



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:06 PM UTC

PDB ID : 8CVL / pdb_00008cvl
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Phe-NH-tRNA^{phe}, peptidyl P-site fMTTHSMRC-NH-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.30Å resolution
Authors : Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
Deposited on : 2022-05-18
Resolution : 2.30 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

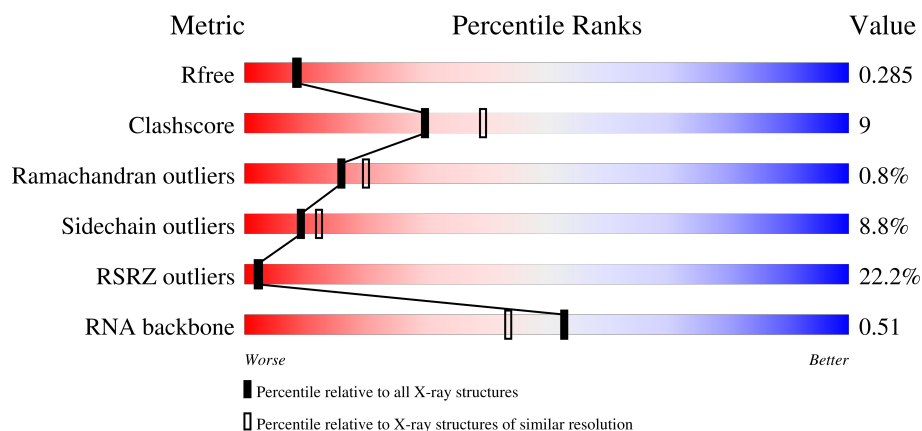
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)
RNA backbone	3983	1090 (2.60-2.00)

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	54% 58% 34% 7%
40	2i	128	73% 52% 45% ..
41	1j	105	45% 56% 32% 8%
41	2j	105	71% 50% 38% 9%
42	1k	129	30% 67% 19% 12%
42	2k	129	52% 59% 27% 12%
43	1l	132	17% 73% 19% 8%
43	2l	132	28% 71% 19% 8%
44	1m	126	34% 59% 33% 6%
44	2m	126	56% 59% 34% ..
45	1n	61	39% 80% 16% ..
45	2n	61	85% 59% 38% ..
46	1o	89	33% 69% 27% ..
46	2o	89	72% 67% 28% ..
47	1p	88	68% 70% 20% 7%
47	2p	88	50% 66% 24% 7%
48	1q	105	39% 74% 18% 6%
48	2q	105	50% 72% 20% 6%
49	1r	88	9% 65% 13% 23%
49	2r	88	40% 45% 30% 23%
50	1s	93	39% 59% 27% 11%
50	2s	93	52% 39% 43% 6%
51	1t	106	47% 58% 28% 9%
51	2t	106	35% 66% 23% 9%
52	1u	27	48% 67% 15% 15%

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	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1z	7	
56	2z	7	
57	1y	76	
57	2y	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	MG	1A	3442	-	-	-	X
58	MG	1a	1742	-	-	-	X
58	MG	2A	3156	-	-	-	X
58	MG	2n	101	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299898 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Phe-NH-tRNA_{Phe}.

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

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA_{met} RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA_{met} Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	7	Total	C	N	O	S	0	0	0
			58	33	12	10	3			
56	2z	7	Total	C	N	O	S	0	0	0
			58	33	12	10	3			

- Molecule 57 is a RNA chain called E-site Deacylated tRNA_{Phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
57	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1101	Total Mg 1101 1101	0	0
58	1B	38	Total Mg 38 38	0	0
58	1D	13	Total Mg 13 13	0	0
58	1E	12	Total Mg 12 12	0	0
58	1F	12	Total Mg 12 12	0	0
58	1G	5	Total Mg 5 5	0	0
58	1H	1	Total Mg 1 1	0	0
58	1I	1	Total Mg 1 1	0	0
58	1N	5	Total Mg 5 5	0	0
58	1O	5	Total Mg 5 5	0	0
58	1P	7	Total Mg 7 7	0	0
58	1Q	8	Total Mg 8 8	0	0
58	1R	4	Total Mg 4 4	0	0
58	1S	3	Total Mg 3 3	0	0
58	1T	2	Total Mg 2 2	0	0
58	1U	10	Total Mg 10 10	0	0
58	1V	7	Total Mg 7 7	0	0
58	1W	4	Total Mg 4 4	0	0
58	1X	4	Total Mg 4 4	0	0
58	1Y	4	Total Mg 4 4	0	0
58	1Z	4	Total Mg 4 4	0	0
58	10	9	Total Mg 9 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	11	6	Total 6	Mg 6	0	0
58	12	2	Total 2	Mg 2	0	0
58	13	4	Total 4	Mg 4	0	0
58	14	1	Total 1	Mg 1	0	0
58	15	7	Total 7	Mg 7	0	0
58	16	1	Total 1	Mg 1	0	0
58	17	5	Total 5	Mg 5	0	0
58	18	7	Total 7	Mg 7	0	0
58	19	1	Total 1	Mg 1	0	0
58	1a	210	Total 210	Mg 210	0	0
58	1b	1	Total 1	Mg 1	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	2	Total 2	Mg 2	0	0
58	1f	2	Total 2	Mg 2	0	0
58	1l	2	Total 2	Mg 2	0	0
58	1m	1	Total 1	Mg 1	0	0
58	1n	2	Total 2	Mg 2	0	0
58	1t	1	Total 1	Mg 1	0	0
58	1w	7	Total 7	Mg 7	0	0
58	1x	12	Total 12	Mg 12	0	0
58	2A	851	Total 851	Mg 851	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2B	20	Total 20	Mg 20	0	0
58	2D	7	Total 7	Mg 7	0	0
58	2E	10	Total 10	Mg 10	0	0
58	2F	6	Total 6	Mg 6	0	0
58	2G	1	Total 1	Mg 1	0	0
58	2N	1	Total 1	Mg 1	0	0
58	2O	2	Total 2	Mg 2	0	0
58	2P	2	Total 2	Mg 2	0	0
58	2Q	4	Total 4	Mg 4	0	0
58	2R	4	Total 4	Mg 4	0	0
58	2T	4	Total 4	Mg 4	0	0
58	2U	1	Total 1	Mg 1	0	0
58	2V	2	Total 2	Mg 2	0	0
58	2W	1	Total 1	Mg 1	0	0
58	2X	1	Total 1	Mg 1	0	0
58	2Y	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	2	Total 2	Mg 2	0	0
58	21	1	Total 1	Mg 1	0	0
58	23	3	Total 3	Mg 3	0	0
58	25	3	Total 3	Mg 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	27	2	Total Mg 2 2	0	0
58	28	4	Total Mg 4 4	0	0
58	29	1	Total Mg 1 1	0	0
58	2a	220	Total Mg 220 220	0	0
58	2d	3	Total Mg 3 3	0	0
58	2e	1	Total Mg 1 1	0	0
58	2f	2	Total Mg 2 2	0	0
58	2i	1	Total Mg 1 1	0	0
58	2j	2	Total Mg 2 2	0	0
58	2k	1	Total Mg 1 1	0	0
58	2l	3	Total Mg 3 3	0	0
58	2n	1	Total Mg 1 1	0	0
58	2q	3	Total Mg 3 3	0	0
58	2r	1	Total Mg 1 1	0	0
58	2t	2	Total Mg 2 2	0	0
58	2v	4	Total Mg 4 4	0	0
58	2w	4	Total Mg 4 4	0	0
58	2x	6	Total Mg 6 6	0	0

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total K 1 1	0	0

Continued on next page...

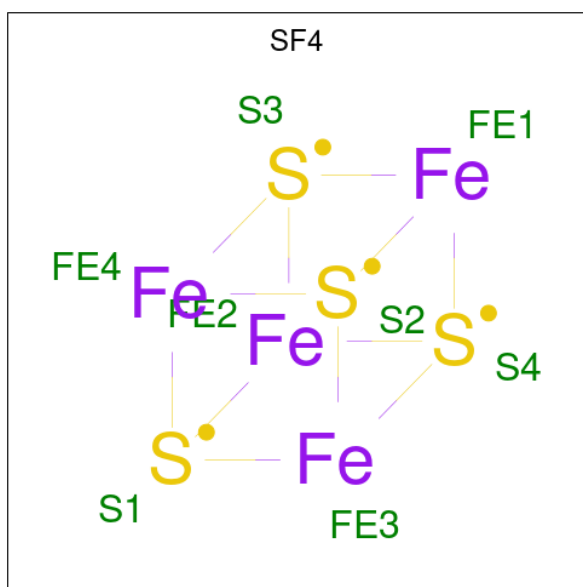
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2A	1	Total K 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1949	Total	O	0	0
			1949	1949		
62	1B	58	Total	O	0	0
			58	58		
62	1D	26	Total	O	0	0
			26	26		
62	1E	28	Total	O	0	0
			28	28		
62	1F	18	Total	O	0	0
			18	18		
62	1G	3	Total	O	0	0
			3	3		
62	1H	2	Total	O	0	0
			2	2		
62	1N	6	Total	O	0	0
			6	6		
62	1O	6	Total	O	0	0
			6	6		
62	1P	19	Total	O	0	0
			19	19		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1Q	7	Total 7	O 7	0	0
62	1R	10	Total 10	O 10	0	0
62	1S	4	Total 4	O 4	0	0
62	1T	7	Total 7	O 7	0	0
62	1U	13	Total 13	O 13	0	0
62	1V	9	Total 9	O 9	0	0
62	1W	7	Total 7	O 7	0	0
62	1X	5	Total 5	O 5	0	0
62	1Y	3	Total 3	O 3	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	13	Total 13	O 13	0	0
62	11	7	Total 7	O 7	0	0
62	12	3	Total 3	O 3	0	0
62	13	6	Total 6	O 6	0	0
62	15	8	Total 8	O 8	0	0
62	16	2	Total 2	O 2	0	0
62	17	8	Total 8	O 8	0	0
62	18	12	Total 12	O 12	0	0
62	1a	301	Total 301	O 301	0	0
62	1b	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1f	1	Total 1	O 1	0	0
62	1i	1	Total 1	O 1	0	0
62	1l	5	Total 5	O 5	0	0
62	1m	1	Total 1	O 1	0	0
62	1o	2	Total 2	O 2	0	0
62	1q	2	Total 2	O 2	0	0
62	1v	5	Total 5	O 5	0	0
62	1w	9	Total 9	O 9	0	0
62	1x	7	Total 7	O 7	0	0
62	1z	3	Total 3	O 3	0	0
62	2A	1047	Total 1047	O 1047	0	0
62	2B	20	Total 20	O 20	0	0
62	2D	26	Total 26	O 26	0	0
62	2E	15	Total 15	O 15	0	0
62	2F	14	Total 14	O 14	0	0
62	2N	1	Total 1	O 1	0	0
62	2O	2	Total 2	O 2	0	0
62	2P	10	Total 10	O 10	0	0
62	2Q	2	Total 2	O 2	0	0
62	2R	3	Total 3	O 3	0	0
62	2T	6	Total 6	O 6	0	0

Continued on next page...

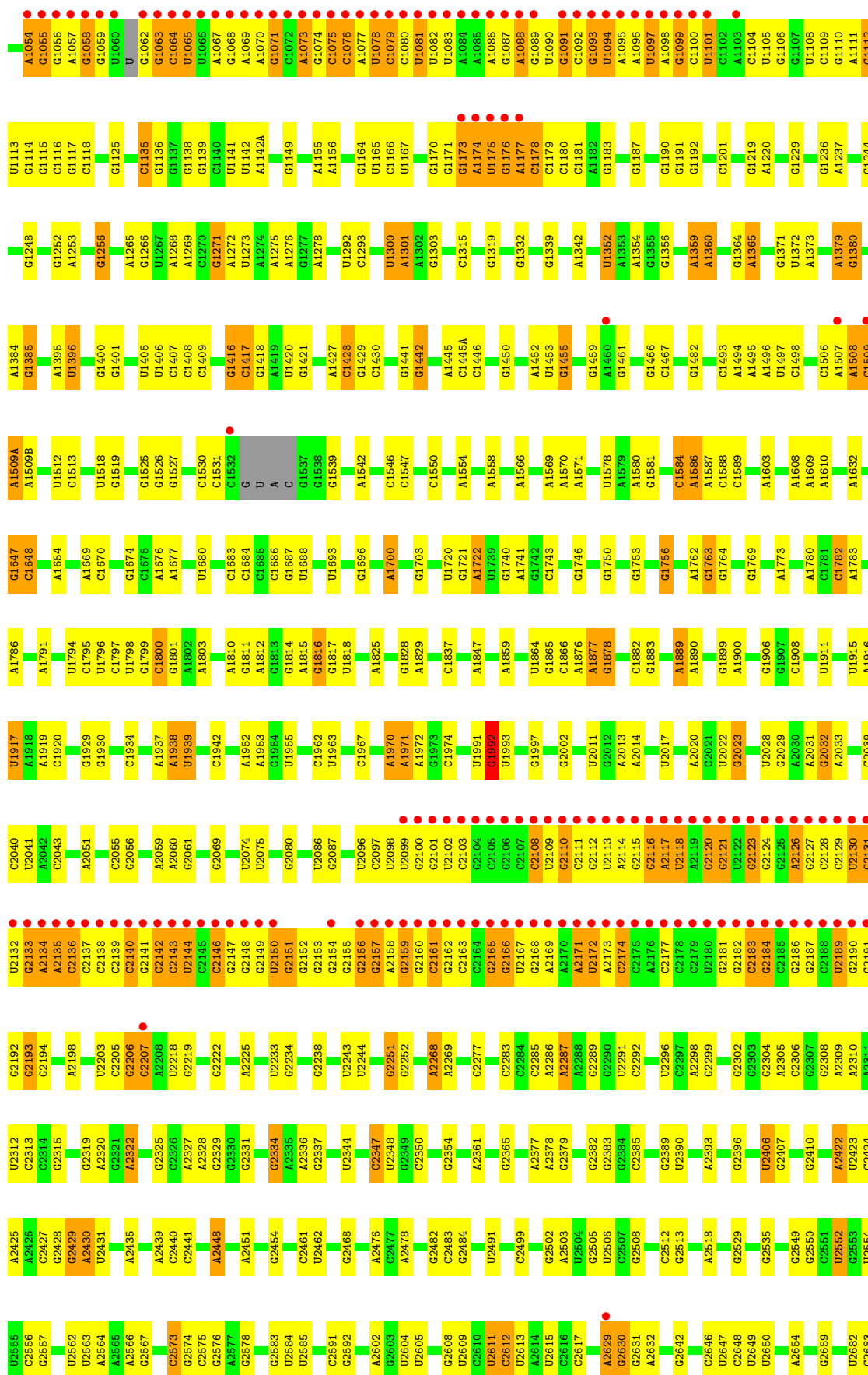
Continued from previous page...

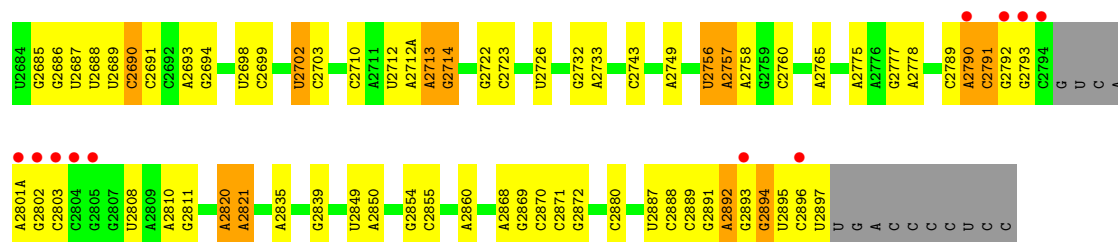
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2U	1	Total 1	O 1	0	0
62	2V	1	Total 1	O 1	0	0
62	2W	3	Total 3	O 3	0	0
62	2X	5	Total 5	O 5	0	0
62	20	2	Total 2	O 2	0	0
62	21	7	Total 7	O 7	0	0
62	22	1	Total 1	O 1	0	0
62	23	2	Total 2	O 2	0	0
62	25	2	Total 2	O 2	0	0
62	27	5	Total 5	O 5	0	0
62	28	3	Total 3	O 3	0	0
62	29	1	Total 1	O 1	0	0
62	2a	196	Total 196	O 196	0	0
62	2c	1	Total 1	O 1	0	0
62	2d	1	Total 1	O 1	0	0
62	2e	2	Total 2	O 2	0	0
62	2g	1	Total 1	O 1	0	0
62	2i	1	Total 1	O 1	0	0
62	2j	2	Total 2	O 2	0	0
62	2l	5	Total 5	O 5	0	0
62	2r	1	Total 1	O 1	0	0

Continued on next page...

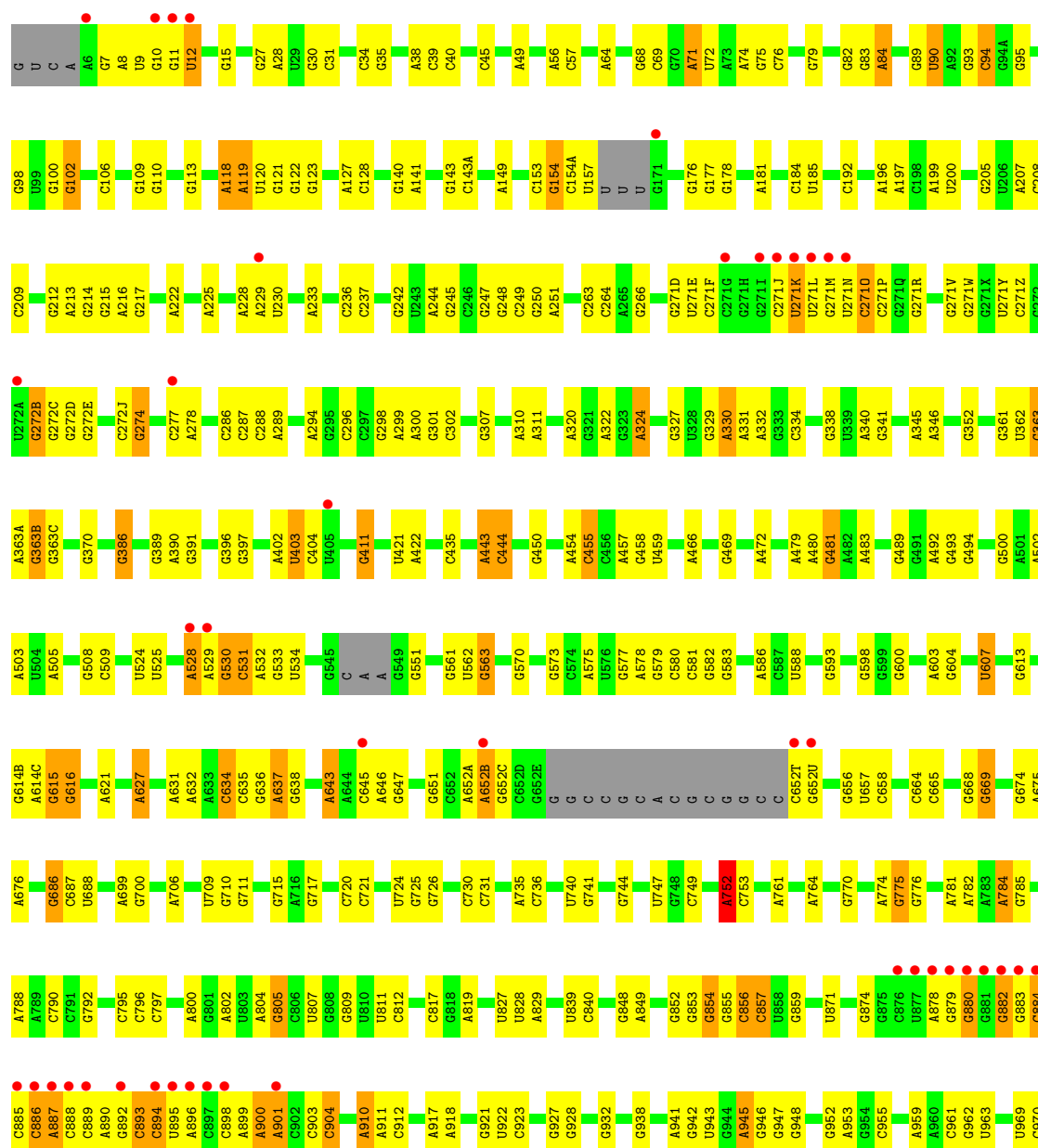
Continued from previous page...

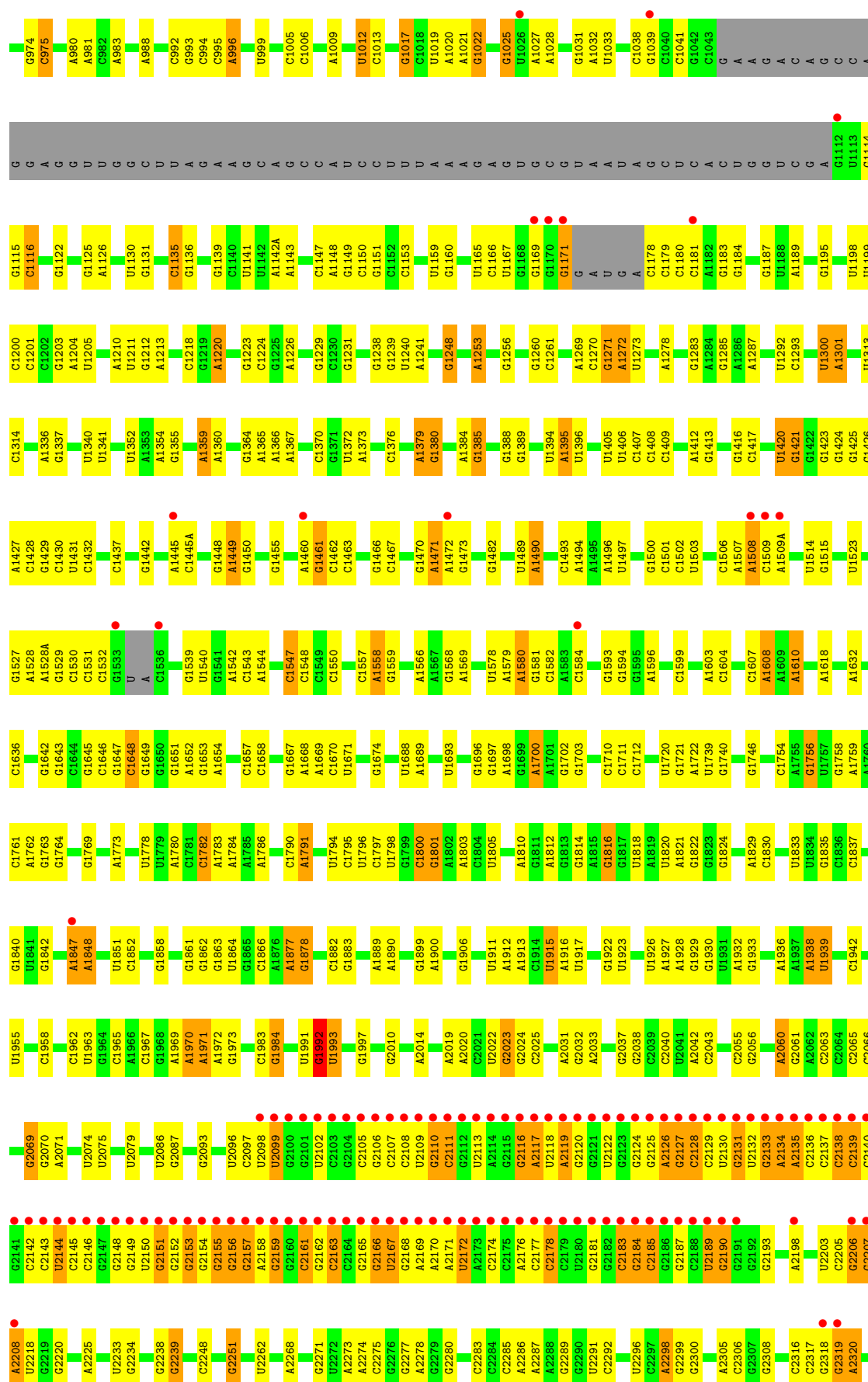
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2t	1	Total 1	O 1	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	6	Total 6	O 6	0	0
62	2x	4	Total 4	O 4	0	0
62	2z	1	Total 1	O 1	0	0

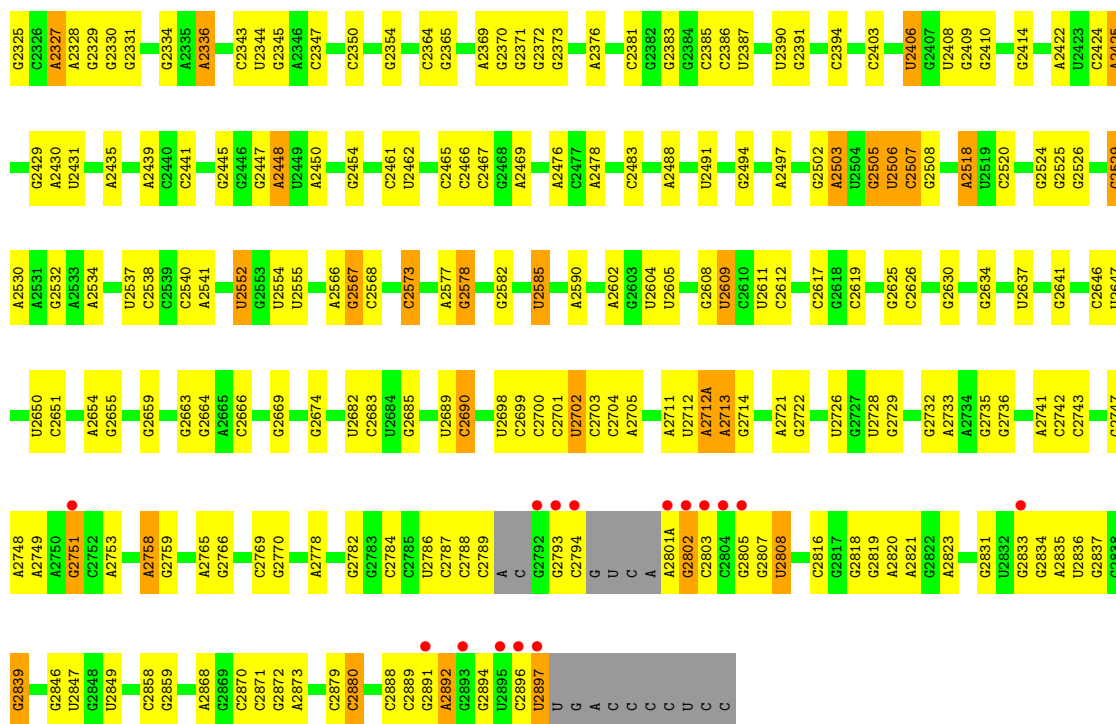




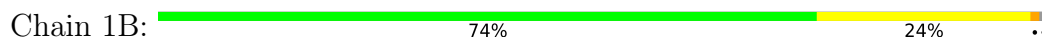
● Molecule 1: 23S Ribosomal RNA



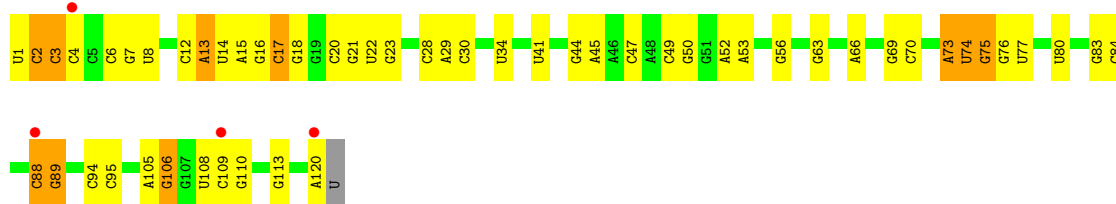




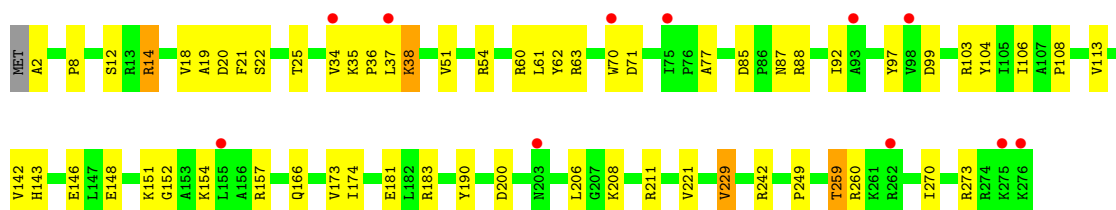
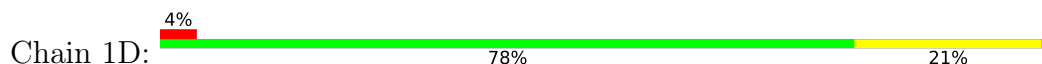
• Molecule 2: 5S Ribosomal RNA



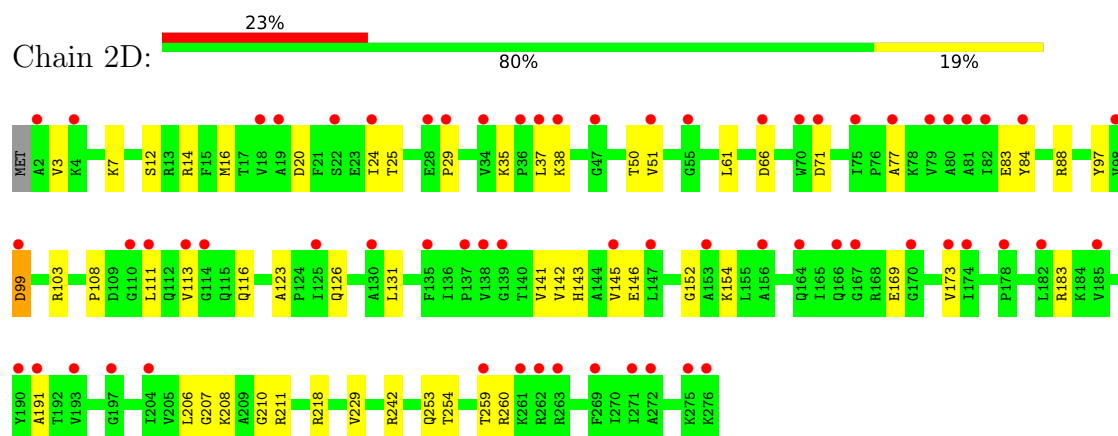
• Molecule 2: 5S Ribosomal RNA



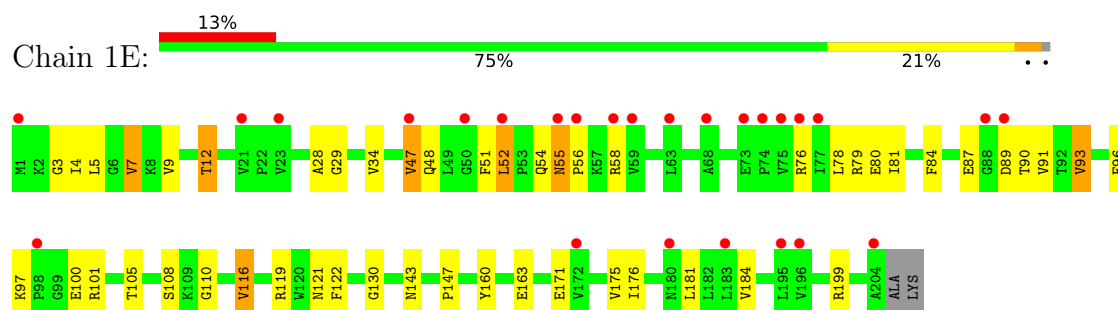
• Molecule 3: 50S ribosomal protein L2



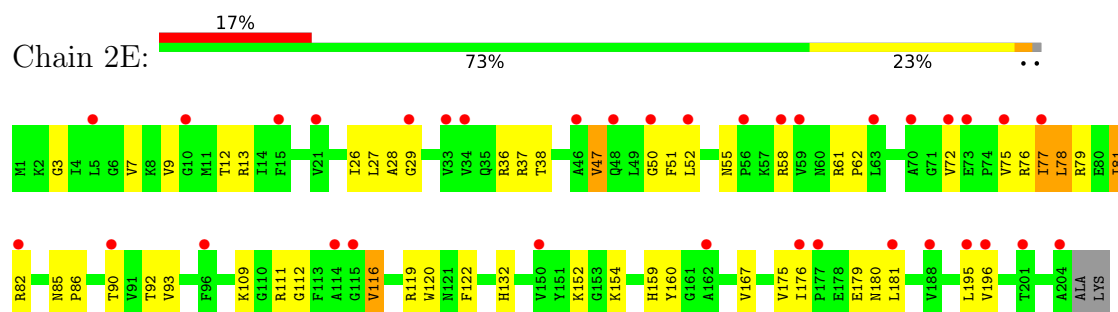
- Molecule 3: 50S ribosomal protein L2



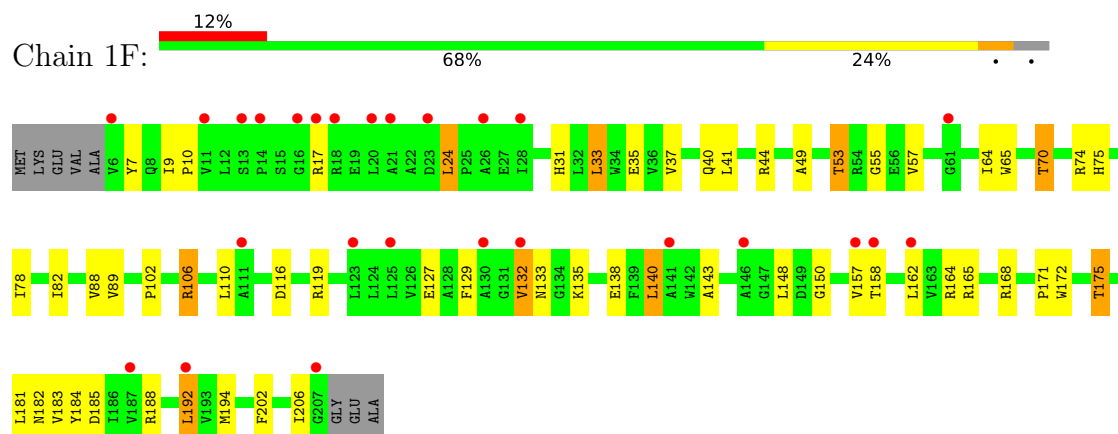
- Molecule 4: 50S ribosomal protein L3



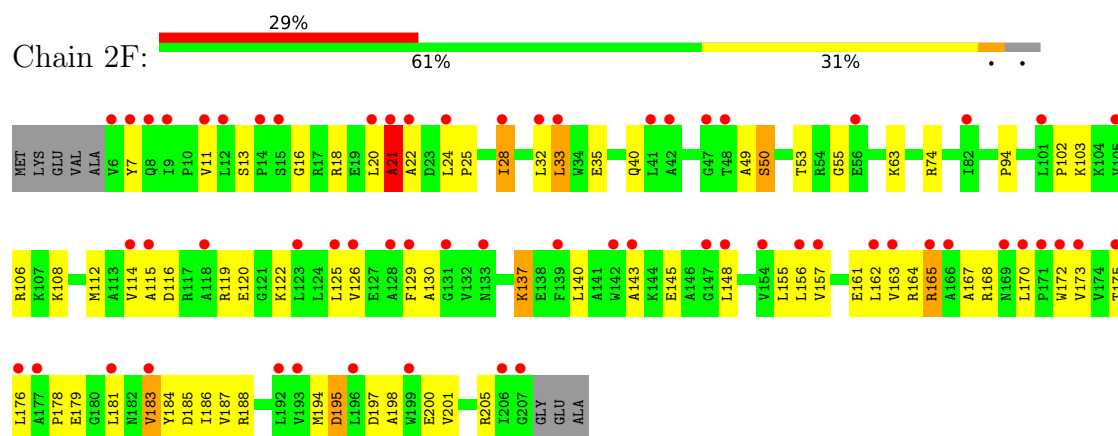
- Molecule 4: 50S ribosomal protein L3



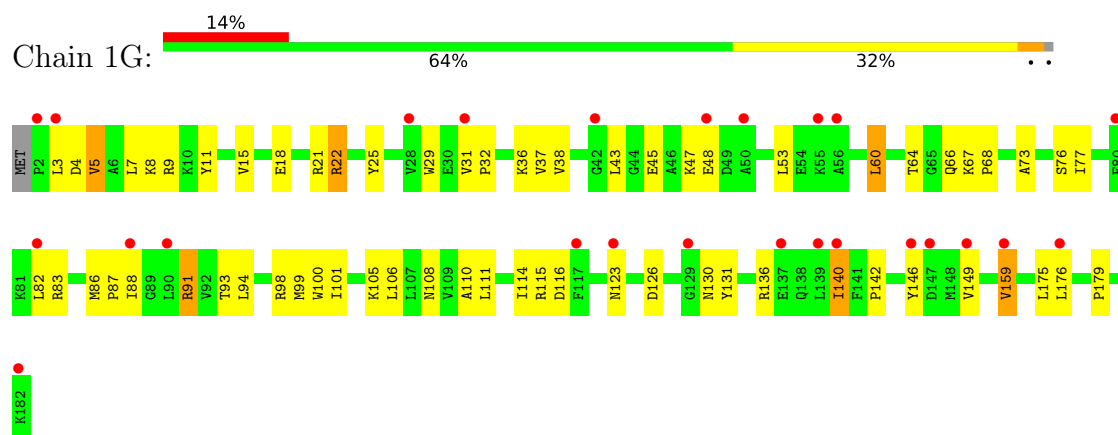
- Molecule 5: 50S ribosomal protein L4



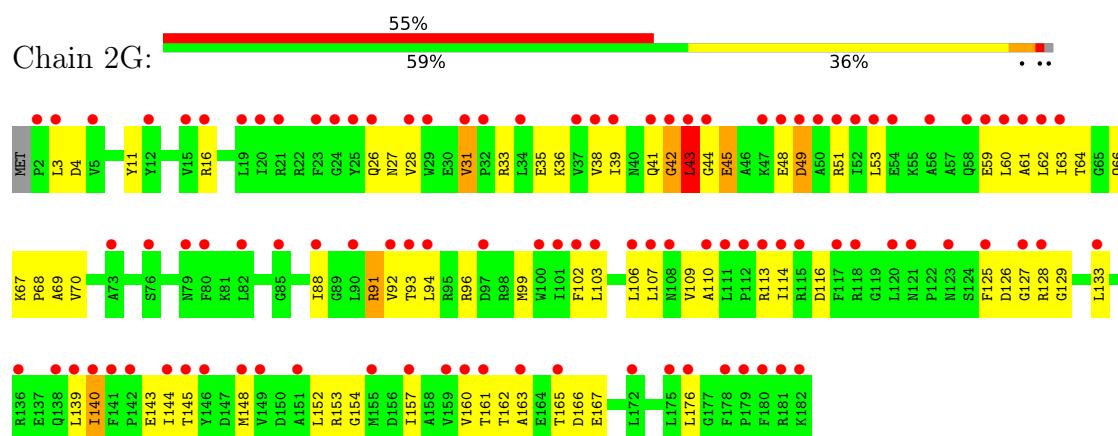
- Molecule 5: 50S ribosomal protein L4



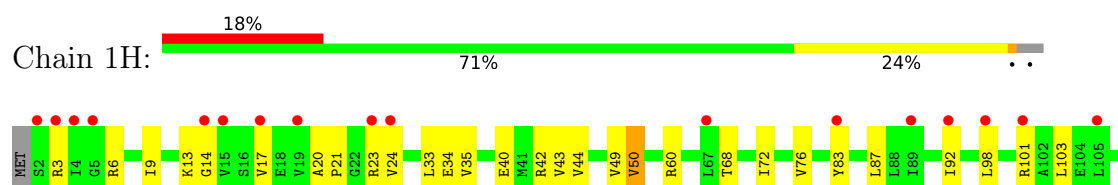
- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5

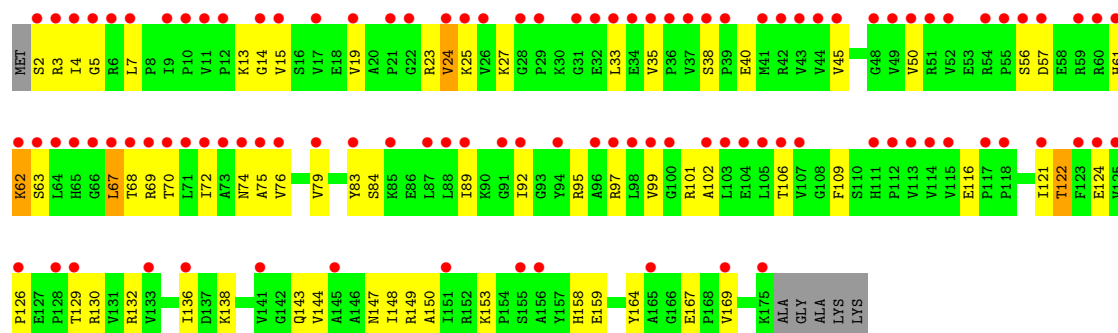


- Molecule 7: 50S ribosomal protein L6

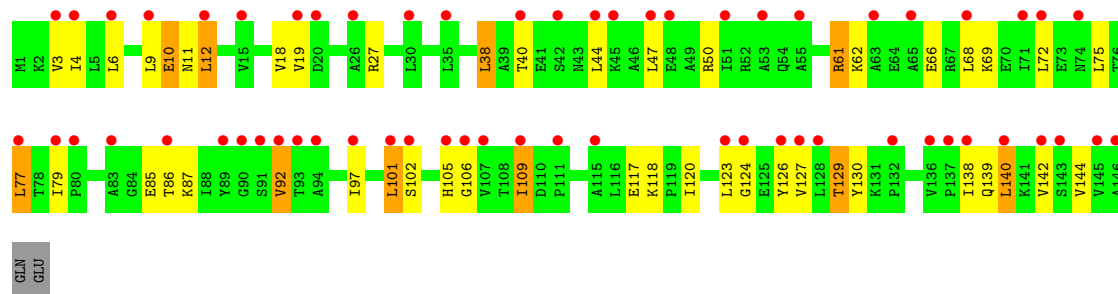
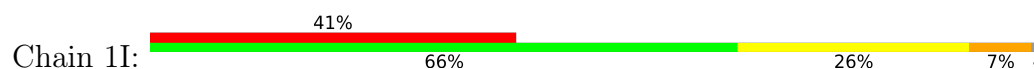




• Molecule 7: 50S ribosomal protein L6



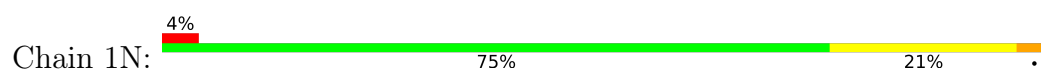
• Molecule 8: 50S ribosomal protein L9

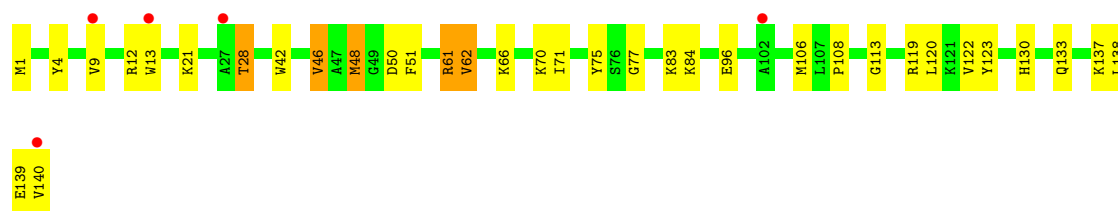


• Molecule 8: 50S ribosomal protein L9

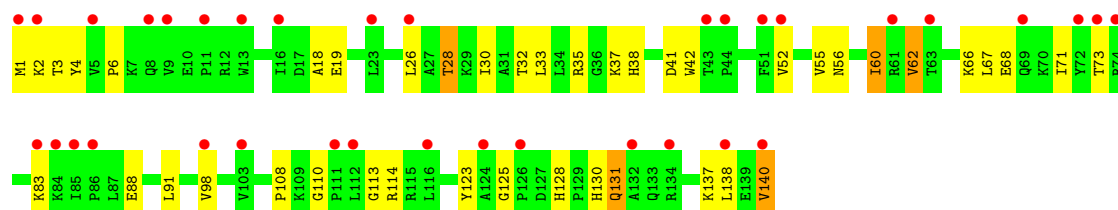
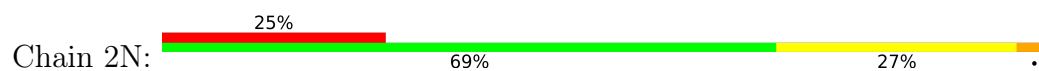


• Molecule 9: 50S ribosomal protein L13

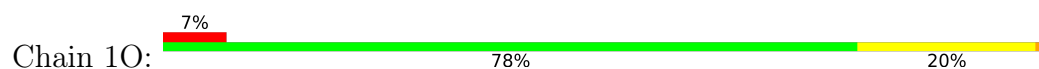




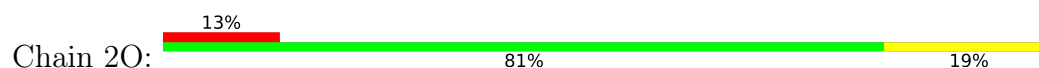
- Molecule 9: 50S ribosomal protein L13



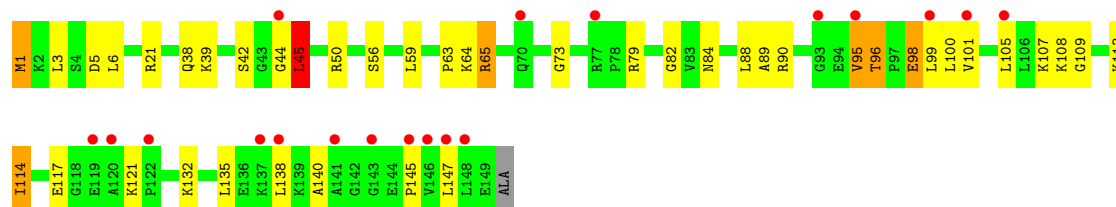
- Molecule 10: 50S ribosomal protein L14



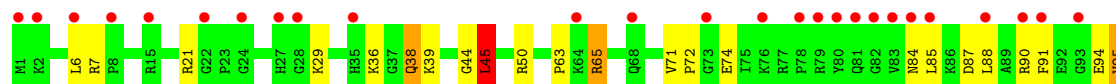
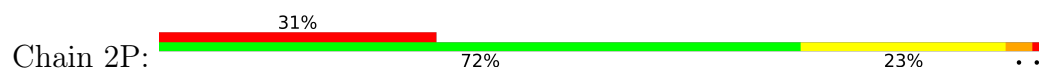
- Molecule 10: 50S ribosomal protein L14



- Molecule 11: 50S ribosomal protein L15

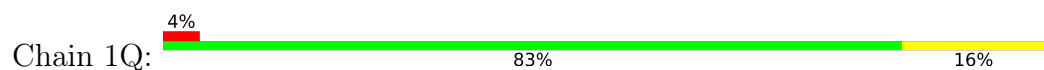


- Molecule 11: 50S ribosomal protein L15

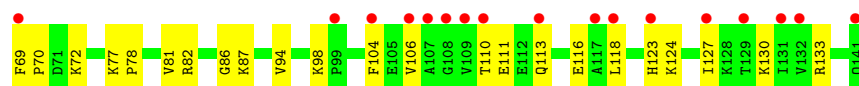
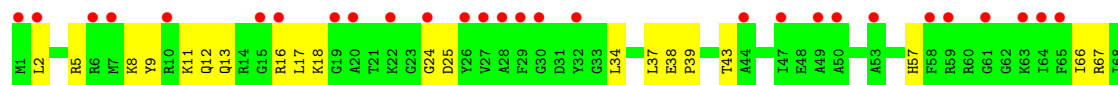




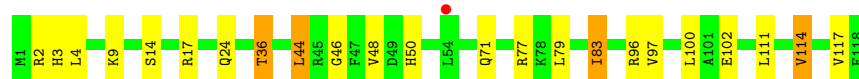
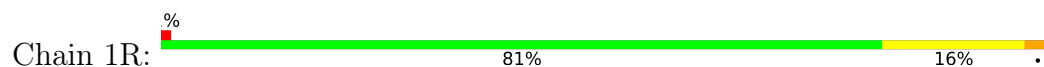
- Molecule 12: 50S ribosomal protein L16



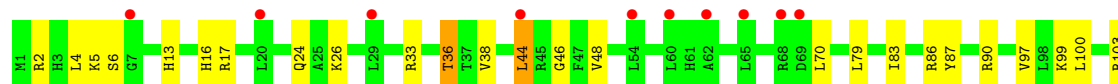
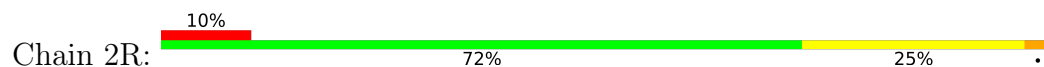
- Molecule 12: 50S ribosomal protein L16



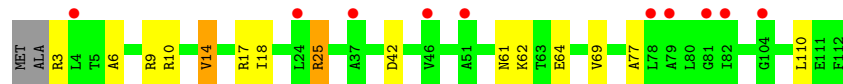
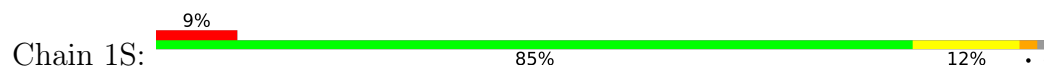
- Molecule 13: 50S ribosomal protein L17



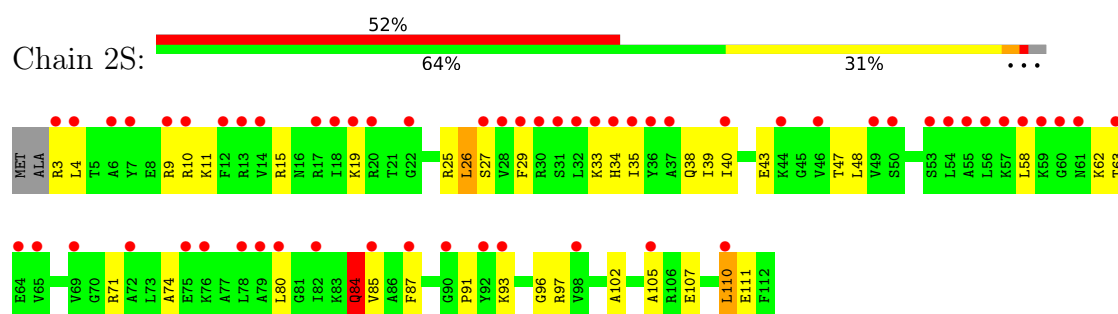
- Molecule 13: 50S ribosomal protein L17



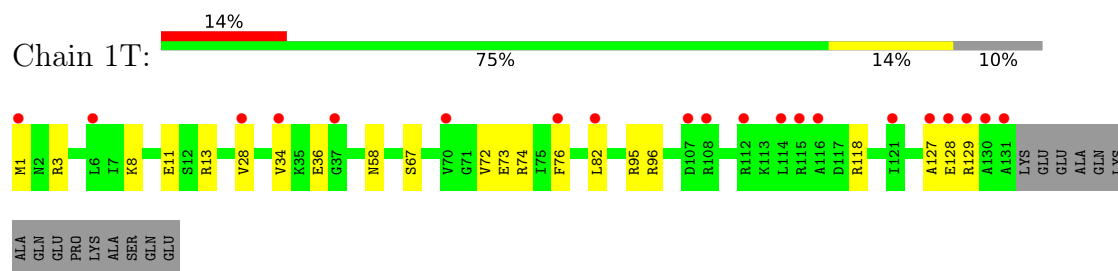
- Molecule 14: 50S ribosomal protein L18



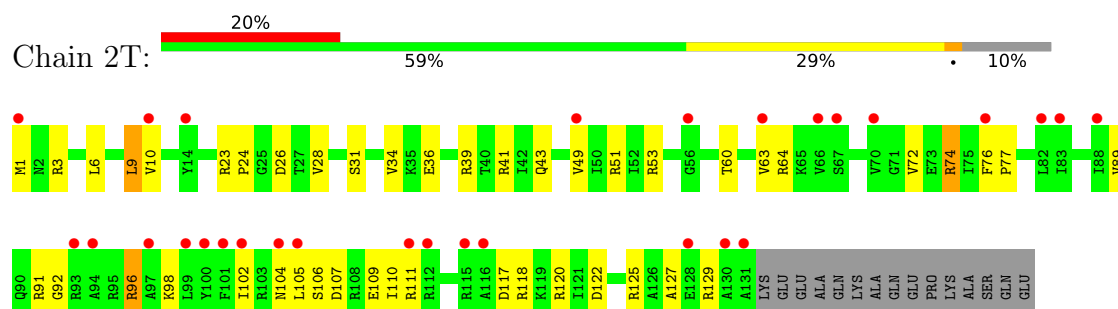
- Molecule 14: 50S ribosomal protein L18



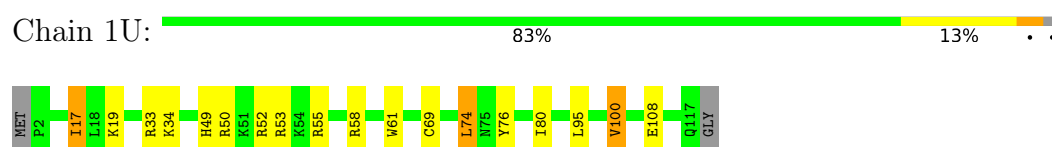
- Molecule 15: 50S ribosomal protein L19



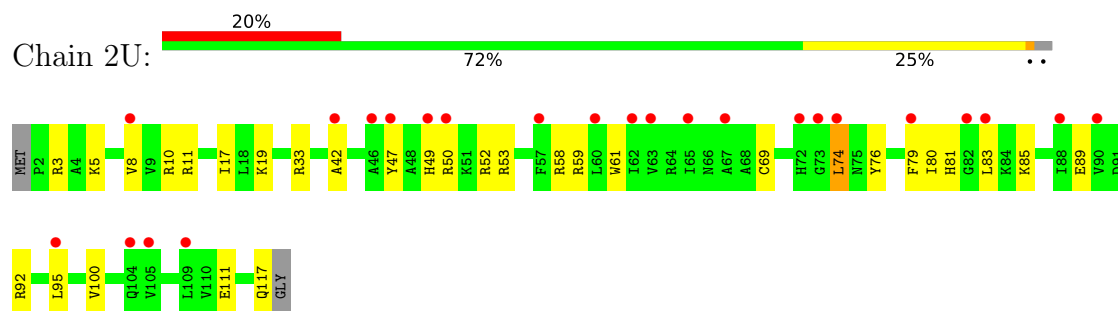
- Molecule 15: 50S ribosomal protein L19



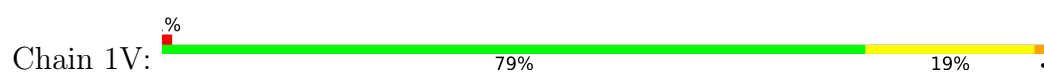
- Molecule 16: 50S ribosomal protein L20



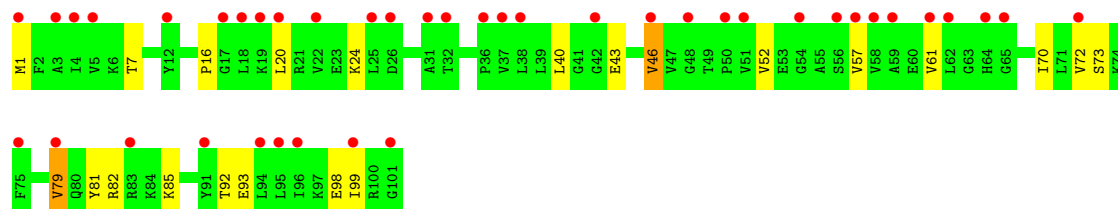
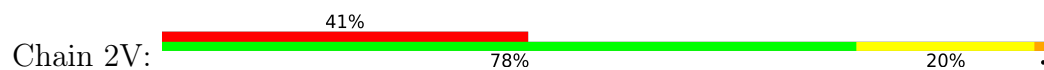
- Molecule 16: 50S ribosomal protein L20



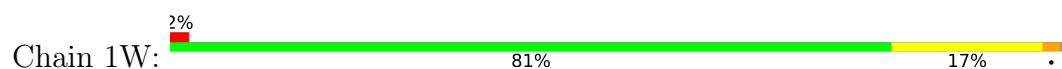
- Molecule 17: 50S ribosomal protein L21



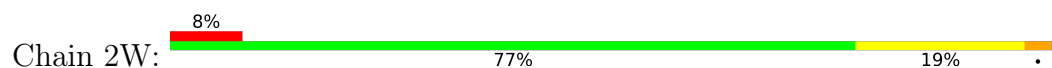
- Molecule 17: 50S ribosomal protein L21



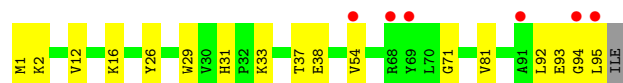
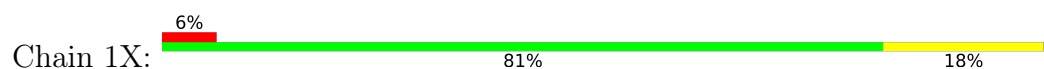
- Molecule 18: 50S ribosomal protein L22



