1	0.97	0.15	38,38,38,38	0
57	MG	2A	3174	1/1	0.97	0.09	53,53,53,53	0
57	MG	2A	3175	1/1	0.97	0.14	43,43,43,43	0
57	MG	2E	303	1/1	0.97	0.17	44,44,44,44	0
57	MG	2A	3627	1/1	0.97	0.13	53,53,53,53	0
59	ZN	14	501	1/1	0.97	0.07	98,98,98,98	0
57	MG	1A	3222	1/1	0.97	0.22	33,33,33,33	0
59	ZN	2Y	501	1/1	0.97	0.06	91,91,91,91	0
57	MG	1A	3443	1/1	0.97	0.11	37,37,37,37	0
59	ZN	2n	102	1/1	0.97	0.06	88,88,88,88	0
60	SF4	1d	302	8/8	0.97	0.06	71,78,83,88	0
57	MG	2A	3035	1/1	0.98	0.13	33,33,33,33	0
57	MG	1A	3425	1/1	0.98	0.13	34,34,34,34	0
57	MG	1A	3494	1/1	0.98	0.21	42,42,42,42	0
57	MG	1A	4075	1/1	0.98	0.06	51,51,51,51	0
57	MG	2A	3186	1/1	0.98	0.05	56,56,56,56	0
57	MG	1A	3495	1/1	0.98	0.11	41,41,41,41	0
57	MG	1A	3188	1/1	0.98	0.20	28,28,28,28	0
57	MG	1A	3189	1/1	0.98	0.13	39,39,39,39	0
57	MG	1A	3005	1/1	0.98	0.06	43,43,43,43	0
57	MG	1A	3244	1/1	0.98	0.07	27,27,27,27	0
57	MG	1P	201	1/1	0.98	0.18	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3968	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	3364	1/1	0.98	0.09	27,27,27,27	0
57	MG	1A	3111	1/1	0.98	0.07	41,41,41,41	0
57	MG	2A	3049	1/1	0.98	0.07	66,66,66,66	0
57	MG	1A	3585	1/1	0.98	0.07	48,48,48,48	0
57	MG	2A	3499	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3144	1/1	0.98	0.05	35,35,35,35	0
57	MG	2A	3052	1/1	0.98	0.06	50,50,50,50	0
57	MG	2A	3502	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3768	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3868	1/1	0.98	0.03	40,40,40,40	0
57	MG	1A	3869	1/1	0.98	0.07	41,41,41,41	0
57	MG	1Q	203	1/1	0.98	0.09	45,45,45,45	0
57	MG	2A	3057	1/1	0.98	0.07	42,42,42,42	0
57	MG	1A	3247	1/1	0.98	0.17	34,34,34,34	0
57	MG	1A	3045	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3024	1/1	0.98	0.10	41,41,41,41	0
57	MG	1A	3438	1/1	0.98	0.23	55,55,55,55	0
57	MG	1A	3591	1/1	0.98	0.07	37,37,37,37	0
57	MG	1A	3679	1/1	0.98	0.05	43,43,43,43	0
57	MG	1A	3196	1/1	0.98	0.06	35,35,35,35	0
57	MG	1A	3036	1/1	0.98	0.26	35,35,35,35	0
57	MG	2A	3843	1/1	0.98	0.08	57,57,57,57	0
57	MG	2A	3214	1/1	0.98	0.52	44,44,44,44	0
57	MG	1A	3777	1/1	0.98	0.04	22,22,22,22	0
57	MG	1A	3778	1/1	0.98	0.05	45,45,45,45	0
57	MG	2A	3068	1/1	0.98	0.05	55,55,55,55	0
57	MG	2A	3520	1/1	0.98	0.07	48,48,48,48	0
57	MG	1A	3373	1/1	0.98	0.18	29,29,29,29	0
57	MG	1A	3008	1/1	0.98	0.10	25,25,25,25	0
57	MG	2A	3071	1/1	0.98	0.05	40,40,40,40	0
57	MG	2A	3524	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3017	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3990	1/1	0.98	0.10	52,52,52,52	0
57	MG	1U	201	1/1	0.98	0.29	35,35,35,35	0
57	MG	1A	3200	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	3117	1/1	0.98	0.11	39,39,39,39	0
57	MG	1A	3886	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3887	1/1	0.98	0.09	34,34,34,34	0
57	MG	1A	3599	1/1	0.98	0.05	50,50,50,50	0
57	MG	1A	3050	1/1	0.98	0.07	28,28,28,28	0
57	MG	1A	3119	1/1	0.98	0.24	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3094	1/1	0.98	0.06	44,44,44,44	0
57	MG	1A	3205	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	3206	1/1	0.98	0.16	41,41,41,41	0