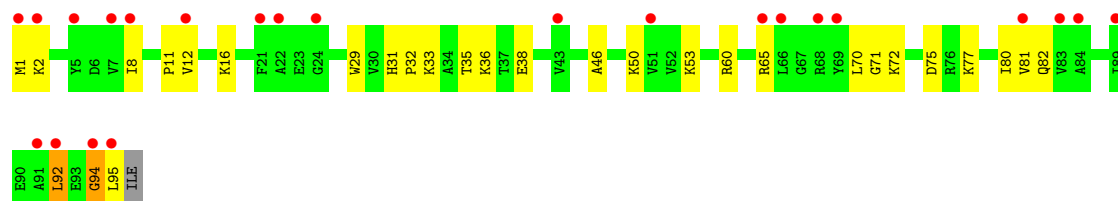
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



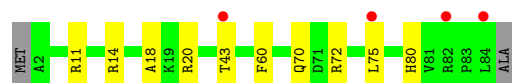
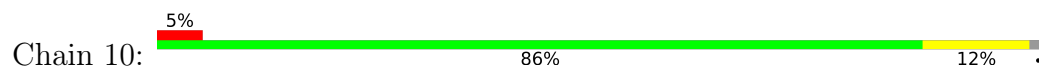
- Molecule 19: 50S ribosomal protein L23



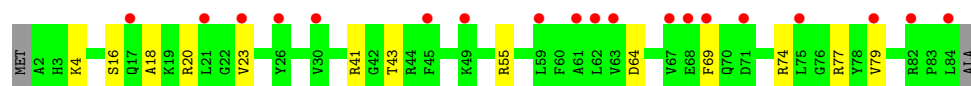
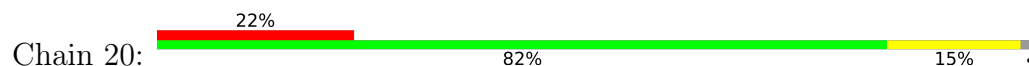
- Molecule 20: 50S ribosomal protein L24

VAL
ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU

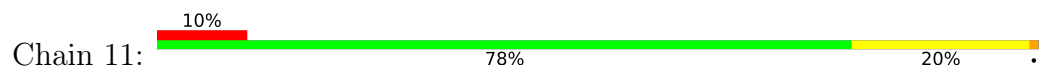
- Molecule 22: 50S ribosomal protein L27



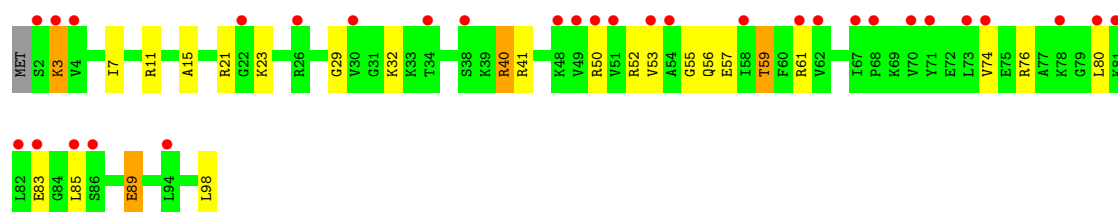
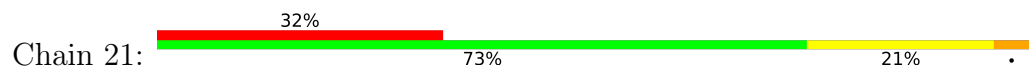
- Molecule 22: 50S ribosomal protein L27



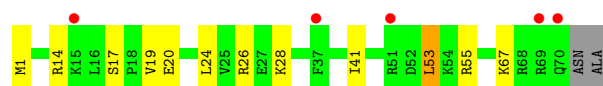
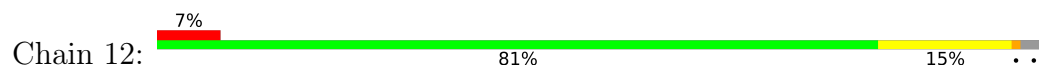
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



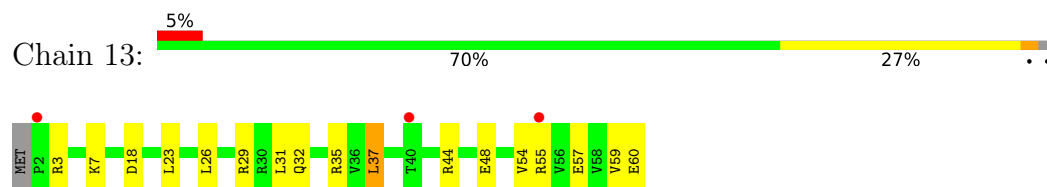
- Molecule 24: 50S ribosomal protein L29



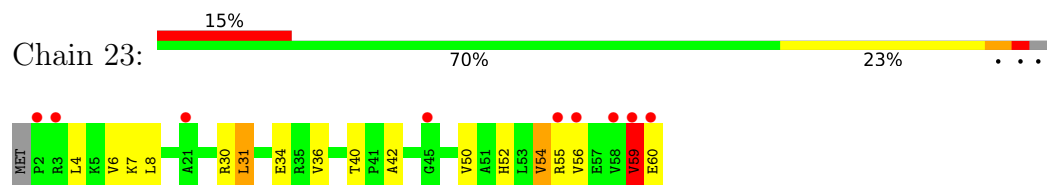
- Molecule 24: 50S ribosomal protein L29



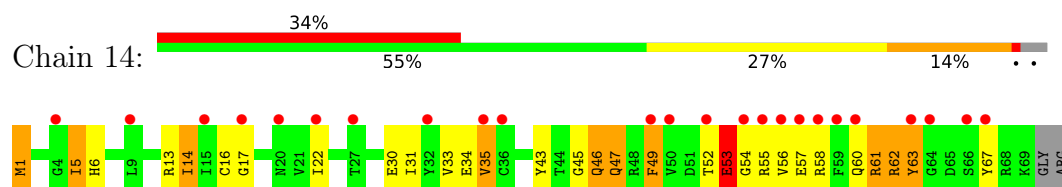
- Molecule 25: 50S ribosomal protein L30



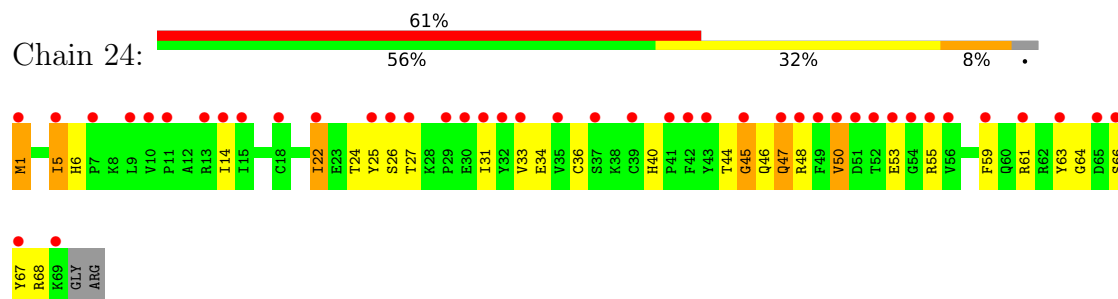
- Molecule 25: 50S ribosomal protein L30



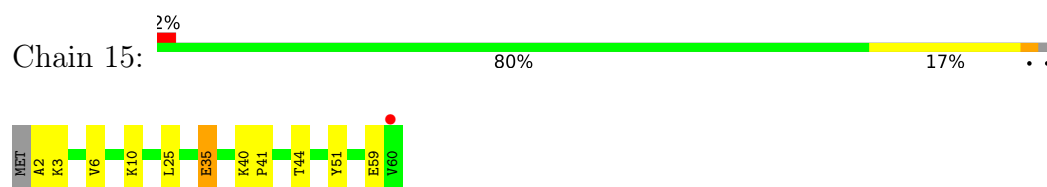
- Molecule 26: 50S ribosomal protein L31



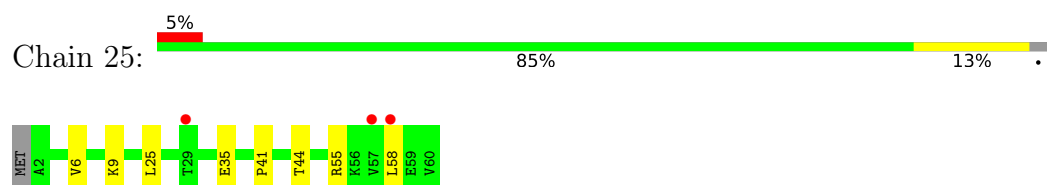
- Molecule 26: 50S ribosomal protein L31



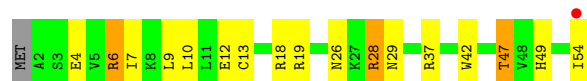
- Molecule 27: 50S ribosomal protein L32



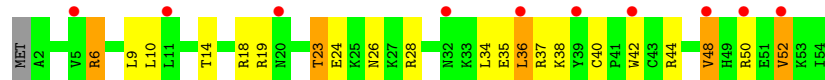
- Molecule 27: 50S ribosomal protein L32



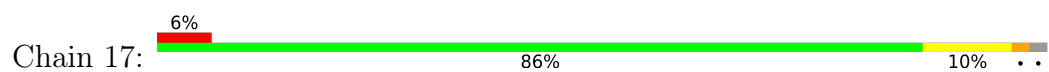
- Molecule 28: 50S ribosomal protein L33



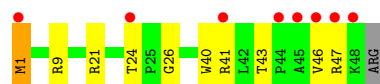
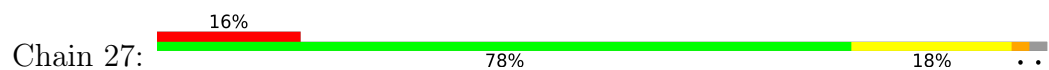
- Molecule 28: 50S ribosomal protein L33



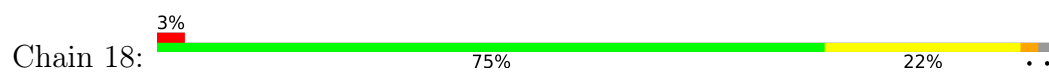
- Molecule 29: 50S ribosomal protein L34



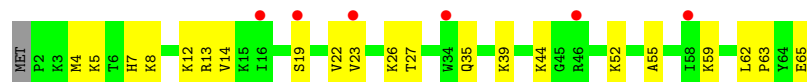
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



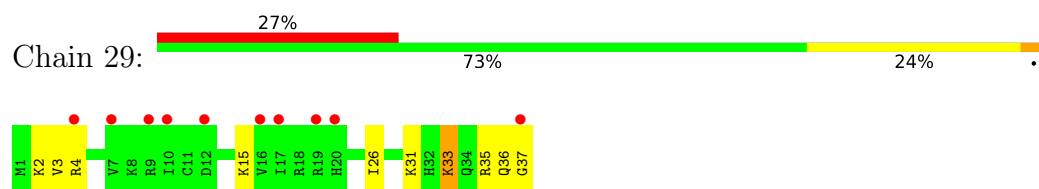
- Molecule 30: 50S ribosomal protein L35



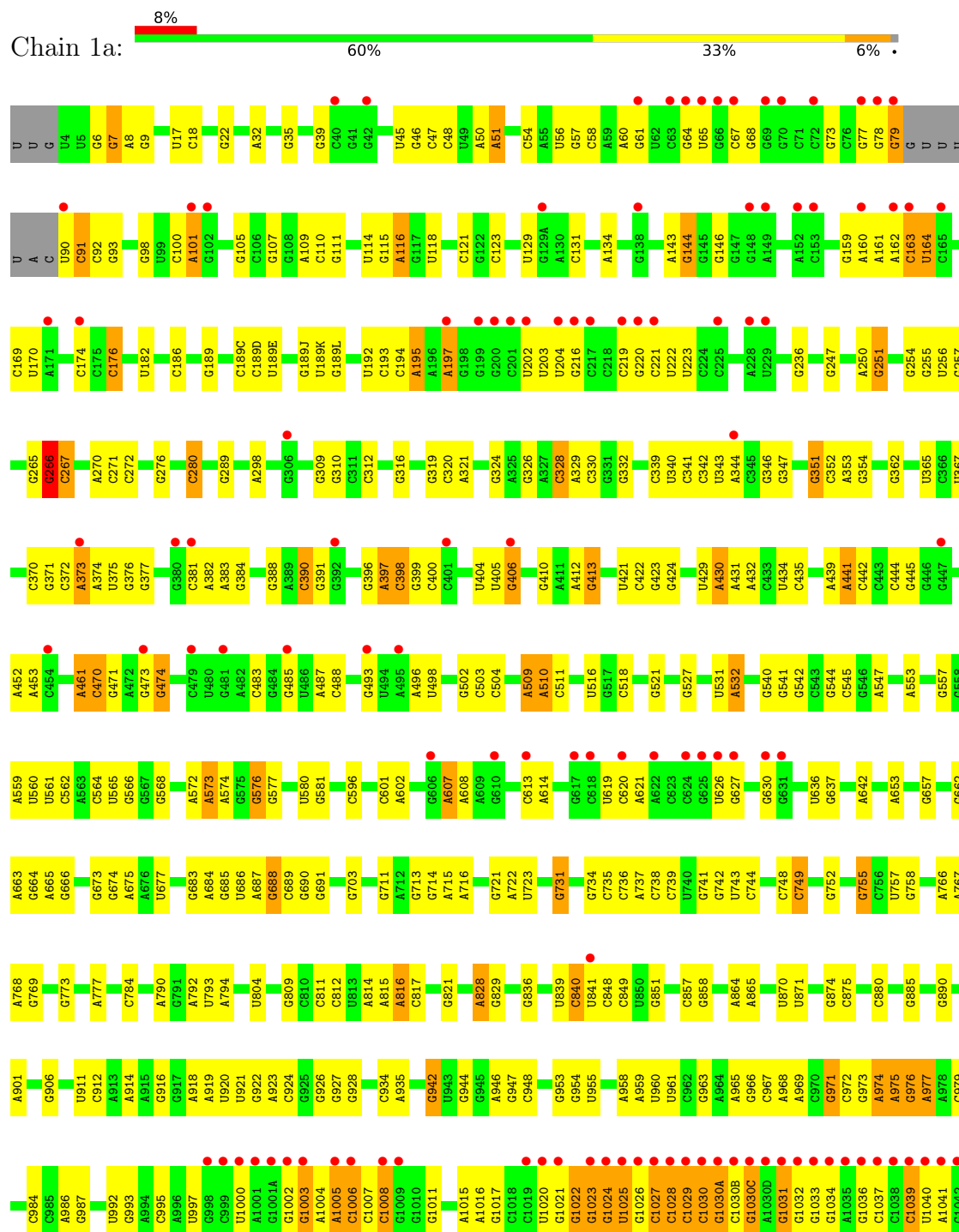
- Molecule 31: 50S ribosomal protein L36

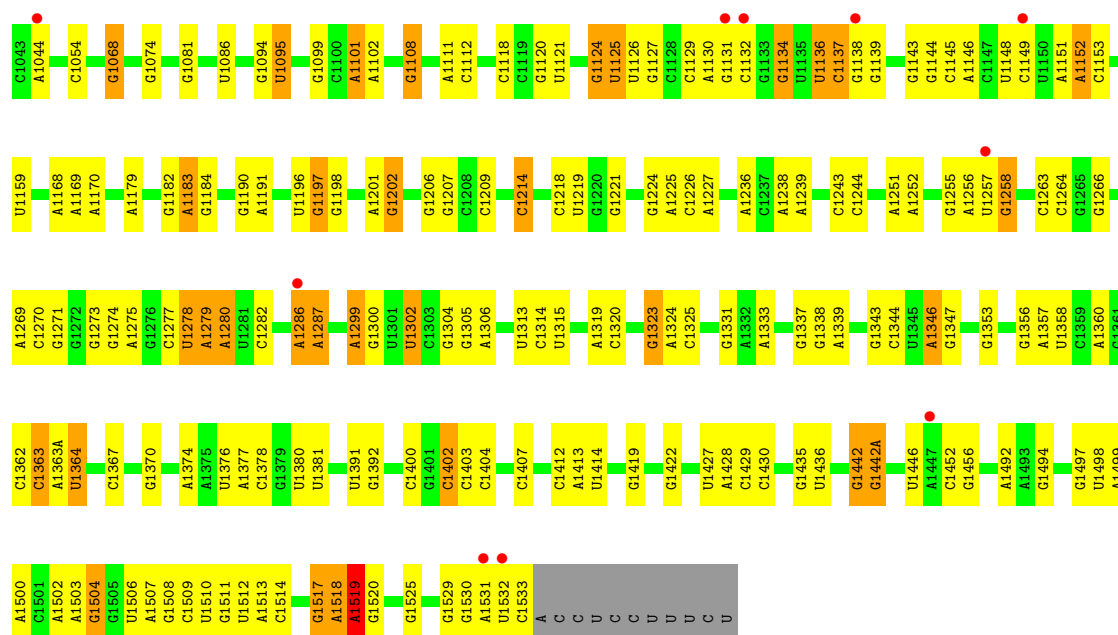


- Molecule 31: 50S ribosomal protein L36

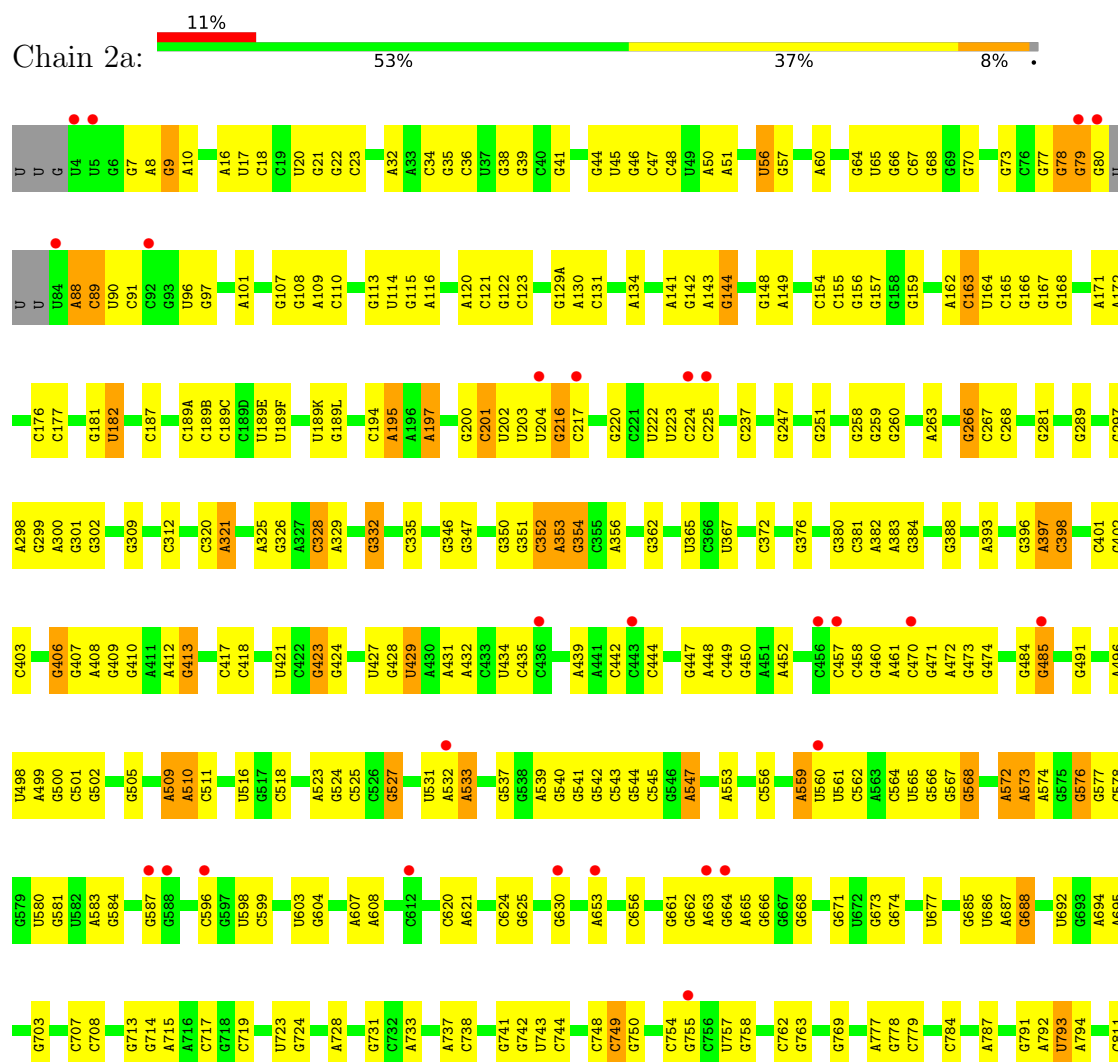


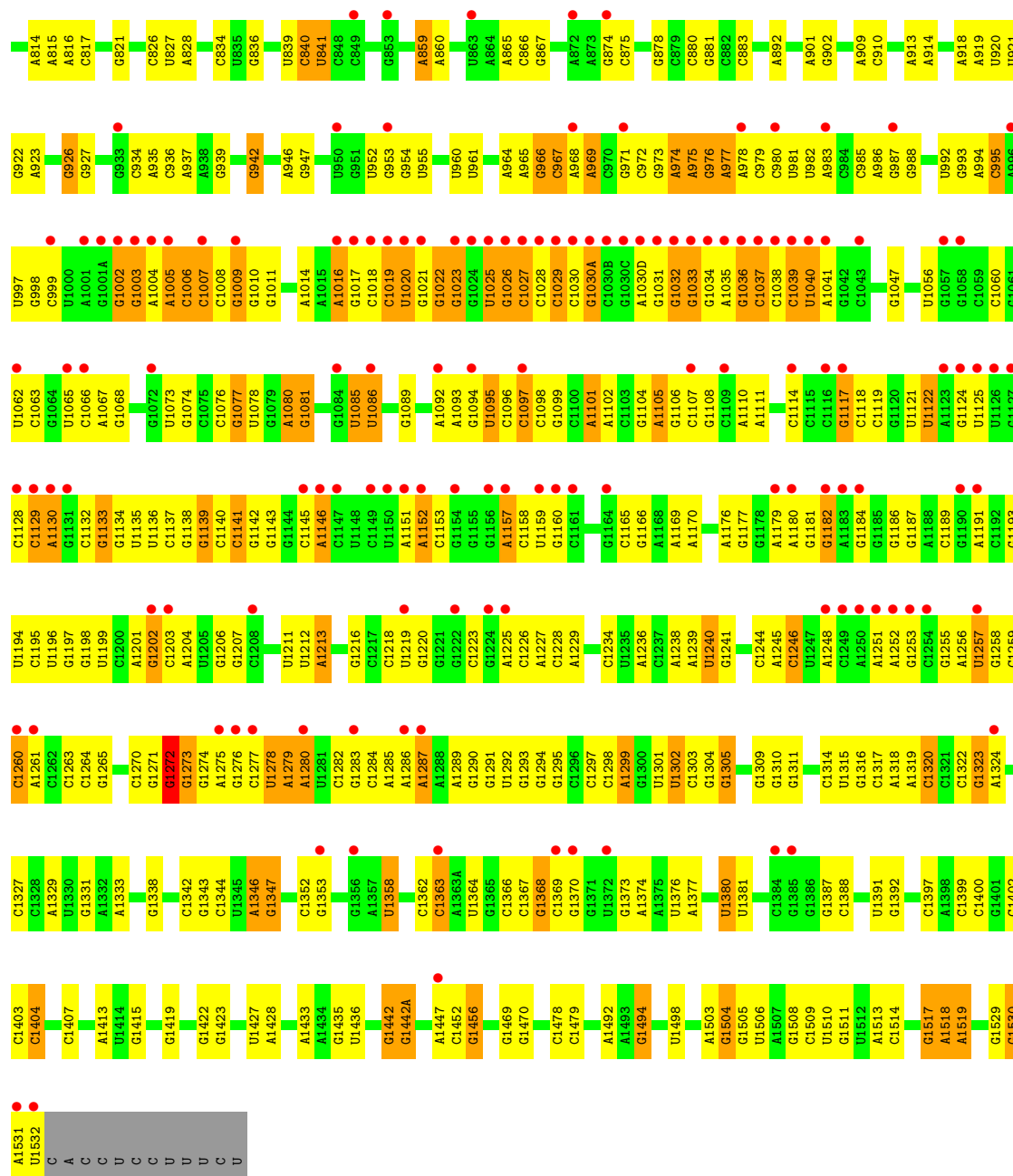
- Molecule 32: 16S Ribosomal RNA





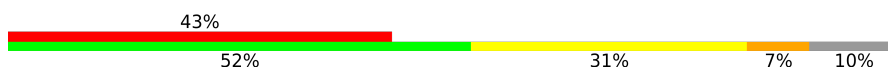
• Molecule 32: 16S Ribosomal RNA

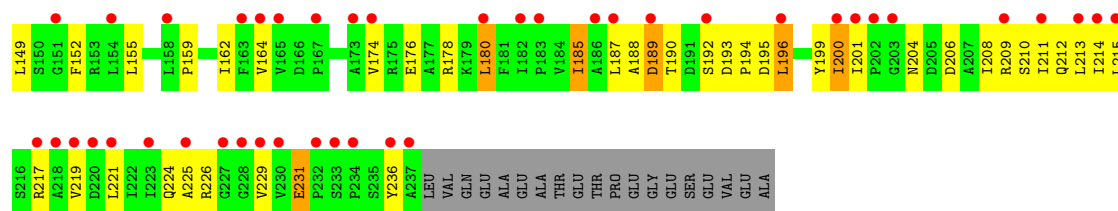




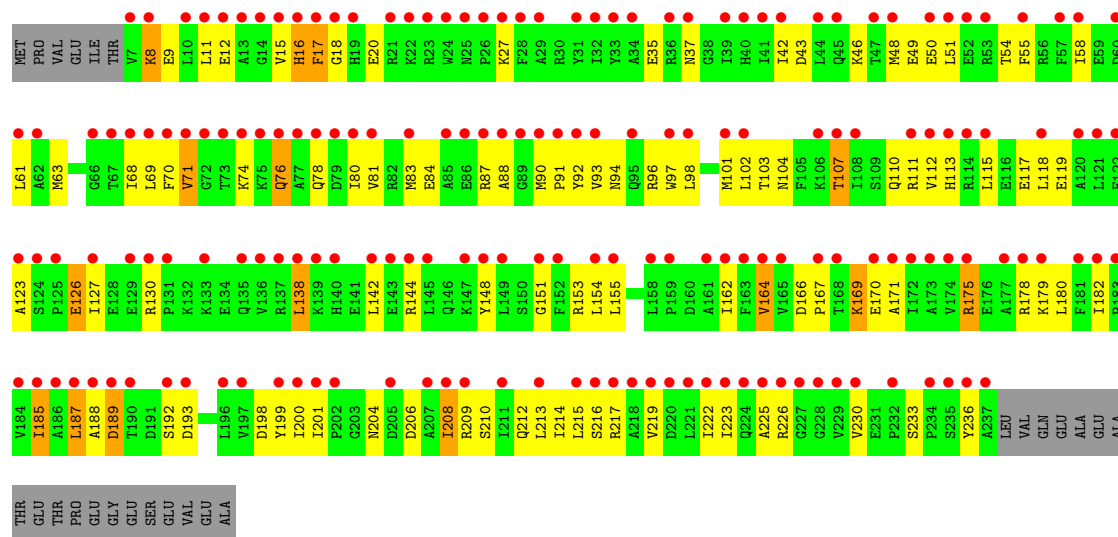
• Molecule 33: 30S ribosomal protein S2

Chain 1b:

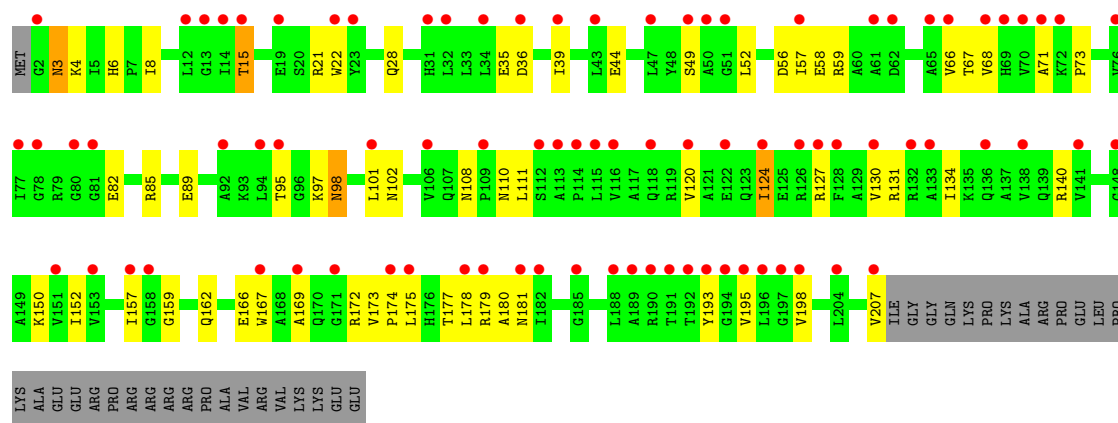




• Molecule 33: 30S ribosomal protein S2

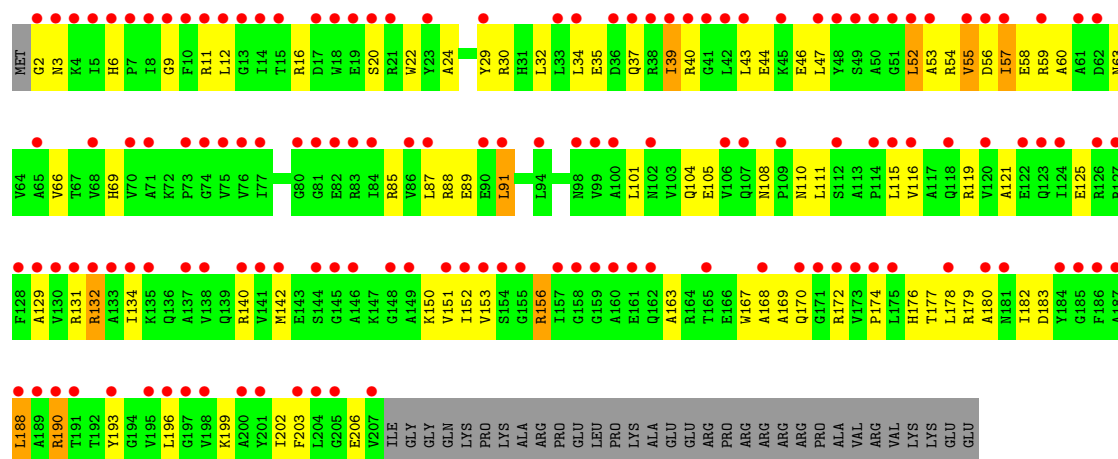


• Molecule 34: 30S ribosomal protein S3



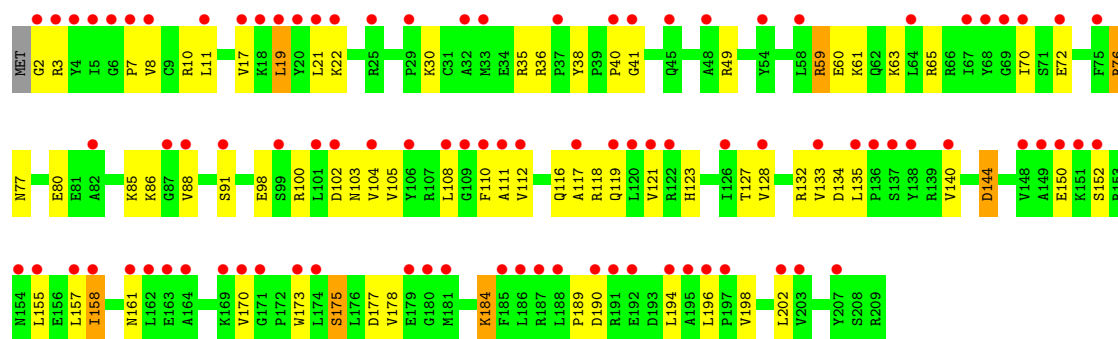
• Molecule 34: 30S ribosomal protein S3





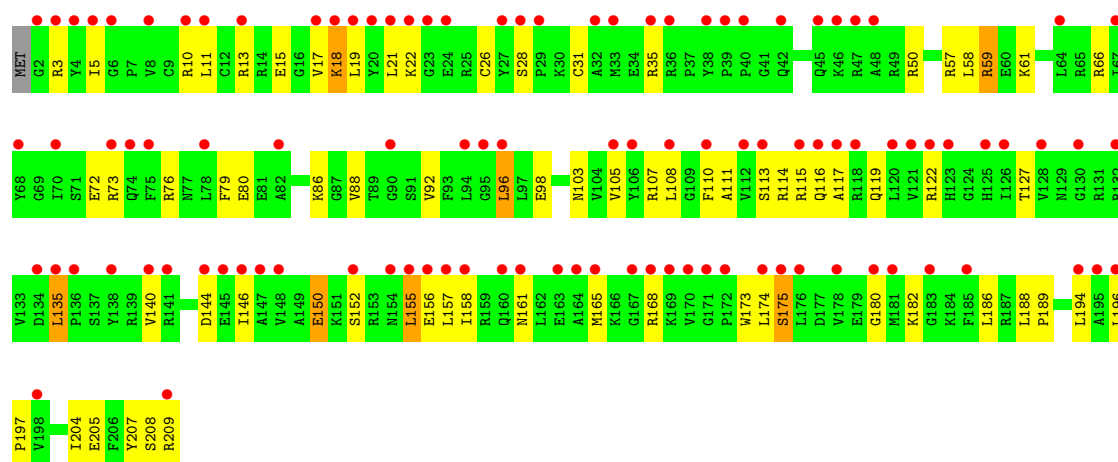
• Molecule 35: 30S ribosomal protein S4

Chain 1d: 45% 65% 32%



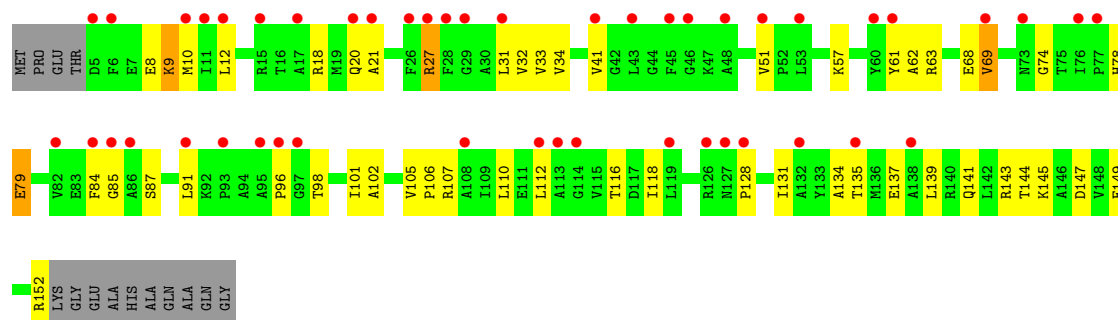
• Molecule 35: 30S ribosomal protein S4

Chain 2d: 50% 64% 32%

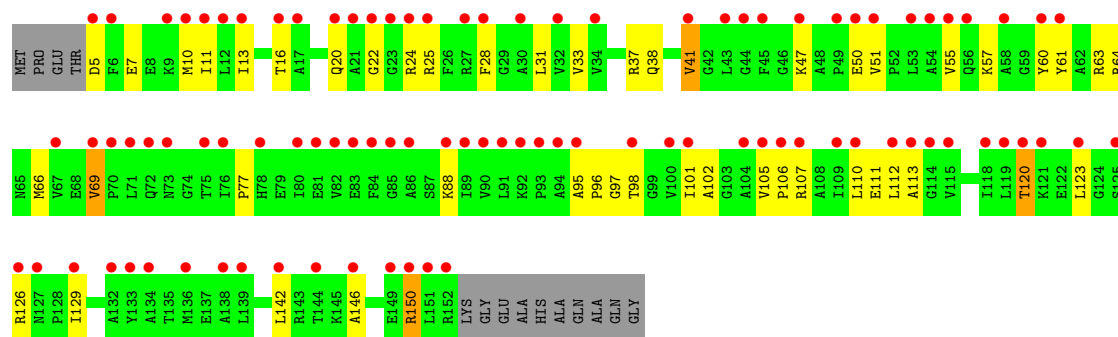


• Molecule 36: 30S ribosomal protein S5

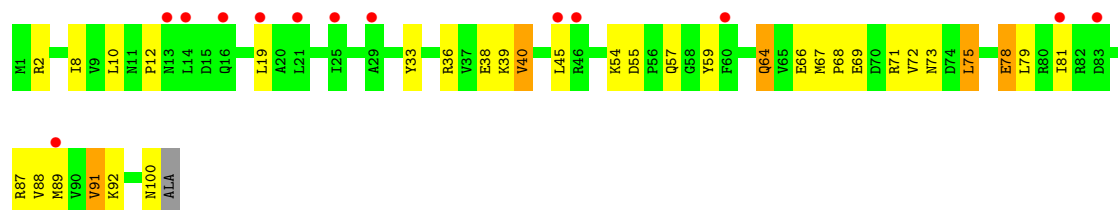
Chain 1e: 29% 60% 29% 9%



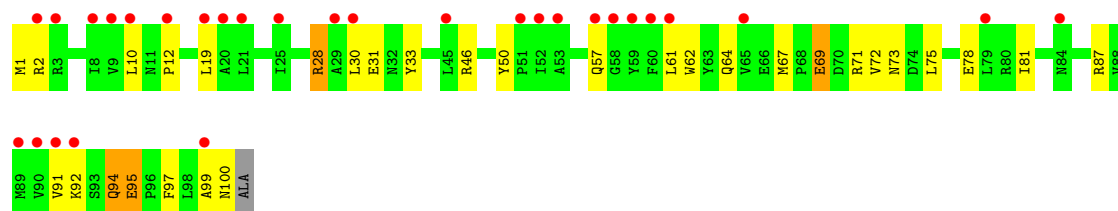
• Molecule 36: 30S ribosomal protein S5



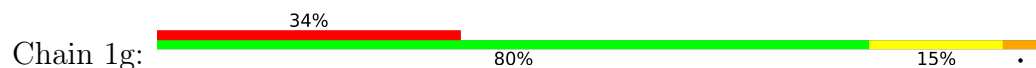
• Molecule 37: 30S ribosomal protein S6

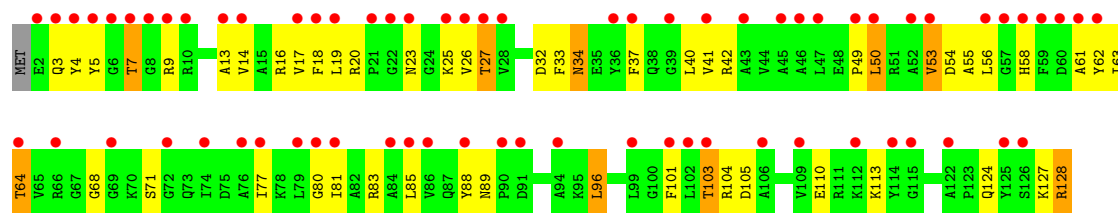


• Molecule 37: 30S ribosomal protein S6

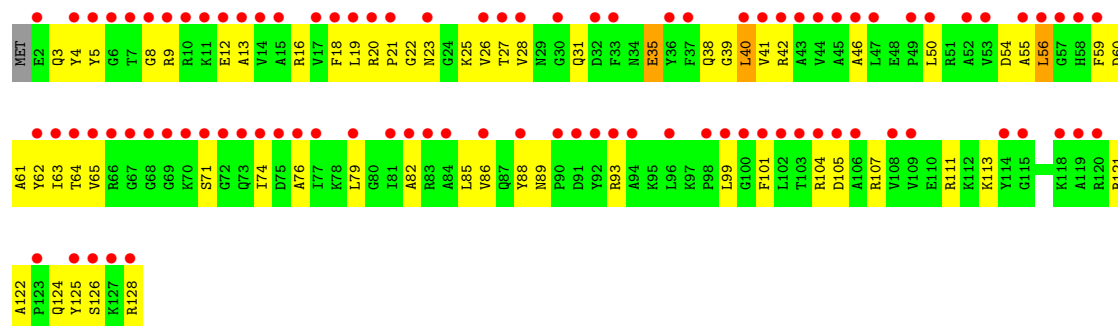
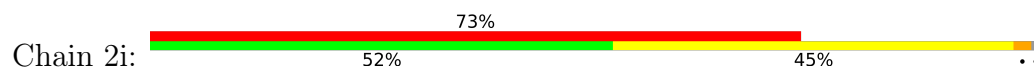


• Molecule 38: 30S ribosomal protein S7

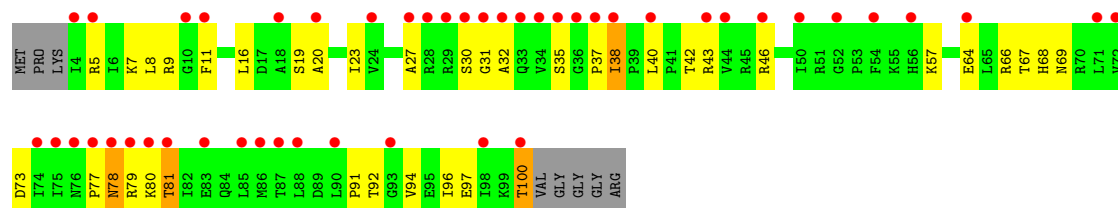




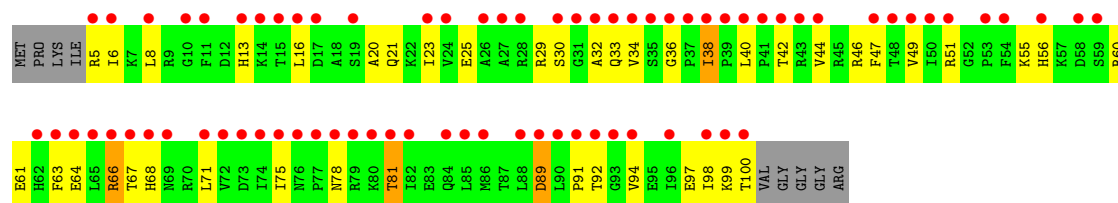
• Molecule 40: 30S ribosomal protein S9



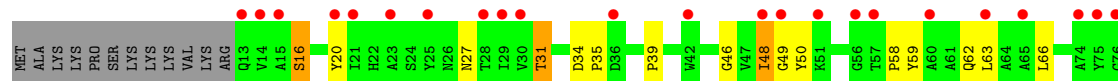
• Molecule 41: 30S ribosomal protein S10

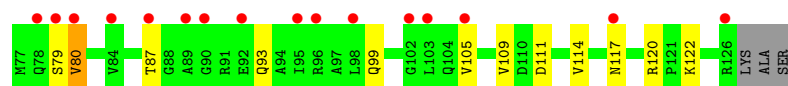


• Molecule 41: 30S ribosomal protein S10

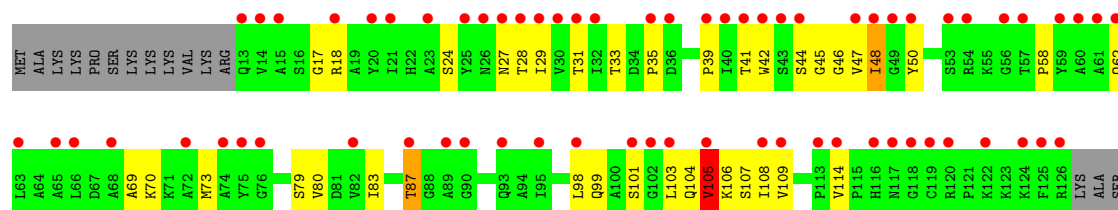


• Molecule 42: 30S ribosomal protein S11

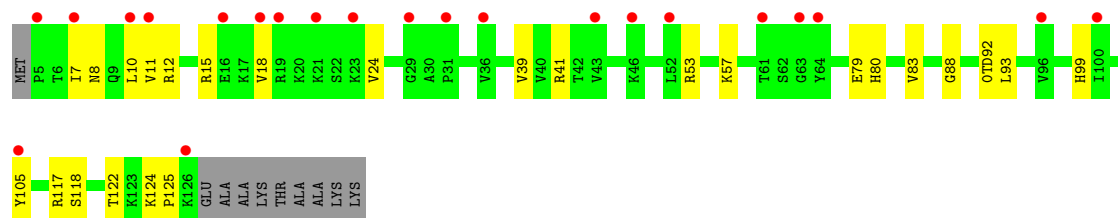
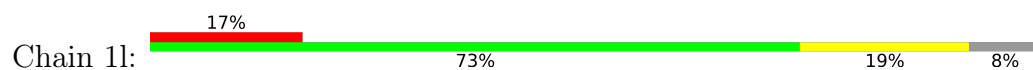




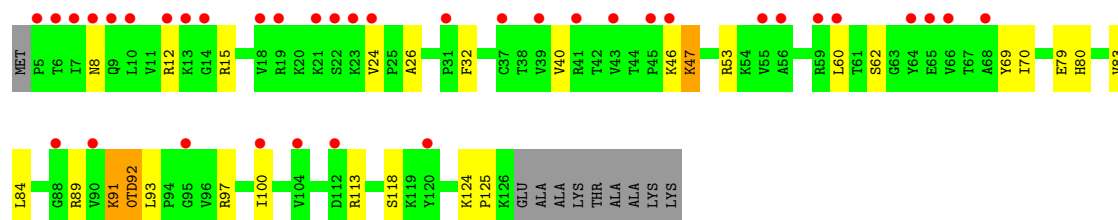
- Molecule 42: 30S ribosomal protein S11



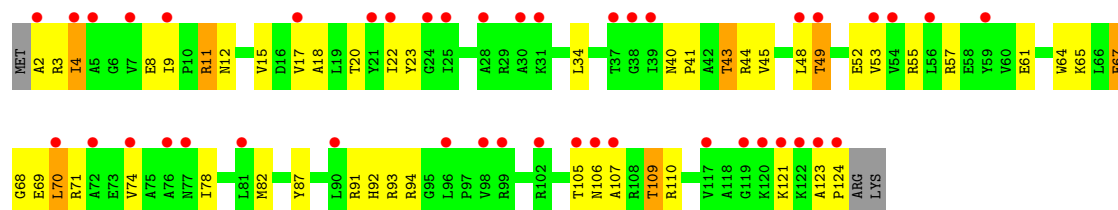
- Molecule 43: 30S ribosomal protein S12



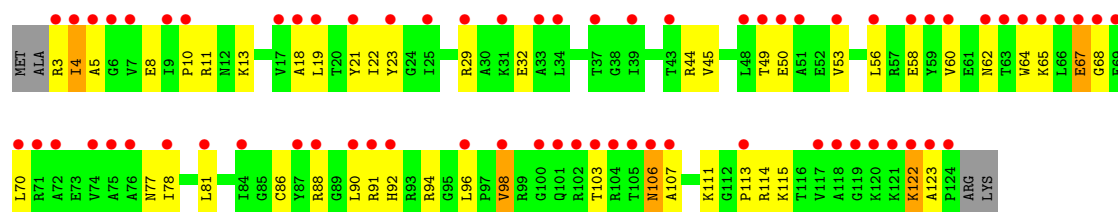
- Molecule 43: 30S ribosomal protein S12



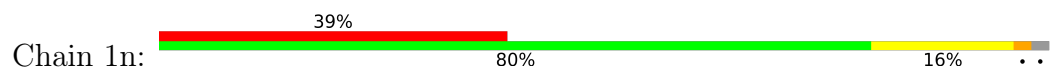
- Molecule 44: 30S ribosomal protein S13



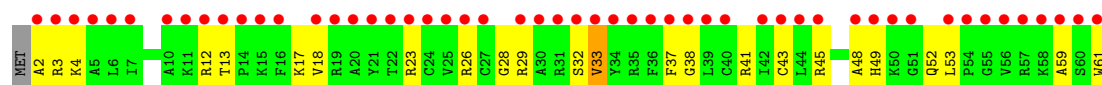
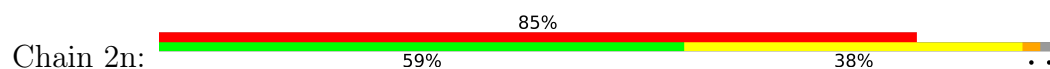
- Molecule 44: 30S ribosomal protein S13



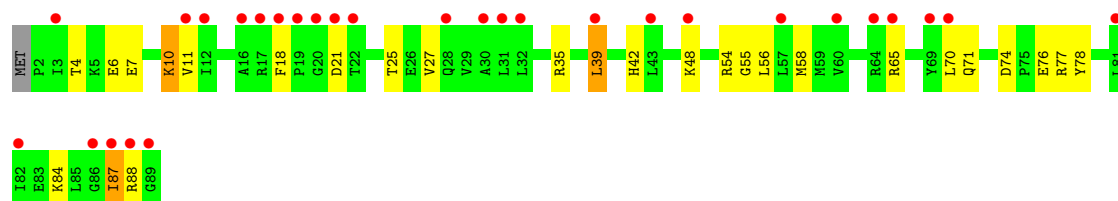
- Molecule 45: 30S ribosomal protein S14 type Z



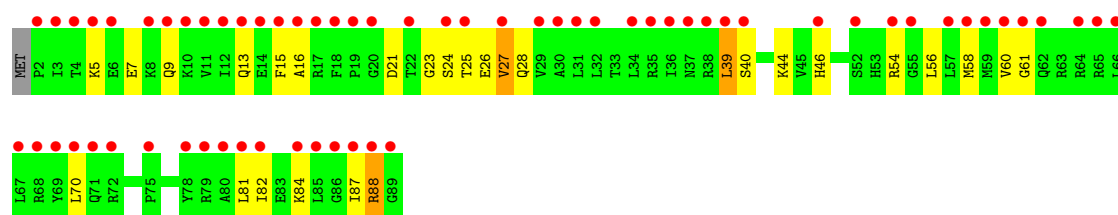
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

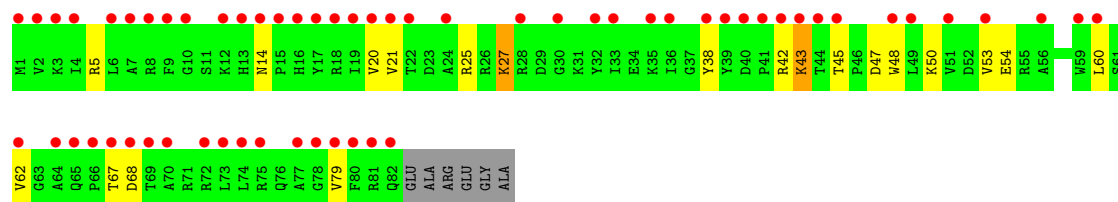


- Molecule 46: 30S ribosomal protein S15

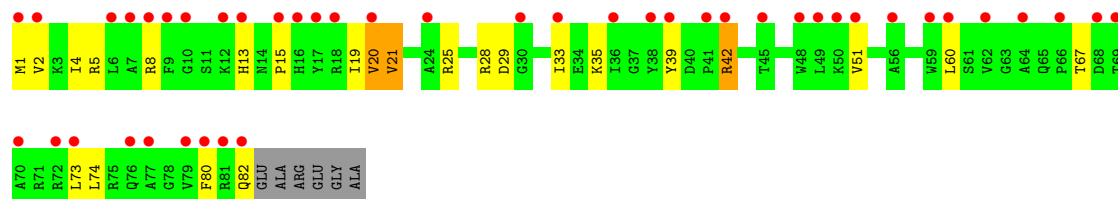


- Molecule 47: 30S ribosomal protein S16

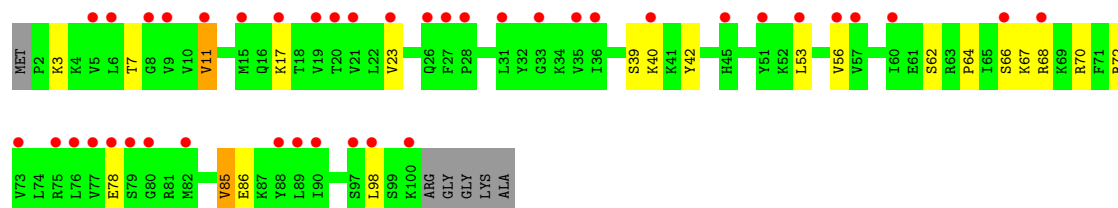
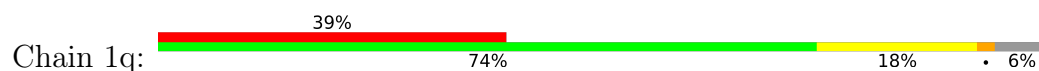




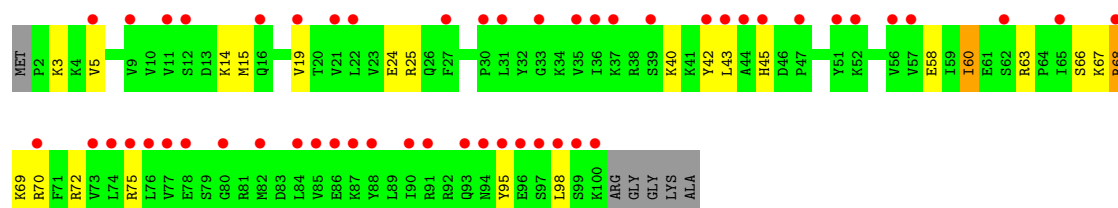
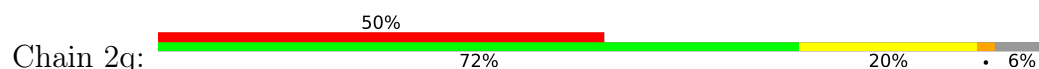
• Molecule 47: 30S ribosomal protein S16



• Molecule 48: 30S ribosomal protein S17



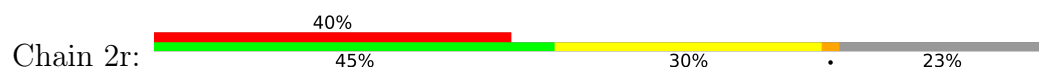
• Molecule 48: 30S ribosomal protein S17

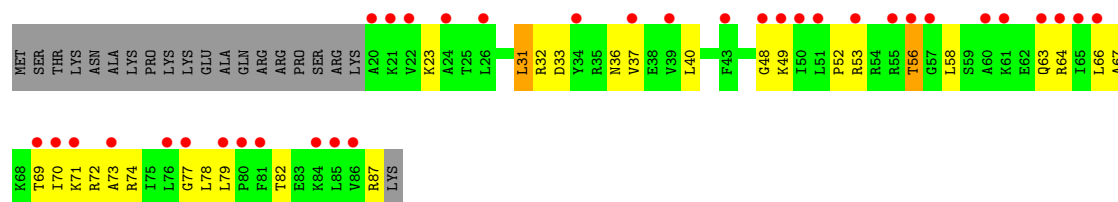


• Molecule 49: 30S ribosomal protein S18

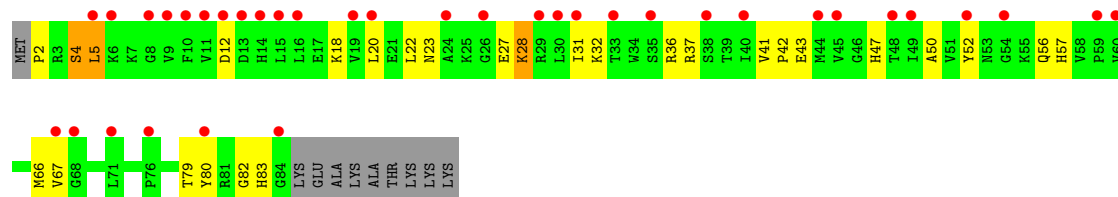
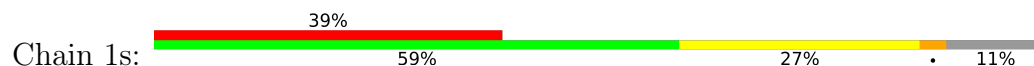


• Molecule 49: 30S ribosomal protein S18

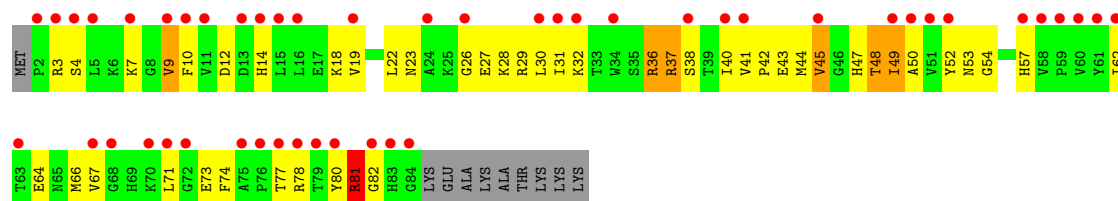




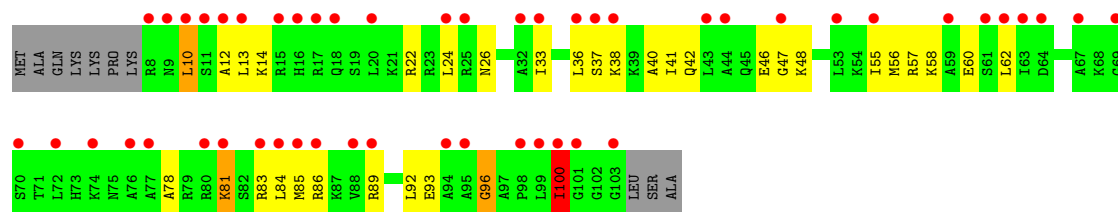
• Molecule 50: 30S ribosomal protein S19



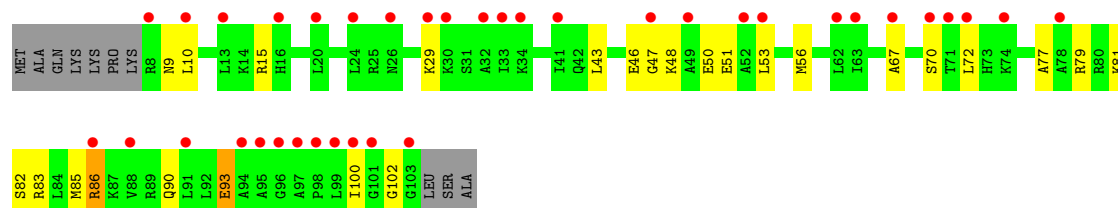
• Molecule 50: 30S ribosomal protein S19



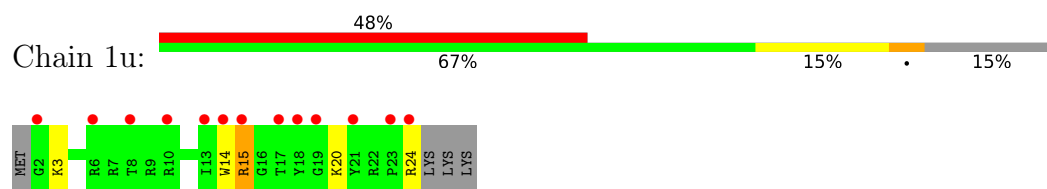
• Molecule 51: 30S ribosomal protein S20



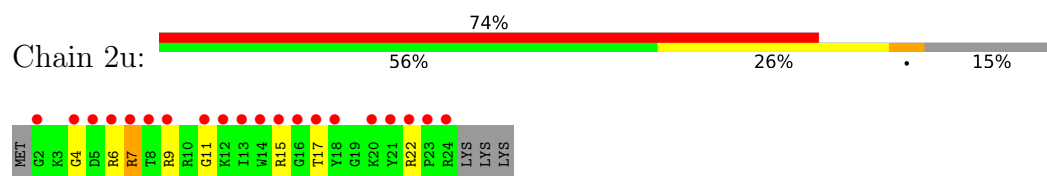
• Molecule 51: 30S ribosomal protein S20



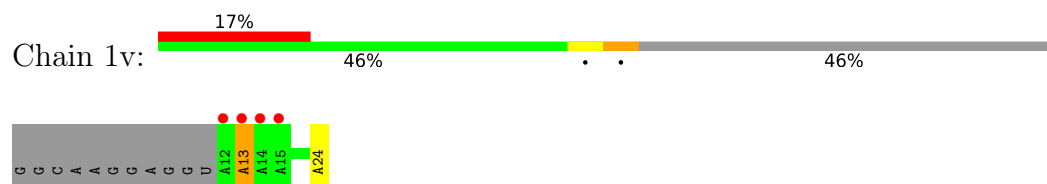
- Molecule 52: 30S ribosomal protein Thx



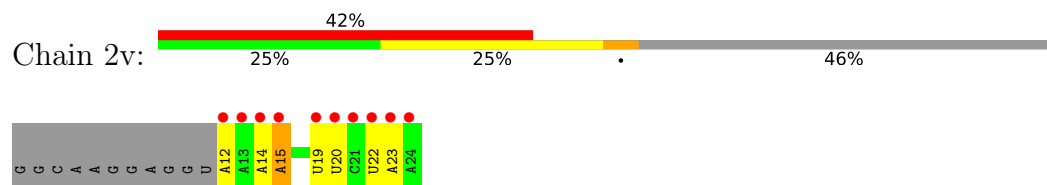
- Molecule 52: 30S ribosomal protein Thx



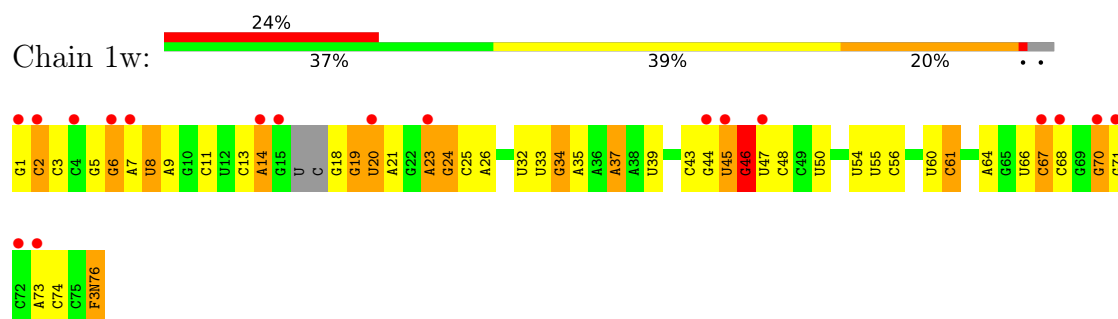
- Molecule 53: MF-mRNA



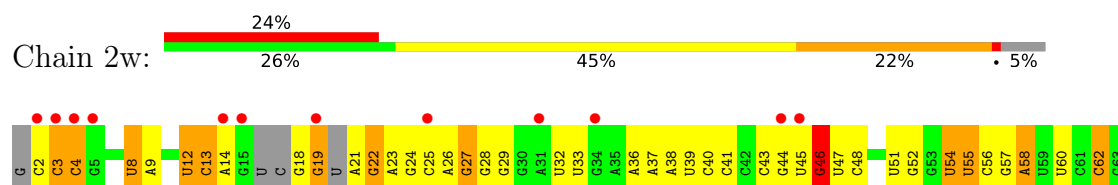
- Molecule 53: MF-mRNA

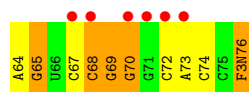


- Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNA_{phe}

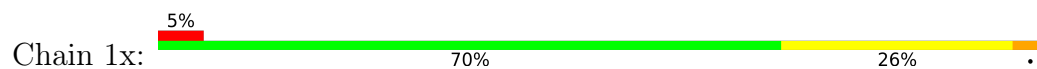


- Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNA_{phe}

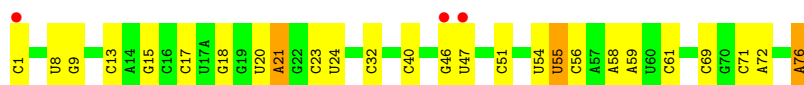




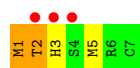
- Molecule 55: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA^{met} RNA-part



- Molecule 55: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA^{met} RNA-part



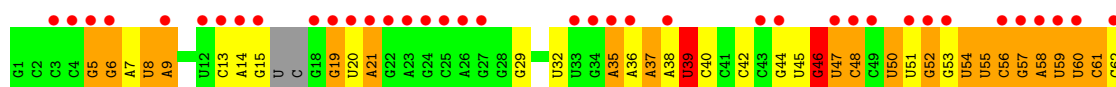
- Molecule 56: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA^{met} Peptide-part



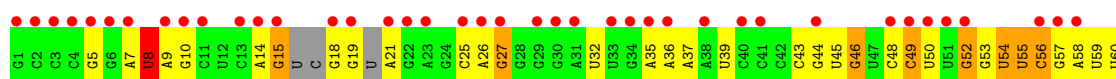
- Molecule 56: P-site Peptidyl-tRNA fMTHSMRC-NH-tRNA^{met} Peptide-part



- Molecule 57: E-site Deacylated tRNA^{phe}



- Molecule 57: E-site Deacylated tRNA^{phe}





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.43Å 447.70Å 618.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.53 – 2.30 121.53 – 2.47	Depositor EDS
% Data completeness (in resolution range)	97.5 (121.53-2.30) 98.6 (121.53-2.47)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.237 , 0.281 (Not available) , 0.285	Depositor DCC
R_{free} test set	101013 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	299898	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: 5MU, OMG, MIA, FME, ZN, OMU, K, MG, 0TD, MA6, UR3, 4SU, 2MG, PSU, SF4, M2G, 8AN, G7M, 4OC, 2MA, F3N, 5MC, 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	0.28	1/69011 (0.0%)	0.48	2/107720 (0.0%)
1	2A	0.22	0/67295	0.41	2/105042 (0.0%)
2	1B	0.22	0/2882	0.41	0/4494
2	2B	0.19	0/2879	0.37	0/4487
3	1D	0.27	0/2186	0.51	0/2944
3	2D	0.22	0/2186	0.44	0/2944
4	1E	0.28	0/1592	0.53	0/2149
4	2E	0.21	0/1592	0.44	0/2149
5	1F	0.26	0/1618	0.49	0/2191
5	2F	0.20	0/1614	0.45	2/2186 (0.1%)
6	1G	0.21	0/1448	0.44	0/1957
6	2G	0.19	0/1453	0.42	0/1963
7	1H	0.21	0/1356	0.44	0/1834
7	2H	0.18	0/1356	0.37	0/1834
8	1I	0.19	0/1112	0.43	0/1514
8	2I	0.20	0/1079	0.43	0/1475
9	1N	0.25	0/1144	0.45	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.26	0/943	0.49	0/1269
10	2O	0.22	0/943	0.44	0/1269
11	1P	0.26	0/1152	0.50	0/1533
11	2P	0.20	0/1152	0.48	0/1533
12	1Q	0.25	0/1143	0.49	0/1527
12	2Q	0.20	0/1143	0.43	0/1527
13	1R	0.27	0/982	0.48	0/1312
13	2R	0.21	0/982	0.46	0/1312
14	1S	0.22	0/883	0.47	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.22	0/1105	0.46	0/1477
15	2T	0.21	0/1097	0.45	0/1468
16	1U	0.27	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.41	0/1301
17	1V	0.25	0/782	0.50	0/1049
17	2V	0.18	0/782	0.40	0/1049
18	1W	0.28	0/897	0.46	0/1205
18	2W	0.22	0/897	0.43	0/1205
19	1X	0.25	0/764	0.51	0/1025
19	2X	0.20	0/764	0.51	2/1025 (0.2%)
20	1Y	0.21	0/819	0.47	0/1095
20	2Y	0.18	0/819	0.42	0/1095
21	1Z	0.22	0/1267	0.48	0/1717
21	2Z	0.21	0/1299	0.44	0/1763
22	10	0.24	0/662	0.46	0/881
22	20	0.20	0/662	0.45	0/881
23	11	0.23	0/762	0.43	0/1014
23	21	0.21	0/762	0.42	0/1014
24	12	0.21	0/590	0.43	0/781
24	22	0.19	0/590	0.42	0/781
25	13	0.24	0/474	0.46	0/635
25	23	0.18	0/469	0.42	0/630
26	14	0.23	0/565	0.53	0/761
26	24	0.24	0/545	0.56	1/737 (0.1%)
27	15	0.25	0/469	0.48	0/635
27	25	0.23	0/469	0.48	0/635
28	16	0.25	0/460	0.48	0/613
28	26	0.20	0/456	0.41	0/608
29	17	0.29	0/426	0.55	0/561
29	27	0.23	0/426	0.50	0/561
30	18	0.27	0/525	0.46	0/691
30	28	0.21	0/525	0.39	0/691
31	19	0.27	0/310	0.52	0/407
31	29	0.21	0/310	0.44	0/407
32	1a	0.20	0/35795	0.40	1/55864 (0.0%)
32	2a	0.19	0/35886	0.38	1/56005 (0.0%)
33	1b	0.20	0/1881	0.46	0/2542
33	2b	0.21	0/1860	0.48	0/2518
34	1c	0.18	0/1572	0.41	0/2126
34	2c	0.19	0/1566	0.41	0/2119
35	1d	0.19	0/1685	0.45	0/2262
35	2d	0.19	0/1704	0.45	0/2284
36	1e	0.20	0/1145	0.45	0/1543
36	2e	0.20	0/1149	0.46	0/1548
37	1f	0.18	0/823	0.39	0/1115
37	2f	0.19	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.40	0/1679
38	2g	0.19	0/1254	0.40	0/1683
39	1h	0.19	0/1108	0.39	0/1494
39	2h	0.18	0/1108	0.39	0/1494
40	1i	0.20	0/1002	0.49	0/1346
40	2i	0.21	0/997	0.52	0/1343
41	1j	0.20	0/722	0.47	0/982
41	2j	0.21	0/727	0.43	0/988
42	1k	0.18	0/844	0.41	0/1145
42	2k	0.18	0/848	0.38	0/1149
43	1l	0.22	0/937	0.43	0/1260
43	2l	0.18	0/937	0.41	0/1260
44	1m	0.20	0/969	0.51	0/1302
44	2m	0.18	0/961	0.45	0/1291
45	1n	0.21	0/501	0.47	0/664
45	2n	0.20	0/501	0.44	0/664
46	1o	0.18	0/739	0.35	0/985
46	2o	0.17	0/739	0.38	0/985
47	1p	0.20	0/697	0.45	0/939
47	2p	0.19	0/693	0.43	0/935
48	1q	0.20	0/836	0.43	0/1117
48	2q	0.17	0/836	0.43	0/1117
49	1r	0.21	0/560	0.41	0/746
49	2r	0.17	0/560	0.41	0/746
50	1s	0.25	0/667	0.48	0/900
50	2s	0.23	0/661	0.55	0/893
51	1t	0.20	0/730	0.47	0/965
51	2t	0.19	0/729	0.44	0/965
52	1u	0.19	0/203	0.43	0/266
52	2u	0.21	0/203	0.45	0/266
53	1v	0.22	0/310	0.33	0/480
53	2v	0.27	0/310	0.47	0/480
54	1w	0.30	1/1581 (0.1%)	0.43	0/2458
54	2w	0.29	1/1531 (0.1%)	0.42	0/2379
55	1x	0.27	0/1723	0.41	0/2684
55	2x	0.25	0/1723	0.40	0/2684
56	1z	0.45	0/48	0.58	0/62
56	2z	0.33	0/48	0.55	0/62
57	1y	0.31	2/1606 (0.1%)	0.41	0/2497
57	2y	0.32	2/1583 (0.1%)	0.42	0/2459
All	All	0.23	7/316730 (0.0%)	0.43	11/474161 (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
12	1Q	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2y	46	G7M	O3'-P	5.60	1.61	1.56
54	1w	46	G7M	O3'-P	5.43	1.61	1.56
54	2w	46	G7M	O3'-P	5.36	1.61	1.56
1	1A	2552	OMU	O3'-P	5.20	1.61	1.56
57	1y	8	4SU	O3'-P	5.12	1.61	1.56
57	2y	8	4SU	O3'-P	5.12	1.61	1.56
57	1y	46	G7M	O3'-P	5.10	1.61	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	6.85	119.77	109.50
26	24	5	ILE	N-CA-C	-6.11	107.91	113.71
1	2A	1992	G	C2'-C3'-O3'	5.76	118.14	109.50
19	2X	94	GLY	CA-C-N	5.67	131.91	121.70
19	2X	94	GLY	C-N-CA	5.67	131.91	121.70
1	2A	752	A	C2'-C3'-O3'	5.48	117.72	109.50
1	1A	512	G	O4'-C1'-N9	5.30	116.16	108.20
32	1a	266	G	C2'-C3'-O3'	5.28	117.42	109.50
5	2F	21	ALA	CA-C-N	5.11	130.90	121.70
5	2F	21	ALA	C-N-CA	5.11	130.90	121.70
32	2a	1272	G	N1-C2-N2	-5.00	101.19	116.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	1Q	15	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31196	627	0
1	2A	60322	0	30425	699	0
2	1B	2577	0	1305	18	0
2	2B	2575	0	1303	36	0
3	1D	2136	0	2218	42	0
3	2D	2136	0	2218	40	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	33	0
5	1F	1583	0	1625	38	0
5	2F	1579	0	1619	53	0
6	1G	1423	0	1436	44	0
6	2G	1428	0	1438	45	0
7	1H	1330	0	1407	26	0
7	2H	1330	0	1407	36	0
8	1I	1097	0	1140	32	0
8	2I	1064	0	1082	36	0
9	1N	1117	0	1184	22	0
9	2N	1117	0	1184	22	0
10	1O	933	0	996	21	0
10	2O	933	0	996	15	0
11	1P	1135	0	1212	35	0
11	2P	1135	0	1212	27	0
12	1Q	1122	0	1179	15	0
12	2Q	1122	0	1179	31	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	19	0
14	1S	873	0	927	14	0
14	2S	870	0	923	26	0
15	1T	1091	0	1151	17	0
15	2T	1083	0	1136	27	0
16	1U	959	0	1019	17	0
16	2U	959	0	1019	22	0
17	1V	771	0	830	10	0
17	2V	771	0	830	8	0
18	1W	886	0	940	12	0
18	2W	886	0	940	13	0
19	1X	750	0	814	12	0
19	2X	750	0	814	28	0
20	1Y	806	0	881	19	0
20	2Y	806	0	881	26	0
21	1Z	1240	0	1240	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	2Z	1271	0	1273	44	0
22	10	653	0	674	8	0
22	20	653	0	674	12	0
23	11	755	0	826	14	0
23	21	755	0	826	21	0
24	12	588	0	643	4	0
24	22	588	0	643	17	0
25	13	469	0	518	10	0
25	23	464	0	514	12	0
26	14	552	0	533	28	0
26	24	532	0	503	18	0
27	15	455	0	465	6	0
27	25	455	0	464	3	0
28	16	453	0	473	10	0
28	26	449	0	469	14	0
29	17	418	0	467	3	0
29	27	418	0	467	10	0
30	18	517	0	582	13	0
30	28	517	0	582	15	0
31	19	307	0	335	3	0
31	29	307	0	335	10	0
32	1a	32246	0	16295	362	0
32	2a	32327	0	16338	486	0
33	1b	1846	0	1867	63	0
33	2b	1825	0	1828	70	0
34	1c	1548	0	1535	38	0
34	2c	1542	0	1517	60	0
35	1d	1655	0	1672	40	0
35	2d	1674	0	1714	52	0
36	1e	1129	0	1185	30	0
36	2e	1133	0	1191	34	0
37	1f	810	0	804	17	0
37	2f	816	0	808	20	0
38	1g	1231	0	1238	17	0
38	2g	1235	0	1249	39	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	19	0
40	1i	983	0	986	38	0
40	2i	978	0	966	40	0
41	1j	709	0	650	26	0
41	2j	714	0	672	29	0
42	1k	829	0	825	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	2k	833	0	835	19	0
43	1l	932	0	981	13	0
43	2l	932	0	980	20	0
44	1m	958	0	1002	29	0
44	2m	950	0	988	33	0
45	1n	492	0	529	7	0
45	2n	492	0	529	27	0
46	1o	728	0	760	14	0
46	2o	728	0	760	19	0
47	1p	681	0	697	12	0
47	2p	677	0	686	17	0
48	1q	823	0	891	15	0
48	2q	823	0	891	12	0
49	1r	555	0	618	8	0
49	2r	555	0	618	24	0
50	1s	652	0	662	21	0
50	2s	646	0	644	34	0
51	1t	728	0	798	21	0
51	2t	727	0	796	18	0
52	1u	199	0	208	3	0
52	2u	199	0	208	6	0
53	1v	277	0	140	2	0
53	2v	277	0	140	8	0
54	1w	1603	0	828	22	0
54	2w	1555	0	797	37	0
55	1x	1646	0	838	15	0
55	2x	1646	0	838	12	0
56	1z	58	0	56	3	0
56	2z	58	0	56	3	0
57	1y	1585	0	803	40	0
57	2y	1565	0	793	34	0
58	10	9	0	0	0	0
58	11	6	0	0	0	0
58	12	2	0	0	0	0
58	13	4	0	0	0	0
58	14	1	0	0	0	0
58	15	7	0	0	0	0
58	16	1	0	0	0	0
58	17	5	0	0	0	0
58	18	7	0	0	0	0
58	19	1	0	0	0	0
58	1A	1101	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	1B	38	0	0	0	0
58	1D	13	0	0	0	0
58	1E	12	0	0	0	0
58	1F	12	0	0	0	0
58	1G	5	0	0	0	0
58	1H	1	0	0	0	0
58	1I	1	0	0	0	0
58	1N	5	0	0	0	0
58	1O	5	0	0	0	0
58	1P	7	0	0	0	0
58	1Q	8	0	0	0	0
58	1R	4	0	0	0	0
58	1S	3	0	0	0	0
58	1T	2	0	0	0	0
58	1U	10	0	0	0	0
58	1V	7	0	0	0	0
58	1W	4	0	0	0	0
58	1X	4	0	0	0	0
58	1Y	4	0	0	0	0
58	1Z	4	0	0	0	0
58	1a	210	0	0	0	0
58	1b	1	0	0	0	0
58	1d	1	0	0	0	0
58	1e	2	0	0	0	0
58	1f	2	0	0	0	0
58	1l	2	0	0	0	0
58	1m	1	0	0	0	0
58	1n	2	0	0	0	0
58	1t	1	0	0	0	0
58	1w	7	0	0	0	0
58	1x	12	0	0	0	0
58	20	2	0	0	0	0
58	21	1	0	0	0	0
58	23	3	0	0	0	0
58	25	3	0	0	0	0
58	27	2	0	0	0	0
58	28	4	0	0	0	0
58	29	1	0	0	0	0
58	2A	851	0	0	0	0
58	2B	20	0	0	0	0
58	2D	7	0	0	0	0
58	2E	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	2F	6	0	0	0	0
58	2G	1	0	0	0	0
58	2N	1	0	0	0	0
58	2O	2	0	0	0	0
58	2P	2	0	0	0	0
58	2Q	4	0	0	0	0
58	2R	4	0	0	0	0
58	2T	4	0	0	0	0
58	2U	1	0	0	0	0
58	2V	2	0	0	0	0
58	2W	1	0	0	0	0
58	2X	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	220	0	0	0	0
58	2d	3	0	0	0	0
58	2e	1	0	0	0	0
58	2f	2	0	0	0	0
58	2i	1	0	0	0	0
58	2j	2	0	0	0	0
58	2k	1	0	0	0	0
58	2l	3	0	0	0	0
58	2n	1	0	0	0	0
58	2q	3	0	0	0	0
58	2r	1	0	0	0	0
58	2t	2	0	0	0	0
58	2v	4	0	0	0	0
58	2w	4	0	0	0	0
58	2x	6	0	0	0	0
59	1A	1	0	0	0	0
59	2A	1	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	10	13	0	0	0	0
62	11	7	0	0	0	0
62	12	3	0	0	0	0
62	13	6	0	0	0	0
62	15	8	0	0	0	0
62	16	2	0	0	0	0
62	17	8	0	0	0	0
62	18	12	0	0	0	0
62	1A	1949	0	0	79	0
62	1B	58	0	0	3	0
62	1D	26	0	0	0	0
62	1E	28	0	0	3	0
62	1F	18	0	0	2	0
62	1G	3	0	0	1	0
62	1H	2	0	0	0	0
62	1N	6	0	0	0	0
62	1O	6	0	0	0	0
62	1P	19	0	0	2	0
62	1Q	7	0	0	0	0
62	1R	10	0	0	4	0
62	1S	4	0	0	0	0
62	1T	7	0	0	0	0
62	1U	13	0	0	0	0
62	1V	9	0	0	0	0
62	1W	7	0	0	0	0
62	1X	5	0	0	0	0
62	1Y	3	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	301	0	0	21	0
62	1b	1	0	0	0	0
62	1e	1	0	0	0	0
62	1f	1	0	0	0	0
62	1i	1	0	0	0	0
62	1l	5	0	0	0	0
62	1m	1	0	0	0	0
62	1o	2	0	0	0	0
62	1q	2	0	0	0	0
62	1v	5	0	0	0	0
62	1w	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1x	7	0	0	2	0
62	1z	3	0	0	0	0
62	20	2	0	0	0	0
62	21	7	0	0	1	0
62	22	1	0	0	0	0
62	23	2	0	0	0	0
62	25	2	0	0	0	0
62	27	5	0	0	0	0
62	28	3	0	0	0	0
62	29	1	0	0	0	0
62	2A	1047	0	0	73	0
62	2B	20	0	0	1	0
62	2D	26	0	0	0	0
62	2E	15	0	0	1	0
62	2F	14	0	0	0	0
62	2N	1	0	0	0	0
62	2O	2	0	0	0	0
62	2P	10	0	0	1	0
62	2Q	2	0	0	0	0
62	2R	3	0	0	0	0
62	2T	6	0	0	0	0
62	2U	1	0	0	1	0
62	2V	1	0	0	0	0
62	2W	3	0	0	0	0
62	2X	5	0	0	1	0
62	2a	196	0	0	8	0
62	2c	1	0	0	0	0
62	2d	1	0	0	0	0
62	2e	2	0	0	0	0
62	2g	1	0	0	0	0
62	2i	1	0	0	0	0
62	2j	2	0	0	0	0
62	2l	5	0	0	0	0
62	2r	1	0	0	0	0
62	2t	1	0	0	0	0
62	2v	2	0	0	0	0
62	2w	6	0	0	1	0
62	2x	4	0	0	0	0
62	2z	1	0	0	0	0
All	All	299898	0	196836	4043	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (4043) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.23	1.36
1:1A:1082:U:O4	1:1A:1086:A:N1	1.92	1.02
1:1A:1054:A:N6	1:1A:1105:U:H3	1.57	1.01
54:2w:4:C:N4	54:2w:69:G:H1	1.59	1.01
1:1A:2499:C:OP1	62:1A:4204:HOH:O	1.80	1.00
1:1A:2121:G:H1	1:1A:2177:C:H42	1.08	0.96
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.45	0.95
1:1A:2100:G:H1	1:1A:2189:U:H3	0.95	0.93
1:2A:2099:U:H3	1:2A:2190:G:H1	0.95	0.93
1:2A:2138:C:H42	1:2A:2153:G:H1	1.11	0.93
1:1A:1071:G:N2	1:1A:1091:G:N7	2.17	0.92
54:2w:4:C:H42	54:2w:69:G:H1	1.02	0.92
1:1A:1054:A:H61	1:1A:1105:U:H3	0.93	0.90
57:1y:53:G:H1	57:1y:61:C:H42	1.19	0.90
1:1A:2136:C:N3	1:1A:2155:G:C2	2.41	0.89
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.06	0.89
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.12	0.88
54:2w:4:C:N3	54:2w:69:G:N2	2.22	0.88
1:1A:1603:A:OP1	62:1A:4205:HOH:O	1.92	0.87
1:1A:2102:U:H3	1:1A:2187:G:H1	1.18	0.86
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.24	0.85
1:1A:2096:U:H3	1:1A:2193:G:H1	1.25	0.85
1:2A:2138:C:N4	1:2A:2153:G:H1	1.74	0.85
19:2X:60:ARG:HH22	29:27:47:ARG:HH22	1.25	0.85
1:1A:2789:C:O2	1:1A:2894:G:N1	2.11	0.84
32:1a:1027:C:C2	32:1a:1034:G:N2	2.44	0.84
57:1y:19:G:N2	57:1y:56:C:N3	2.26	0.83
32:1a:376:G:H5''	47:1p:5:ARG:HG2	1.58	0.83
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.60	0.83
1:1A:279:C:H42	1:1A:361:G:H1	1.26	0.83
32:2a:73:G:H1	32:2a:96:U:H3	1.26	0.82
1:1A:2427:C:OP1	62:1A:4206:HOH:O	1.95	0.82
1:1A:2448:A:OP1	62:1A:4204:HOH:O	1.98	0.82
34:2c:125:GLU:HB2	34:2c:190:ARG:HH21	1.45	0.82
32:2a:1029:C:C4	32:2a:1032:G:N1	2.47	0.82
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.63	0.81
1:2A:1021:A:H62	1:2A:1141:U:H3	1.28	0.81
1:1A:2128:C:N4	1:1A:2160:G:H1	1.79	0.81
1:1A:2550:G:OP1	62:1A:4208:HOH:O	1.98	0.80
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.45	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.46	0.80
1:1A:1271:G:OP2	62:1A:4207:HOH:O	1.97	0.80
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.15	0.80
1:1A:249:C:O2'	11:1P:64:LYS:NZ	2.14	0.80
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.14	0.80
1:1A:1332:G:OP1	62:1A:4209:HOH:O	1.99	0.80
32:1a:975:A:H4'	32:1a:976:G:H5''	1.62	0.80
32:2a:947:G:H1	32:2a:1234:C:H42	1.28	0.80
1:2A:1604:C:OP2	62:2A:3902:HOH:O	1.99	0.80
1:1A:2121:G:H1	1:1A:2177:C:N4	1.79	0.79
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.15	0.79
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.15	0.79
1:1A:2808:U:O2	1:1A:2892:A:N6	2.16	0.79
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.65	0.79
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.14	0.79
32:1a:875:C:H1'	39:1h:15:ASN:HD21	1.48	0.79
1:1A:2124:G:H1	1:1A:2174:C:H42	1.31	0.79
1:2A:2127:G:N1	1:2A:2161:C:C4	2.51	0.78
32:2a:1114:C:H42	32:2a:1186:G:H1	1.31	0.78
1:2A:2127:G:C6	1:2A:2161:C:N4	2.51	0.78
32:2a:1373:G:H5''	38:2g:36:LYS:HE2	1.66	0.78
1:2A:2637:U:H5''	4:2E:82:ARG:HH12	1.47	0.78
32:2a:1244:C:H42	32:2a:1293:G:H1	1.31	0.78
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.17	0.78
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.64	0.78
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.65	0.78
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.66	0.78
1:2A:2808:U:O2	1:2A:2892:A:N6	2.17	0.78
1:2A:397:G:N7	62:2A:3928:HOH:O	2.16	0.77
1:1A:2575:C:OP2	62:1A:4210:HOH:O	2.02	0.77
57:2y:26:A:N1	57:2y:44:G:O6	2.18	0.77
1:1A:881:G:N2	1:1A:897:C:O2	2.18	0.77
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.67	0.77
32:2a:407:G:H5''	35:2d:115:ARG:HB3	1.67	0.77
1:2A:1830:C:OP2	62:2A:3903:HOH:O	2.02	0.76
7:1H:3:ARG:HG3	7:1H:6:ARG:HE	1.50	0.76
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.18	0.76
1:2A:570:G:O6	62:2A:3905:HOH:O	2.04	0.76
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.18	0.76
1:1A:1452:A:OP2	62:1A:4213:HOH:O	2.04	0.76
1:2A:1031:G:H21	31:29:36:GLN:HE22	1.34	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:963:U:OP2	62:2A:3904:HOH:O	2.04	0.76
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.17	0.76
32:2a:1060:C:H5'	45:2n:45:ARG:HH12	1.51	0.76
32:1a:664:G:H22	32:1a:741:G:H1	1.34	0.76
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.49	0.76
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.17	0.76
1:1A:376:C:OP1	62:1A:4211:HOH:O	2.03	0.76
19:2X:72:LYS:NZ	19:2X:75:ASP:OD1	2.18	0.76
1:1A:826:U:OP1	62:1A:4206:HOH:O	2.04	0.76
1:1A:467:G:OP1	29:17:33:ARG:NH1	2.19	0.75
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.68	0.75
1:2A:1271:G:OP2	62:2A:3908:HOH:O	2.04	0.75
1:2A:1970:A:OP1	62:2A:3909:HOH:O	2.05	0.75
1:1A:1315:C:OP2	62:1A:4209:HOH:O	2.03	0.75
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.19	0.75
32:2a:662:G:O2'	32:2a:836:G:OP1	2.04	0.75
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.68	0.75
6:1G:114:ILE:HG13	6:1G:140:ILE:HG12	1.68	0.75
1:2A:2712(A):A:OP2	62:2A:3907:HOH:O	2.04	0.75
1:1A:2612:C:OP2	27:15:2:ALA:N	2.20	0.75
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.69	0.75
37:1f:8:ILE:HG12	37:1f:88:VAL:HG22	1.67	0.75
26:14:55:ARG:H	26:14:56:VAL:HA	1.50	0.75
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.20	0.75
2:2B:20:C:N4	2:2B:63:G:O6	2.15	0.74
32:2a:1029:C:N3	32:2a:1032:G:N2	2.35	0.74
1:1A:1970:A:OP1	62:1A:4212:HOH:O	2.03	0.74
1:2A:962:G:OP1	62:2A:3904:HOH:O	2.05	0.74
32:1a:1500:A:OP2	62:1a:1902:HOH:O	2.05	0.74
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.32	0.74
32:2a:176:C:OP1	51:2t:29:LYS:NZ	2.18	0.74
54:2w:52:G:H1	54:2w:62:C:H42	1.35	0.74
38:2g:99:LEU:HD23	38:2g:102:ARG:HH12	1.52	0.74
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.21	0.74
23:21:50:ARG:HG2	23:21:59:THR:HG23	1.70	0.74
26:14:16:CYS:SG	26:14:17:GLY:N	2.61	0.74
57:1y:8:4SU:O2'	57:1y:21:A:N1	2.20	0.74
1:2A:2127:G:N2	1:2A:2161:C:C2	2.56	0.74
1:1A:382:G:O6	62:1A:4214:HOH:O	2.05	0.74
1:2A:1670:C:OP1	62:2A:3906:HOH:O	2.04	0.74
1:1A:1669:A:OP2	62:1A:4208:HOH:O	2.05	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2135:A:N6	1:1A:2156:G:O2'	2.21	0.73
1:1A:2508:G:OP1	62:1A:4215:HOH:O	2.05	0.73
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.21	0.73
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.70	0.73
1:1A:884:C:H42	1:1A:892:G:H1	1.36	0.73
1:2A:1671:U:OP2	62:2A:3906:HOH:O	2.04	0.73
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.34	0.73
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.21	0.73
1:2A:2127:G:C2	1:2A:2161:C:N3	2.57	0.73
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.21	0.73
8:2I:40:THR:OG1	8:2I:41:GLU:N	2.18	0.73
1:1A:2130:U:O2'	1:1A:2131:G:N2	2.22	0.73
1:1A:2306:C:O2	62:1A:4218:HOH:O	2.07	0.73
1:1A:2615:U:OP1	62:1A:4216:HOH:O	2.06	0.73
32:2a:953:G:H5'	32:2a:965:A:H61	1.53	0.73
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.21	0.73
33:2b:189:ASP:N	33:2b:189:ASP:OD1	2.22	0.73
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.71	0.73
32:1a:574:A:OP2	62:1a:1903:HOH:O	2.07	0.72
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.22	0.72
34:2c:30:ARG:HH21	45:2n:38:GLY:HA2	1.54	0.72
22:10:11:ARG:O	22:10:14:ARG:NH2	2.19	0.72
1:2A:2127:G:N1	1:2A:2161:C:N4	2.37	0.72
1:2A:2682:U:OP2	62:2A:3911:HOH:O	2.06	0.72
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.71	0.72
32:1a:953:G:H5'	32:1a:965:A:H61	1.54	0.72
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.71	0.72
1:1A:1023:U:OP2	62:1A:4217:HOH:O	2.07	0.72
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.22	0.72
1:1A:271(K):U:H1'	8:1I:50:ARG:HD2	1.72	0.72
4:1E:110:GLY:O	62:1R:301:HOH:O	2.07	0.72
55:1x:76:8AN:O2P	62:1x:201:HOH:O	2.08	0.72
1:2A:1313:U:OP1	62:2A:3912:HOH:O	2.07	0.72
32:2a:266:G:H5''	32:2a:268:C:H41	1.55	0.72
1:2A:582:G:OP2	62:2A:3910:HOH:O	2.06	0.72
1:1A:2128:C:N3	1:1A:2160:G:N2	2.38	0.72
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.23	0.72
29:17:24:THR:HG22	29:17:27:GLY:H	1.55	0.72
1:1A:2080:G:O6	62:1A:4219:HOH:O	2.07	0.72
32:1a:642:A:N3	39:1h:113:SER:OG	2.21	0.72
21:1Z:156:LYS:HD2	21:1Z:158:PRO:HD3	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2794:C:N4	1:2A:2802:G:O6	2.23	0.71
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.71	0.71
32:2a:1187:G:OP1	40:2i:113:LYS:NZ	2.23	0.71
32:1a:1197:G:OP2	62:1a:1904:HOH:O	2.07	0.71
23:21:32:LYS:O	62:21:201:HOH:O	2.07	0.71
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	1.71	0.71
19:1X:1:MET:HE1	24:12:26:ARG:HH21	1.55	0.71
14:2S:71:ARG:NH1	14:2S:107:GLU:OE1	2.22	0.71
1:1A:2142:C:N3	1:1A:2149:G:O6	2.23	0.71
1:2A:948:G:OP1	62:2A:3904:HOH:O	2.08	0.71
28:16:13:CYS:SG	28:16:47:THR:HG21	2.30	0.71
1:2A:651:G:OP1	30:28:19:SER:OG	2.09	0.71
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.23	0.71
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.24	0.71
24:22:35:LEU:HD11	24:22:49:LYS:HE2	1.73	0.71
21:2Z:106:GLY:HA3	21:2Z:141:VAL:HB	1.73	0.71
32:2a:1397:C:N4	53:2v:22:U:OP2	2.24	0.71
1:1A:2573:C:OP1	62:1A:4210:HOH:O	2.09	0.71
5:1F:164:ARG:HD2	5:1F:175:THR:HG23	1.72	0.71
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.70	0.71
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.56	0.71
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.24	0.70
32:1a:1414:U:O4	62:1a:1905:HOH:O	2.09	0.70
1:2A:245:G:O6	30:28:8:LYS:NZ	2.24	0.70
57:1y:53:G:H1	57:1y:61:C:N4	1.88	0.70
1:2A:1568:G:N7	62:2A:3958:HOH:O	2.24	0.70
1:2A:1800:C:OP1	3:2D:260:ARG:NH2	2.24	0.70
32:2a:1029:C:N4	32:2a:1032:G:N1	2.39	0.70
54:2w:18:G:O2'	54:2w:57:G:N2	2.24	0.70
1:1A:668:G:N7	62:1A:4264:HOH:O	2.23	0.70
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.25	0.70
33:1b:78:GLN:NE2	33:1b:94:ASN:O	2.23	0.70
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.73	0.70
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.73	0.70
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.73	0.70
28:16:12:GLU:OE1	28:16:19:ARG:NH1	2.25	0.70
1:2A:2163:C:OP1	1:2A:2165:G:N2	2.25	0.70
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.71	0.70
1:1A:1183:G:O2'	25:13:29:ARG:NH2	2.25	0.70
33:1b:32:ILE:HD13	33:1b:40:HIS:HD2	1.55	0.70
42:1k:16:SER:HB2	42:1k:79:SER:HB3	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:943:U:OP2	62:2A:3917:HOH:O	2.10	0.70
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.21	0.70
32:2a:1076:C:H2'	32:2a:1077:G:H5''	1.74	0.70
32:1a:1362:C:OP2	62:1a:1906:HOH:O	2.09	0.70
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.25	0.70
1:2A:1993:U:OP2	62:2A:3915:HOH:O	2.09	0.70
1:1A:2632:A:HO2'	1:1A:2811:G:HO2'	1.39	0.69
1:2A:217:G:OP2	62:2A:3914:HOH:O	2.09	0.69
1:1A:11:G:H2'	1:1A:12:U:H5'	1.74	0.69
1:1A:668:G:OP2	62:1A:4220:HOH:O	2.09	0.69
1:2A:1253:A:OP1	62:2A:3919:HOH:O	2.10	0.69
57:2y:18:G:N2	57:2y:55:PSU:N3	2.40	0.69
57:2y:18:G:N2	57:2y:55:PSU:C4	2.60	0.69
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.17	0.69
23:21:50:ARG:NH1	23:21:57:GLU:OE2	2.23	0.69
1:1A:1082:U:N3	1:1A:1086:A:N6	2.00	0.69
57:1y:19:G:N1	57:1y:56:C:N4	2.40	0.69
1:2A:422:A:OP2	62:2A:3918:HOH:O	2.10	0.69
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.25	0.69
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	1.74	0.69
18:2W:88:ARG:HB2	18:2W:92:ARG:HG2	1.74	0.69
1:2A:2759:G:OP2	62:2A:3916:HOH:O	2.10	0.69
25:23:7:LYS:NZ	25:23:34:GLU:OE1	2.24	0.69
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.40	0.69
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.56	0.69
1:1A:760:G:OP1	62:1A:4222:HOH:O	2.10	0.69
32:1a:1054:C:OP2	62:1a:1904:HOH:O	2.09	0.69
1:2A:1647:G:OP1	62:2A:3908:HOH:O	2.11	0.69
1:1A:1062:G:H8	1:1A:1070:A:H4'	1.57	0.69
1:1A:2702:U:OP2	62:1A:4221:HOH:O	2.09	0.69
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.10	0.69
1:2A:878:A:N6	1:2A:899:A:O2'	2.26	0.69
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.39	0.69
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.26	0.69
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.26	0.69
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.26	0.69
32:2a:148:G:H2'	32:2a:149:A:H8	1.58	0.69
1:1A:1041:C:H42	1:1A:1114:G:H1	1.41	0.69
55:1x:12:G:OP2	62:1x:202:HOH:O	2.10	0.69
1:2A:804:A:OP1	62:2A:3920:HOH:O	2.11	0.69
1:2A:1648:C:OP1	62:2A:3908:HOH:O	2.10	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1014:U:OP2	62:1A:4225:HOH:O	2.12	0.68
42:1k:48:ILE:O	42:1k:50:TYR:N	2.25	0.68
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.76	0.68
1:1A:2136:C:C2	1:1A:2155:G:N2	2.60	0.68
1:2A:2134:A:OP2	1:2A:2157:G:N2	2.27	0.68
32:2a:1302:U:OP2	44:2m:21:TYR:OH	2.08	0.68
1:2A:2127:G:N2	1:2A:2161:C:N3	2.40	0.68
33:2b:74:LYS:O	33:2b:78:GLN:HG2	1.93	0.68
24:12:14:ARG:O	24:12:67:LYS:NZ	2.25	0.68
21:2Z:72:ARG:HH22	21:2Z:97:GLU:HB2	1.59	0.68
21:2Z:100:VAL:HG21	21:2Z:134:PRO:HG2	1.76	0.68
23:21:40:ARG:NH2	23:21:41:ARG:O	2.24	0.68
38:2g:16:LEU:HD22	40:2i:42:ARG:HA	1.75	0.68
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.26	0.68
35:1d:100:ARG:NH2	35:1d:102:ASP:OD2	2.27	0.68
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.75	0.68
32:2a:157:G:H1	32:2a:164:U:H3	1.39	0.68
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.27	0.68
1:1A:2141:G:O6	1:1A:2150:U:O2	2.11	0.68
1:1A:2429:G:OP1	62:1A:4206:HOH:O	2.12	0.68
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.27	0.68
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.26	0.68
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.27	0.68
32:2a:1025:U:H3	32:2a:1036:G:H1	1.42	0.68
1:1A:2059:A:OP2	62:1A:4224:HOH:O	2.11	0.68
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.11	0.68
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.27	0.68
32:1a:1030(A):G:N2	32:1a:1031:G:O6	2.19	0.68
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.42	0.68
35:2d:50:ARG:HH12	36:2e:10:MET:HG3	1.58	0.68
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.28	0.67
1:1A:2821:A:OP2	62:1R:301:HOH:O	2.12	0.67
1:2A:711:G:N2	1:2A:720:C:O2	2.19	0.67
1:2A:2218:U:N3	23:21:55:GLY:O	2.27	0.67
4:2E:77:ILE:HD13	4:2E:195:LEU:HD22	1.75	0.67
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.75	0.67
47:2p:60:LEU:HD21	47:2p:80:PHE:HE1	1.59	0.67
21:2Z:154:ASP:OD1	21:2Z:154:ASP:N	2.24	0.67
40:2i:31:GLN:HB3	40:2i:35:GLU:HG2	1.76	0.67
44:2m:23:TYR:HE2	44:2m:70:LEU:HD22	1.59	0.67
26:14:55:ARG:N	26:14:56:VAL:HA	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.29	0.67
1:2A:2038:G:O6	62:2A:3913:HOH:O	2.08	0.67
32:1a:1224:G:OP1	62:1a:1907:HOH:O	2.11	0.67
1:2A:249:C:O2	30:28:12:LYS:NZ	2.27	0.67
1:1A:2871:C:N3	62:1A:4276:HOH:O	2.26	0.67
1:2A:83:G:H1	1:2A:102:G:HO2'	1.42	0.67
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.23	0.67
1:1A:2128:C:N4	1:1A:2160:G:N1	2.43	0.67
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.75	0.67
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.77	0.67
32:1a:812:C:N3	62:1a:1922:HOH:O	2.27	0.67
1:2A:143(A):C:O2'	19:2X:2:LYS:NZ	2.26	0.67
1:2A:2135:A:N1	1:2A:2156:G:O2'	2.25	0.67
14:2S:84:GLN:H	14:2S:111:GLU:HB2	1.59	0.67
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.77	0.67
1:1A:2136:C:N4	1:1A:2155:G:C6	2.63	0.67
54:2w:68:C:H2'	54:2w:69:G:H8	1.60	0.67
1:1A:1648:C:OP1	62:1A:4207:HOH:O	2.13	0.67
7:2H:121:ILE:HG13	7:2H:144:VAL:HG21	1.76	0.67
50:2s:18:LYS:HB3	50:2s:31:ILE:HD13	1.76	0.67
1:1A:1024:G:OP2	62:1A:4217:HOH:O	2.12	0.67
62:1A:4218:HOH:O	6:1G:45:GLU:OE2	2.12	0.67
7:2H:149:ARG:NH1	7:2H:167:GLU:OE1	2.27	0.67
8:2I:55:ALA:HA	8:2I:58:LEU:HB3	1.77	0.67
44:2m:10:PRO:HD2	44:2m:18:ALA:HB1	1.76	0.67
49:2r:73:ALA:HB1	49:2r:78:LEU:HB2	1.77	0.67
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.59	0.66
45:2n:23:ARG:NH1	45:2n:28:GLY:O	2.28	0.66
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.31	0.66
1:1A:570:G:O6	62:1A:4204:HOH:O	2.10	0.66
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.42	0.66
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.76	0.66
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.26	0.66
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.60	0.66
32:2a:533:A:OP1	62:2a:1902:HOH:O	2.14	0.66
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.27	0.66
20:2Y:39:VAL:HB	20:2Y:42:VAL:HB	1.76	0.66
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.78	0.66
1:2A:10:G:O2'	1:2A:2801(A):A:N7	2.28	0.66
32:1a:573:A:OP2	62:1a:1903:HOH:O	2.13	0.66
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:12:THR:OG1	20:1Y:26:LYS:NZ	2.28	0.66
32:1a:613:C:H2'	32:1a:614:A:H8	1.60	0.66
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.75	0.66
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.28	0.66
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.76	0.66
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.13	0.66
1:1A:1647:G:OP1	62:1A:4207:HOH:O	2.13	0.66
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.19	0.66
1:2A:975:C:OP1	62:2A:3921:HOH:O	2.14	0.66
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.77	0.66
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	1.78	0.66
50:1s:27:GLU:HG3	50:1s:28:LYS:HE3	1.77	0.66
1:2A:1031:G:N2	31:29:36:GLN:HE22	1.92	0.66
1:1A:1058:G:H1	1:1A:1080:C:H42	1.42	0.66
1:2A:370:G:N7	62:2A:3975:HOH:O	2.29	0.66
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.61	0.66
32:2a:1133:G:H1	32:2a:1141:C:H42	1.43	0.66
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.60	0.66
1:1A:1237:A:OP1	62:1A:4228:HOH:O	2.14	0.65
40:1i:96:LEU:HD13	40:1i:101:PHE:HD2	1.60	0.65
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.76	0.65
4:2E:12:THR:HG22	4:2E:13:ARG:H	1.61	0.65
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.28	0.65
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.30	0.65
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.78	0.65
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.76	0.65
32:2a:995:C:O2	45:2n:4:LYS:NZ	2.26	0.65
4:1E:9:VAL:HG13	15:1T:3:ARG:HG2	1.78	0.65
33:1b:178:ARG:HH22	39:1h:74:PRO:HB3	1.61	0.65
1:2A:2619:C:OP1	4:2E:152:LYS:NZ	2.29	0.65
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.29	0.65
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.78	0.65
32:1a:1320:C:O2	50:1s:36:ARG:NH2	2.28	0.65
1:2A:531:C:OP1	1:2A:561:G:N1	2.30	0.65
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.29	0.65
33:2b:18:GLY:HA2	33:2b:42:ILE:HG13	1.79	0.65
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.13	0.65
1:1A:2252:G:OP2	62:1A:4227:HOH:O	2.13	0.65
32:1a:324:G:N7	62:1a:1926:HOH:O	2.28	0.65
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.79	0.65
32:2a:1129:C:H5'	40:2i:16:ARG:HH22	1.60	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1192:G:OP2	62:1A:4229:HOH:O	2.14	0.65
1:2A:1971:A:OP1	62:2A:3909:HOH:O	2.14	0.65
8:2I:101:LEU:HB2	8:2I:107:VAL:HB	1.76	0.65
32:2a:1009:G:O6	32:2a:1020:U:O2	2.15	0.65
49:2r:52:PRO:O	49:2r:56:THR:OG1	2.14	0.65
1:1A:1971:A:OP1	62:1A:4212:HOH:O	2.13	0.65
32:1a:557:G:OP1	62:1a:1909:HOH:O	2.14	0.65
1:2A:2138:C:N3	1:2A:2153:G:N2	2.40	0.65
1:2A:2448:A:OP1	62:2A:3905:HOH:O	2.14	0.65
1:2A:481:G:N7	62:2A:3979:HOH:O	2.30	0.65
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.78	0.65
1:1A:1265:A:OP2	62:1A:4216:HOH:O	2.14	0.65
25:13:55:ARG:HH22	25:13:57:GLU:HB2	1.62	0.64
35:1d:60:GLU:OE2	35:1d:63:LYS:NZ	2.22	0.64
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.22	0.64
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.78	0.64
1:2A:2127:G:C2	1:2A:2161:C:C4	2.86	0.64
32:2a:376:G:O2'	47:2p:5:ARG:NH2	2.30	0.64
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.79	0.64
41:2j:8:LEU:HD11	41:2j:20:ALA:HB2	1.79	0.64
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.79	0.64
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.79	0.64
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.32	0.64
32:2a:1026:G:O6	32:2a:1036:G:N2	2.31	0.64
54:2w:29:G:H1	54:2w:41:C:H42	1.42	0.64
1:2A:1689:A:H62	1:2A:1698:A:H2	1.45	0.64
1:2A:1973:G:OP1	62:2A:3924:HOH:O	2.15	0.64
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.24	0.64
32:2a:978:A:O2'	32:2a:1322:C:N3	2.27	0.64
32:2a:1086:U:H3	32:2a:1099:G:H22	1.43	0.64
33:2b:16:HIS:O	33:2b:18:GLY:N	2.30	0.64
1:1A:607:U:OP1	5:1F:102:PRO:HA	1.97	0.64
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.32	0.64
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.31	0.64
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.78	0.64
54:2w:40:C:OP1	62:2w:201:HOH:O	2.14	0.64
1:1A:2124:G:H1	1:1A:2174:C:N4	1.95	0.64
32:1a:1182:G:H4'	32:1a:1183:A:H5''	1.79	0.64
1:2A:2431:U:OP2	62:2A:3925:HOH:O	2.15	0.64
32:2a:335:C:O2'	32:2a:1433:A:N3	2.30	0.64
33:2b:104:ASN:OD1	33:2b:107:THR:OG1	2.14	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:9:LEU:HD23	8:1I:12:LEU:HD12	1.80	0.64
1:2A:805:G:OP1	62:2A:3920:HOH:O	2.14	0.64
32:2a:457:C:H2'	32:2a:458:C:H6	1.62	0.64
32:2a:1272:G:N2	32:2a:1273:G:C5	2.65	0.64
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.80	0.64
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.14	0.64
35:2d:18:LYS:NZ	35:2d:26:CYS:O	2.31	0.64
1:1A:1865:G:OP1	62:1A:4231:HOH:O	2.15	0.64
1:1A:2142:C:O2	1:1A:2149:G:N1	2.25	0.64
47:1p:53:VAL:HG13	47:1p:79:VAL:HG22	1.78	0.64
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.31	0.64
1:1A:897:C:N3	1:1A:898:C:N4	2.46	0.64
34:1c:36:ASP:OD1	34:1c:59:ARG:NH2	2.30	0.64
57:1y:53:G:H2'	57:1y:54:5MU:H6	1.63	0.64
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.31	0.64
26:24:50:VAL:HG22	44:2m:65:LYS:HB3	1.79	0.64
39:2h:4:ASP:OD1	39:2h:7:ALA:N	2.29	0.64
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.33	0.63
14:2S:105:ALA:HB1	14:2S:110:LEU:HD23	1.79	0.63
54:2w:19:G:H1	54:2w:56:C:H42	1.46	0.63
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.45	0.63
28:16:47:THR:HG22	28:16:49:HIS:CE1	2.33	0.63
32:1a:739:C:HO2'	46:1o:42:HIS:HD1	1.46	0.63
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.80	0.63
1:2A:1376:C:OP2	62:2A:3922:HOH:O	2.14	0.63
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.80	0.63
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.31	0.63
11:2P:121:LYS:O	11:2P:123:LEU:N	2.31	0.63
1:1A:1062:G:H2'	1:1A:1063:G:C8	2.33	0.63
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	1.79	0.63
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.31	0.63
32:2a:661:G:H1	32:2a:744:C:H42	1.45	0.63
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.31	0.63
1:1A:2165:G:H2'	1:1A:2166:G:C4	2.34	0.63
1:1A:2428:G:OP1	62:1A:4206:HOH:O	2.16	0.63
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.80	0.63
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.78	0.63
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.63	0.63
32:1a:1025:U:O2	32:1a:1036:G:O6	2.16	0.63
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.32	0.63
57:2y:18:G:H4'	57:2y:60:U:C5	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:13:ARG:HB3	26:14:30:GLU:HG2	1.81	0.63
28:16:28:ARG:NH1	28:16:29:ASN:OD1	2.31	0.63
1:1A:674:G:O2'	5:1F:74:ARG:HD3	1.99	0.63
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.33	0.63
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.63	0.63
57:2y:63:G:H2'	57:2y:64:A:H8	1.64	0.63
11:1P:38:GLN:O	11:1P:39:LYS:HB3	1.99	0.63
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.80	0.63
32:1a:396:G:O2'	32:1a:398:C:OP1	2.11	0.63
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.33	0.63
4:2E:9:VAL:HG13	15:2T:3:ARG:HG2	1.81	0.63
36:1e:91:LEU:HB3	36:1e:118:ILE:HD11	1.81	0.62
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.79	0.62
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.80	0.62
32:2a:142:G:H2'	32:2a:143:A:C8	2.34	0.62
40:1i:53:VAL:O	40:1i:55:ALA:N	2.27	0.62
1:2A:598:G:N2	5:2F:35:GLU:OE2	2.32	0.62
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.17	0.62
1:2A:1833:U:OP1	62:2A:3929:HOH:O	2.16	0.62
26:24:53:GLU:HG2	26:24:55:ARG:H	1.63	0.62
32:2a:407:G:OP1	35:2d:115:ARG:NH2	2.32	0.62
35:2d:150:GLU:H	35:2d:150:GLU:CD	2.06	0.62
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.82	0.62
41:1j:27:ALA:HA	41:1j:81:THR:HG21	1.81	0.62
32:2a:1003:G:N2	32:2a:1025:U:O4	2.32	0.62
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.16	0.62
1:1A:2344:U:OP1	28:16:37:ARG:NH1	2.31	0.62
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.15	0.62
1:2A:1204:A:H2	1:2A:1241:A:H62	1.46	0.62
4:1E:55:ASN:HB3	4:1E:58:ARG:HB2	1.81	0.62
32:1a:118:U:O4	62:1a:1908:HOH:O	2.12	0.62
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.18	0.62
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.65	0.62
1:1A:530:G:N1	1:1A:2023:G:OP1	2.22	0.62
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.48	0.62
6:2G:64:THR:HG22	6:2G:94:LEU:HD11	1.80	0.62
33:2b:118:LEU:HD11	33:2b:138:LEU:HD23	1.82	0.62
37:2f:100:ASN:HD21	49:2r:23:LYS:HG2	1.63	0.62
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.65	0.62
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.33	0.62
41:1j:64:GLU:OE2	41:1j:66:ARG:NE	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.30	0.62
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.33	0.62
44:1m:12:ASN:O	44:1m:44:ARG:NH1	2.33	0.62
41:2j:21:GLN:HE22	41:2j:25:GLU:HG2	1.65	0.62
44:2m:94:ARG:HB3	44:2m:96:LEU:HD12	1.81	0.62
5:1F:89:VAL:O	62:1F:401:HOH:O	2.16	0.62
38:1g:15:ASP:HB3	38:1g:24:THR:HG23	1.82	0.62
41:1j:46:ARG:HB2	41:1j:46:ARG:HH11	1.65	0.62
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.34	0.62
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.82	0.62
53:2v:22:U:O4	53:2v:23:A:N6	2.31	0.62
1:1A:184:C:H2'	1:1A:185:U:C6	2.34	0.62
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.80	0.62
1:2A:2711:A:OP2	62:2A:3907:HOH:O	2.16	0.62
39:2h:39:LEU:HG	39:2h:44:PHE:HB2	1.81	0.62
57:2y:26:A:N1	57:2y:44:G:C6	2.67	0.62
1:2A:882:G:H22	1:2A:894:C:H42	1.46	0.61
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.65	0.61
54:2w:72:C:H2'	54:2w:73:A:C8	2.35	0.61
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.35	0.61
21:2Z:77:ASP:OD2	21:2Z:80:ARG:NH1	2.32	0.61
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.36	0.61
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.36	0.61
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.35	0.61
32:2a:402:G:N7	62:2a:1920:HOH:O	2.31	0.61
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.33	0.61
52:2u:6:ARG:HB3	52:2u:15:ARG:HE	1.65	0.61
1:1A:621:A:OP2	11:1P:108:LYS:NZ	2.34	0.61
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.82	0.61
32:1a:17:U:H2'	32:1a:18:C:C6	2.35	0.61
1:2A:247:G:H4'	1:2A:386:G:C5	2.35	0.61
9:2N:18:ALA:HB1	9:2N:60:ILE:HD12	1.82	0.61
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.81	0.61
34:2c:35:GLU:O	34:2c:39:ILE:HG13	2.00	0.61
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.65	0.61
1:1A:2337:G:OP1	62:1A:4232:HOH:O	2.16	0.61
32:1a:809:G:OP2	46:1o:48:LYS:NZ	2.31	0.61
32:2a:975:A:H4'	32:2a:976:G:H5''	1.83	0.61
1:1A:2165:G:H1	1:1A:2171:A:H2'	1.65	0.61
32:1a:1004:A:H5''	32:1a:1025:U:H5	1.66	0.61
1:2A:921:G:O6	62:2A:3930:HOH:O	2.16	0.61