57	MG	1A	3694	1/1	0.98	0.03	28,28,28,28	0
57	MG	1A	3520	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3383	1/1	0.98	0.13	30,30,30,30	0
57	MG	1A	3261	1/1	0.98	0.12	38,38,38,38	0
57	MG	1A	3207	1/1	0.98	0.15	32,32,32,32	0
57	MG	1A	3121	1/1	0.98	0.16	33,33,33,33	0
57	MG	2D	301	1/1	0.98	0.21	40,40,40,40	0
57	MG	1A	3156	1/1	0.98	0.18	31,31,31,31	0
57	MG	1A	3122	1/1	0.98	0.21	33,33,33,33	0
57	MG	2D	304	1/1	0.98	0.05	26,26,26,26	0
57	MG	1W	203	1/1	0.98	0.10	35,35,35,35	0
57	MG	1A	3266	1/1	0.98	0.12	39,39,39,39	0
57	MG	1A	3123	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3124	1/1	0.98	0.11	36,36,36,36	0
57	MG	1a	1804	1/1	0.98	0.04	61,61,61,61	0
57	MG	1A	3095	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	3096	1/1	0.98	0.07	52,52,52,52	0
57	MG	1A	3804	1/1	0.98	0.07	42,42,42,42	0
57	MG	1A	3215	1/1	0.98	0.18	45,45,45,45	0
57	MG	1A	3273	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	4019	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3164	1/1	0.98	0.17	43,43,43,43	0
57	MG	2A	3720	1/1	0.98	0.07	49,49,49,49	0
57	MG	1A	3535	1/1	0.98	0.05	32,32,32,32	0
57	MG	2A	3559	1/1	0.98	0.06	39,39,39,39	0
57	MG	1A	3334	1/1	0.98	0.21	38,38,38,38	0
57	MG	2A	3561	1/1	0.98	0.12	59,59,59,59	0
57	MG	1A	3335	1/1	0.98	0.18	38,38,38,38	0
57	MG	10	101	1/1	0.98	0.04	45,45,45,45	0
57	MG	1A	3013	1/1	0.98	0.06	23,23,23,23	0
57	MG	2A	3112	1/1	0.98	0.11	33,33,33,33	0
57	MG	1A	3080	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3625	1/1	0.98	0.08	57,57,57,57	0
57	MG	2A	3115	1/1	0.98	0.07	54,54,54,54	0
57	MG	1A	3626	1/1	0.98	0.10	43,43,43,43	0
57	MG	1A	3540	1/1	0.98	0.16	36,36,36,36	0
57	MG	1A	3720	1/1	0.98	0.06	53,53,53,53	0
57	MG	1A	3277	1/1	0.98	0.10	43,43,43,43	0
57	MG	1k	201	1/1	0.98	0.07	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	4032	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	3020	1/1	0.98	0.06	26,26,26,26	0
57	MG	2A	3417	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3169	1/1	0.98	0.15	33,33,33,33	0
57	MG	1A	3545	1/1	0.98	0.17	38,38,38,38	0
57	MG	1D	305	1/1	0.98	0.05	20,20,20,20	0
57	MG	1r	101	1/1	0.98	0.10	65,65,65,65	0
57	MG	1A	3926	1/1	0.98	0.05	57,57,57,57	0
57	MG	1A	3223	1/1	0.98	0.23	30,30,30,30	0
57	MG	1A	3405	1/1	0.98	0.08	42,42,42,42	0
57	MG	1A	3727	1/1	0.98	0.06	27,27,27,27	0
57	MG	1A	3548	1/1	0.98	0.14	31,31,31,31	0
57	MG	1w	401	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3224	1/1	0.98	0.17	51,51,51,51	0
57	MG	1A	3172	1/1	0.98	0.15	31,31,31,31	0
57	MG	2A	3135	1/1	0.98	0.15	57,57,57,57	0
57	MG	1A	3552	1/1	0.98	0.11	43,43,43,43	0
57	MG	1A	3100	1/1	0.98	0.05	33,33,33,33	0
57	MG	16	101	1/1	0.98	0.09	46,46,46,46	0
57	MG	25	103	1/1	0.98	0.13	46,46,46,46	0
57	MG	2A	3434	1/1	0.98	0.11	49,49,49,49	0
57	MG	2A	3139	1/1	0.98	0.08	36,36,36,36	0
57	MG	2A	3758	1/1	0.98	0.04	56,56,56,56	0
57	MG	1A	3131	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	3065	1/1	0.98	0.03	32,32,32,32	0
57	MG	17	102	1/1	0.98	0.07	30,30,30,30	0
57	MG	2A	3600	1/1	0.98	0.16	65,65,65,65	0