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	1.81	0.61
21:2Z:129:SER:OG	21:2Z:131:ARG:NH1	2.33	0.61
1:1A:192:C:OP1	62:1A:4233:HOH:O	2.16	0.61
7:2H:101:ARG:HH12	7:2H:122:THR:HG22	1.65	0.61
26:24:44:THR:O	26:24:46:GLN:N	2.29	0.61
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.19	0.61
46:2o:24:SER:HB3	46:2o:27:VAL:HG13	1.81	0.61
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.81	0.61
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.01	0.61
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.83	0.61
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.36	0.61
12:2Q:37:LEU:HD11	12:2Q:130:LYS:HB2	1.83	0.61
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.34	0.61
26:24:46:GLN:C	26:24:48:ARG:H	2.09	0.61
47:2p:15:PRO:HD2	47:2p:42:ARG:HD3	1.83	0.61
1:1A:2103:C:H42	1:1A:2186:G:H1	1.49	0.61
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.28	0.61
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.83	0.61
1:1A:2099:U:H3	1:1A:2190:G:H1	1.46	0.60
33:1b:30:ARG:HH21	33:1b:194:PRO:HB2	1.65	0.60
32:2a:947:G:H1	32:2a:1234:C:N4	1.97	0.60
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.34	0.60
32:1a:1264:C:H42	32:1a:1271:G:H1	1.48	0.60
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.33	0.60
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.34	0.60
40:2i:40:LEU:HD13	40:2i:74:ILE:HD11	1.83	0.60
54:2w:68:C:H2'	54:2w:69:G:C8	2.35	0.60
15:1T:1:MET:HE2	15:1T:3:ARG:HG3	1.81	0.60
34:1c:172:ARG:HG3	34:1c:174:PRO:HD3	1.84	0.60
1:2A:2518:A:OP2	62:2A:3927:HOH:O	2.16	0.60
11:1P:89:ALA:O	11:1P:121:LYS:NZ	2.33	0.60
26:14:34:GLU:HG2	26:14:35:VAL:HG12	1.83	0.60
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.83	0.60
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.84	0.60
32:2a:1007:C:N3	32:2a:1022:G:O6	2.34	0.60
45:2n:59:ALA:HB1	45:2n:61:TRP:HZ3	1.66	0.60
6:1G:11:TYR:OH	6:1G:32:PRO:O	2.18	0.60
7:1H:101:ARG:HH22	7:1H:122:THR:HA	1.65	0.60
41:2j:47:PHE:N	41:2j:63:PHE:O	2.21	0.60
26:14:61:ARG:NE	26:14:61:ARG:O	2.35	0.60
1:2A:586:A:N1	1:2A:809:G:O2'	2.29	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:857:C:H4'	22:20:23:VAL:HG21	1.84	0.60
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.35	0.60
32:1a:159:G:N2	32:1a:162:A:OP2	2.35	0.60
32:1a:1003:G:C4	32:1a:1004:A:H2	2.20	0.60
40:1i:27:THR:HG23	40:1i:62:TYR:HA	1.84	0.60
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.67	0.60
50:1s:12:ASP:OD1	50:1s:37:ARG:NH2	2.33	0.60
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.01	0.60
57:2y:46:G7M:O2'	57:2y:48:C:OP2	2.19	0.60
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.01	0.60
1:2A:994:C:O2'	1:2A:996:A:OP1	2.16	0.60
1:2A:2478:A:OP2	31:29:2:LYS:NZ	2.32	0.60
28:26:10:LEU:HB2	28:26:52:VAL:HG12	1.82	0.60
54:2w:43:C:H2'	54:2w:44:G:C8	2.37	0.60
1:1A:1013:C:OP2	62:1A:4225:HOH:O	2.16	0.60
1:1A:2136:C:N4	1:1A:2155:G:N1	2.50	0.60
41:1j:5:ARG:NH2	41:1j:73:ASP:OD2	2.25	0.60
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.84	0.60
1:2A:981:A:OP1	62:2A:3932:HOH:O	2.17	0.60
1:2A:2666:C:H42	7:2H:109:PHE:HA	1.67	0.60
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.67	0.60
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.84	0.60
51:2t:50:GLU:HG3	51:2t:100:ILE:HD13	1.84	0.60
1:1A:763:G:OP1	62:1A:4234:HOH:O	2.17	0.59
1:1A:1371:G:O6	62:1A:4226:HOH:O	2.13	0.59
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.66	0.59
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.83	0.59
1:2A:1502:C:H2'	1:2A:1503:U:H6	1.67	0.59
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.67	0.59
34:2c:40:ARG:HA	34:2c:43:LEU:HB2	1.84	0.59
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.35	0.59
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.34	0.59
32:1a:920:U:H2'	32:1a:921:U:C6	2.37	0.59
32:1a:976:G:OP2	32:1a:1358:U:O2'	2.20	0.59
6:2G:35:GLU:HB3	6:2G:160:VAL:HG12	1.83	0.59
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.37	0.59
47:1p:47:ASP:OD1	47:1p:47:ASP:N	2.36	0.59
20:2Y:30:VAL:HG13	20:2Y:37:VAL:HG12	1.85	0.59
32:2a:1128:C:O2'	32:2a:1129:C:OP1	2.16	0.59
1:1A:602:G:O2'	1:1A:655:A:N6	2.35	0.59
32:1a:748:C:H4'	32:1a:749:C:O5'	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.16	0.59
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.83	0.59
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.85	0.59
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.02	0.59
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.85	0.59
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.35	0.59
38:2g:69:VAL:HG11	38:2g:134:ALA:HB1	1.84	0.59
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.27	0.59
32:1a:1036:G:H5''	32:1a:1037:C:C5	2.37	0.59
33:1b:82:ARG:NH1	33:1b:86:GLU:OE2	2.36	0.59
51:1t:83:ARG:HG2	51:1t:86:ARG:HH12	1.67	0.59
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.34	0.59
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.38	0.59
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.37	0.59
13:2R:87:TYR:OH	13:2R:117:VAL:O	2.17	0.59
32:2a:1047:G:H5''	45:2n:4:LYS:HD3	1.84	0.59
1:1A:1057:A:H61	1:1A:1081:U:H3	1.48	0.59
32:1a:677:U:H3	32:1a:713:G:H22	1.51	0.59
32:1a:1004:A:H5''	32:1a:1025:U:C5	2.37	0.59
33:1b:80:ILE:HD12	33:1b:211:ILE:HG22	1.85	0.59
57:1y:55:PSU:C4	57:1y:57:G:H5'	2.38	0.59
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.36	0.59
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.85	0.59
32:1a:673:G:O3'	37:1f:87:ARG:NH2	2.35	0.59
32:1a:946:A:H2'	32:1a:947:G:C8	2.38	0.59
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.38	0.59
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.38	0.59
1:2A:2394:C:N3	57:2y:76:A:O2'	2.31	0.59
8:2I:26:ALA:HA	8:2I:30:LEU:HB2	1.85	0.59
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.36	0.59
32:2a:1244:C:N4	32:2a:1293:G:H1	2.01	0.59
34:2c:104:GLN:NE2	34:2c:105:GLU:O	2.33	0.59
1:1A:2136:C:N3	1:1A:2155:G:N2	2.50	0.59
36:1e:102:ALA:O	36:1e:107:ARG:NH2	2.35	0.59
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.35	0.59
44:2m:86:CYS:HB2	50:2s:73:GLU:HG2	1.84	0.59
47:2p:28:ARG:NH1	47:2p:29:ASP:OD1	2.36	0.59
57:2y:8:4SU:O4'	57:2y:48:C:O2'	2.21	0.59
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.03	0.58
36:1e:10:MET:HA	36:1e:32:VAL:HG22	1.84	0.58
2:2B:3:C:H2'	2:2B:4:C:C6	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:6:VAL:HG13	25:23:56:VAL:HG22	1.85	0.58
32:2a:38:G:H22	32:2a:397:A:H5''	1.67	0.58
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.17	0.58
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.36	0.58
54:2w:52:G:H1	54:2w:62:C:N4	1.99	0.58
57:2y:14:A:O2'	57:2y:15:G:OP1	2.19	0.58
36:1e:102:ALA:HB1	36:1e:106:PRO:HG2	1.85	0.58
1:2A:947:G:O6	62:2A:3923:HOH:O	2.15	0.58
1:2A:2319:G:N2	14:2S:3:ARG:HA	2.17	0.58
19:2X:1:MET:HE1	24:22:26:ARG:HH21	1.68	0.58
32:2a:692:U:O2'	32:2a:694:A:N7	2.30	0.58
1:1A:700:G:O2'	1:1A:1632:A:N3	2.33	0.58
2:1B:88:C:H2'	2:1B:89:G:O4'	2.03	0.58
32:1a:1198:G:N7	62:1a:1930:HOH:O	2.32	0.58
1:2A:2431:U:OP1	62:2A:3926:HOH:O	2.15	0.58
1:2A:2524:G:N7	62:2A:3985:HOH:O	2.32	0.58
6:2G:133:LEU:HG	6:2G:157:ILE:HB	1.84	0.58
31:29:15:LYS:HD3	31:29:26:ILE:HD11	1.84	0.58
32:2a:1139:G:N2	32:2a:1142:G:O6	2.23	0.58
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.15	0.58
6:1G:5:VAL:HG21	6:1G:100:TRP:HB3	1.86	0.58
32:1a:1040:U:H2'	32:1a:1041:A:H8	1.68	0.58
1:2A:1354:A:H5''	3:2D:38:LYS:HD3	1.84	0.58
1:2A:1603:A:OP1	62:2A:3933:HOH:O	2.17	0.58
1:2A:2136:C:N4	1:2A:2155:G:H1	2.01	0.58
1:2A:2207:G:H3'	1:2A:2208:A:H5''	1.84	0.58
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.38	0.58
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.85	0.58
13:2R:33:ARG:NH2	13:2R:115:GLU:OE1	2.34	0.58
32:2a:114:U:H2'	32:2a:115:G:C8	2.39	0.58
32:2a:447:G:O6	32:2a:485:G:O2'	2.21	0.58
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.68	0.58
1:1A:2126:A:N6	1:1A:2163:C:O4'	2.37	0.58
2:1B:66:A:H61	2:1B:109:C:H5'	1.68	0.58
26:14:54:GLY:N	26:14:55:ARG:HA	2.17	0.58
32:1a:64:G:H4'	32:1a:65:U:H5''	1.86	0.58
50:1s:31:ILE:O	50:1s:50:ALA:N	2.28	0.58
57:1y:57:G:H2'	57:1y:58:A:H5'	1.85	0.58
1:2A:2130:U:H3	1:2A:2159:G:H1	1.51	0.58
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.24	0.58
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:69:HIS:CD2	34:2c:104:GLN:HG2	2.38	0.58
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.68	0.58
32:1a:1239:A:H62	32:1a:1299:A:N6	2.01	0.58
1:2A:2751:G:H8	7:2H:2:SER:HA	1.67	0.58
15:2T:127:ALA:C	15:2T:129:ARG:H	2.10	0.58
32:2a:473:G:H2'	32:2a:474:G:H8	1.68	0.58
33:2b:71:VAL:HB	33:2b:164:VAL:HG13	1.86	0.58
1:1A:893:C:H2'	1:1A:894:C:C6	2.38	0.58
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.69	0.58
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.85	0.58
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.86	0.58
32:2a:148:G:H2'	32:2a:149:A:C8	2.37	0.58
32:2a:181:G:H4'	32:2a:182:U:H5'	1.85	0.58
34:2c:30:ARG:NH2	45:2n:38:GLY:HA2	2.18	0.58
32:1a:1143:G:H2'	32:1a:1144:G:H8	1.69	0.58
33:1b:12:GLU:HB2	33:1b:213:LEU:HD21	1.85	0.58
39:1h:49:GLU:HG3	39:1h:51:VAL:HG22	1.86	0.58
1:2A:2552:OMU:H6	1:2A:2552:OMU:O5'	2.03	0.58
26:24:24:THR:OG1	26:24:25:TYR:N	2.37	0.58
32:2a:9:G:H2'	32:2a:10:A:H8	1.68	0.58
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.37	0.58
40:1i:9:ARG:HG3	40:1i:14:VAL:HG12	1.86	0.58
32:2a:1111:A:N1	34:2c:177:THR:OG1	2.28	0.58
33:2b:187:LEU:HD12	33:2b:214:ILE:HG21	1.86	0.58
36:2e:60:TYR:OH	36:2e:64:ARG:NH1	2.37	0.58
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.85	0.58
40:1i:17:VAL:HG23	40:1i:63:ILE:HG12	1.86	0.58
1:2A:1352:U:OP2	62:2A:3922:HOH:O	2.17	0.58
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.04	0.58
32:2a:1366:C:O2'	41:2j:60:ARG:NH2	2.36	0.58
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.19	0.58
1:1A:2136:C:C4	1:1A:2155:G:C2	2.92	0.57
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.39	0.57
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.26	0.57
1:2A:627:A:N7	11:2P:84:ASN:ND2	2.52	0.57
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.19	0.57
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.13	0.57
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.85	0.57
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.85	0.57
57:2y:66:U:H2'	57:2y:67:C:O4'	2.03	0.57
1:1A:120:U:OP2	62:1A:4237:HOH:O	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.86	0.57
12:1Q:78:PRO:HD3	55:1x:1:C:N3	2.20	0.57
18:1W:67:ASP:OD1	18:1W:67:ASP:N	2.33	0.57
32:1a:673:G:H2'	32:1a:674:G:C8	2.40	0.57
32:1a:984:C:H42	32:1a:1221:G:H1	1.52	0.57
41:1j:100:THR:O	41:1j:100:THR:OG1	2.21	0.57
12:2Q:111:GLU:OE1	12:2Q:133:ARG:NH2	2.36	0.57
35:2d:175:SER:HB3	35:2d:186:LEU:HD21	1.86	0.57
44:2m:5:ALA:HB3	44:2m:22:ILE:HD12	1.86	0.57
56:2z:2:THR:HG23	56:2z:3:HIS:H	1.68	0.57
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.29	0.57
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.33	0.57
2:2B:66:A:N6	2:2B:108:U:H3'	2.19	0.57
32:2a:677:U:H3	32:2a:713:G:H22	1.51	0.57
32:2a:1309:G:OP1	44:2m:88:ARG:NH2	2.37	0.57
37:2f:94:GLN:HE22	49:2r:72:ARG:HH12	1.52	0.57
6:1G:15:VAL:HG21	6:1G:176:LEU:HD23	1.85	0.57
32:1a:79:G:C6	32:1a:90:U:O2	2.56	0.57
1:2A:2343:C:O2'	1:2A:2373:G:O2'	2.21	0.57
6:2G:59:GLU:OE1	6:2G:153:ARG:NH2	2.36	0.57
20:2Y:83:THR:HG21	20:2Y:99:CYS:HB2	1.85	0.57
32:2a:664:G:H22	32:2a:741:G:H1	1.52	0.57
33:2b:54:THR:HG21	33:2b:201:ILE:HD11	1.85	0.57
46:2o:82:ILE:HB	46:2o:87:ILE:HB	1.86	0.57
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.38	0.57
1:1A:1418:G:OP2	62:1A:4236:HOH:O	2.17	0.57
1:1A:2123:G:H2'	1:1A:2124:G:H8	1.68	0.57
1:1A:2790:A:H5'	1:1A:2893:G:H21	1.68	0.57
8:1I:79:ILE:HB	8:1I:144:VAL:HG12	1.86	0.57
9:1N:137:LYS:NZ	9:1N:139:GLU:OE2	2.30	0.57
32:1a:735:C:H2'	32:1a:736:C:H6	1.70	0.57
32:1a:1136:U:H5''	32:1a:1137:C:N3	2.19	0.57
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.85	0.57
32:2a:1077:G:N2	32:2a:1080:A:OP2	2.35	0.57
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.04	0.57
18:1W:86:LEU:HD22	18:1W:96:ILE:HD11	1.87	0.57
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.86	0.57
32:2a:64:G:H4'	32:2a:65:U:H3'	1.86	0.57
32:2a:572:A:OP1	62:2a:1903:HOH:O	2.16	0.57
32:2a:1114:C:N4	32:2a:1186:G:H1	2.00	0.57
37:2f:12:PRO:HG3	37:2f:57:GLN:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:68:THR:O	7:1H:72:ILE:HG12	2.04	0.57
23:11:59:THR:O	23:11:91:LYS:NZ	2.38	0.57
23:11:77:ALA:HB1	23:11:82:LEU:HD11	1.87	0.57
33:1b:16:HIS:CD2	33:1b:204:ASN:H	2.23	0.57
33:1b:92:TYR:CE1	33:1b:94:ASN:HB2	2.40	0.57
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.87	0.57
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.86	0.57
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.19	0.57
21:2Z:61:LEU:HB2	21:2Z:65:GLN:HB2	1.87	0.57
32:2a:909:A:N3	32:2a:1413:A:O2'	2.36	0.57
41:2j:6:ILE:HG12	41:2j:98:ILE:HG13	1.86	0.57
2:1B:51:G:N7	14:1S:62:LYS:NZ	2.45	0.57
32:1a:1095:U:P	32:1a:1108:G:H1	2.28	0.57
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.39	0.57
32:2a:748:C:H4'	32:2a:749:C:O5'	2.05	0.57
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.19	0.57
37:2f:33:TYR:HE2	37:2f:78:GLU:HG2	1.70	0.57
1:2A:122:G:N3	62:2A:3986:HOH:O	2.32	0.57
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.03	0.57
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.86	0.57
21:2Z:155:LEU:HB2	21:2Z:157:LEU:HD12	1.86	0.57
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.87	0.57
11:1P:79:ARG:NH1	11:1P:109:GLY:O	2.36	0.57
20:1Y:92:ASN:HD21	20:1Y:94:LYS:HG2	1.70	0.57
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.70	0.57
44:1m:49:THR:HB	44:1m:52:GLU:H	1.70	0.57
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.40	0.57
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.40	0.57
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.40	0.57
5:2F:24:LEU:HD21	5:2F:114:VAL:HG12	1.87	0.57
33:2b:97:TRP:HH2	33:2b:102:LEU:HG	1.68	0.57
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.86	0.56
36:1e:84:PHE:HB2	36:1e:134:ALA:HB2	1.86	0.56
1:2A:1223:G:N2	1:2A:1226:A:OP2	2.30	0.56
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.40	0.56
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.40	0.56
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.40	0.56
1:1A:588:U:H2'	1:1A:589:C:C6	2.40	0.56
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.69	0.56
1:1A:2322:A:N6	62:1A:4230:HOH:O	2.14	0.56
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.78	0.56
32:1a:601:C:H2'	32:1a:602:A:H8	1.70	0.56
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.20	0.56
1:2A:307:G:H21	1:2A:330:A:H62	1.53	0.56
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	1.86	0.56
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.40	0.56
33:2b:178:ARG:HH22	39:2h:68:ARG:HH22	1.52	0.56
34:2c:57:ILE:HG12	34:2c:66:VAL:HG22	1.88	0.56
1:1A:528:A:O2'	1:1A:529:A:H5'	2.05	0.56
1:1A:1062:G:P	1:1A:1070:A:H1'	2.45	0.56
1:1A:2115:G:H2'	1:1A:2116:G:H5''	1.86	0.56
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.20	0.56
32:1a:1304:G:OP2	62:1a:1913:HOH:O	2.18	0.56
57:1y:51:U:H2'	57:1y:52:G:C8	2.41	0.56
1:2A:300:A:P	20:2Y:86:ARG:HH12	2.28	0.56
1:2A:894:C:O2'	1:2A:895:U:H5''	2.05	0.56
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.40	0.56
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.86	0.56
62:2A:4644:HOH:O	11:2P:44:GLY:HA2	2.05	0.56
32:2a:1074:G:O2'	32:2a:1101:A:N1	2.31	0.56
33:2b:80:ILE:HG12	33:2b:215:LEU:HD12	1.86	0.56
32:1a:193:C:H2'	32:1a:194:C:C6	2.40	0.56
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.87	0.56
2:2B:106:G:H5'	21:2Z:31:ARG:HB3	1.87	0.56
5:2F:137:LYS:HA	5:2F:140:LEU:HD12	1.87	0.56
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.87	0.56
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.38	0.56
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.40	0.56
42:2k:70:LYS:HA	42:2k:73:MET:HE2	1.87	0.56
12:1Q:16:ARG:HG2	12:1Q:18:LYS:HE3	1.87	0.56
1:2A:212:G:H2'	1:2A:213:A:O4'	2.05	0.56
32:2a:1317:C:O2	50:2s:37:ARG:NH2	2.39	0.56
57:2y:63:G:H2'	57:2y:64:A:C8	2.40	0.56
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.41	0.56
32:1a:92:C:H2'	32:1a:93:G:C8	2.40	0.56
32:1a:973:G:OP1	41:1j:57:LYS:NZ	2.30	0.56
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.41	0.56
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.05	0.56
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.39	0.56
20:2Y:28:LYS:HD2	20:2Y:40:GLU:HG3	1.87	0.56
32:2a:457:C:H2'	32:2a:458:C:C6	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	1.87	0.56
33:1b:224:GLN:HG2	33:1b:229:VAL:HG22	1.86	0.56
1:2A:796:C:H2'	1:2A:797:C:C6	2.40	0.56
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.88	0.56
2:2B:7:G:H21	14:2S:38:GLN:NE2	1.94	0.56
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.29	0.56
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.40	0.56
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	1.88	0.56
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.41	0.56
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.19	0.56
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.40	0.56
6:1G:18:GLU:O	6:1G:22:ARG:HB2	2.06	0.56
7:1H:23:ARG:NH2	7:1H:34:GLU:OE2	2.30	0.56
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.88	0.56
33:1b:60:ASP:OD2	33:1b:64:ARG:NH2	2.39	0.56
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.37	0.56
38:1g:12:LEU:HD12	38:1g:12:LEU:H	1.71	0.56
1:2A:675:A:OP1	5:2F:63:LYS:NZ	2.38	0.56
1:2A:2099:U:O2	1:2A:2190:G:N2	2.33	0.56
6:2G:36:LYS:HE3	6:2G:160:VAL:HG21	1.88	0.56
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.18	0.56
1:1A:579:G:H2'	1:1A:580:C:C6	2.41	0.56
1:1A:1039:G:H1	1:1A:1116:C:H42	1.54	0.56
32:1a:6:G:H1	36:1e:98:THR:HG21	1.70	0.56
32:1a:78:G:N2	32:1a:91:C:N3	2.53	0.56
39:1h:39:LEU:HB3	39:1h:45:ILE:HG12	1.86	0.56
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.88	0.56
46:1o:71:GLN:HG3	46:1o:78:TYR:CD2	2.41	0.56
54:1w:1:G:H2'	54:1w:2:C:C6	2.41	0.56
1:2A:458:G:O2'	1:2A:469:G:O6	2.20	0.56
1:2A:643:A:N1	1:2A:2369:A:O2'	2.38	0.56
1:2A:1218:C:H42	1:2A:1231:G:H1	1.52	0.56
1:2A:2102:U:O2	1:2A:2187:G:O6	2.24	0.56
1:2A:2651:C:H42	1:2A:2669:G:H1	1.53	0.56
32:2a:920:U:H2'	32:2a:921:U:C6	2.41	0.56
32:2a:1272:G:N2	32:2a:1273:G:N7	2.53	0.56
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.13	0.56
44:2m:78:ILE:HA	44:2m:81:LEU:HD12	1.87	0.56
1:1A:2123:G:H2'	1:1A:2124:G:C8	2.41	0.56
32:1a:1273:G:H3'	32:1a:1274:G:H8	1.69	0.56
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:13:C:H2'	54:1w:14:A:H5''	1.86	0.56
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.20	0.56
32:2a:352:C:O2'	32:2a:354:G:OP1	2.23	0.56
32:2a:1134:G:C2	32:2a:1135:U:H1'	2.40	0.56
49:2r:48:GLY:O	49:2r:74:ARG:NH2	2.39	0.56
1:1A:1095:A:H2'	1:1A:1096:A:H8	1.70	0.55
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.40	0.55
2:1B:96:U:O4	62:1B:301:HOH:O	2.17	0.55
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.88	0.55
51:1t:40:ALA:HB2	51:1t:55:ILE:HG22	1.88	0.55
1:2A:752:A:H3'	29:27:1:MET:HE1	1.87	0.55
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.06	0.55
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.06	0.55
32:2a:1263:C:N3	32:2a:1272:G:O6	2.39	0.55
39:2h:86:ILE:HD12	39:2h:133:LEU:HD22	1.87	0.55
40:2i:3:GLN:NE2	40:2i:20:ARG:HE	2.00	0.55
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.06	0.55
32:1a:276:G:O2'	48:1q:68:ARG:NH1	2.38	0.55
32:1a:828:A:H2'	32:1a:829:G:O4'	2.05	0.55
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.88	0.55
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.39	0.55
21:2Z:70:LEU:HD12	21:2Z:71:VAL:H	1.69	0.55
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.40	0.55
26:24:26:SER:OG	26:24:27:THR:N	2.40	0.55
32:2a:403:C:N4	62:2a:1918:HOH:O	2.39	0.55
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.70	0.55
33:2b:81:VAL:HB	33:2b:94:ASN:HD21	1.72	0.55
1:1A:278:A:O2'	1:1A:279:C:OP1	2.18	0.55
1:1A:2134:A:N3	1:1A:2159:G:O2'	2.33	0.55
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.71	0.55
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.88	0.55
32:1a:45:U:H2'	32:1a:46:G:C8	2.40	0.55
32:1a:78:G:C6	32:1a:91:C:N4	2.75	0.55
2:2B:83:G:N7	62:2B:302:HOH:O	2.33	0.55
5:2F:103:LYS:HA	5:2F:106:ARG:HD3	1.87	0.55
32:2a:673:G:H2'	32:2a:674:G:C8	2.40	0.55
34:2c:40:ARG:HE	34:2c:55:VAL:HG13	1.71	0.55
34:2c:110:ASN:HD21	34:2c:140:ARG:HE	1.54	0.55
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.71	0.55
3:1D:37:LEU:HD12	3:1D:62:TYR:HB2	1.88	0.55
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.88	0.55
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.88	0.55
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.06	0.55
32:2a:165:C:H2'	32:2a:166:G:C8	2.42	0.55
32:2a:973:G:H3'	32:2a:974:A:H5''	1.88	0.55
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.07	0.55
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.70	0.55
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.41	0.55
32:1a:576:G:O6	32:1a:880:C:O2'	2.22	0.55
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.04	0.55
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	1.89	0.55
32:2a:1060:C:C5	34:2c:2:GLY:HA2	2.41	0.55
1:1A:536:A:H2'	1:1A:537:C:C6	2.41	0.55
62:1A:5715:HOH:O	11:1P:44:GLY:HA2	2.07	0.55
14:1S:61:ASN:HB3	14:1S:64:GLU:HB2	1.89	0.55
21:1Z:7:ALA:HB2	21:1Z:59:LEU:HD22	1.88	0.55
33:1b:112:VAL:HG12	33:1b:149:LEU:HD13	1.89	0.55
7:2H:89:ILE:H	7:2H:89:ILE:HD12	1.72	0.55
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.89	0.55
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.39	0.55
48:2q:67:LYS:O	48:2q:68:ARG:HB2	2.05	0.55
54:2w:27:G:H2'	54:2w:28:G:H8	1.72	0.55
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.05	0.55
6:1G:123:ASN:O	62:1G:301:HOH:O	2.18	0.55
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.89	0.55
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.22	0.55
34:1c:57:ILE:HG12	34:1c:66:VAL:HG12	1.88	0.55
38:1g:113:GLU:HB2	38:1g:119:ARG:HG2	1.89	0.55
1:2A:8:A:H2'	1:2A:9:U:C6	2.42	0.55
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.42	0.55
41:2j:33:GLN:HG2	41:2j:34:VAL:H	1.71	0.55
1:1A:278:A:H2'	1:1A:279:C:C6	2.41	0.55
1:1A:636:G:OP1	11:1P:132:LYS:NZ	2.34	0.55
1:1A:2222:G:O6	62:1A:4235:HOH:O	2.17	0.55
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.22	0.55
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.24	0.55
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.41	0.55
38:1g:50:ILE:HG13	38:1g:61:VAL:HG11	1.89	0.55
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.06	0.55
1:1A:1058:G:H1	1:1A:1080:C:N4	2.03	0.55
1:1A:2422:A:O4'	57:1y:76:A:N6	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.38	0.55
32:1a:192:U:H2'	32:1a:193:C:C6	2.42	0.55
32:1a:1507:A:OP2	53:1v:13:A:N6	2.40	0.55
1:2A:2126:A:N7	1:2A:2163:C:O2'	2.38	0.55
6:2G:41:GLN:O	6:2G:43:LEU:N	2.40	0.55
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.89	0.55
32:2a:165:C:H2'	32:2a:166:G:H8	1.71	0.55
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.39	0.55
38:2g:146:GLU:OE2	38:2g:149:ARG:NE	2.40	0.55
55:2x:55:PSU:N3	55:2x:58:A:OP2	2.30	0.55
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.42	0.55
32:1a:56:U:H2'	32:1a:57:G:C8	2.42	0.55
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.89	0.55
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.15	0.55
54:2w:27:G:H1	54:2w:43:C:H42	1.53	0.55
6:1G:60:LEU:HB3	6:1G:68:PRO:HG3	1.89	0.54
6:1G:98:ARG:NE	26:14:1:MET:HE3	2.23	0.54
7:1H:42:ARG:HG2	7:1H:44:VAL:HG13	1.87	0.54
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.40	0.54
32:1a:865:A:H2	32:1a:918:A:H4'	1.71	0.54
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.88	0.54
40:1i:49:PRO:HG2	40:1i:81:ILE:HG23	1.88	0.54
51:1t:33:ILE:O	51:1t:37:SER:OG	2.13	0.54
1:2A:307:G:N1	1:2A:310:A:OP2	2.40	0.54
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.07	0.54
32:2a:674:G:N2	32:2a:717:C:O2	2.40	0.54
32:2a:964:A:N3	32:2a:969:A:O2'	2.39	0.54
1:1A:1062:G:C8	1:1A:1070:A:H4'	2.40	0.54
32:1a:193:C:H2'	32:1a:194:C:H6	1.72	0.54
32:1a:1108:G:O6	62:1a:1912:HOH:O	2.18	0.54
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.89	0.54
34:1c:98:ASN:N	34:1c:98:ASN:OD1	2.40	0.54
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.89	0.54
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.90	0.54
57:1y:53:G:H2'	57:1y:54:5MU:C6	2.41	0.54
1:2A:2422:A:O4'	57:2y:76:A:N6	2.41	0.54
1:2A:2609:U:O2'	56:2z:1:FME:HG2	2.07	0.54
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.08	0.54
32:2a:163:C:H2'	32:2a:164:U:C6	2.43	0.54
32:2a:1258:G:H2'	32:2a:1259:C:C6	2.42	0.54
1:1A:279:C:N4	1:1A:361:G:H1	2.01	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.89	0.54
34:1c:35:GLU:OE2	34:1c:59:ARG:NH1	2.36	0.54
1:2A:636:G:O2'	1:2A:638:G:O2'	2.22	0.54
1:2A:1445(A):C:H42	1:2A:1466:G:H1	1.56	0.54
1:2A:2134:A:H62	1:2A:2157:G:H4'	1.72	0.54
1:2A:2506:U:O2'	54:2w:76:F3N:H4'	2.08	0.54
19:2X:60:ARG:HH22	29:27:47:ARG:NH2	1.99	0.54
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.90	0.54
23:21:56:GLN:NE2	23:21:85:LEU:O	2.40	0.54
32:2a:542:G:P	35:2d:10:ARG:HH22	2.30	0.54
35:2d:17:VAL:HG11	35:2d:197:PRO:HG3	1.89	0.54
1:1A:271(K):U:O2'	1:1A:271(M):G:N2	2.41	0.54
32:1a:880:C:OP1	43:1l:8:ASN:ND2	2.33	0.54
32:1a:1190:G:O6	62:1a:1911:HOH:O	2.17	0.54
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.41	0.54
46:1o:4:THR:OG1	46:1o:7:GLU:OE2	2.19	0.54
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.72	0.54
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.90	0.54
32:2a:393:A:OP1	62:2a:1905:HOH:O	2.18	0.54
32:2a:913:A:OP1	43:2l:46:LYS:NZ	2.40	0.54
32:2a:1259:C:C4	32:2a:1260:C:H1'	2.42	0.54
34:2c:152:ILE:HG13	34:2c:199:LYS:HB2	1.88	0.54
51:2t:86:ARG:O	51:2t:90:GLN:HB2	2.07	0.54
20:1Y:8:LYS:HD3	20:1Y:97:ARG:NH1	2.23	0.54
30:18:23:VAL:HG13	30:18:47:LYS:HB3	1.89	0.54
32:1a:57:G:H2'	32:1a:58:C:C6	2.43	0.54
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.28	0.54
1:2A:72:U:OP2	24:22:29:LYS:NZ	2.38	0.54
1:2A:307:G:N7	62:2A:3990:HOH:O	2.33	0.54
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.72	0.54
14:2S:25:ARG:HB3	14:2S:40:ILE:HB	1.90	0.54
19:2X:94:GLY:CA	19:2X:95:LEU:HB2	2.36	0.54
27:25:41:PRO:O	27:25:44:THR:OG1	2.23	0.54
32:2a:16:A:N3	32:2a:1080:A:O2'	2.32	0.54
32:2a:1073:U:O2'	33:2b:104:ASN:OD1	2.23	0.54
32:2a:1239:A:H4'	32:2a:1240:U:H5''	1.90	0.54
32:2a:1278:U:H5'	32:2a:1279:A:OP1	2.07	0.54
32:2a:1316:G:H22	32:2a:1319:A:H5''	1.72	0.54
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.22	0.54
1:1A:502:A:OP1	62:1A:4238:HOH:O	2.18	0.54
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:910:A:N1	1:1A:2277:G:H1'	2.21	0.54
5:1F:7:TYR:CD2	5:1F:24:LEU:HB2	2.43	0.54
8:1I:38:LEU:HG	8:1I:40:THR:HG23	1.90	0.54
23:11:75:GLU:OE1	23:11:78:LYS:NZ	2.30	0.54
32:1a:975:A:H5'	32:1a:975:A:H8	1.72	0.54
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.90	0.54
1:2A:1017:G:O6	62:2A:3931:HOH:O	2.16	0.54
11:2P:121:LYS:HE2	11:2P:123:LEU:HD11	1.90	0.54
32:2a:603:U:H2'	32:2a:604:G:H8	1.73	0.54
32:2a:1290:G:O2'	38:2g:37:ASN:ND2	2.41	0.54
38:2g:45:ASP:O	38:2g:49:ILE:HG12	2.06	0.54
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.07	0.54
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.33	0.54
46:1o:18:PHE:CE2	46:1o:21:ASP:HB2	2.43	0.54
8:2I:82:ARG:HB2	8:2I:89:TYR:HD2	1.72	0.54
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.89	0.54
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.89	0.54
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.43	0.54
33:2b:16:HIS:C	33:2b:18:GLY:H	2.14	0.54
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.89	0.54
50:2s:53:ASN:OD1	50:2s:54:GLY:N	2.40	0.54
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.23	0.54
2:1B:43:C:H5''	26:14:1:MET:HE2	1.89	0.54
23:11:76:ARG:NH1	23:11:97:LEU:O	2.41	0.54
32:1a:7:G:H5'	32:1a:298:A:O4'	2.08	0.54
32:1a:544:G:P	35:1d:59:ARG:HH22	2.30	0.54
32:1a:1006:C:H2'	32:1a:1007:C:C6	2.43	0.54
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.08	0.54
54:1w:2:C:H2'	54:1w:3:C:C6	2.42	0.54
5:2F:7:TYR:O	5:2F:22:ALA:N	2.41	0.54
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.89	0.54
32:2a:1133:G:H1	32:2a:1141:C:N4	2.05	0.54
54:2w:4:C:N4	54:2w:69:G:N1	2.26	0.54
1:1A:1139:G:OP2	9:1N:70:LYS:NZ	2.40	0.54
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.43	0.54
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.42	0.54
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.89	0.54
12:1Q:78:PRO:HG2	12:1Q:81:VAL:HG11	1.88	0.54
1:2A:299:A:N1	1:2A:322:A:O2'	2.39	0.54
1:2A:320:A:O2'	1:2A:322:A:OP2	2.25	0.54
1:2A:775:G:O2'	62:2A:3936:HOH:O	2.19	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:882:G:H22	1:2A:894:C:N4	2.05	0.54
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.43	0.54
1:2A:2299:G:H2'	1:2A:2300:G:C8	2.42	0.54
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	1.89	0.54
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.89	0.54
25:23:40:THR:HG22	25:23:42:ALA:H	1.73	0.54
54:2w:33:U:N3	54:2w:36:A:OP2	2.38	0.54
1:1A:1062:G:H22	1:1A:1077:A:H61	1.56	0.54
1:1A:1508:A:O2'	1:1A:1509:C:H5''	2.08	0.54
1:2A:706:A:OP1	3:2D:7:LYS:NZ	2.40	0.54
1:2A:720:C:H2'	1:2A:721:C:C6	2.42	0.54
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.08	0.54
1:2A:2506:U:H1'	54:2w:76:F3N:HD2	1.90	0.54
1:2A:2802:G:H8	1:2A:2802:G:O5'	1.91	0.54
19:2X:60:ARG:HH12	29:27:47:ARG:HH21	1.56	0.54
32:2a:448:A:OP2	32:2a:485:G:N2	2.33	0.54
32:2a:473:G:H2'	32:2a:474:G:C8	2.43	0.54
32:2a:839:U:H3'	32:2a:840:C:H5'	1.90	0.54
44:2m:91:ARG:HB2	44:2m:98:VAL:HG13	1.89	0.54
48:2q:3:LYS:HD3	48:2q:60:ILE:HD11	1.89	0.54
1:1A:489:G:N7	18:1W:49:LYS:NZ	2.56	0.53
41:1j:20:ALA:HB1	41:1j:37:PRO:HB3	1.91	0.53
1:2A:330:A:HO2'	1:2A:331:A:H8	1.55	0.53
5:2F:155:LEU:HD11	5:2F:176:LEU:HD12	1.90	0.53
32:2a:580:U:H5''	46:2o:58:MET:HG2	1.89	0.53
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.42	0.53
1:1A:81:G:H21	20:1Y:1:MET:HE1	1.73	0.53
1:1A:888:C:H2'	1:1A:889:C:C5	2.44	0.53
1:1A:899:A:H2'	1:1A:899:A:N3	2.23	0.53
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.23	0.53
1:2A:582:G:H2'	1:2A:583:G:C8	2.43	0.53
1:2A:2262:U:OP2	22:20:16:SER:OG	2.11	0.53
2:2B:105:A:H5'	2:2B:106:G:OP2	2.08	0.53
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.89	0.53
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.41	0.53
32:2a:539:A:H2'	32:2a:540:G:C8	2.43	0.53
32:2a:976:G:OP2	32:2a:1358:U:O2'	2.24	0.53
32:2a:979:C:H42	45:2n:18:VAL:HG22	1.73	0.53
38:2g:50:ILE:HG22	38:2g:125:MET:HG3	1.89	0.53
47:2p:39:TYR:CD2	47:2p:73:LEU:HD21	2.43	0.53
1:1A:2136:C:C4	1:1A:2155:G:N1	2.76	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.90	0.53
8:1I:12:LEU:HD22	8:1I:19:VAL:HG21	1.90	0.53
57:1y:8:4SU:H4'	57:1y:48:C:H4'	1.90	0.53
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.23	0.53
1:2A:2497:A:O2'	62:2A:3935:HOH:O	2.18	0.53
8:2I:101:LEU:HD13	8:2I:107:VAL:HB	1.90	0.53
38:2g:68:ASN:ND2	38:2g:127:ALA:O	2.36	0.53
42:2k:79:SER:HA	42:2k:104:GLN:HB3	1.89	0.53
42:2k:98:LEU:O	42:2k:101:SER:OG	2.26	0.53
57:2y:14:A:H61	57:2y:21:A:H2	1.57	0.53
7:1H:50:VAL:HG11	7:1H:72:ILE:HG21	1.89	0.53
44:1m:23:TYR:HE2	44:1m:70:LEU:HB3	1.74	0.53
7:2H:121:ILE:HG21	7:2H:144:VAL:HG11	1.90	0.53
32:2a:969:A:OP1	41:2j:55:LYS:NZ	2.41	0.53
54:2w:72:C:H2'	54:2w:73:A:H8	1.73	0.53
1:1A:886:C:OP1	1:1A:886:C:H4'	2.08	0.53
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.90	0.53
32:1a:78:G:N1	32:1a:91:C:N4	2.56	0.53
32:1a:662:G:H2'	32:1a:663:A:C8	2.44	0.53
32:1a:1025:U:C2	32:1a:1036:G:O6	2.62	0.53
33:1b:178:ARG:NH2	39:1h:74:PRO:HB3	2.23	0.53
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.15	0.53
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.56	0.53
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.43	0.53
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	1.90	0.53
8:1I:69:LYS:HA	8:1I:138:ILE:HG12	1.91	0.53
38:1g:78:ARG:HG3	38:1g:79:ARG:H	1.73	0.53
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.33	0.53
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.39	0.53
4:2E:26:ILE:HD13	4:2E:196:VAL:HG21	1.91	0.53
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.43	0.53
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.41	0.53
32:2a:1271:G:C2	32:2a:1272:G:N7	2.77	0.53
32:2a:1305:G:O2'	32:2a:1331:G:N2	2.42	0.53
33:2b:102:LEU:HD13	33:2b:182:ILE:HD12	1.91	0.53
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.55	0.53
54:1w:18:G:H4'	54:1w:60:U:C5	2.43	0.53
4:2E:176:ILE:HB	4:2E:181:LEU:HB2	1.91	0.53
32:2a:918:A:H2'	32:2a:919:A:C8	2.44	0.53
32:2a:1040:U:H2'	32:2a:1041:A:C8	2.44	0.53
54:2w:45:U:H5''	54:2w:46:G7M:OP2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:247:G:H4'	1:1A:386:G:C5	2.43	0.53
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.08	0.53
1:1A:2121:G:N2	1:1A:2177:C:N3	2.50	0.53
28:16:10:LEU:HG	28:16:54:ILE:HG13	1.90	0.53
48:1q:62:SER:OG	48:1q:72:ARG:NE	2.35	0.53
1:2A:118:A:N3	1:2A:178:G:H1'	2.24	0.53
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.73	0.53
4:2E:7:VAL:HG23	4:2E:51:PHE:HE2	1.74	0.53
8:2I:105:HIS:HB2	8:2I:107:VAL:HG23	1.91	0.53
9:2N:30:ILE:HA	9:2N:33:LEU:HD12	1.91	0.53
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.42	0.53
15:2T:41:ARG:NH1	32:2a:346:G:OP1	2.42	0.53
38:2g:22:LEU:HD21	38:2g:66:VAL:HG11	1.90	0.53
38:2g:78:ARG:HG3	38:2g:156:TRP:CZ3	2.44	0.53
39:2h:96:GLY:N	39:2h:99:GLU:OE1	2.35	0.53
1:1A:55:G:O2'	1:1A:127:A:N1	2.37	0.53
8:1I:10:GLU:O	8:1I:12:LEU:N	2.42	0.53
40:1i:77:ILE:O	40:1i:81:ILE:HG22	2.08	0.53
44:1m:92:HIS:CD2	44:1m:110:ARG:HH22	2.27	0.53
1:2A:492:A:H2'	1:2A:493:G:O4'	2.09	0.53
1:2A:770:G:OP2	62:2A:3938:HOH:O	2.19	0.53
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.55	0.53
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.24	0.53
33:2b:43:ASP:OD2	33:2b:46:LYS:N	2.35	0.53
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.08	0.53
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.44	0.53
49:1r:56:THR:HG22	49:1r:58:LEU:HG	1.90	0.53
1:2A:1020:A:N1	1:2A:1141:U:O2'	2.40	0.53
4:2E:119:ARG:HG2	4:2E:120:TRP:NE1	2.24	0.53
28:26:23:THR:OG1	28:26:24:GLU:N	2.41	0.53
32:2a:113:G:N3	32:2a:353:A:O2'	2.41	0.53
32:2a:737:A:H2'	32:2a:738:C:C6	2.44	0.53
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.09	0.53
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.49	0.53
1:1A:821:A:H2'	1:1A:946:G:H5''	1.91	0.52
1:1A:1054:A:N6	1:1A:1105:U:N3	2.37	0.52
32:1a:22:G:H4'	32:1a:885:G:C8	2.44	0.52
32:1a:192:U:H4'	51:1t:57:ARG:HD3	1.91	0.52
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.44	0.52
35:1d:65:ARG:NH1	35:1d:72:GLU:HB2	2.24	0.52
1:2A:271(P):C:HO2'	8:2I:42:SER:HG	1.56	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:17:U:H2'	32:2a:18:C:C6	2.44	0.52
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.44	0.52
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.39	0.52
4:1E:176:ILE:HB	4:1E:181:LEU:HB2	1.91	0.52
10:1O:104:ARG:NE	15:1T:36:GLU:OE2	2.34	0.52
32:1a:35:G:N3	43:1l:118:SER:OG	2.42	0.52
32:1a:1030:C:O2'	32:1a:1030(C):G:O6	2.14	0.52
32:1a:1143:G:H2'	32:1a:1144:G:C8	2.44	0.52
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.44	0.52
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.75	0.52
57:1y:29:G:N2	57:1y:42:C:O2	2.41	0.52
1:2A:646:A:H2'	1:2A:647:G:O4'	2.09	0.52
1:2A:1287:A:H8	13:2R:104:ARG:HD3	1.73	0.52
1:2A:2298:A:H62	1:2A:2318:G:H8	1.57	0.52
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.09	0.52
10:2O:98:VAL:HG21	10:2O:114:ILE:HG23	1.90	0.52
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.91	0.52
32:2a:9:G:H2'	32:2a:10:A:C8	2.44	0.52
32:2a:573:A:N3	32:2a:883:C:O2'	2.41	0.52
32:2a:952:U:H2'	32:2a:953:G:H8	1.73	0.52
32:2a:1033:G:H2'	32:2a:1034:G:H8	1.73	0.52
32:2a:1258:G:H2'	32:2a:1259:C:H6	1.74	0.52
33:2b:58:ILE:HA	33:2b:61:LEU:HB3	1.90	0.52
34:2c:178:LEU:O	34:2c:180:ALA:N	2.41	0.52
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.41	0.52
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.27	0.52
33:1b:59:GLU:HB2	33:1b:221:LEU:HD21	1.90	0.52
54:1w:33:U:O4'	54:1w:37:MIA:H151	2.08	0.52
1:2A:852:G:H2'	1:2A:853:G:H8	1.75	0.52
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.24	0.52
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.41	0.52
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.09	0.52
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.43	0.52
32:2a:7:G:H5'	32:2a:298:A:O4'	2.08	0.52
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.75	0.52
41:2j:8:LEU:HD12	41:2j:16:LEU:HD22	1.91	0.52
50:2s:80:TYR:O	50:2s:81:ARG:HG2	2.08	0.52
1:1A:2193:G:H2'	1:1A:2194:G:H8	1.74	0.52
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.91	0.52
4:1E:54:GLN:HB2	4:1E:76:ARG:HG2	1.91	0.52
32:1a:192:U:H2'	32:1a:193:C:H6	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:108:ASN:HB3	34:1c:111:LEU:HB2	1.92	0.52
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.90	0.52
1:2A:450:G:OP1	62:2A:3937:HOH:O	2.19	0.52
32:2a:56:U:H2'	32:2a:57:G:C8	2.44	0.52
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.08	0.52
1:1A:263:C:H2'	1:1A:264:C:O4'	2.09	0.52
1:1A:593:G:H4'	30:18:4:MET:HE2	1.90	0.52
6:1G:111:LEU:HA	6:1G:114:ILE:HD12	1.90	0.52
32:1a:250:A:H4'	32:1a:251:G:O5'	2.09	0.52
32:1a:755:G:OP2	46:1o:65:ARG:HD2	2.10	0.52
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	1.90	0.52
35:2d:111:ALA:HA	35:2d:116:GLN:HE21	1.75	0.52
37:2f:62:TRP:CH2	37:2f:64:GLN:HB2	2.45	0.52
41:2j:46:ARG:HA	41:2j:64:GLU:HA	1.90	0.52
51:2t:56:MET:HE3	51:2t:85:MET:HG2	1.90	0.52
57:2y:5:G:H1	57:2y:68:C:H42	1.58	0.52
57:2y:55:PSU:N1	57:2y:57:G:H5''	2.24	0.52
1:1A:897:C:H5'	54:1w:56:C:OP1	2.10	0.52
1:1A:1041:C:N4	1:1A:1114:G:H1	2.06	0.52
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.27	0.52
1:1A:1889:A:H2'	1:1A:1890:A:C8	2.45	0.52
1:1A:2379:G:O2'	14:1S:17:ARG:NH2	2.43	0.52
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.75	0.52
32:1a:92:C:H2'	32:1a:93:G:H8	1.74	0.52
32:1a:381:C:H2'	32:1a:382:A:O4'	2.10	0.52
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.45	0.52
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.92	0.52
54:1w:19:G:H4'	54:1w:20:U:OP1	2.10	0.52
1:2A:500:G:N1	1:2A:503:A:OP2	2.43	0.52
1:2A:911:A:N6	12:2Q:11:LYS:O	2.40	0.52
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.44	0.52
5:2F:33:LEU:HB3	11:2P:6:LEU:HD21	1.92	0.52
6:2G:127:GLY:H	6:2G:166:ASP:CG	2.18	0.52
15:2T:24:PRO:HA	15:2T:49:VAL:HG12	1.91	0.52
20:2Y:5:MET:HE1	20:2Y:35:TYR:HA	1.92	0.52
44:2m:13:LYS:O	44:2m:45:VAL:N	2.36	0.52
55:2x:17:C:OP1	55:2x:61:C:H5'	2.09	0.52
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.91	0.52
6:1G:116:ASP:OD2	44:1m:68:GLY:HA3	2.10	0.52
32:1a:674:G:H2'	32:1a:675:A:H8	1.74	0.52
36:1e:137:GLU:HG3	36:1e:141:GLN:HE21	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.10	0.52
1:2A:668:G:H5'	1:2A:669:G:OP2	2.09	0.52
1:2A:988:A:N7	62:2A:3993:HOH:O	2.34	0.52
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.44	0.52
32:2a:1239:A:H62	32:2a:1299:A:N6	2.08	0.52
32:2a:1397:C:OP2	36:2e:24:ARG:NH2	2.42	0.52
57:2y:55:PSU:HN1	57:2y:57:G:H5''	1.75	0.52
3:1D:34:VAL:HG12	3:1D:63:ARG:HG3	1.91	0.52
9:1N:21:LYS:NZ	9:1N:140:VAL:OXT	2.42	0.52
57:1y:37:MIA:H2'	57:1y:38:A:C8	2.44	0.52
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.73	0.52
4:2E:76:ARG:NH1	62:2E:401:HOH:O	2.42	0.52
12:2Q:77:LYS:NZ	12:2Q:86:GLY:O	2.35	0.52
32:2a:1004:A:C8	32:2a:1005:A:H4'	2.44	0.52
50:2s:28:LYS:CB	50:2s:29:ARG:HA	2.39	0.52
1:1A:625:G:O6	11:1P:107:LYS:NZ	2.42	0.52
1:1A:1837:C:OP1	32:1a:784:C:H4'	2.10	0.52
1:1A:2118:U:OP1	1:1A:2148:G:O2'	2.27	0.52
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	1.91	0.52
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.27	0.52
32:1a:973:G:H3'	32:1a:974:A:H5''	1.92	0.52
32:1a:1112:C:H1'	34:1c:179:ARG:HH11	1.75	0.52
57:1y:15:G:H22	57:1y:48:C:H42	1.58	0.52
1:2A:84:A:N1	1:2A:98:G:O2'	2.35	0.52
1:2A:244:A:H4'	11:2P:74:GLU:HB2	1.92	0.52
1:2A:637:A:OP1	11:2P:133:SER:OG	2.24	0.52
1:2A:2166:G:O6	1:2A:2171:A:N6	2.35	0.52
5:2F:197:ASP:O	5:2F:200:GLU:HB3	2.10	0.52
12:2Q:16:ARG:HG2	12:2Q:18:LYS:HE2	1.92	0.52
32:2a:977:A:O2'	32:2a:981:U:N3	2.42	0.52
32:2a:1010:G:N2	32:2a:1020:U:HO2'	2.08	0.52
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.92	0.52
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.58	0.52
19:1X:26:TYR:HB3	19:1X:92:LEU:HD12	1.93	0.52
1:2A:652(A):A:H3'	1:2A:652(B):A:H5''	1.91	0.52
3:2D:25:THR:HG21	3:2D:113:VAL:HG21	1.91	0.52
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	1.91	0.52
32:2a:501:C:H2'	32:2a:502:G:C8	2.45	0.52
32:2a:1274:G:N2	32:2a:1275:A:N7	2.58	0.52
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.25	0.51
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:178:ARG:HH12	39:1h:68:ARG:HH22	1.58	0.51
1:2A:2298:A:N6	1:2A:2318:G:H8	2.08	0.51
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.44	0.51
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.92	0.51
32:2a:673:G:O3'	37:2f:87:ARG:NH2	2.43	0.51
32:2a:926:G:N2	53:2v:15:A:OP2	2.40	0.51
32:2a:1004:A:N6	32:2a:1037:C:O2	2.39	0.51
49:2r:40:LEU:HD13	49:2r:79:LEU:HD11	1.92	0.51
1:1A:1062:G:H22	1:1A:1077:A:N6	2.08	0.51
1:1A:1877:A:H5''	1:1A:1878:G:OP2	2.09	0.51
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.45	0.51
1:1A:2393:A:H5''	11:1P:63:PRO:HB3	1.92	0.51
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.25	0.51
32:1a:100:C:H2'	32:1a:101:A:C8	2.45	0.51
32:1a:735:C:H2'	32:1a:736:C:C6	2.45	0.51
34:1c:120:VAL:O	34:1c:124:ILE:HG12	2.10	0.51
1:2A:910:A:N1	1:2A:2277:G:H1'	2.25	0.51
1:2A:2118:U:OP1	1:2A:2148:G:H4'	2.10	0.51
7:2H:76:VAL:HA	7:2H:79:VAL:HG22	1.91	0.51
17:2V:72:VAL:HB	17:2V:85:LYS:HB3	1.91	0.51
24:22:24:LEU:HD23	24:22:60:LEU:HD21	1.92	0.51
29:27:24:THR:HG22	29:27:26:GLY:H	1.74	0.51
32:2a:979:C:OP1	32:2a:1223:C:N4	2.43	0.51
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.25	0.51
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.92	0.51
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.92	0.51
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.91	0.51
1:1A:27:G:N2	1:1A:512:G:H1'	2.25	0.51
1:1A:272(J):C:H2'	1:1A:274:G:C8	2.43	0.51
1:1A:1512:U:H2'	1:1A:1513:C:C6	2.45	0.51
32:1a:911:U:H2'	32:1a:912:C:C6	2.45	0.51
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.45	0.51
40:1i:50:LEU:HG	40:1i:81:ILE:HD11	1.91	0.51
40:1i:55:ALA:HA	40:1i:58:HIS:CD2	2.46	0.51
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.43	0.51
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.75	0.51
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.46	0.51
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.91	0.51
32:2a:67:C:H2'	32:2a:68:G:C8	2.45	0.51
32:2a:448:A:P	32:2a:485:G:H22	2.32	0.51
32:2a:952:U:H2'	32:2a:953:G:C8	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:28:ARG:HA	37:2f:31:GLU:HG2	1.93	0.51
57:2y:9:A:H5'	57:2y:46:G7M:N3	2.25	0.51
1:1A:918:A:N3	2:1B:80:U:O2'	2.42	0.51
2:1B:58:A:OP2	62:1B:303:HOH:O	2.19	0.51
32:1a:444:C:H2'	32:1a:445:G:H8	1.74	0.51
35:1d:117:ALA:O	35:1d:121:VAL:HG23	2.11	0.51
57:1y:71:G:H2'	57:1y:72:C:H6	1.76	0.51
1:2A:893:C:H5'	1:2A:894:C:C5	2.46	0.51
1:2A:2721:A:OP1	62:2A:3911:HOH:O	2.19	0.51
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.39	0.51
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.44	0.51
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.43	0.51
32:2a:472:A:HO2'	47:2p:82:GLN:H	1.59	0.51
32:2a:524:G:H2'	32:2a:525:C:C6	2.46	0.51
32:2a:707:C:H2'	32:2a:708:C:C6	2.46	0.51
32:2a:1252:A:H2'	32:2a:1253:G:O4'	2.11	0.51
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.76	0.51
33:2b:185:ILE:HG22	33:2b:199:TYR:HD2	1.73	0.51
43:2l:53:ARG:HD2	43:2l:93:LEU:HD11	1.92	0.51
1:1A:1057:A:N6	1:1A:1081:U:H3	2.08	0.51
2:1B:23:G:O6	62:1B:302:HOH:O	2.19	0.51
32:1a:143:A:O2'	32:1a:144:G:OP2	2.24	0.51
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.46	0.51
47:1p:48:TRP:CD1	47:1p:48:TRP:H	2.27	0.51
55:1x:68:C:H2'	55:1x:69:C:C6	2.46	0.51
1:2A:1783:A:H5'	1:2A:2608:G:H4'	1.93	0.51
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.09	0.51
4:2E:29:GLY:H	4:2E:180:ASN:HB3	1.75	0.51
5:2F:13:SER:OG	5:2F:16:GLY:O	2.25	0.51
5:2F:50:SER:HB2	5:2F:94:PRO:HD3	1.92	0.51
6:2G:165:THR:OG1	6:2G:167:GLU:OE1	2.15	0.51
8:2I:140:LEU:HD23	8:2I:142:VAL:HG22	1.91	0.51
23:21:50:ARG:HD2	23:21:57:GLU:OE2	2.11	0.51
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.26	0.51
3:1D:20:ASP:OD2	3:1D:22:SER:OG	2.28	0.51
32:1a:143:A:HO2'	32:1a:144:G:P	2.33	0.51
32:1a:636:U:H2'	32:1a:637:G:H8	1.76	0.51
50:1s:28:LYS:HB3	50:1s:47:HIS:CD2	2.45	0.51
1:2A:76:C:O3'	24:22:59:ARG:HG2	2.10	0.51
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.93	0.51
32:2a:598:U:H2'	32:2a:599:C:H6	1.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.46	0.51
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.92	0.51
1:1A:185:U:H2'	1:1A:186:G:C8	2.46	0.51
1:1A:1453:U:OP1	13:1R:77:ARG:HD3	2.11	0.51
1:1A:1580:A:OP2	1:1A:1580:A:H8	1.93	0.51
3:1D:166:GLN:HB2	3:1D:174:ILE:HG22	1.92	0.51
7:1H:40:GLU:CD	7:1H:60:ARG:HH21	2.18	0.51
32:1a:129:U:H5'	48:1q:3:LYS:HZ1	1.76	0.51
32:1a:948:C:OP1	44:1m:109:THR:OG1	2.28	0.51
32:1a:1027:C:N4	32:1a:1034:G:H1	2.09	0.51
8:2I:130:TYR:N	8:2I:138:ILE:O	2.38	0.51
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.92	0.51
1:1A:1071:G:N1	1:1A:1091:G:O6	2.44	0.51
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.75	0.51
18:1W:18:ARG:HG3	18:1W:76:VAL:HB	1.92	0.51
32:1a:963:G:H5'	62:1a:1978:HOH:O	2.11	0.51
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.10	0.51
1:2A:1269:A:H2'	1:2A:1270:C:C6	2.46	0.51
1:2A:1364:G:P	23:21:3:LYS:HG3	2.51	0.51
1:2A:2577:A:H5''	1:2A:2578:G:H5'	1.92	0.51
5:2F:32:LEU:HD22	5:2F:112:MET:HE2	1.93	0.51
23:21:83:GLU:OE1	23:21:83:GLU:N	2.44	0.51
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.10	0.51
41:2j:44:VAL:HG22	41:2j:66:ARG:HB3	1.93	0.51
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.45	0.51
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.92	0.51
1:1A:2629:A:H1'	1:1A:2630:G:O5'	2.10	0.51
26:14:61:ARG:NH1	50:1s:42:PRO:HD3	2.25	0.51
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.34	0.51
33:1b:8:LYS:O	33:1b:217:ARG:NH2	2.44	0.51
42:1k:34:ASP:HB2	42:1k:35:PRO:HD2	1.92	0.51
50:1s:28:LYS:HB3	50:1s:47:HIS:HD2	1.75	0.51
1:2A:271(Y):U:O3'	1:2A:271(Z):C:H6	1.94	0.51
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.40	0.51
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.46	0.51
1:2A:1489:U:O2'	1:2A:1490:A:H8	1.94	0.51
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.27	0.51
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.25	0.51
32:2a:381:C:H2'	32:2a:382:A:O4'	2.10	0.51
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.75	0.51
7:1H:87:LEU:HD23	7:1H:164:TYR:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.75	0.51
32:1a:1006:C:H42	32:1a:1023:G:H1	1.59	0.51
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.46	0.51
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.91	0.51
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.93	0.51
1:2A:731:C:H5''	62:2A:4110:HOH:O	2.11	0.51
1:2A:890:A:H2'	1:2A:892:G:H8	1.75	0.51
32:2a:60:A:N6	32:2a:110:C:N3	2.57	0.51
32:2a:560:U:H5'	32:2a:566:G:N2	2.26	0.51
1:1A:1364:G:P	23:11:3:LYS:HG3	2.51	0.50
36:1e:57:LYS:HG2	36:1e:61:TYR:CE2	2.46	0.50
1:2A:93:G:H2'	1:2A:94:C:C6	2.47	0.50
1:2A:127:A:H5''	1:2A:128:C:C6	2.46	0.50
1:2A:340:A:H2'	1:2A:341:G:O4'	2.11	0.50
1:2A:2063:C:H5''	62:2A:3962:HOH:O	2.11	0.50
1:2A:2162:G:H2'	1:2A:2163:C:O4'	2.11	0.50
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.46	0.50
8:2I:77:LEU:HD22	8:2I:101:LEU:HB3	1.92	0.50
18:2W:4:LYS:HE2	18:2W:6:ILE:HD11	1.92	0.50
32:2a:45:U:H2'	32:2a:46:G:C8	2.46	0.50
32:2a:663:A:O3'	49:2r:64:ARG:NH2	2.34	0.50
32:2a:946:A:O2'	32:2a:1333:A:N3	2.30	0.50
32:2a:1314:C:H2'	32:2a:1315:U:C6	2.46	0.50
34:2c:24:ALA:HB3	34:2c:29:TYR:HD1	1.76	0.50
46:2o:82:ILE:HD12	46:2o:88:ARG:HB2	1.93	0.50
3:1D:62:TYR:HA	3:1D:87:ASN:OD1	2.10	0.50
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.92	0.50
11:1P:95:VAL:HA	11:1P:99:LEU:HD23	1.92	0.50
43:1l:7:ILE:HD13	43:1l:10:LEU:HD12	1.94	0.50
49:1r:53:ARG:HH21	49:1r:59:SER:HA	1.76	0.50
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.46	0.50
21:2Z:31:ARG:HG3	21:2Z:32:HIS:CD2	2.46	0.50
24:22:7:ARG:HA	24:22:10:LEU:HD12	1.93	0.50
36:2e:102:ALA:O	36:2e:107:ARG:NH2	2.44	0.50
42:2k:44:SER:OG	42:2k:47:VAL:HG23	2.11	0.50
50:2s:22:LEU:O	50:2s:26:GLY:N	2.40	0.50
1:1A:1176:G:H21	1:1A:1178:C:P	2.35	0.50
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.46	0.50
7:1H:17:VAL:HG11	7:1H:50:VAL:HG21	1.92	0.50
34:1c:52:LEU:HD13	34:1c:68:VAL:HG13	1.93	0.50
44:1m:65:LYS:HD3	44:1m:69:GLU:HG2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:362:U:O2'	1:2A:363:G:H5''	2.11	0.50
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.93	0.50
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.11	0.50
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.10	0.50
32:2a:1347:G:H22	32:2a:1374:A:P	2.34	0.50
57:2y:21:A:N6	57:2y:48:C:O4'	2.44	0.50
1:1A:185:U:H4'	1:1A:218:A:H4'	1.94	0.50
1:1A:218:A:C2	1:1A:235:U:H4'	2.46	0.50
1:1A:880:G:H2'	1:1A:881:G:C8	2.46	0.50
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.23	0.50
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.10	0.50
27:15:41:PRO:O	27:15:44:THR:OG1	2.30	0.50
1:2A:324:A:N6	1:2A:338:G:O2'	2.43	0.50
1:2A:686:G:N2	1:2A:788:A:H61	2.09	0.50
1:2A:700:G:O2'	1:2A:1632:A:N3	2.34	0.50
1:2A:900:A:O2'	1:2A:901:A:OP1	2.28	0.50
1:2A:1912:A:HO2'	32:2a:1494:G:HO2'	1.59	0.50
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	1.92	0.50
41:2j:44:VAL:HA	41:2j:66:ARG:HB3	1.93	0.50
44:2m:19:LEU:HD11	44:2m:56:LEU:HD21	1.92	0.50
54:2w:51:U:H2'	54:2w:52:G:C8	2.46	0.50
1:1A:271(I):G:N7	1:1A:271(J):C:N4	2.59	0.50
1:1A:1007:C:OP2	62:1A:4240:HOH:O	2.19	0.50
1:1A:2032:G:OP2	1:1A:2454:G:O2'	2.23	0.50
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.11	0.50
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.93	0.50
17:1V:61:VAL:HA	17:1V:94:LEU:HD23	1.93	0.50
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.08	0.50
32:1a:955:U:O2'	50:1s:83:HIS:HD2	1.95	0.50
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.12	0.50
32:1a:1118:C:OP1	40:1i:104:ARG:NH1	2.33	0.50
32:1a:1125:U:C4	41:1j:38:ILE:HD13	2.46	0.50
32:1a:1255:G:O2'	32:1a:1258:G:N3	2.40	0.50
1:2A:1354:A:H4'	3:2D:38:LYS:HE3	1.93	0.50
1:2A:2117:A:N6	1:2A:2171:A:N1	2.59	0.50
1:2A:2749:A:O3'	7:2H:62:LYS:NZ	2.42	0.50
2:2B:15:A:OP2	2:2B:69:G:N2	2.44	0.50
32:2a:222:U:H2'	32:2a:223:U:C6	2.47	0.50
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.44	0.50
33:2b:78:GLN:O	33:2b:94:ASN:ND2	2.45	0.50
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:106:PRO:O	36:2e:110:LEU:HG	2.10	0.50
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.44	0.50
1:1A:668:G:H5'	1:1A:669:G:OP2	2.11	0.50
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.11	0.50
4:1E:29:GLY:HA3	62:1E:402:HOH:O	2.11	0.50
42:1k:80:VAL:HG23	42:1k:105:VAL:HA	1.94	0.50
2:2B:1:U:O2'	2:2B:2:C:O5'	2.23	0.50
12:2Q:78:PRO:HD3	55:2x:1:C:N3	2.27	0.50
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.93	0.50
17:2V:24:LYS:HA	17:2V:92:THR:OG1	2.11	0.50
21:2Z:145:GLU:O	21:2Z:147:GLY:N	2.45	0.50
32:2a:1056:U:H5'	34:2c:163:ALA:HB2	1.93	0.50
32:2a:1263:C:C4	32:2a:1272:G:O6	2.64	0.50
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.40	0.50
33:2b:119:GLU:CD	33:2b:153:ARG:HH22	2.20	0.50
1:1A:811:U:H2'	11:1P:21:ARG:HA	1.94	0.50
1:1A:1466:G:O2'	1:1A:1546:C:O2'	2.12	0.50
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.46	0.50
16:1U:50:ARG:HG2	16:1U:53:ARG:NH2	2.27	0.50
43:1l:8:ASN:O	43:1l:12:ARG:HG3	2.11	0.50
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.76	0.50
46:1o:6:GLU:O	46:1o:10:LYS:HD2	2.11	0.50
1:2A:300:A:OP2	20:2Y:86:ARG:NH1	2.45	0.50
1:2A:2135:A:C4	1:2A:2136:C:H5	2.30	0.50
1:2A:2818:G:OP1	1:2A:2837:G:O2'	2.28	0.50
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.11	0.50
32:2a:197:A:O2'	32:2a:220:G:N2	2.45	0.50
32:2a:376:G:H4'	47:2p:5:ARG:HH21	1.77	0.50
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.94	0.50
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.12	0.50
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.46	0.50
40:2i:8:GLY:HA2	40:2i:79:LEU:HD23	1.93	0.50
55:2x:21:A:N6	55:2x:46:G:H2'	2.27	0.50
1:1A:1584:C:O2'	1:1A:1586:A:H5'	2.12	0.50
7:1H:3:ARG:HG3	7:1H:6:ARG:NE	2.23	0.50
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.46	0.50
1:2A:271(P):C:O2'	8:2I:42:SER:OG	2.24	0.50
1:2A:2203:U:H2'	1:2A:2205:C:H6	1.77	0.50
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.11	0.50
10:2O:2:ILE:O	10:2O:33:ALA:N	2.41	0.50
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.93	0.50
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.94	0.50
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.14	0.50
32:2a:1056:U:OP1	34:2c:163:ALA:N	2.44	0.50
32:2a:1110:A:H8	32:2a:1110:A:O5'	1.94	0.50
32:2a:1239:A:O2'	38:2g:114:ARG:O	2.26	0.50
38:2g:74:GLU:HG2	38:2g:91:VAL:HG22	1.94	0.50
47:2p:19:ILE:HD13	47:2p:51:VAL:HG22	1.94	0.50
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.94	0.50
1:1A:2151:G:H2'	1:1A:2152:G:C8	2.47	0.50
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.18	0.50
32:1a:256:U:OP1	48:1q:17:LYS:NZ	2.36	0.50
32:1a:316:G:OP2	32:1a:351:G:O2'	2.23	0.50
32:1a:509:A:O2'	32:1a:510:A:OP1	2.25	0.50
45:1n:33:VAL:HA	45:1n:40:CYS:HA	1.94	0.50
1:2A:1840:G:OP2	62:2A:3934:HOH:O	2.18	0.50
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.47	0.50
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.93	0.50
32:2a:1005:A:H5''	32:2a:1006:C:H5	1.77	0.50
32:2a:1029:C:N4	32:2a:1032:G:C6	2.79	0.50
32:2a:1404:5MC:O2	32:2a:1519:MA6:O2'	2.27	0.50
34:2c:11:ARG:NH2	34:2c:182:ILE:HD11	2.27	0.50
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.94	0.50
47:2p:8:ARG:HB3	47:2p:28:ARG:NH1	2.27	0.50
47:2p:21:VAL:HG22	47:2p:33:ILE:HB	1.93	0.50
1:1A:1069:A:H4'	1:1A:1070:A:H5''	1.94	0.49
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.47	0.49
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.47	0.49
32:1a:601:C:H2'	32:1a:602:A:C8	2.47	0.49
33:1b:88:ALA:O	33:1b:226:ARG:NH1	2.44	0.49
34:1c:44:GLU:HA	34:1c:52:LEU:HD23	1.94	0.49
44:1m:3:ARG:HG3	44:1m:4:ILE:N	2.25	0.49
1:2A:113:G:OP1	62:2A:3940:HOH:O	2.20	0.49
1:2A:1394:U:OP1	62:2A:3939:HOH:O	2.20	0.49
1:2A:1711:C:H2'	1:2A:1712:C:H6	1.76	0.49
5:2F:20:LEU:HG	5:2F:21:ALA:H	1.77	0.49
16:2U:58:ARG:HA	16:2U:61:TRP:CE3	2.47	0.49
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.45	0.49
32:2a:297:G:N2	32:2a:300:A:OP2	2.44	0.49
32:2a:427:U:OP1	35:2d:13:ARG:NH1	2.42	0.49
32:2a:607:A:H2'	32:2a:608:A:O4'	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:78:ARG:HB2	38:2g:87:VAL:HG21	1.94	0.49
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.44	0.49
1:1A:2552:OMU:O5'	1:1A:2552:OMU:H6	2.12	0.49
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.93	0.49
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.12	0.49
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.13	0.49
33:1b:19:HIS:HA	33:1b:39:ILE:HG23	1.92	0.49
37:1f:39:LYS:HB2	37:1f:64:GLN:HB3	1.94	0.49
51:1t:92:LEU:O	51:1t:96:GLY:HA2	2.12	0.49
1:2A:271(J):C:O2'	1:2A:271(K):U:OP2	2.25	0.49
1:2A:774:A:H2'	1:2A:774:A:N3	2.28	0.49
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.47	0.49
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.76	0.49
26:24:64:GLY:C	26:24:66:SER:H	2.20	0.49
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.12	0.49
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.46	0.49
38:2g:24:THR:HA	38:2g:27:ILE:HD12	1.93	0.49
1:1A:1356:G:OP2	62:1A:4249:HOH:O	2.20	0.49
1:1A:2682:U:O2'	15:1T:58:ASN:ND2	2.45	0.49
12:1Q:89:ASN:HB2	55:1x:1:C:N3	2.27	0.49
32:1a:8:A:H5'	36:1e:101:ILE:HG22	1.93	0.49
32:1a:373:A:H2'	32:1a:374:A:H8	1.77	0.49
32:1a:1008:C:N3	32:1a:1021:G:O6	2.45	0.49
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.26	0.49
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.94	0.49
35:1d:144:ASP:OD1	35:1d:144:ASP:N	2.45	0.49
40:1i:55:ALA:HB1	40:1i:58:HIS:HB2	1.95	0.49
1:2A:140:G:N2	1:2A:1596:A:H4'	2.28	0.49
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.26	0.49
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.44	0.49
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.11	0.49
19:2X:32:PRO:O	19:2X:77:LYS:HE3	2.13	0.49
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.47	0.49
33:2b:97:TRP:CH2	33:2b:102:LEU:HG	2.46	0.49
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	1.94	0.49
54:2w:29:G:H1	54:2w:41:C:N4	2.09	0.49
1:1A:586:A:N1	1:1A:809:G:O2'	2.40	0.49
4:1E:5:LEU:HD11	4:1E:79:ARG:HB2	1.94	0.49
6:1G:108:ASN:HD22	26:14:22:ILE:HD13	1.77	0.49
33:1b:37:ASN:C	33:1b:39:ILE:H	2.18	0.49
33:1b:131:PRO:O	33:1b:135:GLN:N	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:886:C:H2'	1:2A:887:A:O4'	2.11	0.49
2:2B:13:A:N1	2:2B:69:G:O2'	2.40	0.49
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.47	0.49
32:2a:1310:G:H2'	32:2a:1311:G:C8	2.48	0.49
41:2j:47:PHE:CZ	45:2n:37:PHE:HE2	2.31	0.49
42:2k:73:MET:HG2	42:2k:103:LEU:HD21	1.93	0.49
42:2k:87:THR:O	42:2k:87:THR:OG1	2.24	0.49
1:1A:1093:G:H3'	1:1A:1094:U:H5''	1.95	0.49
32:1a:266:G:N3	32:1a:266:G:H5''	2.28	0.49
33:1b:132:LYS:HA	33:1b:135:GLN:HB3	1.94	0.49
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.93	0.49
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.77	0.49
51:1t:42:GLN:NE2	51:1t:46:GLU:OE2	2.43	0.49
1:2A:969:U:H2'	1:2A:970:C:C6	2.48	0.49
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.48	0.49
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.47	0.49
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.48	0.49
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.21	0.49
1:2A:2319:G:H21	14:2S:3:ARG:HD2	1.77	0.49
2:2B:88:C:H2'	2:2B:89:G:O4'	2.12	0.49
3:2D:123:ALA:HB3	3:2D:131:LEU:HG	1.94	0.49
32:2a:1130:A:H5''	40:2i:18:PHE:CE2	2.47	0.49
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.93	0.49
42:2k:108:ILE:HB	49:2r:87:ARG:HD2	1.95	0.49
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.48	0.49
1:1A:2613:U:OP1	62:1A:4248:HOH:O	2.20	0.49
32:1a:890:G:O2'	32:1a:906:G:O6	2.29	0.49
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.38	0.49
44:1m:82:MET:O	44:1m:93:ARG:NH2	2.35	0.49
1:2A:1645:G:H5''	1:2A:1646:C:H5'	1.95	0.49
1:2A:2239:G:OP2	62:2A:3941:HOH:O	2.20	0.49
1:2A:2390:U:P	30:28:35:GLN:HE22	2.35	0.49
2:2B:83:G:H1	2:2B:94:C:H42	1.61	0.49
7:2H:68:THR:O	7:2H:72:ILE:HG12	2.12	0.49
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.94	0.49
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.44	0.49
57:2y:61:C:H2'	57:2y:62:C:C6	2.47	0.49
1:1A:272(A):U:O2'	1:1A:272(B):G:O5'	2.17	0.49
1:1A:1498:C:OP1	62:1A:4250:HOH:O	2.20	0.49
1:1A:2712:U:O2'	1:1A:2713:A:H5'	2.13	0.49
1:1A:2777:G:O6	62:1A:4244:HOH:O	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.27	0.49
32:1a:1025:U:O2	32:1a:1036:G:C6	2.66	0.49
35:1d:65:ARG:HH11	35:1d:72:GLU:HB2	1.77	0.49
41:1j:64:GLU:HG2	45:1n:59:ALA:HB2	1.95	0.49
54:1w:9:A:H8	54:1w:11:C:H41	1.61	0.49
57:1y:9:A:H4'	57:1y:46:G7M:OP2	2.13	0.49
57:1y:38:A:H2'	57:1y:39:PSU:O4'	2.12	0.49
1:2A:764:A:H5''	3:2D:210:GLY:HA2	1.93	0.49
1:2A:1490:A:O2'	3:2D:99:ASP:OD1	2.29	0.49
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.93	0.49
1:2A:2238:G:H5''	62:2A:4277:HOH:O	2.12	0.49
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.48	0.49
8:2I:88:ILE:HG12	8:2I:123:LEU:HD12	1.94	0.49
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.47	0.49
32:2a:266:G:H2'	32:2a:266:G:N3	2.26	0.49
32:2a:565:U:OP2	32:2a:566:G:O2'	2.28	0.49
32:2a:598:U:H2'	32:2a:599:C:C6	2.47	0.49
32:2a:1076:C:OP1	33:2b:179:LYS:NZ	2.46	0.49
1:1A:72:U:OP1	62:1A:4243:HOH:O	2.19	0.49
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.13	0.49
1:1A:1054:A:OP1	1:1A:1054:A:H4'	2.13	0.49
32:1a:341:C:H2'	32:1a:342:C:H6	1.78	0.49
34:1c:150:LYS:HE2	34:1c:152:ILE:HD11	1.95	0.49
1:2A:800:A:H8	1:2A:800:A:OP1	1.96	0.49
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.13	0.49
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.35	0.49
1:2A:2466:C:OP1	31:29:4:ARG:HB2	2.13	0.49
8:2I:102:SER:O	8:2I:106:GLY:HA2	2.13	0.49
9:2N:62:VAL:HG11	9:2N:66:LYS:HB2	1.95	0.49
26:24:45:GLY:C	26:24:47:GLN:H	2.20	0.49
32:2a:79:G:H1	32:2a:90:U:H3	1.61	0.49
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.46	0.49
35:2d:180:GLY:O	35:2d:182:LYS:HG3	2.13	0.49
41:2j:36:GLY:O	41:2j:38:ILE:HD13	2.12	0.49
46:2o:15:PHE:CZ	46:2o:84:LYS:HD2	2.47	0.49
49:2r:31:LEU:HD23	49:2r:31:LEU:H	1.77	0.49
1:1A:1058:G:N2	1:1A:1080:C:N3	2.55	0.49
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.26	0.49
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.95	0.49
20:1Y:17:SER:OG	20:1Y:71:LYS:NZ	2.39	0.49
39:1h:9:MET:SD	39:1h:26:VAL:HG11	2.53	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:9:ARG:NH2	41:1j:97:GLU:OE1	2.46	0.49
49:1r:31:LEU:HD23	49:1r:31:LEU:H	1.77	0.49
1:2A:1147:C:H2'	1:2A:1148:A:C8	2.48	0.49
1:2A:2131:G:C8	1:2A:2133:G:C2	3.01	0.49
12:2Q:82:ARG:NH2	22:20:4:LYS:HG3	2.28	0.49
14:2S:26:LEU:HD13	14:2S:85:VAL:HG11	1.94	0.49
32:2a:954:G:H2'	32:2a:955:U:O4'	2.12	0.49
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.48	0.49
1:1A:1509(A):A:H3'	1:1A:1509(B):A:H8	1.78	0.49
4:1E:28:ALA:HB3	4:1E:93:VAL:HG13	1.94	0.49
5:1F:10:PRO:HB3	5:1F:17:ARG:HH21	1.77	0.49
32:1a:405:U:O4	35:1d:2:GLY:N	2.46	0.49
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.40	0.49
32:1a:814:A:H2'	32:1a:816:A:H5''	1.95	0.49
32:1a:1027:C:C4	32:1a:1034:G:N1	2.79	0.49
33:1b:21:ARG:HB3	33:1b:39:ILE:HD12	1.95	0.49
54:1w:34:G:H2'	54:1w:35:A:C8	2.47	0.49
1:2A:903:C:H2'	1:2A:904:C:C6	2.48	0.49
1:2A:2130:U:O2	1:2A:2134:A:O2'	2.29	0.49
4:2E:3:GLY:HA3	4:2E:81:ILE:HD12	1.94	0.49
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	1.94	0.49
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.95	0.49
28:26:35:GLU:HG3	28:26:50:ARG:HD3	1.95	0.49
32:2a:407:G:H2'	32:2a:408:A:C8	2.47	0.49
32:2a:757:U:H2'	32:2a:758:G:O4'	2.13	0.49
34:2c:129:ALA:HB3	34:2c:132:ARG:HD2	1.94	0.49
44:2m:50:GLU:HA	44:2m:53:VAL:HG22	1.93	0.49
47:2p:39:TYR:CG	47:2p:73:LEU:HD21	2.48	0.49
54:2w:67:C:H2'	54:2w:68:C:C6	2.48	0.49
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.13	0.48
1:1A:1991:U:H2'	1:1A:1992:G:H5''	1.95	0.48
32:1a:690:G:H2'	32:1a:691:G:O4'	2.12	0.48
57:1y:5:G:H1'	57:1y:69:G:N2	2.28	0.48
1:2A:242:G:C8	30:28:5:LYS:HG2	2.48	0.48
1:2A:1151:G:H4'	16:2U:81:HIS:CG	2.48	0.48
1:2A:2110:G:H8	1:2A:2110:G:OP2	1.95	0.48
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.77	0.48
1:2A:2336:A:H61	22:20:43:THR:HG21	1.76	0.48
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.47	0.48
39:2h:28:ALA:HB3	39:2h:57:PRO:HB2	1.94	0.48
1:1A:226:G:H21	1:1A:228:A:H62	1.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.48	0.48
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.12	0.48
6:1G:98:ARG:CZ	26:14:1:MET:HE3	2.43	0.48
32:1a:743:U:H2'	32:1a:744:C:C6	2.48	0.48
1:2A:479:A:N3	1:2A:481:G:H5''	2.28	0.48
1:2A:709:U:H2'	1:2A:710:G:C8	2.48	0.48
1:2A:848:G:H2'	1:2A:849:A:C8	2.48	0.48
6:2G:127:GLY:N	6:2G:166:ASP:OD1	2.46	0.48
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.95	0.48
32:2a:189(A):C:H2'	32:2a:189(B):C:C6	2.48	0.48
32:2a:460:G:O6	62:2a:1906:HOH:O	2.19	0.48
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.47	0.48
35:2d:57:ARG:NH1	35:2d:205:GLU:HB3	2.28	0.48
39:2h:103:VAL:HG21	39:2h:109:ILE:C	2.37	0.48
44:2m:122:LYS:HD3	44:2m:123:ALA:H	1.77	0.48
1:1A:774:A:N3	1:1A:774:A:H2'	2.28	0.48
1:1A:808:G:OP1	62:1A:4246:HOH:O	2.20	0.48
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.12	0.48
32:1a:715:A:H2'	32:1a:716:A:C8	2.47	0.48
32:1a:870:U:H4'	32:1a:871:U:H5''	1.96	0.48
32:1a:1314:C:H2'	32:1a:1315:U:C6	2.48	0.48
33:1b:92:TYR:HE1	33:1b:94:ASN:HB2	1.77	0.48
40:1i:3:GLN:HE21	40:1i:20:ARG:CZ	2.26	0.48
54:1w:43:C:H2'	54:1w:44:G:C8	2.48	0.48
1:2A:500:G:N2	1:2A:502:A:H3'	2.27	0.48
1:2A:1283:G:O2'	1:2A:1285:G:N7	2.43	0.48
1:2A:1805:U:O2	3:2D:50:THR:HB	2.13	0.48
1:2A:2163:C:H5'	1:2A:2172:U:OP2	2.14	0.48
6:2G:63:ILE:HD11	6:2G:144:ILE:HG13	1.96	0.48
6:2G:152:LEU:H	6:2G:152:LEU:HD12	1.78	0.48
32:2a:109:A:H5'	32:2a:110:C:C5	2.47	0.48
32:2a:224:C:H2'	32:2a:225:C:H6	1.78	0.48
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.44	0.48
32:2a:826:C:H4'	39:2h:12:ARG:HG2	1.96	0.48
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.35	0.48
35:2d:31:CYS:O	35:2d:35:ARG:HG3	2.14	0.48
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.78	0.48
46:2o:56:LEU:O	46:2o:60:VAL:HG22	2.13	0.48
57:2y:26:A:H2'	57:2y:27:G:H5'	1.95	0.48
57:2y:57:G:N3	57:2y:57:G:H2'	2.28	0.48
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1859:A:N6	1:1A:1883:G:O2'	2.47	0.48
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.48	0.48
32:1a:431:A:H2'	32:1a:432:A:O4'	2.14	0.48
33:1b:54:THR:HG23	33:1b:199:TYR:HB3	1.95	0.48
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.96	0.48
1:2A:7:G:H2'	1:2A:8:A:C8	2.47	0.48
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.46	0.48
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.56	0.48
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.28	0.48
33:2b:16:HIS:CB	33:2b:210:SER:HB2	2.43	0.48
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.95	0.48
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.12	0.48
40:2i:126:SER:C	40:2i:128:ARG:H	2.21	0.48
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.46	0.48
50:2s:4:SER:HB3	50:2s:7:LYS:HG3	1.95	0.48
1:1A:1055:G:H1	1:1A:1104:C:H42	1.62	0.48
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.13	0.48
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.37	0.48
6:1G:179:PRO:HG3	26:14:43:TYR:CZ	2.48	0.48
10:1O:120:GLU:OE1	15:1T:67:SER:OG	2.27	0.48
21:1Z:23:LYS:HD3	21:1Z:40:ASP:HA	1.95	0.48
32:1a:399:G:H2'	32:1a:400:C:C6	2.49	0.48
32:1a:502:G:H2'	32:1a:503:C:O4'	2.13	0.48
32:1a:1179:A:H4'	40:1i:103:THR:HA	1.93	0.48
1:2A:184:C:H2'	1:2A:185:U:C6	2.49	0.48
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.47	0.48
1:2A:1472:A:H2'	1:2A:1473:G:O4'	2.13	0.48
3:2D:12:SER:HB3	3:2D:208:LYS:HB3	1.95	0.48
15:2T:106:SER:N	15:2T:109:GLU:OE1	2.35	0.48
21:2Z:166:SER:C	21:2Z:168:GLU:H	2.21	0.48
33:2b:8:LYS:HB3	33:2b:217:ARG:HG3	1.96	0.48
38:2g:111:ARG:HD3	38:2g:113:GLU:OE2	2.13	0.48
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.49	0.48
18:1W:27:LYS:HD2	18:1W:31:GLU:HG2	1.95	0.48
34:1c:56:ASP:HB2	34:1c:67:THR:HB	1.95	0.48
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.22	0.48
14:2S:62:LYS:HB3	14:2S:97:ARG:HD2	1.95	0.48
19:2X:60:ARG:NH2	29:27:47:ARG:HH22	2.03	0.48
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.13	0.48
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.48	0.48
32:2a:1373:G:H5''	38:2g:36:LYS:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	1.94	0.48
50:2s:80:TYR:O	50:2s:82:GLY:N	2.40	0.48
1:1A:686:G:N2	1:1A:788:A:H61	2.12	0.48
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.14	0.48
15:1T:127:ALA:C	15:1T:129:ARG:H	2.21	0.48
25:13:26:LEU:O	25:13:35:ARG:NE	2.43	0.48
54:1w:5:G:H2'	54:1w:6:G:H8	1.78	0.48
1:2A:740:U:H2'	1:2A:741:G:C8	2.49	0.48
1:2A:781:A:P	3:2D:218:ARG:HH22	2.36	0.48
2:2B:76:G:H2'	2:2B:77:U:O4'	2.13	0.48
2:2B:94:C:H2'	2:2B:95:C:C6	2.49	0.48
30:28:14:VAL:HG13	30:28:22:VAL:HG13	1.95	0.48
32:2a:1198:G:H2'	32:2a:1199:U:C6	2.48	0.48
1:1A:484:C:H2'	1:1A:485:C:C6	2.49	0.48
1:1A:1138:G:N3	9:1N:106:MET:HE2	2.29	0.48
1:1A:1508:A:H5'	1:1A:1509(A):A:N7	2.29	0.48
1:1A:1647:G:H3'	1:1A:1647:G:OP2	2.14	0.48
1:1A:1882:C:H2'	1:1A:1883:G:O4'	2.14	0.48
1:1A:2101:G:H2'	1:1A:2102:U:C6	2.49	0.48
1:1A:2110:G:C2	1:1A:2120:G:H1'	2.48	0.48
62:1A:4277:HOH:O	13:1R:50:HIS:ND1	2.35	0.48
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.67	0.48
21:1Z:6:LYS:HD3	21:1Z:8:TYR:OH	2.14	0.48
28:16:26:ASN:HD21	28:16:28:ARG:NH2	2.12	0.48
1:2A:1009:A:O4'	16:2U:59:ARG:HD2	2.14	0.48
1:2A:2205:C:H1'	1:2A:2220:G:N2	2.29	0.48
1:2A:2319:G:N2	14:2S:3:ARG:HH11	2.12	0.48
13:2R:79:LEU:HA	13:2R:83:ILE:HD12	1.95	0.48
24:22:1:MET:HE3	24:22:1:MET:HB2	1.81	0.48
25:23:7:LYS:N	25:23:55:ARG:O	2.45	0.48
32:2a:88:A:H5''	32:2a:89:C:C6	2.48	0.48
32:2a:302:G:N3	32:2a:556:C:H4'	2.29	0.48
32:2a:1469:G:H2'	32:2a:1470:G:H8	1.79	0.48
33:2b:76:GLN:HB2	33:2b:208:ILE:HG12	1.96	0.48
37:2f:99:ALA:HB1	49:2r:23:LYS:NZ	2.29	0.48
53:2v:22:U:H2'	53:2v:23:A:C8	2.49	0.48
1:1A:1092:C:C2'	1:1A:1093:G:H5'	2.44	0.48
1:1A:1352:U:OP2	62:1A:4245:HOH:O	2.20	0.48
4:1E:4:ILE:HD12	4:1E:91:VAL:HG12	1.96	0.48
32:1a:1003:G:H2'	32:1a:1004:A:N3	2.28	0.48
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:67:GLU:HG3	44:1m:71:ARG:NH2	2.29	0.48
54:1w:70:G:H2'	54:1w:71:G:O4'	2.13	0.48
1:2A:839:U:H2'	1:2A:840:C:C6	2.49	0.48
1:2A:1184:G:P	25:23:30:ARG:HE	2.37	0.48
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.48	0.48
32:2a:130:A:N3	32:2a:263:A:O2'	2.41	0.48
32:2a:299:G:H2'	32:2a:300:A:C8	2.48	0.48
32:2a:624:C:H2'	32:2a:625:G:H8	1.79	0.48
32:2a:1085:U:H3'	32:2a:1086:U:C5	2.49	0.48
32:2a:1106:G:H5''	34:2c:172:ARG:HB3	1.95	0.48
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.96	0.48
31:19:16:VAL:HG22	31:19:25:VAL:HG22	1.96	0.48
50:1s:52:TYR:HA	50:1s:56:GLN:O	2.14	0.48
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.38	0.48
57:1y:59:U:H3'	57:1y:60:U:H6	1.79	0.48
1:2A:616:G:H4'	5:2F:205:ARG:HH21	1.79	0.48
1:2A:764:A:H5''	3:2D:210:GLY:CA	2.44	0.48
1:2A:829:A:N7	1:2A:2248:C:H5'	2.29	0.48
6:2G:33:ARG:NH2	6:2G:162:THR:HG21	2.29	0.48
15:2T:26:ASP:OD1	15:2T:92:GLY:N	2.38	0.48
32:2a:123:C:OP1	32:2a:312:C:H5'	2.14	0.48
32:2a:1039:C:C2	32:2a:1040:U:H1'	2.49	0.48
32:2a:1236:A:O2'	32:2a:1304:G:H4'	2.13	0.48
32:2a:1376:U:OP1	38:2g:98:SER:OG	2.31	0.48
1:1A:1114:G:H2'	1:1A:1115:G:O4'	2.14	0.47
1:1A:1219:G:OP2	16:1U:19:LYS:NZ	2.47	0.47
1:1A:1339:G:H5''	19:1X:16:LYS:HD3	1.95	0.47
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.78	0.47
1:1A:2140:C:N3	1:1A:2151:G:O6	2.47	0.47
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.13	0.47
32:1a:362:G:N1	32:1a:365:U:OP2	2.44	0.47
34:1c:162:GLN:NE2	53:1v:24:A:O2'	2.47	0.47
54:1w:66:U:O4	54:1w:67:C:N4	2.47	0.47
57:1y:19:G:H5''	57:1y:60:U:O4	2.14	0.47
1:2A:1200:C:H5'	62:2A:3960:HOH:O	2.13	0.47
1:2A:1649:G:O2'	13:2R:107:ASP:OD2	2.25	0.47
1:2A:2128:C:H2'	1:2A:2129:C:O4'	2.14	0.47
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.29	0.47
1:2A:2336:A:H61	22:20:43:THR:CG2	2.27	0.47
5:2F:170:LEU:HD22	5:2F:172:TRP:HE1	1.79	0.47
8:2I:93:THR:N	8:2I:96:ASP:HB2	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.13	0.47
17:2V:40:LEU:HB2	17:2V:46:VAL:HG23	1.96	0.47
42:2k:83:ILE:HA	42:2k:109:VAL:HG12	1.96	0.47
1:1A:2710:C:OP2	62:1A:4241:HOH:O	2.19	0.47
38:1g:136:LYS:O	38:1g:140:ASP:HB2	2.14	0.47
40:1i:37:PHE:HA	40:1i:40:LEU:HD12	1.95	0.47
51:1t:38:LYS:HA	51:1t:41:ILE:HD12	1.95	0.47
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.14	0.47
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.15	0.47
32:2a:1145:C:H4'	32:2a:1146:A:H8	1.78	0.47
33:2b:74:LYS:HG2	33:2b:169:LYS:HG3	1.94	0.47
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.97	0.47
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.47	0.47
18:1W:23:LEU:HD21	27:15:25:LEU:HB2	1.96	0.47
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.46	0.47
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.95	0.47
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.83	0.47
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.67	0.47
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.79	0.47
41:1j:42:THR:HG23	41:1j:68:HIS:HA	1.96	0.47
43:1l:53:ARG:HB2	43:1l:93:LEU:HD11	1.95	0.47
56:1z:2:THR:HG23	56:1z:3:HIS:H	1.78	0.47
1:2A:1019:U:O2'	1:2A:1021:A:H2	1.97	0.47
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.45	0.47
1:2A:1927:A:H2'	1:2A:1928:A:C8	2.48	0.47
6:2G:68:PRO:HB3	6:2G:92:VAL:HB	1.95	0.47
6:2G:69:ALA:HB3	6:2G:91:ARG:NH2	2.29	0.47
32:2a:1298:C:N4	38:2g:114:ARG:HB3	2.29	0.47
32:2a:1309:G:O3'	44:2m:77:ASN:ND2	2.46	0.47
36:2e:5:ASP:N	36:2e:5:ASP:OD1	2.47	0.47
38:2g:20:ASP:HB3	38:2g:23:VAL:HB	1.95	0.47
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	1.95	0.47
1:1A:1063:G:H2'	1:1A:1064:C:H5	1.79	0.47
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.44	0.47
1:1A:1156:A:OP1	16:1U:55:ARG:NH1	2.47	0.47
1:1A:1180:C:H2'	1:1A:1181:C:C6	2.49	0.47
1:1A:2642:G:P	9:1N:83:LYS:HZ3	2.38	0.47
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.50	0.47
32:1a:194:C:H2'	32:1a:195:A:H5''	1.95	0.47
32:1a:453:A:O2'	47:1p:68:ASP:O	2.31	0.47
32:1a:689:C:OP1	42:1k:27:ASN:ND2	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:811:C:O2'	32:1a:901:A:N1	2.44	0.47
54:1w:60:U:H5''	54:1w:61:C:H5	1.78	0.47
1:2A:10:G:H2'	1:2A:11:G:C8	2.49	0.47
7:2H:70:THR:HG22	7:2H:74:ASN:HD21	1.80	0.47
29:27:24:THR:HG22	29:27:26:GLY:N	2.30	0.47
38:2g:51:GLN:O	38:2g:55:GLY:HA2	2.14	0.47
43:2l:26:ALA:HB1	43:2l:60:LEU:HD12	1.97	0.47
44:2m:113:PRO:O	44:2m:115:LYS:NZ	2.47	0.47
52:2u:17:THR:O	52:2u:22:ARG:NH1	2.47	0.47
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.29	0.47
1:1A:1092:C:H2'	1:1A:1093:G:H5'	1.96	0.47
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.49	0.47
1:1A:1670:C:OP1	62:1A:4251:HOH:O	2.21	0.47
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.43	0.47
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.44	0.47
6:1G:115:ARG:HG2	6:1G:136:ARG:NH2	2.30	0.47
16:1U:50:ARG:HG2	16:1U:53:ARG:HH22	1.80	0.47
18:1W:62:HIS:O	18:1W:64:MET:HG3	2.15	0.47
32:1a:79:G:H1'	32:1a:91:C:O2	2.14	0.47
1:2A:89:G:H3'	1:2A:90:U:H5''	1.97	0.47
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.50	0.47
1:2A:600:G:O3'	5:2F:108:LYS:HE3	2.14	0.47
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.50	0.47
1:2A:1710:C:H5'	1:2A:2859:G:H1'	1.96	0.47
1:2A:2137:C:N4	1:2A:2154:G:H1	2.12	0.47
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.15	0.47
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.96	0.47
8:2I:48:GLU:HG3	8:2I:52:ARG:NH1	2.30	0.47
12:2Q:24:GLY:HA2	12:2Q:67:ARG:NH2	2.30	0.47
16:2U:8:VAL:HG23	16:2U:11:ARG:HH21	1.79	0.47
32:2a:77:G:H2'	32:2a:78:G:O4'	2.14	0.47
32:2a:189(A):C:H2'	32:2a:189(B):C:H6	1.80	0.47
32:2a:406:G:H21	35:2d:119:GLN:NE2	2.11	0.47
32:2a:1004:A:N3	32:2a:1038:C:C2	2.82	0.47
33:2b:178:ARG:NH2	39:2h:68:ARG:HH22	2.13	0.47
34:2c:119:ARG:HE	34:2c:140:ARG:NH2	2.13	0.47
40:2i:99:LEU:HB3	40:2i:101:PHE:HE2	1.78	0.47
1:1A:27:G:C2	1:1A:512:G:N3	2.83	0.47
1:1A:185:U:H2'	1:1A:186:G:H8	1.78	0.47
1:1A:2028:U:H2'	1:1A:2029:G:O4'	2.14	0.47
32:1a:58:C:O2'	32:1a:388:G:N7	2.42	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.40	0.47
32:1a:953:G:H5'	32:1a:965:A:N6	2.27	0.47
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.97	0.47
32:1a:1251:A:H2'	32:1a:1252:A:C8	2.49	0.47
34:1c:21:ARG:HG3	34:1c:58:GLU:HG2	1.97	0.47
37:1f:67:MET:HE1	37:1f:75:LEU:HD12	1.96	0.47
48:1q:56:VAL:HB	48:1q:78:GLU:HB3	1.97	0.47
1:2A:2461:C:H2'	1:2A:2462:U:H6	1.77	0.47
2:2B:6:C:H4'	2:2B:28:C:H5'	1.96	0.47
6:2G:129:GLY:O	6:2G:161:THR:HB	2.15	0.47
12:2Q:43:THR:HA	12:2Q:94:VAL:HG12	1.95	0.47
32:2a:542:G:OP1	35:2d:10:ARG:NH2	2.44	0.47
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.80	0.47
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.14	0.47
50:2s:42:PRO:O	50:2s:45:VAL:HG12	2.14	0.47
54:2w:76:F3N:N	55:2x:76:8AN:O2'	2.47	0.47
1:1A:710:G:H2'	1:1A:711:G:C8	2.50	0.47
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.15	0.47
5:1F:129:PHE:HB3	5:1F:132:VAL:HG13	1.97	0.47
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	1.96	0.47
32:1a:430:A:H4'	35:1d:7:PRO:HG3	1.96	0.47
32:1a:626:U:H2'	32:1a:627:G:H8	1.80	0.47
32:1a:1124:G:N7	32:1a:1145:C:O2'	2.48	0.47
33:1b:102:LEU:HB3	33:1b:180:LEU:HD11	1.95	0.47
34:1c:95:THR:C	34:1c:97:LYS:H	2.23	0.47
36:1e:20:GLN:NE2	36:1e:21:ALA:O	2.47	0.47
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.96	0.47
42:1k:20:TYR:HB2	42:1k:31:THR:HG23	1.97	0.47
50:1s:20:LEU:HD21	50:1s:43:GLU:HG2	1.95	0.47
57:1y:51:U:H2'	57:1y:52:G:H8	1.79	0.47
1:2A:121:G:H4'	1:2A:149:A:H5'	1.97	0.47
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.78	0.47
1:2A:1359:A:H2	1:2A:1372:U:O4	1.96	0.47
1:2A:1782:C:O2	1:2A:2608:G:O2'	2.32	0.47
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.30	0.47
1:2A:2782:G:OP2	62:2A:3943:HOH:O	2.20	0.47
4:2E:7:VAL:HG23	4:2E:51:PHE:CE2	2.50	0.47
5:2F:157:VAL:HG21	5:2F:181:LEU:HD13	1.97	0.47
5:2F:195:ASP:HB3	5:2F:197:ASP:OD1	2.14	0.47
7:2H:25:LYS:HE2	7:2H:27:LYS:HE3	1.97	0.47
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.96	0.47
21:2Z:102:LEU:HD13	21:2Z:139:VAL:HG21	1.97	0.47
23:21:7:ILE:HG23	23:21:98:LEU:HD11	1.97	0.47
28:26:40:CYS:O	28:26:44:ARG:N	2.45	0.47
32:2a:8:A:N6	35:2d:209:ARG:HB2	2.30	0.47
32:2a:510:A:N3	32:2a:543:C:H1'	2.30	0.47
32:2a:840:C:H4'	32:2a:841:U:OP1	2.13	0.47
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.63	0.47
33:2b:81:VAL:HB	33:2b:94:ASN:ND2	2.29	0.47
34:2c:47:LEU:HB2	34:2c:52:LEU:HD22	1.96	0.47
34:2c:134:ILE:HG23	34:2c:151:VAL:HB	1.97	0.47
1:1A:795:C:H2'	1:1A:796:C:C6	2.50	0.47
1:1A:862:G:H2'	1:1A:863:A:O4'	2.15	0.47
1:1A:954:G:H5''	12:1Q:13:GLN:HB3	1.97	0.47
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.50	0.47
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.50	0.47
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.50	0.47
11:1P:5:ASP:OD1	62:1P:301:HOH:O	2.20	0.47
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.96	0.47
26:14:14:ILE:HB	26:14:22:ILE:HB	1.97	0.47
32:1a:309:G:H2'	32:1a:310:G:H8	1.80	0.47
32:1a:382:A:H2'	32:1a:383:A:C8	2.50	0.47
32:1a:1040:U:H2'	32:1a:1041:A:C8	2.47	0.47
43:1l:7:ILE:O	43:1l:11:VAL:HG23	2.15	0.47
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.49	0.47
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.15	0.47
1:2A:2119:A:N1	1:2A:2170:A:H2'	2.30	0.47
5:2F:183:VAL:O	5:2F:187:VAL:HG23	2.15	0.47
6:2G:61:ALA:HA	6:2G:66:GLN:O	2.14	0.47
8:2I:93:THR:O	8:2I:97:ILE:N	2.48	0.47
21:2Z:53:ILE:HA	21:2Z:71:VAL:HG23	1.96	0.47
32:2a:34:C:H2'	32:2a:35:G:H8	1.79	0.47
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.96	0.47
34:2c:85:ARG:O	34:2c:89:GLU:N	2.48	0.47
51:2t:43:LEU:HD13	51:2t:51:GLU:HG3	1.96	0.47
57:2y:10:G:H1	57:2y:25:C:H42	1.62	0.47
1:1A:1256:G:H1'	5:1F:82:ILE:HD11	1.96	0.47
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.50	0.47
1:1A:2144:U:H3'	1:1A:2146:C:N4	2.30	0.47
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.15	0.47
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.96	0.47
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.50	0.47
33:1b:15:VAL:HB	33:1b:209:ARG:HG3	1.97	0.47
41:1j:30:SER:HB3	41:1j:81:THR:HG23	1.95	0.47
1:2A:82:G:H5''	1:2A:296:C:H5'	1.97	0.47
1:2A:153:C:H2'	1:2A:154:G:O4'	2.14	0.47
1:2A:250:G:H2'	1:2A:251:A:C8	2.50	0.47
1:2A:402:A:H2'	1:2A:403:U:H5'	1.96	0.47
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.50	0.47
1:2A:2144:U:H2'	1:2A:2146:C:C4	2.50	0.47
1:2A:2317:C:H2'	1:2A:2318:G:H5'	1.96	0.47
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.15	0.47
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.50	0.47
26:24:14:ILE:O	26:24:22:ILE:HD12	2.15	0.47
32:2a:417:C:H2'	32:2a:418:C:H6	1.80	0.47
32:2a:792:A:H4'	32:2a:793:U:H5''	1.97	0.47
32:2a:1342:C:H2'	32:2a:1343:G:C8	2.50	0.47
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.14	0.47
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.96	0.47
54:2w:21:A:O2'	54:2w:22:G:OP1	2.31	0.47
1:1A:1080:C:H5'	1:1A:1081:U:OP2	2.14	0.47
1:1A:1359:A:H2	1:1A:1372:U:O4	1.98	0.47
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.15	0.47
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.48	0.47
4:1E:12:THR:HG21	15:1T:11:GLU:HG2	1.96	0.47
13:1R:2:ARG:HD2	62:1R:307:HOH:O	2.15	0.47
26:14:62:ARG:C	26:14:63:TYR:CG	2.93	0.47
32:1a:404:U:OP1	35:1d:118:ARG:NH1	2.48	0.47
32:1a:553:A:H5''	43:1l:24:VAL:HG21	1.96	0.47
32:1a:636:U:H2'	32:1a:637:G:C8	2.50	0.47
32:1a:1225:A:N6	62:1a:1956:HOH:O	2.48	0.47
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.50	0.47
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.97	0.47
40:1i:19:LEU:HD21	40:1i:81:ILE:HG13	1.97	0.47
1:2A:207:A:H2'	1:2A:208:C:O4'	2.15	0.47
1:2A:736:C:OP1	62:2A:3946:HOH:O	2.20	0.47
1:2A:885:C:H2'	1:2A:886:C:H4'	1.96	0.47
1:2A:2819:G:N7	62:2A:3999:HOH:O	2.35	0.47
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.30	0.47
32:2a:107:G:H2'	32:2a:108:G:O4'	2.15	0.47
32:2a:130:A:H1'	32:2a:263:A:O2'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1073:U:H2'	32:2a:1074:G:C8	2.48	0.47
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.47	0.47
33:2b:54:THR:HA	33:2b:199:TYR:HB3	1.97	0.47
34:2c:156:ARG:N	34:2c:196:LEU:HD22	2.30	0.47
37:2f:10:LEU:HD11	37:2f:61:LEU:HD12	1.96	0.47
1:1A:121:G:H4'	1:1A:149:A:H5'	1.96	0.46
1:1A:191:A:H2'	1:1A:192:C:C6	2.50	0.46
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.97	0.46
1:1A:1365:A:O2'	23:11:11:ARG:NH1	2.48	0.46
1:1A:1753:G:N1	1:1A:1756:G:OP2	2.45	0.46
2:1B:96:U:OP1	21:1Z:14:LYS:NZ	2.48	0.46
6:1G:67:LYS:HD2	26:14:5:ILE:HD12	1.97	0.46
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.97	0.46
11:1P:96:THR:OG1	11:1P:98:GLU:HG3	2.14	0.46
32:1a:219:C:H2'	32:1a:220:G:O4'	2.15	0.46
32:1a:674:G:H2'	32:1a:675:A:C8	2.51	0.46
32:1a:1118:C:OP1	40:1i:9:ARG:NH1	2.46	0.46
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.96	0.46
51:1t:36:LEU:HD13	51:1t:58:LYS:HG3	1.96	0.46
1:2A:615:G:OP1	5:2F:40:GLN:NE2	2.39	0.46
1:2A:656:G:H2'	1:2A:657:U:O4'	2.14	0.46
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.30	0.46
1:2A:1183:G:H5''	25:23:30:ARG:NH2	2.31	0.46
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	1.97	0.46
18:2W:23:LEU:HD21	27:25:25:LEU:HB2	1.96	0.46
21:2Z:158:PRO:O	21:2Z:161:VAL:HG12	2.15	0.46
25:23:4:LEU:O	25:23:36:VAL:HA	2.15	0.46
32:2a:380:G:N2	32:2a:383:A:OP2	2.48	0.46
32:2a:1166:G:H2'	32:2a:1169:A:OP2	2.15	0.46
32:2a:1194:U:H2'	32:2a:1195:C:C6	2.50	0.46
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.50	0.46
38:2g:54:THR:O	38:2g:56:GLN:N	2.47	0.46
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.95	0.46
1:1A:363:G:H2'	1:1A:363(A):A:H8	1.80	0.46
1:1A:2743:C:OP1	31:19:33:LYS:NZ	2.34	0.46
4:1E:121:ASN:ND2	62:1E:403:HOH:O	2.41	0.46
13:1R:96:ARG:NH2	13:1R:117:VAL:HG13	2.30	0.46
15:1T:118:ARG:HG3	32:1a:1442(A):G:O2'	2.15	0.46
32:1a:110:C:H2'	32:1a:111:G:O4'	2.15	0.46
32:1a:1129:C:O2	32:1a:1130:A:N6	2.31	0.46
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:361:G:O6	62:2A:3942:HOH:O	2.20	0.46
1:2A:2319:G:H22	14:2S:3:ARG:NH1	2.13	0.46
2:2B:29:A:H2'	2:2B:30:C:C6	2.50	0.46
7:2H:5:GLY:HA2	7:2H:69:ARG:HB2	1.97	0.46
11:2P:98:GLU:OE1	11:2P:102:ARG:NH1	2.46	0.46
26:24:68:ARG:NE	26:24:68:ARG:HA	2.29	0.46
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.50	0.46
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.81	0.46
1:1A:796:C:H2'	1:1A:797:C:C6	2.50	0.46
1:1A:1512:U:H2'	1:1A:1513:C:H6	1.79	0.46
3:1D:19:ALA:HB3	3:1D:21:PHE:CE1	2.51	0.46
32:1a:721:G:H4'	32:1a:722:A:O4'	2.15	0.46
32:1a:865:A:C2	32:1a:918:A:H4'	2.50	0.46
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.45	0.46
36:1e:34:VAL:HG12	36:1e:62:ALA:HB1	1.97	0.46
39:1h:35:ILE:HD11	39:1h:134:ILE:HG21	1.96	0.46
55:1x:16:C:H4'	55:1x:60:U:H1'	1.97	0.46
1:2A:11:G:C2'	1:2A:12:U:H5'	2.46	0.46
1:2A:38:A:H2'	1:2A:39:C:C6	2.50	0.46
1:2A:361:G:O2'	1:2A:362:U:H5'	2.14	0.46
1:2A:1506:C:H2'	1:2A:1507:A:H5'	1.97	0.46
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.33	0.46
32:2a:603:U:H2'	32:2a:604:G:C8	2.49	0.46
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.50	0.46
35:2d:108:LEU:HD21	35:2d:174:LEU:HB3	1.96	0.46
36:2e:41:VAL:O	36:2e:66:MET:HA	2.15	0.46
39:2h:51:VAL:HB	39:2h:53:VAL:HG23	1.98	0.46
41:2j:30:SER:O	41:2j:81:THR:OG1	2.18	0.46
49:2r:67:ALA:HA	49:2r:70:ILE:HD12	1.96	0.46
1:1A:428:A:H8	1:1A:428:A:OP2	1.98	0.46
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.44	0.46
20:1Y:5:MET:HG2	20:1Y:30:VAL:HG11	1.98	0.46
32:1a:975:A:H5'	32:1a:975:A:C8	2.50	0.46
32:1a:1086:U:H3	32:1a:1099:G:H22	1.64	0.46
32:1a:1278:U:H5'	32:1a:1279:A:O4'	2.16	0.46
33:1b:82:ARG:HD2	33:1b:92:TYR:CZ	2.50	0.46
33:1b:95:GLN:HG3	33:1b:147:LYS:O	2.15	0.46
42:1k:62:GLN:HB2	42:1k:93:GLN:HE21	1.81	0.46
1:2A:493:G:H2'	1:2A:494:G:O4'	2.15	0.46
1:2A:893:C:H2'	1:2A:894:C:N3	2.30	0.46
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2650:U:H2'	1:2A:2651:C:H6	1.80	0.46
2:2B:21:G:H2'	2:2B:22:U:O4'	2.15	0.46
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.97	0.46
7:2H:33:LEU:HD12	7:2H:75:ALA:HA	1.97	0.46
32:2a:96:U:H2'	32:2a:97:G:C8	2.50	0.46
32:2a:986:A:H1'	50:2s:54:GLY:O	2.15	0.46
32:2a:1060:C:HO2'	41:2j:56:HIS:HD1	1.63	0.46
32:2a:1128:C:HO2'	32:2a:1129:C:P	2.35	0.46
32:2a:1508:G:H2'	32:2a:1509:C:O4'	2.15	0.46
35:2d:152:SER:O	35:2d:155:LEU:HB2	2.15	0.46
40:2i:86:VAL:HG11	40:2i:93:ARG:HE	1.79	0.46
48:2q:15:MET:HE1	48:2q:43:LEU:HD22	1.96	0.46
54:2w:27:G:H2'	54:2w:28:G:C8	2.49	0.46
55:2x:23:C:H2'	55:2x:24:U:C6	2.51	0.46
1:1A:84:A:OP2	20:1Y:8:LYS:NZ	2.34	0.46
1:1A:2103:C:N4	1:1A:2186:G:H1	2.14	0.46
1:1A:2118:U:O4	1:1A:2149:G:H1'	2.16	0.46
1:1A:2251:OMG:HM23	1:1A:2251:OMG:H1'	1.58	0.46
10:1O:78:ARG:NH2	15:1T:73:GLU:OE1	2.42	0.46
42:1k:16:SER:O	42:1k:35:PRO:HD3	2.15	0.46
44:1m:49:THR:O	44:1m:53:VAL:HG23	2.16	0.46
1:2A:345:A:N3	1:2A:346:A:N6	2.63	0.46
1:2A:883:G:H8	1:2A:883:G:O5'	1.98	0.46
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.15	0.46
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.47	0.46
1:2A:2135:A:N9	1:2A:2136:C:H5	2.14	0.46
29:27:9:ARG:CZ	29:27:47:ARG:HD3	2.46	0.46
32:2a:865:A:H5'	32:2a:1078:U:C5	2.49	0.46
38:2g:22:LEU:HG	38:2g:62:PHE:HE2	1.79	0.46
1:1A:30:G:H2'	1:1A:31:C:C6	2.51	0.46
1:1A:125:G:N2	29:17:48:LYS:HA	2.31	0.46
1:1A:875:G:H2'	1:1A:876:C:C6	2.51	0.46
1:1A:2111:C:O2	1:1A:2118:U:H5'	2.15	0.46
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.15	0.46
23:11:3:LYS:HB2	23:11:61:ARG:HH12	1.81	0.46
32:1a:254:G:OP1	48:1q:67:LYS:O	2.34	0.46
32:1a:270:A:H2'	32:1a:271:C:O4'	2.16	0.46
32:1a:565:U:H3'	32:1a:566:G:H2'	1.98	0.46
36:1e:78:HIS:HD2	36:1e:79:GLU:O	1.98	0.46
41:1j:38:ILE:O	41:1j:38:ILE:HG13	2.15	0.46
57:1y:53:G:N2	57:1y:61:C:N3	2.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2728:U:H2'	1:2A:2729:G:C8	2.51	0.46
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	1.98	0.46
6:2G:48:GLU:O	6:2G:51:ARG:HG3	2.15	0.46
6:2G:63:ILE:HD13	6:2G:143:GLU:HB2	1.97	0.46
21:2Z:52:SER:C	21:2Z:54:HIS:H	2.23	0.46
21:2Z:130:PRO:HA	21:2Z:133:ILE:HG13	1.97	0.46
32:2a:985:C:H2'	32:2a:986:A:C8	2.50	0.46
32:2a:1206:G:O2'	34:2c:193:TYR:HA	2.14	0.46
32:2a:1310:G:H1	32:2a:1327:C:H42	1.64	0.46
44:2m:3:ARG:HH22	44:2m:11:ARG:HG3	1.80	0.46
44:2m:107:ALA:HB3	44:2m:111:LYS:HE2	1.96	0.46
54:2w:54:5MU:H2'	54:2w:55:PSU:O4'	2.15	0.46
1:1A:7:G:H2'	1:1A:8:A:O4'	2.16	0.46
1:1A:2584:U:O2	1:1A:2585:U:C4	2.69	0.46
8:1I:62:LYS:O	8:1I:66:GLU:HG2	2.15	0.46
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.37	0.46
32:1a:737:A:H5''	37:1f:92:LYS:HG3	1.98	0.46
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.98	0.46
32:1a:1136:U:H5''	32:1a:1137:C:C4	2.51	0.46
35:1d:102:ASP:OD1	35:1d:103:ASN:N	2.49	0.46
1:2A:747:U:O2	1:2A:2014:A:H1'	2.14	0.46
8:2I:139:GLN:OE1	8:2I:139:GLN:N	2.48	0.46
9:2N:91:LEU:HG	9:2N:98:VAL:HG21	1.96	0.46
12:2Q:2:LEU:HB2	12:2Q:70:PRO:HD2	1.98	0.46
16:2U:76:TYR:HH	16:2U:92:ARG:HE	1.60	0.46
20:2Y:5:MET:HG2	20:2Y:30:VAL:HG11	1.98	0.46
21:2Z:67:LEU:HD12	21:2Z:67:LEU:HA	1.72	0.46
32:2a:587:G:N2	32:2a:754:C:OP2	2.42	0.46
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.31	0.46
57:2y:49:C:O2	57:2y:65:G:N2	2.49	0.46
5:1F:37:VAL:HG21	11:1P:6:LEU:HD11	1.98	0.46
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.98	0.46
25:13:44:ARG:O	25:13:48:GLU:HG3	2.16	0.46
32:1a:160:A:H2'	32:1a:161:A:O4'	2.16	0.46
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.47	0.46
33:1b:101:MET:HA	33:1b:108:ILE:HD12	1.97	0.46
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.14	0.46
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	1.98	0.46
1:2A:200:U:O2	1:2A:386:G:N2	2.48	0.46
1:2A:2116:G:O6	1:2A:2162:G:H5''	2.16	0.46
1:2A:2156:G:H2'	1:2A:2157:G:C5	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:83:TYR:CE2	7:2H:138:LYS:HB2	2.51	0.46
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.14	0.46
32:2a:1358:U:H5''	45:2n:33:VAL:O	2.15	0.46
54:2w:23:A:H2'	54:2w:24:G:C8	2.51	0.46
55:2x:15:G:H2'	55:2x:59:A:N1	2.30	0.46
62:1A:4657:HOH:O	5:1F:70:THR:HG23	2.16	0.46
32:1a:109:A:H2'	32:1a:326:G:N2	2.31	0.46
32:1a:731:G:H5'	32:1a:766:A:H4'	1.97	0.46
35:1d:175:SER:HB3	35:1d:184:LYS:HB2	1.97	0.46
47:1p:38:TYR:CE2	47:1p:50:LYS:HB2	2.51	0.46
1:2A:444:C:H4'	5:2F:49:ALA:HB2	1.98	0.46
1:2A:921:G:H2'	1:2A:922:U:C6	2.50	0.46
1:2A:1204:A:H2	1:2A:1241:A:N6	2.14	0.46
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.16	0.46
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.97	0.46
8:2I:82:ARG:HB2	8:2I:82:ARG:HE	1.60	0.46
12:2Q:57:HIS:CE1	12:2Q:116:GLU:HG2	2.51	0.46
15:2T:36:GLU:OE2	15:2T:41:ARG:NH2	2.45	0.46
28:26:14:THR:HG21	28:26:50:ARG:HH21	1.81	0.46
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.43	0.46
1:1A:299:A:N1	1:1A:322:A:O2'	2.49	0.46
1:1A:717:G:H2'	1:1A:718:A:O4'	2.16	0.46
1:1A:1075:C:H2'	1:1A:1076:C:H5'	1.98	0.46
1:1A:1680:U:O2'	1:1A:1763:G:N7	2.34	0.46
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.31	0.46
3:1D:25:THR:HG21	3:1D:113:VAL:HG21	1.98	0.46
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	1.98	0.46
3:1D:61:LEU:O	3:1D:63:ARG:NH1	2.49	0.46
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.81	0.46
21:1Z:103:ARG:O	21:1Z:138:GLU:HA	2.16	0.46
32:1a:370:C:H2'	32:1a:371:G:C8	2.51	0.46
36:1e:152:ARG:HB3	39:1h:43:GLY:HA3	1.98	0.46
1:2A:192:C:O2'	1:2A:802:A:N3	2.45	0.46
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.16	0.46
1:2A:2330:G:H2'	1:2A:2331:G:O4'	2.16	0.46
5:2F:120:GLU:OE2	5:2F:122:LYS:HG3	2.16	0.46
6:2G:59:GLU:O	6:2G:63:ILE:HG12	2.15	0.46
8:2I:105:HIS:HB2	8:2I:107:VAL:CG2	2.46	0.46
12:2Q:38:GLU:HB2	12:2Q:127:ILE:HB	1.97	0.46
18:2W:1:MET:HE3	18:2W:62:HIS:HB3	1.97	0.46
32:2a:20:U:H2'	32:2a:21:G:O4'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:167:G:H2'	32:2a:168:G:H8	1.80	0.46
32:2a:428:G:OP2	35:2d:10:ARG:NH1	2.48	0.46
32:2a:429:U:O2'	35:2d:22:LYS:NZ	2.38	0.46
32:2a:537:G:H5''	43:2l:113:ARG:NH1	2.31	0.46
32:2a:814:A:H2'	32:2a:816:A:H5''	1.98	0.46
33:2b:63:MET:HG2	33:2b:225:ALA:HB1	1.97	0.46
33:2b:71:VAL:HG12	33:2b:170:GLU:HG2	1.98	0.46
1:1A:11:G:C2'	1:1A:12:U:H5'	2.44	0.45
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.98	0.45
32:1a:1169:A:H2'	32:1a:1170:A:C8	2.51	0.45
32:1a:1499:A:OP2	62:1a:1902:HOH:O	2.21	0.45
40:1i:16:ARG:HH11	40:1i:64:THR:HG21	1.79	0.45
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.97	0.45
41:1j:78:ASN:O	41:1j:80:LYS:N	2.50	0.45
1:2A:143:G:O3'	19:2X:35:THR:HG21	2.16	0.45
1:2A:363(A):A:H2'	1:2A:363(B):G:C8	2.51	0.45
1:2A:1756:G:H4'	1:2A:1758:G:O4'	2.16	0.45
1:2A:2879:C:OP2	62:2A:3945:HOH:O	2.20	0.45
6:2G:116:ASP:CG	44:2m:68:GLY:HA3	2.41	0.45
32:2a:859:A:H2'	32:2a:860:A:O4'	2.16	0.45
32:2a:1366:C:H2'	32:2a:1367:C:H6	1.79	0.45
34:2c:152:ILE:HG22	34:2c:167:TRP:HB3	1.96	0.45
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.49	0.45
38:2g:65:ALA:O	38:2g:69:VAL:HG23	2.16	0.45
44:2m:4:ILE:HG23	44:2m:22:ILE:HD11	1.97	0.45
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.97	0.45
1:1A:818:G:H5'	1:1A:839:U:OP1	2.16	0.45
1:1A:1683:C:H2'	1:1A:1684:C:C6	2.51	0.45
1:1A:2206:G:H8	1:1A:2207:G:N7	2.15	0.45
32:1a:620:C:H2'	32:1a:621:A:O4'	2.16	0.45
32:1a:1266:G:N2	32:1a:1269:A:OP2	2.47	0.45
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.44	0.45
35:1d:112:VAL:HG12	35:1d:116:GLN:NE2	2.31	0.45
38:1g:89:MET:SD	38:1g:155:ARG:HB2	2.56	0.45
40:1i:34:ASN:HD22	40:1i:34:ASN:N	2.14	0.45
1:2A:1607:C:H5''	1:2A:1608:A:H5'	1.99	0.45
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.51	0.45
1:2A:2166:G:H3'	1:2A:2167:U:C5'	2.46	0.45
6:2G:49:ASP:OD1	6:2G:49:ASP:N	2.50	0.45
12:2Q:78:PRO:HD3	55:2x:1:C:C2	2.52	0.45
19:2X:94:GLY:HA3	19:2X:95:LEU:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:14:THR:OG1	28:26:48:VAL:HG13	2.16	0.45
32:2a:109:A:C6	32:2a:326:G:C6	3.04	0.45
32:2a:176:C:H2'	32:2a:177:C:C6	2.51	0.45
32:2a:328:C:H4'	32:2a:329:A:H5'	1.98	0.45
32:2a:815:A:N7	32:2a:1509:C:O2'	2.47	0.45
32:2a:986:A:H2'	32:2a:987:G:C8	2.52	0.45
32:2a:1095:U:OP2	62:2a:1907:HOH:O	2.21	0.45
32:2a:1228:C:H2'	32:2a:1229:A:H8	1.81	0.45
33:2b:111:ARG:HD3	33:2b:111:ARG:HA	1.64	0.45
41:2j:13:HIS:HB3	41:2j:68:HIS:CE1	2.51	0.45
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.97	0.45
1:1A:1062:G:N2	1:1A:1077:A:H61	2.14	0.45
1:1A:1100:C:H5'	1:1A:1101:U:OP2	2.16	0.45
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.50	0.45
1:1A:1825:A:OP1	3:1D:249:PRO:HD3	2.17	0.45
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.31	0.45
1:1A:2451:A:C6	54:1w:76:F3N:HE1	2.51	0.45
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.52	0.45
32:1a:504:C:OP1	62:1a:1914:HOH:O	2.20	0.45
32:1a:690:G:C6	32:1a:691:G:C6	3.04	0.45
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.51	0.45
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.81	0.45
51:1t:37:SER:O	51:1t:41:ILE:HG13	2.16	0.45
57:1y:19:G:C6	57:1y:56:C:N4	2.85	0.45
1:2A:271(R):G:OP1	23:21:76:ARG:NE	2.50	0.45
1:2A:735:A:N7	1:2A:761:A:H2	2.14	0.45
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.35	0.45
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.99	0.45
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.34	0.45
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.47	0.45
16:2U:85:LYS:HB3	16:2U:85:LYS:HE2	1.67	0.45
32:2a:523:A:N1	43:2l:92:OTD:H6	2.31	0.45
32:2a:1040:U:H2'	32:2a:1041:A:H8	1.79	0.45
32:2a:1265:G:C4	32:2a:1271:G:N2	2.85	0.45
32:2a:1342:C:H2'	32:2a:1343:G:H8	1.81	0.45
37:2f:97:PHE:HB2	49:2r:32:ARG:NH1	2.32	0.45
38:2g:70:LYS:O	38:2g:138:LYS:HD2	2.17	0.45
46:2o:5:LYS:H	46:2o:5:LYS:HG3	1.50	0.45
54:2w:12:U:H2'	54:2w:13:C:O4'	2.17	0.45
55:2x:58:A:H4'	55:2x:59:A:OP1	2.17	0.45
1:1A:184:C:H2'	1:1A:185:U:H6	1.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:581:C:H2'	1:1A:582:G:C8	2.51	0.45
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.50	0.45
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.39	0.45
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.81	0.45
2:1B:2:C:H2'	2:1B:3:C:C6	2.52	0.45
6:1G:4:ASP:OD1	6:1G:9:ARG:NH1	2.50	0.45
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.32	0.45
32:1a:1191:A:OP1	34:1c:4:LYS:NZ	2.45	0.45
32:1a:1304:G:C6	32:1a:1305:G:N1	2.85	0.45
54:1w:5:G:H2'	54:1w:6:G:C8	2.51	0.45
1:2A:581:C:H2'	1:2A:582:G:C8	2.51	0.45
1:2A:613:G:O2'	1:2A:614(C):A:N1	2.49	0.45
1:2A:676:A:H2	1:2A:2069:G:N3	2.14	0.45
1:2A:1550:C:OP1	1:2A:1720:U:O2'	2.31	0.45
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.52	0.45
1:2A:2177:C:H2'	1:2A:2178:C:O4'	2.16	0.45
2:2B:77:U:H4'	21:2Z:84:GLU:OE1	2.15	0.45
5:2F:28:ILE:HD11	5:2F:115:ALA:HB3	1.98	0.45
10:2O:49:ARG:HH12	32:2a:1423:G:P	2.38	0.45
15:2T:102:ILE:HB	15:2T:110:ILE:HG12	1.99	0.45
24:22:1:MET:HB3	24:22:5:GLU:OE1	2.16	0.45
28:26:35:GLU:C	28:26:36:LEU:HG	2.41	0.45
32:2a:90:U:H2'	32:2a:91:C:H6	1.81	0.45
32:2a:910:C:OP1	43:2l:97:ARG:NH2	2.43	0.45
36:2e:63:ARG:HA	36:2e:66:MET:HE1	1.98	0.45
57:2y:18:G:C2	57:2y:55:PSU:C4	3.05	0.45
1:1A:1354:A:H4'	3:1D:38:LYS:HE3	1.98	0.45
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.21	0.45
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.51	0.45
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.52	0.45
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.30	0.45
1:1A:2562:U:H4'	10:1O:25:LEU:HD21	1.98	0.45
1:1A:2722:G:H5'	13:1R:4:LEU:HD12	1.98	0.45
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.52	0.45
26:14:57:GLU:HA	26:14:58:ARG:HA	1.55	0.45
32:1a:767:A:H2'	32:1a:768:A:O4'	2.17	0.45
39:1h:96:GLY:N	39:1h:99:GLU:OE1	2.50	0.45
42:1k:99:GLN:HG3	42:1k:105:VAL:HG21	1.99	0.45
1:2A:56:A:H2'	1:2A:57:C:O4'	2.17	0.45
1:2A:2506:U:C2	1:2A:2585:U:O4	2.70	0.45
4:2E:55:ASN:HB3	4:2E:58:ARG:HG3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.41	0.45
32:2a:194:C:H2'	32:2a:195:A:H5''	1.97	0.45
32:2a:423:G:H3'	32:2a:423:G:N3	2.32	0.45
32:2a:499:A:H4'	32:2a:500:G:H5'	1.98	0.45
32:2a:881:G:P	43:2l:12:ARG:HH22	2.39	0.45
32:2a:1097:C:O2'	32:2a:1169:A:N3	2.41	0.45
36:2e:102:ALA:HB2	36:2e:120:THR:HG21	1.99	0.45
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.52	0.45
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.17	0.45
49:2r:56:THR:H	49:2r:56:THR:HG1	1.49	0.45
1:1A:907:U:HO2'	12:1Q:101:ARG:HH22	1.63	0.45
1:1A:1064:C:H2'	1:1A:1065:U:H5'	1.98	0.45
4:1E:7:VAL:HG23	4:1E:51:PHE:HE2	1.81	0.45
18:1W:71:VAL:HA	18:1W:107:LEU:HD23	1.98	0.45
32:1a:163:C:H2'	32:1a:164:U:C6	2.51	0.45
32:1a:532:A:N6	32:1a:1206:G:O2'	2.50	0.45
32:1a:741:G:H2'	32:1a:742:G:O4'	2.16	0.45
32:1a:946:A:O2'	32:1a:1333:A:N3	2.46	0.45
32:1a:1429:C:H2'	32:1a:1430:C:H6	1.80	0.45
39:1h:86:ILE:HD12	39:1h:133:LEU:HD22	1.99	0.45
1:2A:563:G:OP2	62:2A:3944:HOH:O	2.20	0.45
1:2A:593:G:H4'	30:28:63:PRO:HB3	1.99	0.45
1:2A:918:A:C2	2:2B:80:U:H4'	2.52	0.45
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.16	0.45
7:2H:19:VAL:HA	7:2H:24:VAL:HG12	1.97	0.45
8:2I:97:ILE:O	8:2I:101:LEU:HG	2.16	0.45
32:2a:1032:G:H2'	32:2a:1033:G:C8	2.52	0.45
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.16	0.45
32:2a:1240:U:O2'	38:2g:32:ARG:HD2	2.16	0.45
34:2c:131:ARG:NH1	34:2c:167:TRP:O	2.49	0.45
35:2d:122:ARG:HA	35:2d:122:ARG:HD2	1.79	0.45
36:2e:142:LEU:HD23	36:2e:142:LEU:HA	1.80	0.45
38:2g:31:MET:HG3	38:2g:36:LYS:HA	1.99	0.45
42:2k:31:THR:HG23	42:2k:42:TRP:HB3	1.97	0.45
1:1A:150:C:C2'	1:1A:151:C:H5'	2.47	0.45
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.52	0.45
7:1H:116:GLU:HG3	7:1H:117:PRO:HD2	1.97	0.45
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.25	0.45
33:1b:100:GLY:O	33:1b:104:ASN:N	2.34	0.45
33:1b:195:ASP:O	39:1h:74:PRO:HG3	2.17	0.45
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:33:TYR:OH	37:1f:78:GLU:HG3	2.16	0.45
37:1f:38:GLU:HB2	37:1f:64:GLN:HG3	1.98	0.45
1:2A:687:C:H2'	1:2A:688:U:O4'	2.17	0.45
11:2P:94:GLU:HG2	11:2P:95:VAL:N	2.32	0.45
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.90	0.45
32:2a:875:C:O2'	39:2h:14:ARG:HD2	2.17	0.45
32:2a:974:A:H8	32:2a:974:A:OP1	2.00	0.45
32:2a:1076:C:C2'	32:2a:1077:G:H5''	2.45	0.45
32:2a:1265:G:C2	32:2a:1271:G:C2	3.05	0.45
40:2i:9:ARG:HA	40:2i:13:ALA:O	2.17	0.45
1:1A:1070:A:N6	1:1A:1097:U:H4'	2.32	0.45
1:1A:1495:A:C6	1:1A:1496:A:C6	3.04	0.45
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.52	0.45
1:1A:2298:A:H2'	1:1A:2299:G:O4'	2.17	0.45
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.51	0.45
32:1a:815:A:N7	32:1a:1509:C:O2'	2.42	0.45
32:1a:1302:U:C5	44:1m:17:VAL:HG21	2.52	0.45
33:1b:80:ILE:O	33:1b:84:GLU:HG2	2.17	0.45
50:1s:18:LYS:HD3	50:1s:31:ILE:HG23	1.99	0.45
55:1x:37:A:H2'	55:1x:38:A:O4'	2.16	0.45
57:1y:75:C:H5''	57:1y:76:A:H5'	1.98	0.45
1:2A:871:U:OP1	12:2Q:5:ARG:HG3	2.16	0.45
1:2A:2786:U:H2'	1:2A:2787:C:C6	2.52	0.45
3:2D:16:MET:HG3	3:2D:207:GLY:HA3	1.97	0.45
6:2G:96:ARG:H	6:2G:99:MET:HE2	1.81	0.45
8:2I:117:GLU:H	8:2I:117:GLU:HG3	1.56	0.45
10:2O:77:ILE:HB	15:2T:74:ARG:HD2	1.99	0.45
21:2Z:152:ALA:O	21:2Z:155:LEU:HG	2.17	0.45
26:24:36:CYS:O	26:24:40:HIS:HB2	2.17	0.45
32:2a:320:C:H2'	32:2a:321:A:O4'	2.17	0.45
32:2a:1297:C:OP2	44:2m:44:ARG:NH2	2.48	0.45
33:2b:74:LYS:HB3	33:2b:74:LYS:HE2	1.76	0.45
36:2e:69:VAL:HG23	36:2e:142:LEU:HD12	1.98	0.45
38:2g:70:LYS:HG2	38:2g:96:GLN:HB3	1.99	0.45
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.42	0.45
1:1A:196:A:O2'	1:1A:805:G:O6	2.26	0.45
1:1A:639:U:H2'	1:1A:640:C:C6	2.52	0.45
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.51	0.45
1:1A:2165:G:H2'	1:1A:2166:G:C5	2.51	0.45
1:1A:2461:C:H2'	1:1A:2462:U:C6	2.52	0.45
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.52	0.45
21:1Z:44:PHE:CZ	21:1Z:86:VAL:HG11	2.52	0.45
32:1a:222:U:H2'	32:1a:223:U:C6	2.51	0.45
32:1a:265:G:H2'	32:1a:267:C:H5	1.82	0.45
32:1a:1120:G:H2'	32:1a:1121:U:H6	1.82	0.45
33:1b:59:GLU:HG2	33:1b:225:ALA:HB2	1.99	0.45
40:1i:127:LYS:NZ	55:1x:34:C:OP2	2.46	0.45
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.15	0.45
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.52	0.45
1:2A:1599:C:OP1	19:2X:36:LYS:HG3	2.17	0.45
7:2H:35:VAL:HG21	7:2H:72:ILE:HD13	1.98	0.45
11:2P:94:GLU:HG3	11:2P:124:LYS:HE2	1.98	0.45
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.98	0.45
32:2a:974:A:P	45:2n:29:ARG:HH21	2.40	0.45
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.50	0.45
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	1.98	0.45
1:1A:534:U:H2'	1:1A:535:C:C6	2.51	0.45
1:1A:743:G:OP1	4:1E:130:GLY:HA2	2.17	0.45
1:1A:1908:C:O2	55:1x:12:G:H4'	2.16	0.45
8:1I:10:GLU:C	8:1I:12:LEU:H	2.25	0.45
39:1h:20:TYR:HA	39:1h:65:TYR:CZ	2.52	0.45
40:1i:55:ALA:HA	40:1i:58:HIS:HD2	1.81	0.45
42:1k:62:GLN:O	42:1k:66:LEU:HG	2.17	0.45
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.99	0.45
1:2A:715:G:O4'	46:2o:60:VAL:HG11	2.16	0.45
1:2A:795:C:H2'	1:2A:796:C:C6	2.52	0.45
1:2A:1032:A:H2	1:2A:1122:G:H22	1.65	0.45
1:2A:1461:G:H2'	1:2A:1462:C:H6	1.82	0.45
1:2A:1502:C:H2'	1:2A:1503:U:C6	2.50	0.45
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.32	0.45
1:2A:2655:G:O2'	1:2A:2664:G:O6	2.31	0.45
14:2S:87:PHE:CZ	14:2S:102:ALA:HB2	2.52	0.45
32:2a:444:C:N4	32:2a:491:G:O6	2.49	0.45
39:2h:120:THR:O	39:2h:124:ALA:N	2.49	0.45
45:2n:12:ARG:HG2	45:2n:13:THR:N	2.31	0.45
50:2s:27:GLU:H	50:2s:27:GLU:HG3	1.60	0.45
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.14	0.44
1:1A:211:A:H2'	1:1A:212:G:O4'	2.17	0.44
1:1A:744:G:OP1	62:1A:4255:HOH:O	2.21	0.44
1:1A:911:A:N6	12:1Q:11:LYS:O	2.47	0.44
1:1A:1037:G:H1	1:1A:1118:C:H42	1.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1654:A:OP2	62:1A:4247:HOH:O	2.20	0.44
1:1A:2629:A:H1'	1:1A:2630:G:C5'	2.47	0.44
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.51	0.44
1:1A:2775:A:OP2	62:1A:4252:HOH:O	2.21	0.44
10:1O:112:MET:H	10:1O:112:MET:HG2	1.46	0.44
12:1Q:130:LYS:HE2	12:1Q:130:LYS:HB3	1.69	0.44
21:1Z:138:GLU:H	21:1Z:156:LYS:HE3	1.82	0.44
32:1a:78:G:C2	32:1a:91:C:N3	2.85	0.44
36:1e:85:GLY:C	36:1e:87:SER:H	2.24	0.44
43:1l:79:GLU:HG2	43:1l:80:HIS:CD2	2.52	0.44
57:1y:35:A:H2'	57:1y:36:A:C8	2.52	0.44
1:2A:980:A:N3	1:2A:2037:G:O2'	2.44	0.44
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.52	0.44
2:2B:56:G:H5'	6:2G:27:ASN:ND2	2.32	0.44
21:2Z:54:HIS:CD2	21:2Z:101:PRO:HG3	2.52	0.44
25:23:50:VAL:O	25:23:54:VAL:HB	2.17	0.44
26:24:61:ARG:HA	26:24:61:ARG:HH11	1.81	0.44
32:2a:540:G:H2'	32:2a:541:G:O4'	2.18	0.44
32:2a:547:A:H5'	62:2a:1918:HOH:O	2.17	0.44
32:2a:578:C:O2'	32:2a:728:A:N3	2.49	0.44
32:2a:1004:A:H61	32:2a:1037:C:H1'	1.82	0.44
34:2c:39:ILE:HD11	34:2c:59:ARG:NH2	2.32	0.44
35:2d:140:VAL:HG13	35:2d:144:ASP:HB2	2.00	0.44
36:2e:77:PRO:HD2	36:2e:142:LEU:HD13	1.99	0.44
49:2r:66:LEU:HG	49:2r:70:ILE:HD11	1.99	0.44
57:2y:35:A:C6	57:2y:36:A:C2	3.05	0.44
1:1A:7:G:H2'	1:1A:8:A:C8	2.52	0.44
1:1A:746:A:H2'	1:1A:2612:C:H5''	1.98	0.44
1:1A:1177:A:H8	1:1A:1177:A:O5'	2.01	0.44
3:1D:60:ARG:HD3	3:1D:87:ASN:ND2	2.32	0.44
4:1E:108:SER:HG	4:1E:163:GLU:H	1.65	0.44
6:1G:83:ARG:O	6:1G:86:MET:HG3	2.17	0.44
9:1N:4:TYR:CG	16:1U:100:VAL:HG11	2.53	0.44
16:1U:69:CYS:HB3	16:1U:74:LEU:HD13	1.98	0.44
32:1a:790:A:N1	32:1a:1497:G:H5''	2.32	0.44
32:1a:1360:A:H8	32:1a:1360:A:OP1	2.01	0.44
32:1a:1378:C:O2	38:1g:76:ARG:NH1	2.43	0.44
32:1a:1380:U:C4	38:1g:3:ARG:HG2	2.51	0.44
39:1h:121:ASP:OD1	39:1h:121:ASP:N	2.50	0.44
45:1n:58:LYS:HE3	45:1n:58:LYS:HB3	1.69	0.44
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.49	0.44
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.99	0.44
20:2Y:38:ILE:HD13	20:2Y:66:PRO:HA	1.98	0.44
32:2a:545:C:H5'	35:2d:72:GLU:HB2	1.98	0.44
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.31	0.44
32:2a:1391:U:H2'	32:2a:1392:G:H8	1.83	0.44
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.85	0.44
34:2c:172:ARG:NH2	34:2c:174:PRO:HG3	2.32	0.44
41:2j:5:ARG:N	41:2j:99:LYS:O	2.50	0.44
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.49	0.44
50:2s:12:ASP:O	50:2s:14:HIS:N	2.41	0.44
54:2w:18:G:H21	54:2w:58:A:H5'	1.82	0.44
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.36	0.44
1:1A:1069:A:O4'	1:1A:1096:A:O2'	2.34	0.44
1:1A:1445(A):C:H2'	1:1A:1446:C:H6	1.83	0.44
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.53	0.44
1:1A:2659:G:O6	62:1A:4242:HOH:O	2.19	0.44
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.35	0.44
12:1Q:89:ASN:HB2	55:1x:1:C:C4	2.52	0.44
21:1Z:138:GLU:H	21:1Z:156:LYS:CE	2.30	0.44
32:1a:461:A:O2'	32:1a:470:C:H5'	2.16	0.44
32:1a:839:U:H3'	32:1a:840:C:H5'	1.98	0.44
33:1b:55:PHE:CD1	33:1b:221:LEU:HD22	2.52	0.44
34:1c:39:ILE:HG21	34:1c:66:VAL:HG11	2.00	0.44
1:2A:286:C:H2'	1:2A:287:C:H6	1.82	0.44
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.52	0.44
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.28	0.44
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.99	0.44
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.52	0.44
3:2D:146:GLU:HG2	3:2D:152:GLY:C	2.42	0.44
21:2Z:63:ASP:OD1	21:2Z:65:GLN:HG3	2.18	0.44
30:28:62:LEU:HB3	30:28:65:GLU:HG2	2.00	0.44
32:2a:1097:C:H2'	32:2a:1098:C:H6	1.82	0.44
32:2a:1291:G:C6	32:2a:1292:U:C4	3.05	0.44
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.52	0.44
33:2b:102:LEU:HB3	33:2b:180:LEU:HD12	1.99	0.44
35:2d:76:ARG:O	35:2d:80:GLU:HG2	2.17	0.44
35:2d:107:ARG:HH12	35:2d:194:LEU:HD23	1.83	0.44
35:2d:173:TRP:CE2	35:2d:189:PRO:HB3	2.53	0.44
57:2y:18:G:O6	57:2y:56:C:N4	2.51	0.44
1:1A:219:G:O6	62:1A:4239:HOH:O	2.19	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:271(D):G:H2'	1:1A:271(E):U:C6	2.52	0.44
1:1A:272(I):U:H2'	1:1A:272(J):C:O4'	2.17	0.44
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.53	0.44
1:1A:1782:C:H1'	1:1A:2609:U:H5''	1.99	0.44
11:1P:138:LEU:C	11:1P:140:ALA:H	2.25	0.44
17:1V:29:PRO:HA	17:1V:61:VAL:HG22	1.99	0.44
32:1a:1314:C:N4	50:1s:2:PRO:O	2.45	0.44
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.18	0.44
1:2A:236:C:H2'	1:2A:237:C:H6	1.82	0.44
1:2A:390:A:H4'	1:2A:391:G:H5'	1.99	0.44
1:2A:524:U:H2'	1:2A:525:U:C6	2.52	0.44
1:2A:1431:U:H2'	1:2A:1432:C:C6	2.52	0.44
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.52	0.44
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.50	0.44
9:2N:138:LEU:HB3	9:2N:140:VAL:HG13	2.00	0.44
16:2U:8:VAL:HG23	16:2U:11:ARG:NH2	2.31	0.44
17:2V:24:LYS:HE2	17:2V:24:LYS:HB3	1.76	0.44
32:2a:23:C:OP2	32:2a:561:U:N3	2.36	0.44
32:2a:397:A:H3'	32:2a:397:A:N3	2.33	0.44
32:2a:544:G:P	35:2d:59:ARG:HH22	2.38	0.44
32:2a:1006:C:H2'	32:2a:1007:C:O4'	2.17	0.44
35:2d:19:LEU:O	35:2d:21:LEU:HG	2.17	0.44
40:2i:82:ALA:HA	40:2i:85:LEU:HD12	1.98	0.44
43:2l:53:ARG:HB3	43:2l:69:TYR:HE1	1.83	0.44
43:2l:79:GLU:HG2	43:2l:80:HIS:CD2	2.52	0.44
1:1A:620:G:H2'	1:1A:620:G:N3	2.31	0.44
1:1A:710:G:H2'	1:1A:711:G:H8	1.82	0.44
1:1A:1077:A:H2'	1:1A:1078:U:H4'	1.99	0.44
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.17	0.44
3:1D:206:LEU:HA	3:1D:211:ARG:NH1	2.32	0.44
5:1F:33:LEU:HB3	11:1P:6:LEU:HD21	2.00	0.44
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.53	0.44
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.86	0.44
32:1a:256:U:H2'	32:1a:257:G:H8	1.83	0.44
32:1a:560:U:H5'	32:1a:566:G:N2	2.33	0.44
35:1d:10:ARG:HB2	35:1d:40:PRO:HG3	1.99	0.44
57:1y:63:G:H2'	57:1y:64:A:O4'	2.17	0.44
1:2A:272(J):C:H3'	1:2A:274:G:H8	1.82	0.44
1:2A:749:C:O2	1:2A:1618:A:H2'	2.17	0.44
1:2A:893:C:H2'	1:2A:894:C:C4	2.53	0.44
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1810:A:H8	1:2A:1810:A:O5'	2.01	0.44
14:2S:26:LEU:HD12	14:2S:39:ILE:HG12	1.98	0.44
32:2a:1108:G:H5'	34:2c:176:HIS:CD2	2.53	0.44
32:2a:1280:A:H5'	41:2j:40:LEU:HD22	1.98	0.44
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.32	0.44
1:1A:7:G:H2'	1:1A:8:A:H8	1.82	0.44
1:1A:2133:G:C2	1:1A:2157:G:N3	2.86	0.44
1:1A:2482:G:O3'	54:1w:64:A:H4'	2.18	0.44
1:1A:2849:U:P	15:1T:95:ARG:HH12	2.41	0.44
4:1E:52:LEU:O	4:1E:76:ARG:N	2.43	0.44
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.51	0.44
5:1F:135:LYS:HB2	5:1F:138:GLU:HG3	2.00	0.44
5:1F:140:LEU:HD12	5:1F:140:LEU:HA	1.91	0.44
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.98	0.44
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.52	0.44
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.51	0.44
32:1a:60:A:N1	32:1a:107:G:O2'	2.46	0.44
32:1a:197:A:C6	32:1a:221:C:H4'	2.52	0.44
32:1a:1151:A:O2'	32:1a:1152:A:H8	2.00	0.44
32:1a:1338:G:C6	32:1a:1339:A:C6	3.06	0.44
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.18	0.44
33:1b:12:GLU:C	33:1b:14:GLY:H	2.25	0.44
35:1d:76:ARG:NE	35:1d:80:GLU:OE2	2.47	0.44
57:1y:71:G:O2'	57:1y:72:C:H5'	2.17	0.44
1:2A:298:G:H5''	1:2A:299:A:OP1	2.18	0.44
1:2A:1028:A:N6	1:2A:1126:A:OP1	2.50	0.44
1:2A:1260:G:C6	1:2A:1261:C:C4	3.06	0.44
1:2A:1423:G:H2'	1:2A:1424:G:H8	1.83	0.44
1:2A:2156:G:H2'	1:2A:2157:G:C6	2.53	0.44
7:2H:95:ARG:NH2	7:2H:97:ARG:HD3	2.33	0.44
32:2a:719:C:H42	49:2r:71:LYS:HE2	1.82	0.44
32:2a:1074:G:O2'	33:2b:103:THR:OG1	2.34	0.44
35:2d:17:VAL:HG12	35:2d:19:LEU:HD12	1.99	0.44
48:2q:14:LYS:HE3	48:2q:14:LYS:HB3	1.85	0.44
1:1A:909:A:H2'	1:1A:912:C:C5	2.53	0.44
1:1A:1542:A:H8	1:1A:1542:A:OP1	2.01	0.44
1:1A:2017:U:O2	27:15:10:LYS:HB2	2.18	0.44
1:1A:2138:C:C2	1:1A:2154:G:C2	3.05	0.44
1:1A:2506:U:C2	1:1A:2585:U:O4	2.71	0.44
5:1F:74:ARG:HG2	62:1F:412:HOH:O	2.17	0.44
8:1I:38:LEU:H	8:1I:38:LEU:CD2	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:72:LEU:HD12	8:1I:138:ILE:HD13	2.00	0.44
11:1P:84:ASN:HB3	11:1P:117:GLU:O	2.18	0.44
22:10:72:ARG:HB3	22:10:75:LEU:HB2	2.00	0.44
32:1a:111:G:H5''	47:1p:27:LYS:HB3	2.00	0.44
32:1a:473:G:H2'	32:1a:474:G:O4'	2.18	0.44
33:1b:204:ASN:OD1	33:1b:206:ASP:N	2.29	0.44
57:1y:36:A:H2'	57:1y:37:MIA:O4'	2.18	0.44
57:1y:67:C:H2'	57:1y:68:C:C6	2.53	0.44
1:2A:479:A:H4'	1:2A:480:A:OP1	2.17	0.44
1:2A:2316:C:H2'	1:2A:2317:C:C6	2.53	0.44
13:2R:83:ILE:HA	13:2R:86:ARG:HD3	1.99	0.44
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.17	0.44
32:2a:56:U:H2'	32:2a:57:G:H8	1.81	0.44
32:2a:1029:C:C2	32:2a:1032:G:N2	2.74	0.44
32:2a:1067:A:H8	32:2a:1067:A:O5'	2.00	0.44
32:2a:1304:G:C6	32:2a:1305:G:N1	2.86	0.44
33:2b:219:VAL:HA	33:2b:222:ILE:HG12	1.99	0.44
1:1A:603:A:H4'	1:1A:604:G:H5'	1.99	0.44
1:1A:969:U:H2'	1:1A:970:C:C6	2.53	0.44
1:1A:1441:G:H2'	1:1A:1442:G:H8	1.82	0.44
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.18	0.44
1:1A:2756:U:H1'	1:1A:2757:A:H5''	1.99	0.44
11:1P:90:ARG:NH1	11:1P:105:LEU:HD11	2.33	0.44
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.35	0.44
21:1Z:61:LEU:HD22	21:1Z:61:LEU:H	1.82	0.44
26:14:46:GLN:H	26:14:46:GLN:HG2	1.50	0.44
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.33	0.44
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.17	0.44
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.53	0.44
1:2A:579:G:H2'	1:2A:580:C:C6	2.53	0.44
7:2H:38:SER:C	7:2H:40:GLU:H	2.26	0.44
32:2a:8:A:N7	35:2d:208:SER:OG	2.47	0.44
32:2a:620:C:C2	35:2d:135:LEU:HG	2.52	0.44
32:2a:685:G:C2	32:2a:686:U:C4	3.06	0.44
32:2a:936:C:H2'	32:2a:937:A:O4'	2.18	0.44
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.83	0.44
35:2d:10:ARG:HG3	35:2d:11:LEU:HD12	1.99	0.44
41:2j:25:GLU:O	41:2j:29:ARG:HG2	2.17	0.44
1:1A:244:A:C2	1:1A:255:A:C4	3.06	0.44
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.52	0.44
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1818:U:H2'	3:1D:157:ARG:HG3	2.00	0.44
1:1A:2142:C:N3	1:1A:2149:G:C6	2.85	0.44
1:1A:2484:G:H1'	12:1Q:124:LYS:HD2	1.99	0.44
1:1A:2850:A:N7	1:1A:2868:A:O2'	2.45	0.44
2:1B:37:C:H2'	2:1B:38:C:O4'	2.18	0.44
4:1E:34:VAL:HB	4:1E:48:GLN:HE21	1.83	0.44
7:1H:24:VAL:HG11	7:1H:43:VAL:HG11	2.00	0.44
9:1N:138:LEU:HD23	9:1N:138:LEU:HA	1.85	0.44
19:1X:54:VAL:HG22	19:1X:81:VAL:HG12	2.00	0.44
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.18	0.44
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.18	0.44
2:2B:52:A:N6	14:2S:33:LYS:HG2	2.33	0.44
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	2.00	0.44
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.33	0.44
25:23:59:VAL:HG12	25:23:60:GLU:H	1.83	0.44
32:2a:979:C:N4	45:2n:18:VAL:HG22	2.33	0.44
32:2a:1212:U:H5'	32:2a:1213:A:C8	2.52	0.44
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.53	0.44
34:2c:60:ALA:HB3	34:2c:63:ASN:HD21	1.82	0.44
34:2c:111:LEU:HD23	34:2c:111:LEU:HA	1.86	0.44
40:2i:71:SER:HA	40:2i:74:ILE:HD12	2.00	0.44
1:1A:41:C:H2'	1:1A:42:G:O4'	2.17	0.43
1:1A:118:A:C8	1:1A:119:A:C8	3.06	0.43
1:1A:271(V):G:O6	62:1A:4256:HOH:O	2.21	0.43
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.18	0.43
1:1A:2011:U:OP1	18:1W:42:ARG:HD3	2.17	0.43
1:1A:2609:U:C6	56:1z:1:FME:HCN	2.53	0.43
6:1G:126:ASP:HB2	6:1G:130:ASN:O	2.18	0.43
21:1Z:158:PRO:O	21:1Z:161:VAL:HG22	2.18	0.43
30:18:26:LYS:HG2	30:18:46:ARG:O	2.18	0.43
32:1a:487:A:H2'	32:1a:488:C:O4'	2.17	0.43
36:1e:12:LEU:HB3	36:1e:31:LEU:HB3	2.00	0.43
54:1w:23:A:C6	54:1w:24:G:C6	3.06	0.43
1:2A:922:U:H2'	1:2A:923:C:C6	2.53	0.43
1:2A:2166:G:N7	1:2A:2167:U:H2'	2.32	0.43
1:2A:2590:A:N3	62:2A:4008:HOH:O	2.37	0.43
15:2T:34:VAL:HG11	15:2T:43:GLN:NE2	2.33	0.43
16:2U:10:ARG:NH2	62:2U:301:HOH:O	2.51	0.43
21:2Z:55:HIS:HE1	21:2Z:135:GLU:HB2	1.83	0.43
24:22:29:LYS:HE2	24:22:57:ILE:HG21	1.99	0.43
32:2a:1251:A:HO2'	32:2a:1369:C:HO2'	1.63	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:12:GLU:HA	33:2b:213:LEU:HD11	2.00	0.43
1:1A:784:A:C8	1:1A:792:G:C5	3.06	0.43
1:1A:839:U:H2'	1:1A:840:C:C6	2.52	0.43
1:1A:858:U:O2	1:1A:2268:A:H2'	2.18	0.43
1:1A:882:G:H4'	54:1w:19:G:C6	2.53	0.43
1:1A:1075:C:O2	1:1A:1076:C:H2'	2.18	0.43
1:1A:1268:A:C2	1:1A:2013:A:C4	3.06	0.43
1:1A:1815:A:P	3:1D:54:ARG:HH22	2.42	0.43
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.54	0.43
1:1A:2896:C:H2'	1:1A:2897:U:C6	2.53	0.43
11:1P:96:THR:HG1	11:1P:99:LEU:H	1.65	0.43
12:1Q:8:LYS:HB3	12:1Q:9:TYR:CD2	2.53	0.43
13:1R:71:GLN:NE2	62:1R:302:HOH:O	2.40	0.43
21:1Z:151:HIS:CE1	21:1Z:170:THR:HG22	2.52	0.43
30:18:4:MET:HE3	30:18:63:PRO:HG3	2.00	0.43
32:1a:78:G:N1	32:1a:91:C:C4	2.86	0.43
32:1a:684:A:H1'	42:1k:39:PRO:HD2	2.00	0.43
32:1a:737:A:H2'	32:1a:738:C:C6	2.53	0.43
33:1b:189:ASP:HB2	33:1b:190:THR:H	1.58	0.43
34:1c:130:VAL:O	34:1c:134:ILE:HG13	2.18	0.43
34:1c:130:VAL:HG21	34:1c:157:ILE:HG23	2.01	0.43
38:1g:37:ASN:OD1	40:1i:41:VAL:HG12	2.18	0.43
56:1z:1:FME:HB3	56:1z:2:THR:H	1.49	0.43
1:2A:1171:G:H8	1:2A:1171:G:O5'	2.02	0.43
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.53	0.43
1:2A:1203:G:OP2	1:2A:1204:A:O2'	2.23	0.43
1:2A:1642:G:H2'	1:2A:1643:G:O4'	2.18	0.43
1:2A:2134:A:N6	1:2A:2157:G:H4'	2.33	0.43
11:2P:88:LEU:HA	11:2P:91:PHE:HD2	1.83	0.43
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.29	0.43
32:2a:501:C:OP2	43:2l:124:LYS:NZ	2.31	0.43
32:2a:920:U:H2'	32:2a:921:U:H6	1.81	0.43
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.30	0.43
32:2a:966:M2G:HM23	32:2a:967:5MC:H1'	2.00	0.43
32:2a:1165:C:H2'	32:2a:1166:G:O4'	2.17	0.43
36:2e:31:LEU:HD11	36:2e:129:ILE:HA	1.99	0.43
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.18	0.43
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	2.00	0.43
51:2t:53:LEU:HB2	51:2t:100:ILE:HD11	1.99	0.43
1:1A:484:C:H2'	1:1A:485:C:H6	1.83	0.43
1:1A:1416:G:O2'	1:1A:1417:C:OP2	2.28	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2304:G:H22	1:1A:2312:U:H3	1.66	0.43
1:1A:2309:A:N6	1:1A:2310:A:N1	2.67	0.43
1:1A:2365:G:H4'	22:10:60:PHE:CZ	2.54	0.43
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.53	0.43
8:1I:124:GLY:H	8:1I:144:VAL:HG23	1.82	0.43
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	2.00	0.43
21:1Z:54:HIS:HB2	21:1Z:55:HIS:CD2	2.53	0.43
32:1a:922:G:C6	32:1a:923:A:C6	3.06	0.43
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.54	0.43
34:1c:66:VAL:HG23	34:1c:101:LEU:HD13	2.00	0.43
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.29	0.43
44:1m:92:HIS:HA	44:1m:110:ARG:NH2	2.33	0.43
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.32	0.43
1:2A:657:U:H2'	1:2A:658:C:C6	2.54	0.43
1:2A:2650:U:H2'	1:2A:2651:C:C6	2.53	0.43
1:2A:2685:G:P	15:2T:51:ARG:HH12	2.42	0.43
1:2A:2807:G:C2	1:2A:2808:U:H1'	2.53	0.43
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.15	0.43
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.99	0.43
6:2G:16:ARG:NE	6:2G:31:VAL:HG11	2.33	0.43
32:2a:347:G:H8	32:2a:347:G:OP2	2.01	0.43
32:2a:376:G:H5''	47:2p:5:ARG:HB2	1.99	0.43
32:2a:450:G:H8	32:2a:450:G:O5'	2.02	0.43
32:2a:714:G:H2'	32:2a:715:A:C8	2.52	0.43
33:2b:204:ASN:O	33:2b:210:SER:HB3	2.18	0.43
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.18	0.43
49:2r:58:LEU:HD12	49:2r:66:LEU:HD22	1.99	0.43
1:1A:363:G:H2'	1:1A:363(A):A:C8	2.53	0.43
1:1A:875:G:H2'	1:1A:876:C:H6	1.83	0.43
1:1A:877:U:O2'	1:1A:900:A:N6	2.51	0.43
1:1A:893:C:O2'	1:1A:894:C:H5'	2.18	0.43
1:1A:1094:U:H1'	1:1A:1097:U:C4	2.53	0.43
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.99	0.43
1:1A:2576:G:H1'	62:1A:4664:HOH:O	2.19	0.43
2:1B:66:A:N6	2:1B:109:C:H5'	2.31	0.43
4:1E:97:LYS:N	4:1E:100:GLU:OE2	2.40	0.43
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.84	0.43
11:1P:59:LEU:HD13	30:18:58:ILE:HD13	2.00	0.43
32:1a:79:G:O6	32:1a:90:U:O2	2.36	0.43
32:1a:864:A:H2'	32:1a:865:A:C8	2.53	0.43
32:1a:976:G:OP1	45:1n:32:SER:N	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.18	0.43
32:1a:1264:C:N4	32:1a:1271:G:H1	2.13	0.43
44:1m:52:GLU:HG2	44:1m:55:ARG:NH2	2.33	0.43
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.18	0.43
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.54	0.43
1:2A:141:A:H8	1:2A:1409:C:H5'	1.83	0.43
18:2W:5:ALA:O	18:2W:6:ILE:HG13	2.18	0.43
21:2Z:23:LYS:NZ	21:2Z:40:ASP:HB2	2.33	0.43
32:2a:417:C:H2'	32:2a:418:C:C6	2.54	0.43
32:2a:668:G:H21	46:2o:46:HIS:CE1	2.36	0.43
32:2a:762:C:H2'	32:2a:763:G:C8	2.53	0.43
32:2a:1134:G:N1	32:2a:1135:U:H1'	2.33	0.43
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	1.99	0.43
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.54	0.43
36:2e:111:GLU:C	36:2e:113:ALA:H	2.27	0.43
47:2p:1:MET:HE2	47:2p:1:MET:HB3	1.79	0.43
1:1A:518:G:H2'	1:1A:519:U:C6	2.54	0.43
1:1A:647:G:H2'	1:1A:648:G:O4'	2.18	0.43
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.53	0.43
6:1G:37:VAL:HG23	6:1G:99:MET:HG3	1.99	0.43
6:1G:53:LEU:HD11	6:1G:87:PRO:HB2	2.00	0.43
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.18	0.43
17:1V:10:LYS:NZ	17:1V:23:GLU:OE2	2.51	0.43
20:1Y:5:MET:HG3	20:1Y:7:VAL:O	2.18	0.43
26:14:43:TYR:O	26:14:45:GLY:N	2.51	0.43
32:1a:848:C:H2'	32:1a:849:C:C6	2.53	0.43
32:1a:857:C:H2'	32:1a:858:G:O4'	2.19	0.43
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.19	0.43
33:1b:24:TRP:HZ3	33:1b:29:ALA:HB2	1.84	0.43
41:1j:31:GLY:HA3	41:1j:32:ALA:HA	1.87	0.43
1:2A:30:G:H2'	1:2A:31:C:C6	2.53	0.43
1:2A:892:G:H3'	1:2A:893:C:C5'	2.48	0.43
1:2A:1341:U:O2	19:2X:80:ILE:HD12	2.18	0.43
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.54	0.43
1:2A:1912:A:O2'	32:2a:1494:G:O2'	2.31	0.43
1:2A:2663:G:H2'	1:2A:2664:G:O4'	2.17	0.43
13:2R:13:HIS:CE1	13:2R:16:HIS:HB2	2.53	0.43
21:2Z:146:ILE:HG23	21:2Z:174:VAL:O	2.18	0.43
32:2a:1517:G:H2'	32:2a:1518:MA6:H8	2.00	0.43
50:2s:40:ILE:HB	50:2s:67:VAL:O	2.18	0.43
1:1A:1530:C:H2'	1:1A:1531:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.30	0.43
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.18	0.43
16:1U:17:ILE:HD12	16:1U:17:ILE:HA	1.79	0.43
26:14:61:ARG:HD3	50:1s:67:VAL:HG12	2.00	0.43
32:1a:45:U:H2'	32:1a:46:G:H8	1.83	0.43
32:1a:947:G:H2'	32:1a:948:C:O4'	2.17	0.43
32:1a:1325:C:OP1	52:1u:15:ARG:NH1	2.51	0.43
32:1a:1508:G:OP1	62:1a:1915:HOH:O	2.21	0.43
1:2A:68:G:H2'	1:2A:69:C:O4'	2.18	0.43
1:2A:176:G:O2'	1:2A:177:G:H5'	2.18	0.43
1:2A:1862:G:H2'	1:2A:1863:G:H8	1.83	0.43
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.53	0.43
5:2F:137:LYS:H	5:2F:137:LYS:HG2	1.56	0.43
7:2H:150:ALA:HA	7:2H:153:LYS:HG3	2.00	0.43
12:2Q:2:LEU:HB3	12:2Q:69:PHE:CE1	2.54	0.43
24:22:44:LEU:HD12	24:22:44:LEU:HA	1.88	0.43
32:2a:811:C:O2'	32:2a:901:A:N1	2.44	0.43
32:2a:1089:G:H1	32:2a:1096:C:H42	1.65	0.43
32:2a:1260:C:P	32:2a:1284:C:H4'	2.59	0.43
32:2a:1263:C:H3'	32:2a:1263:C:H6	1.84	0.43
32:2a:1271:G:C2	32:2a:1272:G:C8	3.07	0.43
48:2q:40:LYS:HD3	48:2q:42:TYR:OH	2.18	0.43
1:1A:414:C:H2'	1:1A:415:A:C8	2.53	0.43
1:1A:444:C:H4'	5:1F:49:ALA:HB2	2.00	0.43
1:1A:1155:A:P	16:1U:55:ARG:HD2	2.59	0.43
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.41	0.43
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.18	0.43
6:1G:82:LEU:HD11	6:1G:88:ILE:HG21	2.00	0.43
32:1a:444:C:H2'	32:1a:445:G:C8	2.53	0.43
32:1a:977:A:O2'	32:1a:979:C:OP2	2.31	0.43
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.53	0.43
44:1m:2:ALA:N	44:1m:8:GLU:OE1	2.52	0.43
1:2A:208:C:H2'	1:2A:209:C:C6	2.54	0.43
1:2A:885:C:H2'	1:2A:886:C:C4'	2.49	0.43
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.18	0.43
1:2A:1359:A:C2	1:2A:1372:U:O4	2.71	0.43
1:2A:1818:U:O2'	3:2D:154:LYS:O	2.28	0.43
1:2A:2024:G:H2'	1:2A:2025:C:H6	1.83	0.43
1:2A:2108:C:H2'	1:2A:2109:U:C6	2.54	0.43
1:2A:2286:A:C6	28:26:34:LEU:HD21	2.54	0.43
1:2A:2699:C:H2'	1:2A:2700:C: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:2801(A):A:H3'	1:2A:2802:G:H5'	1.99	0.43
2:2B:83:G:H1	2:2B:94:C:N4	2.16	0.43
5:2F:20:LEU:HD22	5:2F:125:LEU:HD13	1.99	0.43
19:2X:35:THR:OG1	19:2X:38:GLU:HB2	2.19	0.43
20:2Y:97:ARG:NH1	20:2Y:106:LEU:O	2.52	0.43
21:2Z:126:VAL:HB	21:2Z:161:VAL:HG23	2.01	0.43
21:2Z:150:LEU:HB2	21:2Z:171:ILE:HD11	2.00	0.43
32:2a:34:C:H2'	32:2a:35:G:C8	2.53	0.43
32:2a:583:A:H2'	32:2a:584:G:O4'	2.19	0.43
32:2a:988:G:C1'	32:2a:1014:A:H61	2.32	0.43
32:2a:1002:G:C2	32:2a:1003:G:C8	3.07	0.43
33:2b:27:LYS:HD3	33:2b:193:ASP:OD1	2.18	0.43
34:2c:182:ILE:HG23	34:2c:203:PHE:HD1	1.83	0.43
36:2e:7:GLU:CD	36:2e:37:ARG:HH21	2.26	0.43
47:2p:13:HIS:C	47:2p:15:PRO:HD3	2.44	0.43
55:2x:21:A:H61	55:2x:46:G:H2'	1.83	0.43
1:1A:71:A:OP2	62:1A:4257:HOH:O	2.21	0.43
1:1A:548:A:H61	17:1V:18:LEU:HA	1.84	0.43
1:1A:555:U:O2'	1:1A:556:G:N7	2.51	0.43
1:1A:576:U:H2'	1:1A:577:G:C8	2.54	0.43
1:1A:1952:A:C6	1:1A:1953:A:N1	2.86	0.43
36:1e:135:THR:O	36:1e:139:LEU:HG	2.19	0.43
39:1h:13:ILE:HD11	39:1h:61:VAL:HG11	2.00	0.43
1:2A:884:C:H3'	1:2A:885:C:H6	1.83	0.43
1:2A:1547:C:H2'	1:2A:1548:C:C6	2.54	0.43
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.51	0.43
1:2A:2659:G:OP1	7:2H:158:HIS:NE2	2.37	0.43
1:2A:2749:A:H1'	7:2H:63:SER:OG	2.19	0.43
28:26:18:ARG:HD3	28:26:42:TRP:CE2	2.54	0.43
32:2a:224:C:H2'	32:2a:225:C:C6	2.54	0.43
32:2a:309:G:O2'	32:2a:607:A:N1	2.52	0.43
32:2a:431:A:H2'	32:2a:432:A:C8	2.54	0.43
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.18	0.43
33:2b:70:PHE:HE2	33:2b:90:MET:HB2	1.83	0.43
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	2.00	0.43
1:1A:1099:G:H2'	1:1A:1100:C:O4'	2.18	0.43
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.54	0.43
62:1A:4914:HOH:O	10:1O:20:MET:HE2	2.18	0.43
6:1G:77:ILE:HD12	6:1G:82:LEU:HD23	2.00	0.43
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	2.00	0.43
32:1a:146:G:H1	32:1a:176:C:H42	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.46	0.43
32:1a:607:A:H2'	32:1a:608:A:C8	2.54	0.43
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.46	0.43
33:1b:185:ILE:HG22	33:1b:199:TYR:HD2	1.84	0.43
34:1c:124:ILE:HG12	34:1c:124:ILE:H	1.54	0.43
54:1w:23:A:N6	54:1w:24:G:O6	2.52	0.43
57:1y:35:A:OP2	57:1y:35:A:H8	2.01	0.43
1:2A:1527:G:O2'	1:2A:1544:A:N6	2.33	0.43
1:2A:1970:A:H4'	1:2A:1971:A:OP1	2.19	0.43
1:2A:2722:G:H5'	13:2R:4:LEU:HD12	2.01	0.43
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	2.00	0.43
20:2Y:15:VAL:HG21	20:2Y:42:VAL:HG11	2.00	0.43
22:20:64:ASP:OD1	22:20:64:ASP:N	2.51	0.43
22:20:69:PHE:CE2	22:20:79:VAL:HG22	2.54	0.43
32:2a:154:C:H2'	32:2a:155:C:H6	1.83	0.43
32:2a:946:A:H2'	32:2a:947:G:C8	2.53	0.43
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.54	0.43
32:2a:1530:G:OP1	32:2a:1530:G:H4'	2.19	0.43
44:2m:92:HIS:CE1	44:2m:98:VAL:HG21	2.54	0.43
54:2w:70:G:H8	54:2w:70:G:OP2	2.01	0.43
1:1A:1071:G:H4'	1:1A:1089:G:OP2	2.19	0.43
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.54	0.43
3:1D:92:ILE:HD12	3:1D:104:TYR:CD1	2.53	0.43
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.84	0.43
5:1F:202:PHE:CZ	5:1F:206:ILE:HD13	2.54	0.43
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.81	0.43
32:1a:280:C:N3	48:1q:39:SER:OG	2.48	0.43
32:1a:1209:C:O2'	32:1a:1214:C:N4	2.52	0.43
33:1b:174:VAL:O	33:1b:178:ARG:HG2	2.19	0.43
34:1c:159:GLY:HA2	34:1c:193:TYR:CD1	2.54	0.43
35:1d:63:LYS:HB2	35:1d:63:LYS:HE3	1.78	0.43
35:1d:155:LEU:HB3	35:1d:158:ILE:HD11	2.01	0.43
41:1j:19:SER:OG	41:1j:91:PRO:HD2	2.18	0.43
44:1m:74:VAL:O	44:1m:78:ILE:HG13	2.19	0.43
57:1y:67:C:H2'	57:1y:68:C:H6	1.84	0.43
1:2A:39:C:H2'	1:2A:40:C:C6	2.54	0.43
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.53	0.43
1:2A:1820:U:H4'	1:2A:1821:A:OP2	2.19	0.43
1:2A:2370:G:C6	1:2A:2371:G:C6	3.07	0.43
1:2A:2391:G:O6	1:2A:2425:A:H8	2.01	0.43
1:2A:2508:G:O3'	1:2A:2555:U:H5'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:17:C:H2'	2:2B:18:G:C8	2.54	0.43
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.46	0.43
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.19	0.43
6:2G:67:LYS:HE3	26:24:5:ILE:HD12	2.01	0.43
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.17	0.43
8:2I:98:ALA:HA	8:2I:101:LEU:HD11	2.01	0.43
9:2N:6:PRO:HG3	9:2N:41:ASP:HB2	2.00	0.43
19:2X:32:PRO:HA	19:2X:77:LYS:HB2	2.01	0.43
32:2a:1314:C:H2'	32:2a:1315:U:H6	1.84	0.43
33:2b:178:ARG:NH2	39:2h:74:PRO:HG3	2.34	0.43
38:2g:47:CYS:O	38:2g:58:PRO:HG3	2.19	0.43
44:2m:49:THR:O	44:2m:53:VAL:HG13	2.19	0.43
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	2.01	0.43
1:1A:141:A:C6	1:1A:142:A:N1	2.87	0.42
1:1A:242:G:C8	30:18:5:LYS:HG2	2.54	0.42
1:1A:2168:G:N1	1:1A:2171:A:N7	2.68	0.42
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.54	0.42
1:1A:2508:G:H5''	62:1A:4215:HOH:O	2.19	0.42
3:1D:18:VAL:HG12	3:1D:211:ARG:NH2	2.34	0.42
10:1O:86:ILE:HG22	10:1O:94:ARG:HD3	2.00	0.42
25:13:59:VAL:O	25:13:60:GLU:HG2	2.19	0.42
32:1a:613:C:H2'	32:1a:614:A:C8	2.46	0.42
32:1a:1239:A:H62	32:1a:1299:A:H62	1.65	0.42
36:1e:68:GLU:HG3	36:1e:69:VAL:N	2.33	0.42
38:1g:78:ARG:HA	38:1g:78:ARG:HD2	1.88	0.42
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.51	0.42
43:1l:117:ARG:HB3	43:1l:122:THR:HB	2.01	0.42
45:1n:3:ARG:HG3	45:1n:4:LYS:N	2.33	0.42
51:1t:13:LEU:HD12	51:1t:14:LYS:N	2.33	0.42
1:2A:307:G:H21	1:2A:330:A:N6	2.17	0.42
1:2A:817:C:O2'	1:2A:839:U:H5''	2.19	0.42
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.54	0.42
1:2A:1759:A:H1'	1:2A:2711:A:C2	2.54	0.42
3:2D:66:ASP:OD2	3:2D:103:ARG:NH1	2.49	0.42
5:2F:156:LEU:HD21	5:2F:163:VAL:HG12	2.01	0.42
6:2G:41:GLN:HG2	6:2G:154:GLY:O	2.19	0.42
8:2I:84:GLY:C	8:2I:86:THR:H	2.25	0.42
18:2W:27:LYS:HA	18:2W:27:LYS:HD2	1.91	0.42
30:28:26:LYS:HB2	30:28:44:LYS:O	2.19	0.42
32:2a:120:A:C6	32:2a:122:G:C2	3.07	0.42
32:2a:1318:A:H5''	50:2s:3:ARG:NH2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1508:A:H5'	1:1A:1509(A):A:C5	2.54	0.42
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	2.01	0.42
4:1E:47:VAL:O	4:1E:80:GLU:HA	2.18	0.42
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	2.01	0.42
10:1O:21:CYS:HB2	10:1O:39:ILE:HD12	2.00	0.42
21:1Z:52:SER:O	21:1Z:52:SER:OG	2.28	0.42
32:1a:714:G:H2'	32:1a:715:A:C8	2.54	0.42
33:1b:200:ILE:HD12	33:1b:200:ILE:H	1.84	0.42
37:1f:10:LEU:HB2	37:1f:59:TYR:HB3	2.00	0.42
40:1i:5:TYR:OH	40:1i:7:THR:OG1	2.33	0.42
1:2A:2024:G:H2'	1:2A:2025:C:C6	2.54	0.42
1:2A:2233:U:H2'	1:2A:2234:G:C8	2.54	0.42
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.34	0.42
1:2A:2306:C:N4	6:2G:42:GLY:O	2.46	0.42
4:2E:27:LEU:HD22	15:2T:1:MET:SD	2.59	0.42
8:2I:88:ILE:HD11	8:2I:144:VAL:HG11	2.02	0.42
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.84	0.42
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.57	0.42
21:2Z:166:SER:O	21:2Z:168:GLU:N	2.52	0.42
32:2a:1152:A:H2'	32:2a:1153:C:C6	2.54	0.42
32:2a:1316:G:H5''	45:2n:17:LYS:HE3	2.01	0.42
34:2c:131:ARG:HH21	36:2e:50:GLU:HG3	1.84	0.42
34:2c:176:HIS:O	34:2c:178:LEU:HD12	2.19	0.42
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.35	0.42
40:2i:18:PHE:O	40:2i:61:ALA:HA	2.20	0.42
40:2i:22:GLY:HA3	40:2i:60:ASP:OD2	2.18	0.42
47:2p:4:ILE:HA	47:2p:20:VAL:O	2.19	0.42
1:1A:71:A:H5''	1:1A:73:A:C8	2.55	0.42
1:1A:1062:G:H1'	1:1A:1088:A:C8	2.54	0.42
1:1A:1400:G:H2'	1:1A:1401:G:C8	2.54	0.42
1:1A:1466:G:H2'	1:1A:1547:C:H41	1.84	0.42
1:1A:1512:U:O2'	1:1A:1513:C:H5'	2.19	0.42
1:1A:1683:C:H2'	1:1A:1684:C:H6	1.85	0.42
1:1A:2165:G:C6	1:1A:2171:A:H8	2.37	0.42
1:1A:2406:U:H6	1:1A:2406:U:H2'	1.66	0.42
1:1A:2690:C:OP2	13:1R:14:SER:HB3	2.19	0.42
4:1E:47:VAL:HG22	4:1E:84:PHE:O	2.19	0.42
6:1G:66:GLN:NE2	6:1G:93:THR:O	2.43	0.42
6:1G:101:ILE:HG22	6:1G:105:LYS:HE2	2.01	0.42
20:1Y:82:PRO:O	20:1Y:101:LYS:NZ	2.38	0.42
23:11:23:LYS:HB3	23:11:29:GLY:HA3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:626:U:H2'	32:1a:627:G:C8	2.54	0.42
32:1a:958:A:C6	32:1a:959:A:N1	2.87	0.42
32:1a:1168:A:H8	32:1a:1168:A:OP1	2.02	0.42
40:1i:7:THR:O	40:1i:83:ARG:HD2	2.19	0.42
1:2A:141:A:C8	1:2A:1408:C:O2'	2.65	0.42
1:2A:403:U:H4'	1:2A:404:C:H5'	2.02	0.42
1:2A:530:G:C5	1:2A:2022:U:H5''	2.54	0.42
1:2A:807:U:O2'	1:2A:2060:A:N1	2.50	0.42
1:2A:1922:G:H2'	1:2A:1923:U:O4'	2.19	0.42
1:2A:2136:C:N4	1:2A:2155:G:N1	2.68	0.42
4:2E:78:LEU:O	4:2E:79:ARG:NH1	2.46	0.42
7:2H:23:ARG:O	7:2H:24:VAL:HG13	2.19	0.42
12:2Q:25:ASP:OD2	21:2Z:78:LYS:HG2	2.20	0.42
32:2a:553:A:H5''	43:2l:24:VAL:HG21	2.01	0.42
32:2a:778:G:H2'	32:2a:779:C:O4'	2.19	0.42
32:2a:1018:C:H2'	32:2a:1019:C:O4'	2.19	0.42
32:2a:1121:U:O2'	32:2a:1122:U:H5'	2.19	0.42
32:2a:1362:C:H2'	32:2a:1363:C:H5''	2.01	0.42
44:2m:60:VAL:HG13	44:2m:64:TRP:CE3	2.54	0.42
52:2u:6:ARG:HA	52:2u:11:GLY:HA3	2.00	0.42
57:2y:66:U:C4	57:2y:67:C:C4	3.07	0.42
1:1A:841:A:H2'	1:1A:842:G:C8	2.55	0.42
1:1A:1803:A:H4'	3:1D:259:THR:HG23	2.01	0.42
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.84	0.42
1:1A:2168:G:N2	1:1A:2171:A:N7	2.67	0.42
32:1a:169:C:H2'	32:1a:170:U:H6	1.83	0.42
32:1a:339:C:H2'	32:1a:340:U:C6	2.54	0.42
32:1a:1391:U:O2'	32:1a:1532:U:OP1	2.34	0.42
33:1b:188:ALA:HB1	33:1b:192:SER:OG	2.19	0.42
37:1f:8:ILE:HD11	37:1f:79:LEU:HD13	2.01	0.42
44:1m:57:ARG:O	44:1m:61:GLU:HG3	2.18	0.42
51:1t:56:MET:HE3	51:1t:85:MET:HG2	2.01	0.42
1:2A:927:G:H2'	1:2A:928:G:O4'	2.19	0.42
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.34	0.42
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.35	0.42
1:2A:2391:G:O2'	1:2A:2422:A:N7	2.53	0.42
2:2B:75:G:H5'	2:2B:76:G:OP2	2.19	0.42
32:2a:434:U:H2'	32:2a:435:C:C6	2.54	0.42
36:2e:20:GLN:OE1	36:2e:25:ARG:NH1	2.52	0.42
44:2m:23:TYR:CE2	44:2m:70:LEU:HD22	2.49	0.42
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2t:77:ALA:O	51:2t:81:LYS:HG3	2.18	0.42
1:1A:622:G:H2'	1:1A:623:G:H8	1.85	0.42
1:1A:1079:C:H2'	1:1A:1080:C:O4'	2.20	0.42
1:1A:1087:G:H2'	1:1A:1089:G:O4'	2.20	0.42
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.84	0.42
1:1A:1417:C:H2'	1:1A:1418:G:O4'	2.19	0.42
1:1A:1720:U:H2'	1:1A:1721:G:O4'	2.19	0.42
1:1A:2193:G:H2'	1:1A:2194:G:C8	2.55	0.42
10:1O:25:LEU:HD23	10:1O:25:LEU:HA	1.88	0.42
32:1a:79:G:O6	32:1a:90:U:C2	2.72	0.42
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.52	0.42
44:1m:123:ALA:HA	44:1m:124:PRO:HD3	1.89	0.42
50:1s:18:LYS:O	50:1s:22:LEU:HG	2.19	0.42
51:1t:83:ARG:HA	51:1t:86:ARG:NH1	2.35	0.42
1:2A:287:C:H2'	1:2A:288:C:H6	1.84	0.42
1:2A:1354:A:H2'	1:2A:1355:G:O4'	2.19	0.42
21:2Z:98:MET:O	21:2Z:126:VAL:HG22	2.20	0.42
32:2a:259:G:H2'	32:2a:260:G:O4'	2.20	0.42
32:2a:791:G:C6	32:2a:792:A:N7	2.87	0.42
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.52	0.42
33:2b:171:ALA:O	33:2b:175:ARG:HB2	2.19	0.42
33:2b:223:ILE:HA	33:2b:226:ARG:HD3	2.01	0.42
35:2d:165:MET:SD	35:2d:168:ARG:HB2	2.59	0.42
44:2m:13:LYS:HA	44:2m:44:ARG:NH1	2.33	0.42
57:2y:49:C:H2'	57:2y:50:U:C6	2.54	0.42
1:1A:69:C:O2'	1:1A:70:G:H5'	2.19	0.42
1:1A:1056:G:H5''	1:1A:1057:A:C4'	2.50	0.42
1:1A:1063:G:H2'	1:1A:1064:C:C5	2.55	0.42
1:1A:2098:U:H3	1:1A:2191:G:H1	1.67	0.42
2:1B:78:A:C2	2:1B:100:A:C4	3.08	0.42
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.55	0.42
16:1U:34:LYS:HA	16:1U:34:LYS:HD2	1.77	0.42
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.54	0.42
26:14:53:GLU:H	26:14:53:GLU:HG3	1.59	0.42
26:14:53:GLU:HB2	26:14:55:ARG:HA	2.01	0.42
32:1a:377:G:OP1	47:1p:5:ARG:HD2	2.19	0.42
32:1a:683:G:H2'	32:1a:684:A:C8	2.55	0.42
32:1a:928:G:O2'	32:1a:1533:C:OP1	2.37	0.42
32:1a:1226:C:H4'	50:1s:80:TYR:CZ	2.55	0.42
32:1a:1518:MA6:H93	32:1a:1519:MA6:C9	2.49	0.42
38:1g:104:LEU:HA	38:1g:104:LEU:HD13	1.74	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:72:U:OP1	62:2A:3947:HOH:O	2.21	0.42
1:2A:577:G:C6	1:2A:578:A:C6	3.08	0.42
1:2A:2674:G:H5''	10:2O:26:LYS:HE3	2.02	0.42
5:2F:137:LYS:HE2	5:2F:137:LYS:HB3	1.53	0.42
6:2G:103:LEU:O	6:2G:107:LEU:HG	2.19	0.42
9:2N:35:ARG:O	9:2N:42:TRP:NE1	2.51	0.42
16:2U:79:PHE:CE2	16:2U:83:LEU:HD11	2.54	0.42
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.18	0.42
30:28:4:MET:HE3	30:28:63:PRO:HG3	2.02	0.42
32:2a:409:G:C6	32:2a:410:G:C4	3.07	0.42
32:2a:1216:G:OP1	45:2n:2:ALA:HA	2.20	0.42
32:2a:1279:A:O2'	32:2a:1282:C:N4	2.52	0.42
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.84	0.42
33:2b:74:LYS:HD2	33:2b:166:ASP:HB3	2.01	0.42
33:2b:87:ARG:CZ	33:2b:233:SER:HB2	2.50	0.42
34:2c:53:ALA:HB2	34:2c:115:LEU:CD1	2.49	0.42
34:2c:156:ARG:H	34:2c:196:LEU:HD22	1.84	0.42
40:2i:18:PHE:HD2	40:2i:62:TYR:HD2	1.66	0.42
40:2i:50:LEU:HB2	40:2i:55:ALA:O	2.19	0.42
1:1A:303:U:H2'	1:1A:304:G:C8	2.54	0.42
1:1A:1406:U:H2'	1:1A:1407:C:H6	1.84	0.42
4:1E:93:VAL:HG22	62:1E:402:HOH:O	2.19	0.42
7:1H:9:ILE:HD12	7:1H:50:VAL:HG12	2.02	0.42
7:1H:113:VAL:HG11	7:1H:151:ILE:HD13	2.01	0.42
10:1O:104:ARG:CZ	15:1T:34:VAL:HG11	2.49	0.42
12:1Q:51:ARG:O	12:1Q:55:VAL:HG23	2.20	0.42
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.53	0.42
23:11:18:ILE:HG12	23:11:37:ILE:HG12	2.01	0.42
23:11:94:LEU:HA	23:11:97:LEU:HD12	2.02	0.42
32:1a:976:G:N2	32:1a:1363:C:OP2	2.51	0.42
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.55	0.42
32:1a:1152:A:H2'	32:1a:1153:C:H6	1.85	0.42
32:1a:1273:G:C2	32:1a:1274:G:H1'	2.55	0.42
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.54	0.42
37:1f:89:MET:HE3	37:1f:91:VAL:HG21	2.00	0.42
41:1j:8:LEU:C	41:1j:16:LEU:HD11	2.44	0.42
1:2A:109:G:H2'	1:2A:110:G:O4'	2.20	0.42
1:2A:1862:G:H2'	1:2A:1863:G:C8	2.55	0.42
1:2A:2743:C:OP1	31:29:33:LYS:NZ	2.38	0.42
2:2B:49:C:H2'	2:2B:50:G:C8	2.54	0.42
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:91:ARG:HD2	15:2T:120:ARG:NH1	2.35	0.42
19:2X:65:ARG:HH11	19:2X:70:LEU:HD21	1.84	0.42
23:21:15:ALA:O	23:21:40:ARG:HG3	2.20	0.42
32:2a:362:G:N2	32:2a:365:U:OP2	2.52	0.42
32:2a:509:A:HO2'	32:2a:510:A:P	2.38	0.42
32:2a:1272:G:H5'	32:2a:1273:G:OP2	2.20	0.42
33:2b:98:LEU:HD12	33:2b:98:LEU:HA	1.86	0.42
34:2c:121:ALA:HB1	34:2c:188:LEU:O	2.19	0.42
35:2d:157:LEU:O	35:2d:161:ASN:ND2	2.52	0.42
37:2f:33:TYR:HA	37:2f:71:ARG:HH11	1.84	0.42
40:2i:125:TYR:HD2	40:2i:126:SER:N	2.18	0.42
50:2s:41:VAL:HG22	50:2s:44:MET:HE3	2.02	0.42
1:1A:271(K):U:H1'	8:1I:50:ARG:NH2	2.35	0.42
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.20	0.42
18:1W:10:VAL:HG12	18:1W:12:ILE:HG22	2.01	0.42
27:15:35:GLU:HG3	27:15:51:TYR:CD1	2.55	0.42
32:1a:540:G:H2'	32:1a:541:G:O4'	2.20	0.42
32:1a:944:G:O6	32:1a:1337:G:H8	2.03	0.42
32:1a:971:G:N2	32:1a:1363(A):A:OP2	2.43	0.42
33:1b:193:ASP:HB3	33:1b:196:LEU:HD22	2.01	0.42
36:1e:18:ARG:HH11	36:1e:27:ARG:HH12	1.67	0.42
39:1h:44:PHE:HB3	39:1h:80:ILE:HD11	2.02	0.42
54:1w:26:A:H61	54:1w:44:G:H1	1.68	0.42
1:2A:992:C:OP1	16:2U:47:TYR:OH	2.31	0.42
1:2A:1115:G:C2	1:2A:1116:C:C2	3.08	0.42
1:2A:1159:U:H2'	1:2A:1160:G:H8	1.85	0.42
1:2A:1429:G:H2'	1:2A:1430:C:H6	1.84	0.42
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.29	0.42
1:2A:2184:G:H2'	1:2A:2185:C:C6	2.55	0.42
1:2A:2507:C:H5''	1:2A:2573:C:C4	2.54	0.42
3:2D:29:PRO:HA	3:2D:83:GLU:OE1	2.20	0.42
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.20	0.42
32:2a:688:G:H5'	42:2k:46:GLY:C	2.45	0.42
32:2a:743:U:H2'	32:2a:744:C:C6	2.55	0.42
32:2a:976:G:N2	32:2a:1363:C:OP2	2.53	0.42
32:2a:1080:A:H5'	36:2e:16:THR:HG21	2.00	0.42
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.55	0.42
32:2a:1503:A:C2	53:2v:12:A:H2	2.37	0.42
33:2b:50:GLU:HB3	33:2b:200:ILE:O	2.20	0.42
33:2b:91:PRO:HG3	33:2b:154:LEU:HB2	2.02	0.42
35:2d:105:VAL:HG13	35:2d:110:PHE:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.55	0.42
41:2j:89:ASP:O	41:2j:91:PRO:HD3	2.19	0.42
1:1A:330:A:H2'	1:1A:330:A:N3	2.35	0.42
1:1A:518:G:H4'	18:1W:18:ARG:NE	2.35	0.42
1:1A:548:A:H1'	1:1A:549:G:OP1	2.20	0.42
1:1A:571:A:O2'	17:1V:78:LYS:HE2	2.20	0.42
1:1A:723:G:H2'	1:1A:724:U:O4'	2.20	0.42
1:1A:1550:C:OP1	1:1A:1720:U:O2'	2.35	0.42
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	2.01	0.42
9:1N:120:LEU:HG	9:1N:122:VAL:HG23	2.01	0.42
15:1T:8:LYS:HE3	15:1T:8:LYS:HB3	1.92	0.42
21:1Z:77:ASP:OD2	21:1Z:80:ARG:NH1	2.47	0.42
23:11:65:SER:OG	23:11:66:HIS:ND1	2.39	0.42
32:1a:114:U:H2'	32:1a:115:G:C8	2.55	0.42
32:1a:441:A:H8	32:1a:441:A:OP2	2.03	0.42
32:1a:1201:A:H4'	32:1a:1202:G:O5'	2.20	0.42
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.33	0.42
39:1h:114:THR:HG22	39:1h:131:GLY:HA3	2.02	0.42
44:1m:15:VAL:HG11	44:1m:48:LEU:HD11	2.02	0.42
44:1m:67:GLU:HB3	44:1m:68:GLY:H	1.76	0.42
48:1q:64:PRO:HB3	48:1q:70:ARG:NH1	2.35	0.42
51:1t:89:ARG:O	51:1t:93:GLU:HG2	2.20	0.42
1:2A:263:C:H2'	1:2A:264:C:O4'	2.20	0.42
1:2A:528:A:N1	1:2A:2042:A:H2'	2.34	0.42
1:2A:1425:G:C6	1:2A:1426:G:C6	3.08	0.42
1:2A:2086:U:H2'	1:2A:2087:G:H8	1.85	0.42
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.20	0.42
1:2A:2748:A:H5'	7:2H:4:ILE:CD1	2.49	0.42
8:2I:26:ALA:O	8:2I:31:LEU:HB2	2.20	0.42
13:2R:26:LYS:HE2	13:2R:70:LEU:O	2.20	0.42
20:2Y:20:TYR:HD1	20:2Y:23:ARG:HG3	1.85	0.42
32:2a:537:G:H5''	43:2l:113:ARG:HH12	1.85	0.42
32:2a:1225:A:H2'	32:2a:1226:C:C5	2.54	0.42
32:2a:1403:C:C2	32:2a:1404:5MC:HM52	2.55	0.42
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.55	0.42
54:2w:64:A:O2'	54:2w:65:G:H5'	2.20	0.42
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.20	0.42
1:1A:422:A:H2'	1:1A:423:A:C8	2.55	0.42
1:1A:593:G:C4'	30:18:4:MET:HE2	2.49	0.42
1:1A:672:C:OP2	11:1P:42:SER:OG	2.33	0.42
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1094:U:H2'	1:1A:1095:A:C8	2.55	0.42
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.55	0.42
1:1A:2269:A:OP1	62:1A:4259:HOH:O	2.22	0.42
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.20	0.42
9:1N:12:ARG:NH2	9:1N:50:ASP:OD2	2.43	0.42
12:1Q:19:GLY:O	12:1Q:98:LYS:HE3	2.20	0.42
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.19	0.42
20:1Y:92:ASN:ND2	20:1Y:94:LYS:HG2	2.35	0.42
25:13:3:ARG:NH2	25:13:60:GLU:OE1	2.45	0.42
32:1a:757:U:H2'	32:1a:758:G:O4'	2.19	0.42
32:1a:1313:U:OP2	50:1s:5:LEU:HG	2.19	0.42
35:1d:111:ALA:HA	35:1d:161:ASN:ND2	2.34	0.42
38:1g:144:MET:HE2	38:1g:144:MET:HB3	1.78	0.42
40:1i:4:TYR:CD1	40:1i:88:TYR:HA	2.55	0.42
40:1i:96:LEU:HD13	40:1i:101:PHE:CD2	2.46	0.42
44:1m:57:ARG:HG3	44:1m:61:GLU:OE2	2.20	0.42
57:1y:47:U:H2'	57:1y:50:U:OP1	2.20	0.42
57:1y:56:C:H2'	57:1y:57:G:O4'	2.20	0.42
1:2A:652(T):C:H5'	1:2A:652(U):G:OP2	2.20	0.42
1:2A:1213:A:N3	1:2A:1238:G:O2'	2.43	0.42
1:2A:1500:G:H2'	1:2A:1501:C:C6	2.55	0.42
1:2A:1851:U:H2'	1:2A:1852:C:O4'	2.20	0.42
1:2A:2189:U:H2'	1:2A:2190:G:C8	2.54	0.42
1:2A:2319:G:O6	14:2S:4:LEU:HD12	2.19	0.42
1:2A:2503:2MA:O2'	1:2A:2505:G:OP2	2.28	0.42
1:2A:2701:C:H2'	1:2A:2702:U:H2'	2.02	0.42
1:2A:2735:G:H2'	1:2A:2736:G:H8	1.85	0.42
2:2B:16:G:C2'	2:2B:17:C:H5'	2.50	0.42
2:2B:44:G:N3	2:2B:47:C:N4	2.62	0.42
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.55	0.42
6:2G:43:LEU:C	6:2G:45:GLU:H	2.28	0.42
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	2.02	0.42
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.48	0.42
10:2O:120:GLU:HG2	10:2O:122:LEU:HG	2.01	0.42
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.35	0.42
19:2X:50:LYS:NZ	62:2X:3601:HOH:O	2.52	0.42
43:2l:89:ARG:NH2	43:2l:91:LYS:HA	2.35	0.42
57:2y:14:A:C6	57:2y:15:G:C6	3.08	0.42
1:1A:747:U:O2	1:1A:2014:A:H1'	2.20	0.41
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.55	0.41
1:1A:2389:G:H5''	1:1A:2390:U:O4'	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:24:G:N7	2:1B:56:G:H2'	2.35	0.41
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	2.02	0.41
7:1H:103:LEU:HB3	7:1H:115:VAL:HB	2.02	0.41
10:1O:112:MET:HE3	10:1O:112:MET:HB3	1.69	0.41
32:1a:255:G:C2	32:1a:272:C:C2	3.08	0.41
32:1a:918:A:H2'	32:1a:919:A:O4'	2.19	0.41
34:1c:150:LYS:HG3	34:1c:169:ALA:HB2	2.02	0.41
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.85	0.41
42:1k:111:ASP:OD1	49:1r:84:LYS:HE3	2.20	0.41
51:1t:57:ARG:HH22	51:1t:100:ILE:CD1	2.32	0.41
1:2A:855:G:C6	1:2A:856:C:C4	3.08	0.41
1:2A:1471:A:H2'	1:2A:1471:A:N3	2.35	0.41
1:2A:1702:G:H2'	1:2A:1703:G:O4'	2.20	0.41
1:2A:2143:C:O2	1:2A:2149:G:N2	2.53	0.41
1:2A:2156:G:H2'	1:2A:2157:G:C4	2.55	0.41
9:2N:55:VAL:HB	9:2N:125:GLY:O	2.19	0.41
11:2P:85:LEU:HD23	11:2P:88:LEU:HD12	2.02	0.41
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.53	0.41
18:2W:6:ILE:HG12	18:2W:104:THR:OG1	2.20	0.41
20:2Y:43:ASN:ND2	20:2Y:65:ALA:O	2.49	0.41
28:26:19:ARG:HH12	28:26:52:VAL:HG21	1.85	0.41
32:2a:986:A:H2'	32:2a:987:G:H8	1.85	0.41
32:2a:1273:G:C6	32:2a:1274:G:C4	3.08	0.41
32:2a:1318:A:H5'	50:2s:10:PHE:CE1	2.55	0.41
33:2b:130:ARG:HA	33:2b:130:ARG:HD3	1.91	0.41
33:2b:153:ARG:C	33:2b:155:LEU:H	2.28	0.41
34:2c:88:ARG:HA	34:2c:91:LEU:HD13	2.00	0.41
35:2d:88:VAL:HG13	36:2e:97:GLY:HA2	2.02	0.41
41:2j:49:VAL:O	41:2j:61:GLU:N	2.52	0.41
1:1A:324:A:N6	1:1A:338:G:O2'	2.53	0.41
1:1A:329:G:H8	1:1A:329:G:OP1	2.03	0.41
1:1A:337:C:H2'	1:1A:338:G:O4'	2.20	0.41
1:1A:593:G:C2	1:1A:665:C:C2	3.08	0.41
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.20	0.41
1:1A:1782:C:O2	1:1A:2608:G:O2'	2.38	0.41
1:1A:2382:G:H21	30:18:42:ARG:NH2	2.18	0.41
62:1A:5767:HOH:O	9:1N:28:THR:HG23	2.20	0.41
8:1I:66:GLU:C	8:1I:68:LEU:H	2.26	0.41
8:1I:109:ILE:HD13	8:1I:109:ILE:HA	1.74	0.41
19:1X:92:LEU:O	19:1X:94:GLY:N	2.53	0.41
32:1a:266:G:O3'	48:1q:67:LYS:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:343:U:O2'	32:1a:346:G:O6	2.24	0.41
32:1a:768:A:OP1	32:1a:804:U:H4'	2.19	0.41
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.50	0.41
35:1d:36:ARG:HB3	35:1d:38:TYR:CZ	2.55	0.41
35:1d:196:LEU:O	35:1d:198:VAL:N	2.45	0.41
36:1e:145:LYS:O	36:1e:149:GLU:HG2	2.19	0.41
41:1j:7:LYS:HD2	41:1j:9:ARG:HH12	1.84	0.41
57:1y:8:4SU:H1'	57:1y:48:C:O2	2.21	0.41
1:2A:271(V):G:H2'	1:2A:271(W):G:O4'	2.20	0.41
1:2A:332:A:O2'	1:2A:334:C:OP2	2.29	0.41
1:2A:581:C:OP2	16:2U:33:ARG:HD2	2.20	0.41
1:2A:1882:C:H2'	1:2A:1883:G:O4'	2.20	0.41
1:2A:2097:C:H2'	1:2A:2098:U:C6	2.55	0.41
1:2A:2207:G:H2'	1:2A:2208:A:H2	1.85	0.41
9:2N:19:GLU:HB2	9:2N:56:ASN:HD22	1.84	0.41
20:2Y:55:TYR:N	20:2Y:56:PRO:HD3	2.35	0.41
20:2Y:90:LEU:HD23	20:2Y:90:LEU:HA	1.91	0.41
23:21:52:ARG:HA	23:21:56:GLN:O	2.20	0.41
30:28:55:ALA:O	30:28:59:LYS:HG3	2.19	0.41
32:2a:1023:G:H8	32:2a:1023:G:OP2	2.03	0.41
35:2d:92:VAL:HG22	35:2d:96:LEU:HD22	2.01	0.41
43:2l:124:LYS:HA	43:2l:125:PRO:HD3	1.96	0.41
1:1A:460:A:H2'	1:1A:461:C:O4'	2.20	0.41
1:1A:2086:U:H2'	1:1A:2087:G:H8	1.84	0.41
4:1E:56:PRO:C	4:1E:58:ARG:H	2.28	0.41
8:1I:101:LEU:O	8:1I:106:GLY:N	2.54	0.41
8:1I:109:ILE:HD12	8:1I:130:TYR:CZ	2.55	0.41
9:1N:51:PHE:CZ	9:1N:119:ARG:HG2	2.56	0.41
9:1N:61:ARG:HA	9:1N:61:ARG:HD3	1.72	0.41
10:1O:19:ILE:HG22	10:1O:43:VAL:HG22	2.02	0.41
25:13:18:ASP:OD1	25:13:18:ASP:N	2.53	0.41
32:1a:339:C:H2'	32:1a:340:U:H6	1.85	0.41
32:1a:405:U:H3'	32:1a:406:G:H5'	2.02	0.41
32:1a:562:C:H1'	43:1l:15:ARG:HB3	2.02	0.41
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.83	0.41
33:1b:102:LEU:HB3	33:1b:180:LEU:CD1	2.50	0.41
33:1b:152:PHE:CE1	33:1b:155:LEU:HD23	2.55	0.41
39:1h:9:MET:HG3	39:1h:26:VAL:HG21	2.01	0.41
54:1w:45:U:H5'	54:1w:46:G7M:OP2	2.21	0.41
57:1y:15:G:N2	57:1y:48:C:H42	2.18	0.41
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:674:G:C1'	5:2F:74:ARG:HD3	2.49	0.41
1:2A:724:U:H2'	1:2A:725:G:O4'	2.21	0.41
1:2A:854:G:C2	1:2A:855:G:C5	3.08	0.41
1:2A:884:C:H3'	1:2A:885:C:C6	2.55	0.41
1:2A:1842:G:O2'	3:2D:253:GLN:OE1	2.30	0.41
26:24:50:VAL:HG11	44:2m:64:TRP:C	2.45	0.41
32:2a:141:A:H1'	32:2a:182:U:O2	2.21	0.41
32:2a:567:G:H2'	32:2a:568:G:O4'	2.19	0.41
32:2a:581:G:OP1	46:2o:61:GLY:HA3	2.20	0.41
32:2a:878:G:OP1	39:2h:88:LYS:HB3	2.21	0.41
32:2a:1273:G:H5'	32:2a:1274:G:OP2	2.19	0.41
32:2a:1275:A:H2'	32:2a:1276:G:O4'	2.20	0.41
33:2b:113:HIS:O	33:2b:117:GLU:HB2	2.19	0.41
34:2c:56:ASP:O	34:2c:57:ILE:HG13	2.20	0.41
36:2e:41:VAL:HG13	36:2e:112:LEU:O	2.20	0.41
40:2i:5:TYR:OH	40:2i:16:ARG:HG2	2.20	0.41
48:2q:95:TYR:HA	48:2q:98:LEU:HD12	2.03	0.41
54:2w:25:C:H2'	54:2w:26:A:C8	2.54	0.41
1:1A:504:U:H5''	1:1A:505:A:OP1	2.20	0.41
1:1A:1003:G:O2'	1:1A:1010:A:N1	2.49	0.41
1:1A:2117:A:H61	1:1A:2172:U:H3	1.68	0.41
1:1A:2336:A:H61	22:10:43:THR:HG22	1.86	0.41
7:1H:3:ARG:HD2	7:1H:3:ARG:HA	1.70	0.41
8:1I:77:LEU:HD12	8:1I:97:ILE:HG23	2.02	0.41
8:1I:109:ILE:HG23	8:1I:130:TYR:CE1	2.56	0.41
13:1R:9:LYS:O	13:1R:17:ARG:HD3	2.21	0.41
26:14:33:VAL:HG12	26:14:35:VAL:H	1.84	0.41
32:1a:986:A:H2'	32:1a:987:G:C8	2.56	0.41
32:1a:1364:U:C6	52:1u:14:TRP:HH2	2.38	0.41
33:1b:32:ILE:HD13	33:1b:40:HIS:CD2	2.44	0.41
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.54	0.41
36:1e:9:LYS:HB2	36:1e:112:LEU:HD11	2.03	0.41
1:2A:534:U:H5'	16:2U:42:ALA:HB1	2.03	0.41
1:2A:880:G:N2	1:2A:898:C:H1'	2.35	0.41
1:2A:945:A:C4	1:2A:2448:A:C2	3.08	0.41
1:2A:1248:G:C5	16:2U:3:ARG:HB2	2.55	0.41
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.86	0.41
1:2A:1668:A:H4'	1:2A:1669:A:O5'	2.20	0.41
1:2A:1790:C:H2'	1:2A:1791:A:C5	2.55	0.41
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.85	0.41
1:2A:2896:C:H2'	1:2A:2897:U:C5	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.21	0.41
15:2T:1:MET:HE2	15:2T:1:MET:HB3	1.80	0.41
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	2.02	0.41
23:21:40:ARG:HE	23:21:40:ARG:HB2	1.74	0.41
26:24:46:GLN:O	26:24:48:ARG:N	2.54	0.41
32:2a:171:A:H2'	32:2a:172:A:C8	2.56	0.41
32:2a:1117:G:H5'	32:2a:1118:C:OP2	2.20	0.41
32:2a:1133:G:H2'	32:2a:1134:G:O4'	2.20	0.41
32:2a:1291:G:H4'	40:2i:39:GLY:HA3	2.02	0.41
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.36	0.41
35:2d:59:ARG:NH1	35:2d:59:ARG:HA	2.35	0.41
36:2e:77:PRO:HG2	36:2e:142:LEU:HD22	2.02	0.41
39:2h:9:MET:HE1	39:2h:32:LYS:HA	2.03	0.41
40:2i:23:ASN:HD21	40:2i:25:LYS:NZ	2.17	0.41
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.81	0.41
45:2n:23:ARG:HG3	45:2n:28:GLY:O	2.20	0.41
46:2o:26:GLU:HG3	46:2o:81:LEU:HD13	2.02	0.41
48:2q:58:GLU:OE2	48:2q:75:ARG:NH2	2.53	0.41
55:2x:40:C:H4'	57:2y:36:A:OP1	2.21	0.41
1:1A:45:C:OP2	1:1A:215:G:H2'	2.19	0.41
1:1A:321:G:N3	5:1F:165:ARG:HD2	2.35	0.41
1:1A:1025:G:O2'	62:1A:4217:HOH:O	2.13	0.41
1:1A:1359:A:N3	1:1A:1359:A:H5'	2.35	0.41
1:1A:1359:A:C2	1:1A:1372:U:O4	2.72	0.41
1:1A:1676:A:H2'	1:1A:1677:A:O4'	2.20	0.41
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	2.02	0.41
1:1A:2203:U:O2'	1:1A:2205:C:H5'	2.20	0.41
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.84	0.41
2:1B:55:U:H2'	2:1B:56:G:O4'	2.20	0.41
3:1D:77:ALA:HA	3:1D:97:TYR:HA	2.01	0.41
3:1D:106:ILE:O	3:1D:108:PRO:HD3	2.20	0.41
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.38	0.41
8:1I:77:LEU:HA	8:1I:77:LEU:HD23	1.81	0.41
14:1S:25:ARG:HB3	14:1S:25:ARG:HH11	1.85	0.41
24:12:17:SER:OG	24:12:20:GLU:OE1	2.18	0.41
32:1a:1030(B):C:H2'	32:1a:1030(C):G:H5'	2.02	0.41
32:1a:1179:A:O3'	40:1i:103:THR:HB	2.20	0.41
33:1b:8:LYS:HB3	33:1b:9:GLU:H	1.63	0.41
34:1c:82:GLU:O	34:1c:85:ARG:HG3	2.21	0.41
37:1f:36:ARG:NH1	37:1f:66:GLU:OE2	2.54	0.41
39:1h:39:LEU:HD12	39:1h:39:LEU:HA	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1l:124:LYS:HA	43:1l:125:PRO:HD3	1.90	0.41
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	2.01	0.41
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.21	0.41
2:2B:22:U:H2'	2:2B:23:G:C8	2.56	0.41
5:2F:165:ARG:HG2	5:2F:168:ARG:NH2	2.35	0.41
8:2I:61:ARG:HD3	8:2I:61:ARG:HA	1.77	0.41
8:2I:82:ARG:NH2	8:2I:90:GLY:H	2.19	0.41
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.19	0.41
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.21	0.41
11:2P:95:VAL:HA	11:2P:99:LEU:HD23	2.03	0.41
14:2S:74:ALA:HB2	14:2S:110:LEU:HD22	2.02	0.41
16:2U:76:TYR:OH	16:2U:92:ARG:NE	2.36	0.41
21:2Z:157:LEU:HD21	21:2Z:163:LEU:HB2	2.02	0.41
32:2a:1294:G:H2'	32:2a:1295:G:H8	1.85	0.41
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.35	0.41
32:2a:1505:G:H2'	53:2v:15:A:OP2	2.19	0.41
33:2b:212:GLN:OE1	33:2b:216:SER:HB3	2.20	0.41
35:2d:61:LYS:HE2	35:2d:61:LYS:HB3	1.90	0.41
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	2.02	0.41
55:2x:71:C:H2'	55:2x:72:A:O4'	2.21	0.41
1:1A:478:A:C6	1:1A:480:A:C6	3.09	0.41
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.21	0.41
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.32	0.41
1:1A:2002:G:OP2	13:1R:9:LYS:NZ	2.51	0.41
1:1A:2118:U:H5	1:1A:2148:G:N3	2.18	0.41
1:1A:2312:U:OP1	6:1G:73:ALA:HA	2.21	0.41
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.20	0.41
1:1A:2563:U:H4'	10:1O:28:SER:HA	2.03	0.41
5:1F:192:LEU:HD22	5:1F:194:MET:HG3	2.02	0.41
7:1H:40:GLU:OE2	7:1H:60:ARG:NH2	2.49	0.41
9:1N:42:TRP:HA	9:1N:48:MET:HE1	2.02	0.41
30:18:58:ILE:HA	30:18:61:LEU:HD12	2.03	0.41
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.20	0.41
33:1b:37:ASN:C	33:1b:39:ILE:N	2.78	0.41
33:1b:64:ARG:H	33:1b:64:ARG:HG2	1.77	0.41
35:1d:196:LEU:C	35:1d:198:VAL:H	2.27	0.41
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	2.03	0.41
42:1k:58:PRO:O	42:1k:93:GLN:HG2	2.20	0.41
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.55	0.41
1:2A:1178:C:P	1:2A:1178:C:H6	2.44	0.41
1:2A:1710:C:H4'	1:2A:2858:C:O2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.21	0.41
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	2.02	0.41
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH22	1.85	0.41
32:2a:237:C:H5''	48:2q:25:ARG:CZ	2.51	0.41
32:2a:413:G:N2	32:2a:428:G:H1'	2.36	0.41
32:2a:620:C:H2'	32:2a:621:A:O4'	2.19	0.41
32:2a:741:G:H2'	32:2a:742:G:O4'	2.21	0.41
32:2a:976:G:OP1	45:2n:32:SER:N	2.53	0.41
32:2a:1259:C:O2'	32:2a:1283:G:N2	2.49	0.41
34:2c:6:HIS:HB3	45:2n:49:HIS:CD2	2.55	0.41
34:2c:108:ASN:HB3	34:2c:111:LEU:HB2	2.02	0.41
34:2c:134:ILE:HG22	34:2c:168:ALA:HB3	2.01	0.41
34:2c:183:ASP:N	34:2c:202:ILE:O	2.46	0.41
36:2e:28:PHE:O	36:2e:47:LYS:HA	2.20	0.41
49:2r:53:ARG:HG2	49:2r:63:GLN:HE21	1.86	0.41
51:2t:10:LEU:HD12	51:2t:10:LEU:HA	1.83	0.41
56:2z:5:MET:HE3	56:2z:5:MET:HB3	1.59	0.41
1:1A:295:G:H4'	20:1Y:1:MET:HE3	2.02	0.41
1:1A:818:G:H4'	1:1A:838:C:O3'	2.20	0.41
1:1A:1073:A:OP2	1:1A:1096:A:H5'	2.21	0.41
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.55	0.41
5:1F:182:ASN:HD21	5:1F:185:ASP:CG	2.27	0.41
6:1G:64:THR:HB	6:1G:94:LEU:HD21	2.03	0.41
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	2.03	0.41
9:1N:123:TYR:HH	9:1N:130:HIS:HE2	1.60	0.41
11:1P:3:LEU:HD23	11:1P:3:LEU:HA	1.91	0.41
11:1P:42:SER:O	62:1P:302:HOH:O	2.22	0.41
32:1a:924:C:O2'	32:1a:1502:A:N1	2.45	0.41
32:1a:1243:C:H2'	32:1a:1244:C:C6	2.56	0.41
35:1d:8:VAL:O	35:1d:11:LEU:HB2	2.21	0.41
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	2.02	0.41
38:1g:79:ARG:HD2	38:1g:80:VAL:N	2.35	0.41
47:1p:43:LYS:HA	47:1p:48:TRP:HB3	2.02	0.41
1:2A:11:G:O5'	1:2A:11:G:H8	2.04	0.41
1:2A:118:A:C8	1:2A:119:A:C8	3.08	0.41
1:2A:271(P):C:H4'	8:2I:42:SER:O	2.21	0.41
1:2A:272(B):G:H2'	1:2A:272(C):G:H8	1.86	0.41
1:2A:411:G:OP2	1:2A:2406:U:O2'	2.36	0.41
1:2A:1372:U:H2'	1:2A:1373:A:O4'	2.21	0.41
1:2A:1394:U:C4	1:2A:1395:A:C5	3.08	0.41
1:2A:1913:A:C6	54:2w:38:A:H5'	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.35	0.41
1:2A:2387:U:H4'	22:20:41:ARG:NH2	2.35	0.41
5:2F:181:LEU:HD11	5:2F:186:ILE:HD11	2.03	0.41
7:2H:124:GLU:HG3	7:2H:132:ARG:HB3	2.03	0.41
11:2P:39:LYS:HG2	62:2P:303:HOH:O	2.20	0.41
14:2S:29:PHE:O	14:2S:35:ILE:HA	2.20	0.41
21:2Z:159:PRO:HA	21:2Z:160:GLY:HA2	1.73	0.41
26:24:1:MET:HE2	26:24:6:HIS:CE1	2.55	0.41
32:2a:187:C:OP1	51:2t:82:SER:OG	2.32	0.41
32:2a:1080:A:H5''	32:2a:1081:G:OP2	2.21	0.41
32:2a:1289:A:OP1	52:2u:9:ARG:NH1	2.50	0.41
34:2c:190:ARG:NE	34:2c:190:ARG:O	2.53	0.41
38:2g:88:PRO:HD2	38:2g:151:TYR:O	2.21	0.41
40:2i:85:LEU:O	40:2i:88:TYR:HB3	2.21	0.41
43:2l:47:LYS:HE2	53:2v:20:U:H4'	2.03	0.41
1:1A:94:C:H2'	1:1A:94(A):G:O4'	2.21	0.41
1:1A:839:U:H1'	1:1A:1191:G:H1'	2.03	0.41
1:1A:870:A:OP1	12:1Q:6:ARG:NH2	2.53	0.41
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.35	0.41
1:1A:1408:C:H2'	1:1A:1409:C:C6	2.56	0.41
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.21	0.41
1:1A:1919:A:O3'	32:1a:1517:G:H1'	2.21	0.41
1:1A:1934:C:H4'	1:1A:1974:C:O3'	2.21	0.41
1:1A:2630:G:H2'	1:1A:2631:G:H8	1.85	0.41
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	2.03	0.41
21:1Z:138:GLU:H	21:1Z:156:LYS:HZ1	1.69	0.41
26:14:34:GLU:HB2	44:1m:57:ARG:CZ	2.51	0.41
32:1a:123:C:OP1	32:1a:312:C:H5'	2.21	0.41
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.19	0.41
35:1d:128:VAL:HB	35:1d:133:VAL:HG21	2.02	0.41
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	2.02	0.41
55:1x:19:G:H4'	55:1x:20:U:OP2	2.21	0.41
1:2A:562:U:H6	1:2A:562:U:H2'	1.73	0.41
1:2A:1272:A:H3'	1:2A:1273:U:H5''	2.03	0.41
1:2A:1388:G:H2'	1:2A:1389:G:C8	2.56	0.41
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.21	0.41
2:2B:17:C:H2'	2:2B:18:G:O4'	2.21	0.41
4:2E:109:LYS:O	4:2E:111:ARG:NH1	2.53	0.41
6:2G:11:TYR:OH	6:2G:33:ARG:HG2	2.20	0.41
7:2H:102:ALA:HB2	7:2H:116:GLU:HG3	2.02	0.41
10:2O:111:PHE:O	10:2O:115:VAL:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:20:LEU:HD12	17:2V:20:LEU:HA	1.80	0.41
21:2Z:53:ILE:HD11	21:2Z:99:TYR:HB2	2.02	0.41
26:24:14:ILE:HA	26:24:31:ILE:O	2.21	0.41
28:26:38:LYS:HE3	28:26:38:LYS:HB3	1.90	0.41
32:2a:266:G:O3'	48:2q:67:LYS:HB2	2.21	0.41
32:2a:866:C:C4	32:2a:867:G:H1'	2.56	0.41
32:2a:1298:C:H2'	38:2g:114:ARG:NH2	2.36	0.41
32:2a:1381:U:O2	38:2g:79:ARG:HB3	2.20	0.41
32:2a:1504:G:H4'	32:2a:1505:G:C4	2.55	0.41
38:2g:153:HIS:ND1	42:2k:58:PRO:HD2	2.36	0.41
50:2s:50:ALA:O	50:2s:57:HIS:ND1	2.52	0.41
54:2w:18:G:H4'	54:2w:60:U:C5	2.55	0.41
1:1A:53:A:H2'	1:1A:54:G:O4'	2.20	0.41
1:1A:245:G:O5'	11:1P:73:GLY:HA2	2.20	0.41
1:1A:675:A:C8	1:1A:804:A:C6	3.09	0.41
1:1A:1022:G:C6	1:1A:1141:U:C5	3.08	0.41
1:1A:1058:G:H4'	1:1A:1058:G:OP1	2.20	0.41
1:1A:2313:C:H4'	6:1G:91:ARG:HG3	2.02	0.41
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.62	0.41
8:1I:61:ARG:HA	8:1I:61:ARG:HD3	1.83	0.41
8:1I:101:LEU:HD21	8:1I:140:LEU:HD11	2.03	0.41
11:1P:1:MET:HE2	11:1P:1:MET:HB2	1.75	0.41
11:1P:88:LEU:HD11	11:1P:114:ILE:HD13	2.03	0.41
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.82	0.41
13:1R:79:LEU:HA	13:1R:83:ILE:HG13	2.03	0.41
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.56	0.41
32:1a:67:C:H2'	32:1a:68:G:C8	2.55	0.41
32:1a:397:A:H3'	32:1a:397:A:N3	2.36	0.41
32:1a:580:U:H2'	32:1a:581:G:O4'	2.21	0.41
32:1a:685:G:C2	32:1a:686:U:C4	3.09	0.41
34:1c:58:GLU:HB3	41:1j:92:THR:HG21	2.02	0.41
34:1c:71:ALA:O	34:1c:73:PRO:HD3	2.21	0.41
34:1c:101:LEU:HD12	34:1c:102:ASN:H	1.85	0.41
34:1c:131:ARG:NH1	34:1c:167:TRP:O	2.45	0.41
34:1c:173:VAL:HG12	34:1c:175:LEU:HD22	2.02	0.41
35:1d:150:GLU:C	35:1d:152:SER:H	2.29	0.41
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.54	0.41
38:1g:57:GLU:OE1	38:1g:59:LEU:HB3	2.21	0.41
55:1x:19:G:H3'	55:1x:20:U:C5	2.56	0.41
55:1x:21:A:H3'	55:1x:46:G:O6	2.20	0.41
1:2A:443:A:H5''	1:2A:444:C:OP1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:631:A:H2'	1:2A:632:A:O4'	2.20	0.41
1:2A:856:C:N4	62:2A:3930:HOH:O	2.53	0.41
1:2A:892:G:H3'	1:2A:893:C:H5''	2.03	0.41
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.55	0.41
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.20	0.41
1:2A:1926:U:H2'	1:2A:1928:A:OP2	2.20	0.41
1:2A:2134:A:H62	1:2A:2157:G:C4'	2.34	0.41
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.20	0.41
1:2A:2370:G:H2'	1:2A:2371:G:C8	2.56	0.41
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.56	0.41
1:2A:2625:G:H2'	1:2A:2626:C:O4'	2.21	0.41
2:2B:14:U:OP2	2:2B:70:C:O2'	2.39	0.41
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.55	0.41
9:2N:26:LEU:HD23	9:2N:60:ILE:HD11	2.02	0.41
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	2.03	0.41
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CD1	2.56	0.41
14:2S:93:LYS:HB2	14:2S:93:LYS:HE2	1.88	0.41
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.35	0.41
20:2Y:52:SER:OG	20:2Y:55:TYR:HB2	2.20	0.41
22:20:18:ALA:HB3	22:20:20:ARG:NH1	2.36	0.41
32:2a:35:G:H2'	32:2a:36:C:C6	2.56	0.41
32:2a:329:A:C5	32:2a:332:G:C6	3.09	0.41
32:2a:396:G:O2'	32:2a:398:C:OP1	2.33	0.41
32:2a:1264:C:C4	32:2a:1272:G:O6	2.73	0.41
32:2a:1380:U:C4	38:2g:3:ARG:HG2	2.55	0.41
34:2c:54:ARG:O	34:2c:69:HIS:ND1	2.53	0.41
36:2e:88:LYS:HB3	36:2e:123:LEU:HB2	2.02	0.41
38:2g:22:LEU:HG	38:2g:62:PHE:CE2	2.56	0.41
40:2i:8:GLY:HA3	40:2i:76:ALA:O	2.21	0.41
41:2j:49:VAL:CG2	45:2n:41:ARG:HB2	2.50	0.41
42:2k:17:GLY:O	42:2k:80:VAL:HA	2.20	0.41
42:2k:33:THR:HG22	42:2k:39:PRO:HA	2.02	0.41
46:2o:40:SER:O	46:2o:44:LYS:HG3	2.21	0.41
50:2s:30:LEU:HD13	50:2s:48:THR:OG1	2.21	0.41
57:2y:7:A:N6	57:2y:65:G:H1	2.19	0.41
1:1A:1252:G:N3	16:1U:33:ARG:HG2	2.36	0.41
1:1A:1550:C:H4'	1:1A:1743:C:O2	2.21	0.41
1:1A:2354:G:O2'	62:1A:4223:HOH:O	2.10	0.41
1:1A:2646:C:OP1	62:1A:4261:HOH:O	2.22	0.41
1:1A:2648:C:H2'	1:1A:2649:U:C6	2.56	0.41
5:1F:110:LEU:HD11	5:1F:181:LEU:HG	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.55	0.41
32:1a:51:A:N7	32:1a:114:U:O2'	2.53	0.41
32:1a:390:C:H2'	32:1a:391:G:C8	2.55	0.41
32:1a:434:U:H2'	32:1a:435:C:C6	2.56	0.41
32:1a:995:C:H1'	45:1n:4:LYS:HE2	2.03	0.41
32:1a:1148:U:O4'	40:1i:16:ARG:HD2	2.20	0.41
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.55	0.41
57:1y:19:G:C2	57:1y:56:C:N3	2.89	0.41
1:2A:27:G:O2'	1:2A:28:A:OP2	2.36	0.41
1:2A:455:C:N3	1:2A:472:A:H2'	2.35	0.41
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.69	0.41
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.56	0.41
1:2A:1657:C:H2'	1:2A:1658:C:H6	1.86	0.41
1:2A:1814:G:C4'	3:2D:51:VAL:HG21	2.51	0.41
1:2A:2119:A:C2	1:2A:2170:A:H2'	2.56	0.41
1:2A:2344:U:OP1	28:26:37:ARG:HD3	2.20	0.41
1:2A:2747:G:O2'	7:2H:67:LEU:HD12	2.21	0.41
5:2F:197:ASP:OD1	5:2F:198:ALA:N	2.54	0.41
8:2I:4:ILE:HD11	8:2I:44:LEU:HD13	2.03	0.41
8:2I:69:LYS:NZ	8:2I:137:PRO:O	2.43	0.41
15:2T:107:ASP:O	15:2T:111:ARG:HG3	2.21	0.41
19:2X:94:GLY:N	19:2X:95:LEU:HB2	2.36	0.41
24:22:1:MET:H1	24:22:52:ASP:CG	2.28	0.41
26:24:67:TYR:HD2	50:2s:9:VAL:HB	1.85	0.41
32:2a:35:G:O2'	43:2l:118:SER:O	2.31	0.41
32:2a:325:A:H2'	32:2a:326:G:O4'	2.20	0.41
32:2a:1005:A:H3'	32:2a:1006:C:H6	1.82	0.41
34:2c:53:ALA:HB2	34:2c:115:LEU:HD11	2.02	0.41
38:2g:42:ILE:HG22	38:2g:120:ILE:HD12	2.03	0.41
53:2v:22:U:H2'	53:2v:23:A:H8	1.84	0.41
1:1A:1814:G:C6	1:1A:1815:A:C6	3.09	0.40
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.57	0.40
5:1F:41:LEU:O	5:1F:44:ARG:HG2	2.21	0.40
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	2.03	0.40
16:1U:49:HIS:HA	16:1U:52:ARG:HB2	2.02	0.40
19:1X:94:GLY:H	19:1X:95:LEU:C	2.28	0.40
32:1a:115:G:H4'	32:1a:116:A:O5'	2.21	0.40
32:1a:375:U:C4	32:1a:376:G:N7	2.90	0.40
32:1a:619:U:O2	35:1d:133:VAL:HA	2.21	0.40
32:1a:748:C:H6	32:1a:748:C:O5'	2.04	0.40
32:1a:953:G:H2'	32:1a:954:G:O4'	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:35:GLU:CD	34:1c:59:ARG:HH12	2.27	0.40
34:1c:110:ASN:ND2	34:1c:140:ARG:HB3	2.36	0.40
37:1f:12:PRO:HG3	37:1f:57:GLN:O	2.21	0.40
40:1i:18:PHE:O	40:1i:61:ALA:HA	2.20	0.40
48:1q:7:THR:O	48:1q:23:VAL:HG13	2.21	0.40
1:2A:83:G:N1	1:2A:102:G:O2'	2.40	0.40
1:2A:811:U:H2'	11:2P:21:ARG:HA	2.02	0.40
1:2A:1125:G:H5'	31:29:37:GLY:HA2	2.02	0.40
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.20	0.40
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.21	0.40
1:2A:2784:C:H1'	4:2E:37:ARG:NH1	2.35	0.40
2:2B:3:C:H2'	2:2B:4:C:H6	1.86	0.40
2:2B:14:U:H1'	2:2B:108:U:O2'	2.22	0.40
5:2F:24:LEU:HD12	5:2F:24:LEU:HA	1.96	0.40
15:2T:74:ARG:HG2	15:2T:76:PHE:CZ	2.55	0.40
16:2U:69:CYS:HB3	16:2U:74:LEU:HD13	2.03	0.40
21:2Z:100:VAL:HA	21:2Z:101:PRO:HD3	1.92	0.40
32:2a:143:A:O2'	32:2a:144:G:OP2	2.34	0.40
32:2a:408:A:H2'	32:2a:409:G:O4'	2.21	0.40
32:2a:576:G:O6	32:2a:880:C:O2'	2.31	0.40
32:2a:892:A:O2'	32:2a:1415:G:H4'	2.21	0.40
32:2a:977:A:O3'	32:2a:980:C:N4	2.54	0.40
32:2a:1016:A:N6	32:2a:1017:G:C2	2.89	0.40
35:2d:114:ARG:HA	35:2d:117:ALA:HB3	2.03	0.40
38:2g:63:LYS:HE3	38:2g:63:LYS:HB2	1.97	0.40
41:2j:42:THR:HG22	41:2j:66:ARG:HB2	2.02	0.40
51:2t:93:GLU:H	51:2t:93:GLU:HG3	1.70	0.40
1:1A:189:G:O6	1:1A:205:G:O2'	2.37	0.40
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.20	0.40
1:1A:2128:C:H6	1:1A:2128:C:O5'	2.04	0.40
1:1A:2583:G:H2'	1:1A:2584:U:O4'	2.21	0.40
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.54	0.40
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.46	0.40
4:1E:96:PHE:O	4:1E:175:VAL:HG21	2.22	0.40
14:1S:77:ALA:HB3	14:1S:110:LEU:HD11	2.03	0.40
17:1V:71:LEU:HD23	17:1V:71:LEU:HA	1.86	0.40
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	2.05	0.40
32:1a:319:G:H2'	32:1a:320:C:O4'	2.22	0.40
32:1a:413:G:O6	35:1d:35:ARG:HD3	2.22	0.40
32:1a:1305:G:O2'	32:1a:1306:A:OP2	2.38	0.40
47:1p:14:ASN:HA	47:1p:42:ARG:NH2	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.56	0.40
1:2A:466:A:H5'	29:27:21:ARG:NH2	2.35	0.40
1:2A:856:C:HO2'	1:2A:857:C:P	2.43	0.40
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.86	0.40
1:2A:1803:A:N1	1:2A:1822:G:O2'	2.44	0.40
1:2A:2133:G:N2	1:2A:2157:G:C8	2.90	0.40
1:2A:2151:G:H2'	1:2A:2152:G:O4'	2.20	0.40
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.22	0.40
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.54	0.40
5:2F:157:VAL:HG12	5:2F:198:ALA:HB1	2.03	0.40
6:2G:43:LEU:HD13	6:2G:43:LEU:HA	1.83	0.40
6:2G:148:MET:HE2	6:2G:148:MET:HB3	1.88	0.40
11:2P:94:GLU:HG2	11:2P:95:VAL:H	1.87	0.40
12:2Q:110:THR:HB	12:2Q:113:GLN:H	1.86	0.40
14:2S:33:LYS:HB2	14:2S:34:HIS:HD2	1.86	0.40
24:22:51:ARG:O	24:22:55:ARG:HG2	2.21	0.40
25:23:4:LEU:HD23	25:23:4:LEU:HA	1.91	0.40
32:2a:1107:C:C4	32:2a:1108:G:C8	3.09	0.40
32:2a:1290:G:H2'	32:2a:1291:G:H8	1.86	0.40
32:2a:1478:C:H2'	32:2a:1479:C:C6	2.57	0.40
48:2q:66:SER:OG	48:2q:69:LYS:HB2	2.20	0.40
50:2s:80:TYR:C	50:2s:82:GLY:H	2.27	0.40
54:2w:2:C:H2'	54:2w:3:C:C6	2.56	0.40
1:1A:81:G:H21	20:1Y:1:MET:CE	2.33	0.40
1:1A:857:C:N4	1:1A:858:U:O4	2.54	0.40
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.22	0.40
1:1A:2302:G:C2	1:1A:2315:G:C2	3.08	0.40
1:1A:2854:G:H2'	1:1A:2855:C:C6	2.57	0.40
5:1F:106:ARG:H	5:1F:106:ARG:HG2	1.70	0.40
6:1G:76:SER:C	6:1G:77:ILE:HG13	2.47	0.40
6:1G:115:ARG:HG2	6:1G:136:ARG:HH22	1.86	0.40
11:1P:59:LEU:HD11	30:18:10:ALA:HA	2.03	0.40
21:1Z:30:ASN:HA	21:1Z:89:PHE:HE1	1.87	0.40
22:10:18:ALA:HB3	22:10:20:ARG:NH1	2.35	0.40
25:13:26:LEU:HD22	25:13:37:LEU:HD13	2.03	0.40
32:1a:1277:C:O2'	32:1a:1279:A:H8	2.04	0.40
34:1c:177:THR:HG22	34:1c:180:ALA:H	1.85	0.40
40:1i:13:ALA:HB2	40:1i:68:GLY:HA3	2.02	0.40
40:1i:50:LEU:HB3	40:1i:85:LEU:HD11	2.03	0.40
41:1j:46:ARG:HB2	41:1j:46:ARG:NH1	2.33	0.40
50:1s:23:ASN:HA	50:1s:27:GLU:OE1	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1t:57:ARG:HH22	51:1t:100:ILE:HD12	1.87	0.40
57:1y:55:PSU:O5'	57:1y:55:PSU:H6	2.04	0.40
1:2A:634:C:H2'	1:2A:635:C:C6	2.56	0.40
1:2A:664:C:H2'	1:2A:665:C:H6	1.87	0.40
1:2A:699:A:H2'	1:2A:700:G:O4'	2.22	0.40
1:2A:942:G:O2'	1:2A:1189:A:N3	2.54	0.40
1:2A:1470:G:H5''	1:2A:1471:A:OP1	2.21	0.40
1:2A:2136:C:N3	1:2A:2155:G:N2	2.56	0.40
1:2A:2712:U:O2'	1:2A:2713:A:H5'	2.21	0.40
2:2B:83:G:H5''	25:23:52:HIS:CD2	2.56	0.40
8:2I:101:LEU:HB2	8:2I:107:VAL:CB	2.49	0.40
10:2O:88:ASN:OD1	10:2O:92:GLU:HB3	2.22	0.40
32:2a:114:U:H2'	32:2a:115:G:H8	1.85	0.40
32:2a:216:G:H2'	32:2a:217:C:O4'	2.21	0.40
32:2a:1077:G:N1	32:2a:1080:A:OP2	2.49	0.40
33:2b:16:HIS:C	33:2b:18:GLY:N	2.78	0.40
33:2b:51:LEU:O	33:2b:55:PHE:HB2	2.21	0.40
34:2c:172:ARG:HH21	34:2c:174:PRO:HG3	1.86	0.40
40:2i:23:ASN:HD21	40:2i:25:LYS:HE2	1.86	0.40
57:2y:52:G:H8	57:2y:52:G:OP2	2.03	0.40
1:1A:388:G:O2'	1:1A:389:G:N7	2.49	0.40
1:1A:674:G:H1'	5:1F:74:ARG:CD	2.52	0.40
1:1A:1721:G:H3'	1:1A:1722:A:H5''	2.03	0.40
1:1A:2296:U:OP2	14:1S:6:ALA:HB2	2.21	0.40
1:1A:2808:U:H5''	1:1A:2891:G:O6	2.21	0.40
1:1A:2820:A:O2'	1:1A:2821:A:OP1	2.38	0.40
7:1H:119:GLU:O	7:1H:140:LYS:NZ	2.39	0.40
10:1O:59:LYS:NZ	10:1O:89:ASN:OD1	2.52	0.40
15:1T:13:ARG:HE	15:1T:13:ARG:HB3	1.64	0.40
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.56	0.40
31:19:25:VAL:HB	31:19:34:GLN:HB2	2.03	0.40
32:1a:688:G:H5'	42:1k:46:GLY:C	2.47	0.40
32:1a:1131:G:O5'	32:1a:1131:G:H8	2.04	0.40
33:1b:103:THR:HG23	33:1b:176:GLU:HB3	2.03	0.40
44:1m:9:ILE:HB	44:1m:18:ALA:HB1	2.04	0.40
44:1m:20:THR:C	44:1m:22:ILE:H	2.29	0.40
57:1y:5:G:C2	57:1y:6:G:C4	3.10	0.40
1:2A:93:G:H2'	1:2A:94:C:H6	1.84	0.40
1:2A:272(D):G:C2	1:2A:272(E):G:C8	3.10	0.40
1:2A:288:C:H2'	1:2A:289:A:H8	1.86	0.40
1:2A:995:C:O2	9:2N:3:THR:OG1	2.33	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1179:C:H2'	1:2A:1180:C:C6	2.57	0.40
1:2A:1336:A:H2'	1:2A:1337:G:H8	1.85	0.40
1:2A:1388:G:H2'	1:2A:1389:G:H8	1.86	0.40
1:2A:1528:A:H2'	1:2A:1528(A):A:C8	2.56	0.40
1:2A:1636:C:H4'	1:2A:1761:C:O4'	2.21	0.40
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.22	0.40
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.20	0.40
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.55	0.40
62:2A:4313:HOH:O	4:2E:167:VAL:HG11	2.20	0.40
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	2.03	0.40
6:2G:39:ILE:HD11	6:2G:102:PHE:CZ	2.56	0.40
6:2G:51:ARG:HD2	6:2G:51:ARG:H	1.85	0.40
15:2T:122:ASP:HA	15:2T:125:ARG:HG2	2.04	0.40
23:21:85:LEU:HD22	23:21:89:GLU:HG2	2.03	0.40
25:23:8:LEU:HG	25:23:31:LEU:HD22	2.03	0.40
32:2a:44:G:C2	32:2a:45:U:H1'	2.57	0.40
32:2a:406:G:O2'	35:2d:3:ARG:NH2	2.54	0.40
32:2a:407:G:H2'	32:2a:408:A:H8	1.87	0.40
32:2a:923:A:O2'	32:2a:1399:C:OP2	2.39	0.40
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.36	0.40
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.22	0.40
34:2c:9:GLY:HA2	34:2c:12:LEU:HG	2.02	0.40
35:2d:17:VAL:HG11	35:2d:197:PRO:CG	2.52	0.40
36:2e:95:ALA:C	36:2e:97:GLY:H	2.29	0.40
42:2k:48:ILE:O	42:2k:50:TYR:N	2.46	0.40
50:2s:38:SER:HB2	50:2s:71:LEU:HD12	2.03	0.40
57:2y:18:G:H1'	57:2y:57:G:O6	2.22	0.40
1:1A:150:C:O2'	1:1A:151:C:H5'	2.21	0.40
1:1A:226:G:N2	1:1A:228:A:H62	2.18	0.40
1:1A:773:U:H2'	1:1A:774:A:H5'	2.02	0.40
1:1A:942:G:H4'	1:1A:1190:G:H5'	2.04	0.40
1:1A:1509:C:H3'	1:1A:1509:C:OP1	2.21	0.40
1:1A:1526:G:C6	1:1A:1527:G:C2	3.09	0.40
1:1A:2161:C:O2'	1:1A:2162:G:H8	2.04	0.40
1:1A:2169:A:H1'	57:1y:56:C:H5'	2.03	0.40
1:1A:2336:A:H61	22:10:43:THR:CG2	2.35	0.40
1:1A:2556:C:H2'	1:1A:2557:G:O4'	2.22	0.40
1:1A:2712:U:H2'	1:1A:2714:G:H5''	2.04	0.40
17:1V:2:PHE:CE2	17:1V:41:GLY:HA3	2.56	0.40
32:1a:186:C:H5'	51:1t:78:ALA:HB1	2.03	0.40
32:1a:236:G:H5''	48:1q:42:TYR:OH	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:328:C:H4'	32:1a:329:A:H5'	2.04	0.40
32:1a:769:G:H4'	32:1a:1513:A:H4'	2.04	0.40
32:1a:975:A:N6	32:1a:1367:C:O4'	2.55	0.40
32:1a:1005:A:OP2	32:1a:1024:G:N2	2.55	0.40
35:1d:19:LEU:O	35:1d:21:LEU:N	2.54	0.40
42:1k:59:TYR:CE2	42:1k:63:LEU:HD11	2.57	0.40
48:1q:11:VAL:HG12	48:1q:85:VAL:HG13	2.02	0.40
1:2A:302:C:OP2	20:2Y:73:ARG:NH1	2.48	0.40
1:2A:911:A:N6	12:2Q:9:TYR:HB3	2.36	0.40
1:2A:1983:C:H2'	1:2A:1984:G:H5''	2.04	0.40
1:2A:2251:OMG:H1'	1:2A:2251:OMG:HM23	1.80	0.40
1:2A:2728:U:H5'	10:2O:70:LYS:NZ	2.36	0.40
2:2B:73:A:C6	2:2B:74:U:C2	3.10	0.40
9:2N:131:GLN:H	9:2N:131:GLN:HG2	1.57	0.40
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.57	0.40
21:2Z:146:ILE:HG23	21:2Z:174:VAL:C	2.47	0.40
31:29:3:VAL:HA	31:29:35:ARG:O	2.22	0.40
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.56	0.40
32:2a:200:G:H2'	32:2a:201:C:O4'	2.22	0.40
32:2a:985:C:H2'	32:2a:986:A:H8	1.85	0.40
32:2a:994:A:N7	32:2a:1216:G:H4'	2.37	0.40
34:2c:69:HIS:HA	34:2c:104:GLN:HB3	2.04	0.40
41:2j:38:ILE:HG12	41:2j:71:LEU:O	2.21	0.40
42:2k:69:ALA:O	42:2k:73:MET:HG3	2.21	0.40
50:2s:52:TYR:HB2	50:2s:57:HIS:CE1	2.57	0.40
51:2t:72:LEU:HD12	51:2t:72:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24	31
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	31
5	1F	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
5	2F	200/210 (95%)	187 (94%)	10 (5%)	3 (2%)	8	8
6	1G	179/182 (98%)	165 (92%)	14 (8%)	0	100	100
6	2G	179/182 (98%)	158 (88%)	19 (11%)	2 (1%)	11	13
7	1H	172/180 (96%)	165 (96%)	6 (4%)	1 (1%)	21	27
7	2H	172/180 (96%)	146 (85%)	24 (14%)	2 (1%)	10	12
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	18	23
8	2I	144/148 (97%)	119 (83%)	23 (16%)	2 (1%)	9	9
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	23
10	1O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	20
10	2O	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	20
11	1P	147/150 (98%)	136 (92%)	10 (7%)	1 (1%)	18	23
11	2P	147/150 (98%)	127 (86%)	15 (10%)	5 (3%)	3	2
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	103 (95%)	3 (3%)	2 (2%)	6	5
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	15
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	15
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	11	13
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	131 (88%)	16 (11%)	1 (1%)	18	23
21	2Z	156/206 (76%)	128 (82%)	23 (15%)	5 (3%)	3	2
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11	13
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	1 (2%)	1 (2%)	8	8
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	6	6
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	0
26	24	67/71 (94%)	51 (76%)	14 (21%)	2 (3%)	3	2
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	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%)	196 (86%)	27 (12%)	6 (3%)	4	3
33	2b	229/256 (90%)	196 (86%)	29 (13%)	4 (2%)	7	7
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	180 (88%)	22 (11%)	2 (1%)	12	15
35	1d	206/209 (99%)	190 (92%)	16 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	188 (91%)	18 (9%)	0	100	100
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	9	9
36	2e	146/162 (90%)	130 (89%)	12 (8%)	4 (3%)	4	3
37	1f	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	12	15
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	18	23
38	2g	153/156 (98%)	133 (87%)	17 (11%)	3 (2%)	6	5
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
40	1i	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	16	20
40	2i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	16	20
41	1j	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	3	2
41	2j	94/105 (90%)	77 (82%)	15 (16%)	2 (2%)	5	4
42	1k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14	17
42	2k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	6	6
43	1l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16	20
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16	20
44	1m	121/126 (96%)	102 (84%)	17 (14%)	2 (2%)	7	7
44	2m	120/126 (95%)	104 (87%)	14 (12%)	2 (2%)	7	7
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	12
47	1p	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
48	2q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	12	15
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	65 (80%)	14 (17%)	2 (2%)	4	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	5	4
51	2t	94/106 (89%)	84 (89%)	9 (10%)	1 (1%)	11	13
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
56	1z	5/7 (71%)	4 (80%)	0	1 (20%)	0	0
56	2z	5/7 (71%)	4 (80%)	0	1 (20%)	0	0
All	All	11378/12142 (94%)	10471 (92%)	817 (7%)	90 (1%)	16	20

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	1Z	53	ILE
26	14	47	GLN
26	14	62	ARG
33	1b	17	PHE
33	1b	124	SER
42	1k	49	GLY
44	1m	67	GLU
44	1m	107	ALA
56	1z	2	THR
5	2F	130	ALA
33	2b	17	PHE
33	2b	20	GLU
33	2b	123	ALA
33	2b	126	GLU
34	2c	179	ARG
38	2g	80	VAL
8	1I	11	ASN
19	1X	93	GLU
26	14	53	GLU
33	1b	126	GLU
40	1i	54	ASP
51	1t	96	GLY
6	2G	42	GLY
6	2G	43	LEU
8	2I	10	GLU
11	2P	38	GLN
21	2Z	146	ILE
23	21	3	LYS
26	24	45	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	2g	55	GLY
41	2j	75	ILE
44	2m	67	GLU
44	2m	106	ASN
46	2o	88	ARG
48	2q	68	ARG
50	2s	9	VAL
50	2s	81	ARG
4	1E	52	LEU
7	1H	126	PRO
26	14	49	PHE
33	1b	8	LYS
41	1j	78	ASN
7	2H	126	PRO
10	2O	29	ASN
14	2S	84	GLN
21	2Z	93	ASP
36	2e	98	THR
42	2k	106	LYS
56	2z	2	THR
17	1V	79	VAL
33	1b	125	PRO
41	1j	77	PRO
41	1j	79	ARG
43	1l	105	TYR
4	2E	52	LEU
5	2F	18	ARG
5	2F	21	ALA
8	2I	41	GLU
9	2N	2	LYS
11	2P	29	LYS
11	2P	36	LYS
11	2P	45	LEU
21	2Z	52	SER
24	22	43	GLN
26	24	47	GLN
36	2e	69	VAL
43	2l	91	LYS
10	1O	5	GLN
11	1P	45	LEU
14	2S	96	GLY
17	2V	79	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2e	11	ILE
38	2g	52	GLU
40	2i	56	LEU
41	2j	78	ASN
33	1b	231	GLU
36	1e	69	VAL
36	1e	96	PRO
38	1g	55	GLY
11	2P	122	PRO
21	2Z	144	LEU
34	2c	156	ARG
21	2Z	167	PRO
7	2H	92	ILE
36	2e	96	PRO
51	1t	100	ILE
51	2t	102	GLY
37	1f	40	VAL
25	23	59	VAL
42	2k	105	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	204 (95%)	11 (5%)	21	32
3	2D	215/218 (99%)	202 (94%)	13 (6%)	17	25
4	1E	164/166 (99%)	153 (93%)	11 (7%)	15	21
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15	21
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6	8
5	2F	159/166 (96%)	147 (92%)	12 (8%)	12	17
6	1G	143/156 (92%)	132 (92%)	11 (8%)	12	16
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5	6
7	1H	144/148 (97%)	136 (94%)	8 (6%)	19	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	2H	144/148 (97%)	131 (91%)	13 (9%)	9	12
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	2
8	2I	105/124 (85%)	85 (81%)	20 (19%)	1	1
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	16
9	2N	118/119 (99%)	106 (90%)	12 (10%)	7	8
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	42
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36	53
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8	10
11	2P	115/116 (99%)	102 (89%)	13 (11%)	5	7
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13	18
12	2Q	111/111 (100%)	110 (99%)	1 (1%)	70	84
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11	15
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14	20
14	1S	86/88 (98%)	83 (96%)	3 (4%)	32	48
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	6
15	1T	115/127 (91%)	112 (97%)	3 (3%)	40	59
15	2T	113/127 (89%)	102 (90%)	11 (10%)	8	10
16	1U	93/94 (99%)	88 (95%)	5 (5%)	20	29
16	2U	93/94 (99%)	86 (92%)	7 (8%)	12	17
17	1V	80/82 (98%)	73 (91%)	7 (9%)	9	12
17	2V	80/82 (98%)	68 (85%)	12 (15%)	3	3
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15	21
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	12
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61	77
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	59
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	13	19
20	2Y	85/91 (93%)	70 (82%)	15 (18%)	2	2
21	1Z	135/179 (75%)	122 (90%)	13 (10%)	8	10
21	2Z	137/179 (76%)	115 (84%)	22 (16%)	2	2
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	64 (98%)	1 (2%)	57	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	11	80/83 (96%)	79 (99%)	1 (1%)	61	77
23	21	80/83 (96%)	75 (94%)	5 (6%)	16	23
24	12	65/67 (97%)	58 (89%)	7 (11%)	6	7
24	22	65/67 (97%)	61 (94%)	4 (6%)	16	24
25	13	51/52 (98%)	48 (94%)	3 (6%)	18	26
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	25
26	14	59/63 (94%)	47 (80%)	12 (20%)	1	1
26	24	53/63 (84%)	46 (87%)	7 (13%)	4	4
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	15
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	15
28	16	51/52 (98%)	45 (88%)	6 (12%)	5	6
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	3
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	18
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	10
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	28
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	45
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	55
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	55
33	1b	192/220 (87%)	164 (85%)	28 (15%)	3	3
33	2b	187/220 (85%)	155 (83%)	32 (17%)	2	2
34	1c	142/188 (76%)	131 (92%)	11 (8%)	12	16
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4	4
35	1d	169/181 (93%)	140 (83%)	29 (17%)	2	2
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	11
36	1e	113/123 (92%)	107 (95%)	6 (5%)	20	30
36	2e	114/123 (93%)	107 (94%)	7 (6%)	17	24
37	1f	84/90 (93%)	73 (87%)	11 (13%)	4	4
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	8
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5	6
38	2g	120/127 (94%)	107 (89%)	13 (11%)	6	7
39	1h	114/119 (96%)	105 (92%)	9 (8%)	11	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	2h	114/119 (96%)	100 (88%)	14 (12%)	4	5
40	1i	90/99 (91%)	77 (86%)	13 (14%)	3	3
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	9
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6	8
41	2j	69/92 (75%)	60 (87%)	9 (13%)	4	4
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	7
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	7
43	1l	96/108 (89%)	93 (97%)	3 (3%)	35	52
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26	40
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5	6
44	2m	92/101 (91%)	83 (90%)	9 (10%)	7	10
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	14
45	2n	49/50 (98%)	47 (96%)	2 (4%)	27	41
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9	12
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	32
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	4
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	8
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20	30
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20	30
49	1r	59/77 (77%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21	32
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9	12
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	6
51	1t	70/82 (85%)	64 (91%)	6 (9%)	10	13
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	27
52	1u	18/22 (82%)	15 (83%)	3 (17%)	2	2
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	28
56	1z	6/6 (100%)	5 (83%)	1 (17%)	2	2
56	2z	6/6 (100%)	5 (83%)	1 (17%)	2	2
All	All	9315/10076 (92%)	8491 (91%)	824 (9%)	9	12