57	MG	1A	3021	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3134	1/1	0.98	0.20	34,34,34,34	0
57	MG	2A	3765	1/1	0.98	0.12	40,40,40,40	0
57	MG	1A	3104	1/1	0.98	0.14	42,42,42,42	0
57	MG	1E	307	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3350	1/1	0.98	0.14	38,38,38,38	0
57	MG	1E	309	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3561	1/1	0.98	0.11	39,39,39,39	0
57	MG	1A	3067	1/1	0.98	0.10	31,31,31,31	0
57	MG	1A	3233	1/1	0.98	0.12	33,33,33,33	0
57	MG	2a	1609	1/1	0.98	0.29	68,68,68,68	0
57	MG	2A	3152	1/1	0.98	0.17	47,47,47,47	0
57	MG	2A	3006	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3650	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3008	1/1	0.98	0.14	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3009	1/1	0.98	0.03	40,40,40,40	0
57	MG	2A	3010	1/1	0.98	0.06	45,45,45,45	0
57	MG	1A	3180	1/1	0.98	0.04	37,37,37,37	0
57	MG	1F	302	1/1	0.98	0.17	34,34,34,34	0
57	MG	2A	3457	1/1	0.98	0.06	25,25,25,25	0
57	MG	1A	3181	1/1	0.98	0.09	42,42,42,42	0
57	MG	1F	304	1/1	0.98	0.22	32,32,32,32	0
57	MG	1A	3566	1/1	0.98	0.11	46,46,46,46	0
57	MG	2A	3016	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	4058	1/1	0.98	0.10	32,32,32,32	0
57	MG	2A	3018	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	3137	1/1	0.98	0.12	34,34,34,34	0
57	MG	1A	3107	1/1	0.98	0.07	33,33,33,33	0
57	MG	2A	3315	1/1	0.98	0.11	47,47,47,47	0
57	MG	1F	309	1/1	0.98	0.03	36,36,36,36	0
57	MG	1F	310	1/1	0.98	0.25	28,28,28,28	0
57	MG	1A	3570	1/1	0.98	0.08	39,39,39,39	0
57	MG	1A	3657	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3847	1/1	0.98	0.26	37,37,37,37	0
57	MG	1A	3751	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3849	1/1	0.98	0.20	36,36,36,36	0
57	MG	2a	1635	1/1	0.98	0.05	47,47,47,47	0
57	MG	2A	3475	1/1	0.98	0.08	59,59,59,59	0
57	MG	2A	3799	1/1	0.98	0.05	52,52,52,52	0
57	MG	1A	3043	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3186	1/1	0.98	0.10	39,39,39,39	0
57	MG	1A	3109	1/1	0.98	0.05	28,28,28,28	0
57	MG	1a	1745	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3424	1/1	0.98	0.18	47,47,47,47	0
57	MG	1A	4071	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	3575	1/1	0.98	0.05	22,22,22,22	0
60	SF4	2d	302	8/8	0.98	0.06	69,73,83,84	0
57	MG	1A	3713	1/1	0.99	0.04	44,44,44,44	0
57	MG	1A	3003	1/1	0.99	0.03	23,23,23,23	0
57	MG	1A	3857	1/1	0.99	0.11	37,37,37,37	0
57	MG	1N	203	1/1	0.99	0.03	34,34,34,34	0
57	MG	2A	3680	1/1	0.99	0.06	35,35,35,35	0
57	MG	2A	3460	1/1	0.99	0.04	28,28,28,28	0
57	MG	1A	3908	1/1	0.99	0.06	47,47,47,47	0
57	MG	1A	3909	1/1	0.99	0.02	14,14,14,14	0
57	MG	1A	3012	1/1	0.99	0.03	33,33,33,33	0
57	MG	1A	4020	1/1	0.99	0.03	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3686	1/1	0.99	0.04	50,50,50,50	0
57	MG	2A	3045	1/1	0.99	0.11	42,42,42,42	0
57	MG	1A	3034	1/1	0.99	0.08	38,38,38,38	0
57	MG	1A	3294	1/1	0.99	0.07	23,23,23,23	0
57	MG	1A	3035	1/1	0.99	0.08	24,24,24,24	0
57	MG	1A	3018	1/1	0.99	0.05	43,43,43,43	0
57	MG	1A	3297	1/1	0.99	0.03	30,30,30,30	0
57	MG	1A	3076	1/1	0.99	0.06	27,27,27,27	0