All (824) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	14	ARG
3	1D	38	LYS
3	1D	99	ASP
3	1D	142	VAL
3	1D	154	LYS
3	1D	173	VAL
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
4	1E	7	VAL
4	1E	12	THR
4	1E	47	VAL
4	1E	55	ASN
4	1E	78	LEU
4	1E	87	GLU
4	1E	89	ASP
4	1E	90	THR
4	1E	93	VAL
4	1E	116	VAL
4	1E	184	VAL
5	1F	9	ILE
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	88	VAL
5	1F	106	ARG
5	1F	127	GLU
5	1F	132	VAL
5	1F	140	LEU
5	1F	158	THR
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	22	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	1G	31	VAL
6	1G	36	LYS
6	1G	43	LEU
6	1G	60	LEU
6	1G	91	ARG
6	1G	140	ILE
6	1G	159	VAL
7	1H	49	VAL
7	1H	50	VAL
7	1H	76	VAL
7	1H	92	ILE
7	1H	98	LEU
7	1H	116	GLU
7	1H	127	GLU
7	1H	160	LYS
8	1I	6	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	27	ARG
8	1I	38	LEU
8	1I	47	LEU
8	1I	61	ARG
8	1I	77	LEU
8	1I	85	GLU
8	1I	86	THR
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	102	SER
8	1I	109	ILE
8	1I	123	LEU
8	1I	127	VAL
8	1I	129	THR
8	1I	140	LEU
9	1N	1	MET
9	1N	9	VAL
9	1N	28	THR
9	1N	46	VAL
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	71	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	1N	84	LYS
10	1O	22	ILE
10	1O	28	SER
10	1O	42	SER
10	1O	112	MET
11	1P	1	MET
11	1P	45	LEU
11	1P	56	SER
11	1P	65	ARG
11	1P	95	VAL
11	1P	96	THR
11	1P	98	GLU
11	1P	100	LEU
11	1P	101	VAL
11	1P	114	ILE
11	1P	147	LEU
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	18	LYS
12	1Q	56	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	115	MET
12	1Q	133	ARG
13	1R	24	GLN
13	1R	36	THR
13	1R	44	LEU
13	1R	83	ILE
13	1R	100	LEU
13	1R	102	GLU
13	1R	111	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	25	ARG
14	1S	69	VAL
15	1T	28	VAL
15	1T	96	ARG
15	1T	128	GLU
16	1U	17	ILE
16	1U	74	LEU
16	1U	95	LEU
16	1U	100	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1U	108	GLU
17	1V	46	VAL
17	1V	53	GLU
17	1V	61	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	95	LEU
17	1V	100	ARG
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	24	ILE
18	1W	67	ASP
19	1X	37	THR
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	31	LEU
20	1Y	72	VAL
20	1Y	92	ASN
20	1Y	106	LEU
21	1Z	42	VAL
21	1Z	53	ILE
21	1Z	61	LEU
21	1Z	69	THR
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	119	GLU
21	1Z	124	ILE
21	1Z	139	VAL
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
23	11	59	THR
24	12	1	MET
24	12	19	VAL
24	12	24	LEU
24	12	28	LYS
24	12	41	ILE
24	12	53	LEU
24	12	55	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	13	23	LEU
25	13	37	LEU
25	13	54	VAL
26	14	1	MET
26	14	5	ILE
26	14	14	ILE
26	14	35	VAL
26	14	46	GLN
26	14	47	GLN
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	61	ARG
26	14	63	TYR
26	14	67	TYR
27	15	6	VAL
27	15	35	GLU
27	15	40	LYS
27	15	59	GLU
28	16	4	GLU
28	16	6	ARG
28	16	7	ILE
28	16	9	LEU
28	16	28	ARG
28	16	47	THR
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	50	LEU
31	19	4	ARG
33	1b	12	GLU
33	1b	20	GLU
33	1b	21	ARG
33	1b	35	GLU
33	1b	37	ASN
33	1b	39	ILE
33	1b	44	LEU
33	1b	54	THR
33	1b	63	MET
33	1b	64	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	73	THR
33	1b	80	ILE
33	1b	101	MET
33	1b	112	VAL
33	1b	127	ILE
33	1b	137	ARG
33	1b	164	VAL
33	1b	180	LEU
33	1b	185	ILE
33	1b	187	LEU
33	1b	189	ASP
33	1b	196	LEU
33	1b	200	ILE
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	231	GLU
33	1b	236	TYR
34	1c	3	ASN
34	1c	15	THR
34	1c	28	GLN
34	1c	49	SER
34	1c	89	GLU
34	1c	98	ASN
34	1c	124	ILE
34	1c	178	LEU
34	1c	195	VAL
34	1c	198	VAL
34	1c	207	VAL
35	1d	3	ARG
35	1d	17	VAL
35	1d	19	LEU
35	1d	22	LYS
35	1d	49	ARG
35	1d	59	ARG
35	1d	70	ILE
35	1d	76	ARG
35	1d	77	ASN
35	1d	85	LYS
35	1d	86	LYS
35	1d	88	VAL
35	1d	91	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	104	VAL
35	1d	108	LEU
35	1d	127	THR
35	1d	132	ARG
35	1d	135	LEU
35	1d	140	VAL
35	1d	144	ASP
35	1d	157	LEU
35	1d	158	ILE
35	1d	170	VAL
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	184	LYS
35	1d	190	ASP
35	1d	194	LEU
36	1e	9	LYS
36	1e	27	ARG
36	1e	41	VAL
36	1e	51	VAL
36	1e	79	GLU
36	1e	131	ILE
37	1f	19	LEU
37	1f	40	VAL
37	1f	45	LEU
37	1f	55	ASP
37	1f	64	GLN
37	1f	72	VAL
37	1f	73	ASN
37	1f	75	LEU
37	1f	78	GLU
37	1f	81	ILE
37	1f	91	VAL
38	1g	10	ARG
38	1g	12	LEU
38	1g	21	VAL
38	1g	24	THR
38	1g	41	ARG
38	1g	50	ILE
38	1g	59	LEU
38	1g	61	VAL
38	1g	85	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	1g	104	LEU
38	1g	110	GLN
38	1g	114	ARG
38	1g	115	ARG
38	1g	155	ARG
39	1h	39	LEU
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	77	GLU
39	1h	86	ILE
39	1h	99	GLU
39	1h	112	LEU
39	1h	133	LEU
40	1i	7	THR
40	1i	23	ASN
40	1i	25	LYS
40	1i	27	THR
40	1i	34	ASN
40	1i	50	LEU
40	1i	53	VAL
40	1i	64	THR
40	1i	89	ASN
40	1i	96	LEU
40	1i	103	THR
40	1i	105	ASP
40	1i	128	ARG
41	1j	23	ILE
41	1j	38	ILE
41	1j	43	ARG
41	1j	81	THR
41	1j	94	VAL
41	1j	96	ILE
41	1j	100	THR
42	1k	16	SER
42	1k	31	THR
42	1k	48	ILE
42	1k	80	VAL
42	1k	87	THR
42	1k	109	VAL
42	1k	114	VAL
42	1k	117	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	1k	122	LYS
43	1l	18	VAL
43	1l	57	LYS
43	1l	83	VAL
44	1m	4	ILE
44	1m	11	ARG
44	1m	43	THR
44	1m	49	THR
44	1m	64	TRP
44	1m	70	LEU
44	1m	94	ARG
44	1m	105	THR
44	1m	106	ASN
44	1m	109	THR
44	1m	121	LYS
45	1n	3	ARG
45	1n	9	LYS
45	1n	13	THR
45	1n	56	VAL
46	1o	10	LYS
46	1o	11	VAL
46	1o	27	VAL
46	1o	39	LEU
46	1o	76	GLU
46	1o	84	LYS
46	1o	87	ILE
47	1p	20	VAL
47	1p	21	VAL
47	1p	27	LYS
47	1p	43	LYS
47	1p	45	THR
47	1p	54	GLU
47	1p	60	LEU
47	1p	62	VAL
47	1p	67	THR
48	1q	11	VAL
48	1q	53	LEU
48	1q	85	VAL
48	1q	86	GLU
48	1q	98	LEU
50	1s	4	SER
50	1s	5	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1s	28	LYS
50	1s	41	VAL
50	1s	66	MET
50	1s	79	THR
51	1t	10	LEU
51	1t	24	LEU
51	1t	62	LEU
51	1t	81	LYS
51	1t	84	LEU
51	1t	100	ILE
52	1u	15	ARG
52	1u	20	LYS
52	1u	24	ARG
56	1z	5	MET
3	2D	3	VAL
3	2D	20	ASP
3	2D	37	LEU
3	2D	61	LEU
3	2D	88	ARG
3	2D	99	ASP
3	2D	116	GLN
3	2D	126	GLN
3	2D	141	VAL
3	2D	142	VAL
3	2D	169	GLU
3	2D	173	VAL
3	2D	242	ARG
4	2E	38	THR
4	2E	47	VAL
4	2E	72	VAL
4	2E	77	ILE
4	2E	78	LEU
4	2E	81	ILE
4	2E	90	THR
4	2E	92	THR
4	2E	116	VAL
4	2E	154	LYS
4	2E	175	VAL
5	2F	28	ILE
5	2F	33	LEU
5	2F	50	SER
5	2F	137	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	2F	145	GLU
5	2F	161	GLU
5	2F	162	LEU
5	2F	165	ARG
5	2F	175	THR
5	2F	179	GLU
5	2F	183	VAL
5	2F	195	ASP
6	2G	3	LEU
6	2G	4	ASP
6	2G	26	GLN
6	2G	28	VAL
6	2G	31	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	49	ASP
6	2G	53	LEU
6	2G	60	LEU
6	2G	62	LEU
6	2G	70	VAL
6	2G	91	ARG
6	2G	109	VAL
6	2G	126	ASP
6	2G	140	ILE
6	2G	145	THR
7	2H	7	LEU
7	2H	15	VAL
7	2H	24	VAL
7	2H	57	ASP
7	2H	62	LYS
7	2H	67	LEU
7	2H	84	SER
7	2H	99	VAL
7	2H	106	THR
7	2H	122	THR
7	2H	129	THR
7	2H	130	ARG
7	2H	136	ILE
8	2I	15	VAL
8	2I	38	LEU
8	2I	40	THR
8	2I	43	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2I	44	LEU
8	2I	58	LEU
8	2I	61	ARG
8	2I	68	LEU
8	2I	72	LEU
8	2I	82	ARG
8	2I	86	THR
8	2I	87	LYS
8	2I	102	SER
8	2I	117	GLU
8	2I	127	VAL
8	2I	129	THR
8	2I	133	HIS
8	2I	140	LEU
8	2I	142	VAL
8	2I	145	VAL
9	2N	1	MET
9	2N	28	THR
9	2N	38	HIS
9	2N	60	ILE
9	2N	62	VAL
9	2N	68	GLU
9	2N	71	ILE
9	2N	73	THR
9	2N	83	LYS
9	2N	131	GLN
9	2N	137	LYS
9	2N	140	VAL
10	2O	71	ARG
10	2O	91	LEU
10	2O	104	ARG
11	2P	7	ARG
11	2P	45	LEU
11	2P	65	ARG
11	2P	71	VAL
11	2P	95	VAL
11	2P	98	GLU
11	2P	100	LEU
11	2P	119	GLU
11	2P	125	VAL
11	2P	133	SER
11	2P	135	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	2P	136	GLU
11	2P	147	LEU
12	2Q	106	VAL
13	2R	6	SER
13	2R	24	GLN
13	2R	36	THR
13	2R	44	LEU
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	11	LYS
14	2S	26	LEU
14	2S	27	SER
14	2S	43	GLU
14	2S	48	LEU
14	2S	58	LEU
14	2S	63	THR
14	2S	80	LEU
14	2S	84	GLN
14	2S	110	LEU
15	2T	9	LEU
15	2T	28	VAL
15	2T	31	SER
15	2T	39	ARG
15	2T	63	VAL
15	2T	64	ARG
15	2T	72	VAL
15	2T	74	ARG
15	2T	89	VAL
15	2T	96	ARG
15	2T	104	ASN
16	2U	5	LYS
16	2U	17	ILE
16	2U	74	LEU
16	2U	89	GLU
16	2U	95	LEU
16	2U	111	GLU
16	2U	117	GLN
17	2V	1	MET
17	2V	7	THR
17	2V	46	VAL
17	2V	52	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	2V	57	VAL
17	2V	61	VAL
17	2V	70	ILE
17	2V	73	SER
17	2V	79	VAL
17	2V	82	ARG
17	2V	93	GLU
17	2V	98	GLU
18	2W	4	LYS
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	39	THR
18	2W	67	ASP
18	2W	78	GLU
18	2W	92	ARG
19	2X	81	VAL
19	2X	92	LEU
20	2Y	1	MET
20	2Y	5	MET
20	2Y	7	VAL
20	2Y	14	LEU
20	2Y	26	LYS
20	2Y	30	VAL
20	2Y	50	ARG
20	2Y	67	LEU
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	90	LEU
20	2Y	91	GLU
20	2Y	97	ARG
20	2Y	98	VAL
20	2Y	99	CYS
21	2Z	33	LEU
21	2Z	35	ARG
21	2Z	41	LEU
21	2Z	42	VAL
21	2Z	53	ILE
21	2Z	63	ASP
21	2Z	67	LEU
21	2Z	70	LEU
21	2Z	71	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	2Z	90	VAL
21	2Z	91	LEU
21	2Z	96	VAL
21	2Z	100	VAL
21	2Z	121	HIS
21	2Z	144	LEU
21	2Z	153	SER
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	169	GLU
21	2Z	170	THR
21	2Z	171	ILE
21	2Z	174	VAL
22	20	74	ARG
23	21	11	ARG
23	21	40	ARG
23	21	59	THR
23	21	80	LEU
23	21	89	GLU
24	22	35	LEU
24	22	45	SER
24	22	54	LYS
24	22	70	GLN
25	23	31	LEU
25	23	54	VAL
25	23	59	VAL
26	24	1	MET
26	24	22	ILE
26	24	33	VAL
26	24	34	GLU
26	24	50	VAL
26	24	59	PHE
26	24	63	TYR
27	25	6	VAL
27	25	35	GLU
27	25	55	ARG
27	25	58	LEU
28	26	6	ARG
28	26	9	LEU
28	26	23	THR
28	26	28	ARG
28	26	36	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	26	48	VAL
28	26	52	VAL
29	27	1	MET
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	13	ARG
30	28	23	VAL
31	29	33	LYS
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	15	VAL
33	2b	16	HIS
33	2b	35	GLU
33	2b	37	ASN
33	2b	48	MET
33	2b	49	GLU
33	2b	68	ILE
33	2b	71	VAL
33	2b	76	GLN
33	2b	83	MET
33	2b	93	VAL
33	2b	107	THR
33	2b	110	GLN
33	2b	112	VAL
33	2b	115	LEU
33	2b	127	ILE
33	2b	138	LEU
33	2b	142	LEU
33	2b	164	VAL
33	2b	169	LYS
33	2b	175	ARG
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP
33	2b	198	ASP
33	2b	208	ILE
33	2b	209	ARG
33	2b	230	VAL
33	2b	236	TYR
34	2c	3	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	16	ARG
34	2c	32	LEU
34	2c	34	LEU
34	2c	39	ILE
34	2c	46	GLU
34	2c	52	LEU
34	2c	55	VAL
34	2c	57	ILE
34	2c	87	LEU
34	2c	91	LEU
34	2c	101	LEU
34	2c	116	VAL
34	2c	132	ARG
34	2c	153	VAL
34	2c	188	LEU
34	2c	190	ARG
34	2c	206	GLU
35	2d	5	ILE
35	2d	18	LYS
35	2d	28	SER
35	2d	58	LEU
35	2d	59	ARG
35	2d	86	LYS
35	2d	96	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	158	ILE
35	2d	175	SER
35	2d	188	LEU
35	2d	196	LEU
36	2e	13	ILE
36	2e	38	GLN
36	2e	41	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	120	THR
36	2e	150	ARG
37	2f	1	MET
37	2f	19	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	2f	28	ARG
37	2f	69	GLU
37	2f	72	VAL
37	2f	81	ILE
37	2f	92	LYS
37	2f	94	GLN
37	2f	95	GLU
38	2g	6	ARG
38	2g	9	VAL
38	2g	13	GLN
38	2g	15	ASP
38	2g	21	VAL
38	2g	24	THR
38	2g	30	ILE
38	2g	79	ARG
38	2g	94	ARG
38	2g	98	SER
38	2g	113	GLU
38	2g	139	GLU
38	2g	144	MET
39	2h	3	THR
39	2h	21	LYS
39	2h	25	ASP
39	2h	29	SER
39	2h	37	ARG
39	2h	51	VAL
39	2h	52	ASP
39	2h	54	ASP
39	2h	68	ARG
39	2h	99	GLU
39	2h	112	LEU
39	2h	113	SER
39	2h	133	LEU
39	2h	137	VAL
40	2i	12	GLU
40	2i	27	THR
40	2i	35	GLU
40	2i	38	GLN
40	2i	40	LEU
40	2i	41	VAL
40	2i	54	ASP
40	2i	65	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	2i	89	ASN
41	2j	23	ILE
41	2j	38	ILE
41	2j	66	ARG
41	2j	67	THR
41	2j	81	THR
41	2j	89	ASP
41	2j	94	VAL
41	2j	97	GLU
41	2j	100	THR
42	2k	24	SER
42	2k	29	ILE
42	2k	41	THR
42	2k	48	ILE
42	2k	62	GLN
42	2k	87	THR
42	2k	105	VAL
42	2k	107	SER
42	2k	114	VAL
43	2l	40	VAL
43	2l	47	LYS
43	2l	62	SER
43	2l	83	VAL
44	2m	4	ILE
44	2m	8	GLU
44	2m	32	GLU
44	2m	90	LEU
44	2m	98	VAL
44	2m	103	THR
44	2m	106	ASN
44	2m	114	ARG
44	2m	122	LYS
45	2n	3	ARG
45	2n	33	VAL
46	2o	7	GLU
46	2o	13	GLN
46	2o	27	VAL
46	2o	39	LEU
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	35	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	2p	42	ARG
47	2p	67	THR
47	2p	74	LEU
48	2q	5	VAL
48	2q	19	VAL
48	2q	24	GLU
48	2q	60	ILE
48	2q	63	ARG
49	2r	31	LEU
49	2r	56	THR
49	2r	82	THR
50	2s	36	ARG
50	2s	37	ARG
50	2s	43	GLU
50	2s	45	VAL
50	2s	47	HIS
50	2s	48	THR
50	2s	49	ILE
50	2s	81	ARG
51	2t	46	GLU
51	2t	70	SER
51	2t	86	ARG
51	2t	93	GLU
52	2u	7	ARG
56	2z	5	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	116	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
6	1G	26	GLN
6	1G	108	ASN
6	1G	132	ASN
8	1I	133	HIS
12	1Q	12	GLN
14	1S	84	GLN
15	1T	58	ASN
15	1T	84	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1U	81	HIS
16	1U	94	ASN
18	1W	60	ASN
19	1X	31	HIS
19	1X	82	GLN
21	1Z	50	GLN
21	1Z	55	HIS
21	1Z	73	GLN
21	1Z	75	ASN
21	1Z	132	ASN
21	1Z	151	HIS
24	12	56	GLN
25	13	32	GLN
29	17	36	GLN
30	18	35	GLN
33	1b	40	HIS
33	1b	94	ASN
33	1b	140	HIS
34	1c	6	HIS
34	1c	102	ASN
34	1c	118	GLN
34	1c	162	GLN
34	1c	170	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	201	GLN
36	1e	20	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	57	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	64	GLN
38	1g	86	GLN
39	1h	15	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	1i	38	GLN
40	1i	58	HIS
40	1i	124	GLN
43	1l	80	HIS
43	1l	99	HIS
44	1m	77	ASN
44	1m	92	HIS
47	1p	13	HIS
49	1r	63	GLN
50	1s	47	HIS
50	1s	83	HIS
51	1t	16	HIS
3	2D	116	GLN
4	2E	48	GLN
5	2F	29	ASN
5	2F	69	HIS
6	2G	27	ASN
7	2H	74	ASN
8	2I	105	HIS
9	2N	131	GLN
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	57	HIS
12	2Q	113	GLN
13	2R	71	GLN
14	2S	38	GLN
15	2T	43	GLN
15	2T	84	GLN
15	2T	90	GLN
15	2T	104	ASN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	32	HIS
21	2Z	55	HIS
24	22	43	GLN
24	22	46	GLN
24	22	70	GLN
25	23	32	GLN
26	24	40	HIS
26	24	46	GLN
28	26	20	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	29	20	HIS
31	29	36	GLN
33	2b	76	GLN
33	2b	110	GLN
33	2b	135	GLN
33	2b	140	HIS
34	2c	37	GLN
34	2c	110	ASN
34	2c	162	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	130	ASN
37	2f	73	ASN
37	2f	94	GLN
37	2f	100	ASN
38	2g	13	GLN
38	2g	37	ASN
38	2g	106	GLN
38	2g	148	ASN
39	2h	82	HIS
40	2i	3	GLN
40	2i	23	ASN
40	2i	31	GLN
40	2i	38	GLN
41	2j	21	GLN
41	2j	33	GLN
41	2j	62	HIS
41	2j	68	HIS
42	2k	26	ASN
43	2l	99	HIS
44	2m	12	ASN
44	2m	77	ASN
48	2q	26	GLN
49	2r	63	GLN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	436 (15%)	30 (1%)
1	2A	2791/2915 (95%)	439 (15%)	21 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	21 (17%)	0
32	1a	1497/1521 (98%)	233 (15%)	0
32	2a	1501/1521 (98%)	273 (18%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	23 (32%)	0
54	2w	68/76 (89%)	20 (29%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	9 (12%)	0
57	1y	72/76 (94%)	29 (40%)	0
57	2y	70/76 (92%)	19 (27%)	0
All	All	9345/9620 (97%)	1520 (16%)	51 (0%)

All (1520) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	140	G
1	1A	151	C
1	1A	154(A)	C
1	1A	181	A
1	1A	182	A
1	1A	188	G
1	1A	196	A
1	1A	197	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	265	A
1	1A	269	U
1	1A	271(B)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	271(X)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	327	G
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	353	G
1	1A	357	A
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	386	G
1	1A	389	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	456	C
1	1A	479	A
1	1A	481	G
1	1A	504	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	505	A
1	1A	508	G
1	1A	509	C
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	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	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	789	A
1	1A	792	G
1	1A	805	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	893	C
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1040	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1044	G
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	1063	G
1	1A	1064	C
1	1A	1065	U
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1083	U
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1097	U
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1111	A
1	1A	1112	G
1	1A	1117	G
1	1A	1135	C
1	1A	1136	G
1	1A	1142	U
1	1A	1149	G
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1220	A
1	1A	1229	G
1	1A	1236	G
1	1A	1244	G
1	1A	1248	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1276	A
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1319	G
1	1A	1342	A
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1461	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1539	G
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1703	G
1	1A	1722	A
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1769	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	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1877	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2097	C
1	1A	2108	C
1	1A	2110	G
1	1A	2112	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2120	G
1	1A	2121	G
1	1A	2123	G
1	1A	2126	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2137	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2193	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2268	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2322	A
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2423	U
1	1A	2424	C
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	2440	C
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2573	C
1	1A	2574	G
1	1A	2602	A
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2686	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2760	C
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	13	A
2	1B	25	A
2	1B	45	A
2	1B	56	G
2	1B	57	A
2	1B	67	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1B	73	A
2	1B	85	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	73	G
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	163	C
32	1a	164	U
32	1a	174	C
32	1a	176	C
32	1a	182	U
32	1a	189	G
32	1a	189(C)	C
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	280	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	330	C
32	1a	332	G
32	1a	344	A
32	1a	347	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	390	C
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	474	G
32	1a	483	C
32	1a	485	G
32	1a	493	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	564	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	630	G
32	1a	653	A
32	1a	657	G
32	1a	665	A
32	1a	666	G
32	1a	687	A
32	1a	688	G
32	1a	703	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	749	C
32	1a	752	G
32	1a	755	G
32	1a	773	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	874	G
32	1a	914	A
32	1a	916	G
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	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1044	A
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1111	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1282	C
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1302	U
32	1a	1319	A
32	1a	1323	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1452	C
32	1a	1456	G
32	1a	1492	A
32	1a	1494	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	13	A
54	1w	2	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	25	C
54	1w	34	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1w	48	C
54	1w	50	U
54	1w	61	C
54	1w	67	C
54	1w	68	C
54	1w	70	G
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	64	G
57	1y	5	G
57	1y	6	G
57	1y	7	A
57	1y	9	A
57	1y	13	C
57	1y	14	A
57	1y	19	G
57	1y	20	U
57	1y	21	A
57	1y	35	A
57	1y	39	PSU
57	1y	40	C
57	1y	44	G
57	1y	45	U
57	1y	46	G7M
57	1y	47	U
57	1y	48	C
57	1y	50	U
57	1y	52	G
57	1y	56	C
57	1y	57	G
57	1y	58	A
57	1y	59	U
57	1y	60	U
57	1y	61	C
57	1y	62	C
57	1y	65	G
57	1y	70	G
57	1y	72	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	49	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	123	G
1	2A	154	G
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	197	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	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	274	G
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	311	A
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	363(C)	G
1	2A	386	G
1	2A	389	G
1	2A	396	G
1	2A	403	U
1	2A	411	G
1	2A	421	U
1	2A	435	C
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	603	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	643	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	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	854	G
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	879	G
1	2A	880	G
1	2A	882	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	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C
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	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1114	G
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1143	A
1	2A	1167	U
1	2A	1169	G
1	2A	1171	G
1	2A	1181	C
1	2A	1195	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1205	U
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1224	C
1	2A	1229	G
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
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	1395	A
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1523	U
1	2A	1531	C
1	2A	1532	C
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1608	A
1	2A	1610	A
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
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	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1861	G
1	2A	1866	C
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	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	2093	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C
1	2A	2113	U
1	2A	2116	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2144	U
1	2A	2145	C
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2163	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2181	G
1	2A	2183	C
1	2A	2184	G
1	2A	2185	C
1	2A	2189	U
1	2A	2190	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2193	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2239	G
1	2A	2268	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2372	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2414	G
1	2A	2424	C
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2530	A
1	2A	2532	G
1	2A	2534	A
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2582	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	2641	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2808	U
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	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	34	U
2	2B	41	U
2	2B	45	A
2	2B	53	A
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	84	C
2	2B	88	C
2	2B	89	G
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	113	G
2	2B	120	A
32	2a	9	G
32	2a	22	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	56	U
32	2a	66	G
32	2a	70	G
32	2a	78	G
32	2a	79	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	156	G
32	2a	159	G
32	2a	162	A
32	2a	163	C
32	2a	182	U
32	2a	189(C)	C
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	301	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	356	A
32	2a	367	U
32	2a	372	C
32	2a	384	G
32	2a	388	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	423	G
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	442	C
32	2a	449	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	703	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	777	A
32	2a	787	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	859	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	934	C
32	2a	935	A
32	2a	939	G
32	2a	942	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	982	U
32	2a	983	A
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1007	C
32	2a	1008	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1019	C
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1080	A
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1104	G
32	2a	1105	A
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1160	G
32	2a	1182	G
32	2a	1184	G
32	2a	1191	A
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1220	G
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1248	A
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1285	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1320	C
32	2a	1323	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1380	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	14	A
53	2v	15	A
53	2v	19	U
54	2w	3	C
54	2w	4	C
54	2w	8	4SU
54	2w	9	A
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	27	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	58	A
54	2w	62	C
54	2w	65	G
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	74	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	20	U
55	2x	21	A
55	2x	47	U
55	2x	51	C
55	2x	56	C
55	2x	69	C
57	2y	8	4SU
57	2y	15	G
57	2y	19	G
57	2y	27	G
57	2y	43	C
57	2y	45	U
57	2y	49	C
57	2y	52	G
57	2y	53	G
57	2y	54	5MU
57	2y	56	C
57	2y	58	A
57	2y	59	U
57	2y	61	C
57	2y	65	G
57	2y	69	G
57	2y	70	G
57	2y	73	A
57	2y	75	C