57	MG	1A	3551	1/1	0.99	0.17	43,43,43,43	0
57	MG	1A	3437	1/1	0.99	0.07	49,49,49,49	0
57	MG	1A	3077	1/1	0.99	0.10	42,42,42,42	0
57	MG	1A	3333	1/1	0.99	0.18	38,38,38,38	0
57	MG	1A	3680	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	3637	1/1	0.99	0.09	37,37,37,37	0
57	MG	1A	3555	1/1	0.99	0.17	32,32,32,32	0
57	MG	1A	3153	1/1	0.99	0.19	35,35,35,35	0
57	MG	1D	311	1/1	0.99	0.10	30,30,30,30	0
57	MG	15	102	1/1	0.99	0.20	28,28,28,28	0
57	MG	1A	3009	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	3269	1/1	0.99	0.20	38,38,38,38	0
57	MG	15	105	1/1	0.99	0.12	29,29,29,29	0
57	MG	1a	1713	1/1	0.99	0.23	46,46,46,46	0
57	MG	15	106	1/1	0.99	0.11	38,38,38,38	0
57	MG	2A	3205	1/1	0.99	0.11	54,54,54,54	0
57	MG	1A	3371	1/1	0.99	0.20	28,28,28,28	0
57	MG	1A	3014	1/1	0.99	0.03	28,28,28,28	0
57	MG	1A	3182	1/1	0.99	0.09	32,32,32,32	0
57	MG	1A	3645	1/1	0.99	0.06	22,22,22,22	0
57	MG	2A	3564	1/1	0.99	0.03	29,29,29,29	0
57	MG	2A	3565	1/1	0.99	0.05	48,48,48,48	0
57	MG	1A	3007	1/1	0.99	0.03	36,36,36,36	0
57	MG	2A	3072	1/1	0.99	0.06	31,31,31,31	0
57	MG	1A	3880	1/1	0.99	0.07	45,45,45,45	0
57	MG	1A	3986	1/1	0.99	0.05	38,38,38,38	0
57	MG	1A	3157	1/1	0.99	0.08	31,31,31,31	0
57	MG	1A	3158	1/1	0.99	0.08	25,25,25,25	0
57	MG	1A	3081	1/1	0.99	0.05	29,29,29,29	0
57	MG	1A	3834	1/1	0.99	0.10	58,58,58,58	0
57	MG	1A	3937	1/1	0.99	0.04	52,52,52,52	0
57	MG	2A	3801	1/1	0.99	0.05	50,50,50,50	0
57	MG	1A	3052	1/1	0.99	0.05	49,49,49,49	0
57	MG	1A	3216	1/1	0.99	0.06	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3217	1/1	0.99	0.08	33,33,33,33	0
57	MG	1U	208	1/1	0.99	0.08	36,36,36,36	0
57	MG	1A	3569	1/1	0.99	0.09	39,39,39,39	0
57	MG	1A	3996	1/1	0.99	0.02	33,33,33,33	0
57	MG	2A	3086	1/1	0.99	0.14	34,34,34,34	0
57	MG	2A	3809	1/1	0.99	0.04	38,38,38,38	0
57	MG	1A	3138	1/1	0.99	0.04	17,17,17,17	0
57	MG	1a	1734	1/1	0.99	0.06	42,42,42,42	0
57	MG	2A	3438	1/1	0.99	0.09	23,23,23,23	0
57	MG	1A	3022	1/1	0.99	0.05	17,17,17,17	0
57	MG	1A	3030	1/1	0.99	0.14	26,26,26,26	0
57	MG	1A	3794	1/1	0.99	0.03	24,24,24,24	0
57	MG	1A	3068	1/1	0.99	0.03	17,17,17,17	0
57	MG	2A	3817	1/1	0.99	0.04	25,25,25,25	0
57	MG	1A	3103	1/1	0.99	0.04	23,23,23,23	0
57	MG	1A	3703	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	4004	1/1	0.99	0.03	56,56,56,56	0
57	MG	1A	3042	1/1	0.99	0.11	42,42,42,42	0
57	MG	1A	4063	1/1	0.99	0.04	31,31,31,31	0
57	MG	1A	3031	1/1	0.99	0.12	31,31,31,31	0
59	ZN	1Y	205	1/1	0.99	0.03	58,58,58,58	0
57	MG	1A	3497	1/1	0.99	0.10	35,35,35,35	0
59	ZN	15	110	1/1	0.99	0.03	47,47,47,47	0
59	ZN	16	103	1/1	0.99	0.05	44,44,44,44	0
59	ZN	19	102	1/1	0.99	0.06	44,44,44,44	0
57	MG	1A	3195	1/1	0.99	0.15	25,25,25,25	0
57	MG	1A	3168	1/1	0.99	0.06	28,28,28,28	0
57	MG	1A	3106	1/1	0.99	0.13	30,30,30,30	0
59	ZN	25	108	1/1	0.99	0.03	58,58,58,58	0
59	ZN	26	102	1/1	0.99	0.04	64,64,64,64	0
59	ZN	29	102	1/1	0.99	0.05	68,68,68,68	0
57	MG	1A	3170	1/1	0.99	0.07	37,37,37,37	0
57	MG	1A	3171	1/1	0.99	0.05	25,25,25,25	0
57	MG	1A	3428	1/1	0.99	0.05	43,43,43,43	0
57	MG	1A	3733	1/1	1.00	0.07	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.