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(J)	C
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	1047	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1275	A
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	1997	G
1	1A	2134	A
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2439	A
1	2A	2689	U

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

90 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
57	4SU	1y	8	57	18,21,22	1.75	4 (22%)	25,30,33	1.96	5 (20%)
55	8AN	2x	76	55,58	21,24,25	1.41	3 (14%)	26,35,38	2.30	11 (42%)
57	PSU	1y	39	57	18,21,22	1.37	2 (11%)	21,30,33	2.04	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.33	4 (22%)	21,30,33	2.00	4 (19%)
54	PSU	1w	32	54,58	18,21,22	1.30	2 (11%)	21,30,33	2.03	4 (19%)
55	4SU	1x	8	55	18,21,22	2.25	5 (27%)	25,30,33	1.74	7 (28%)
1	5MU	2A	1939	1,58	19,22,23	1.36	5 (26%)	27,32,35	2.34	8 (29%)
57	G7M	1y	46	57	23,26,27	1.53	4 (17%)	34,39,42	1.74	5 (14%)
55	5MC	2x	32	55	19,22,23	1.80	3 (15%)	26,32,35	1.20	4 (15%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.03	3 (14%)
54	F3N	2w	76	54,1	33,36,37	1.45	4 (12%)	41,51,54	1.78	10 (24%)
1	PSU	2A	1917	1	18,21,22	1.40	2 (11%)	21,30,33	2.04	4 (19%)
32	PSU	1a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.94	3 (14%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	1.00	1 (4%)
1	5MU	1A	1915	1	19,22,23	1.36	5 (26%)	27,32,35	2.17	7 (25%)
54	MIA	1w	37	54	28,31,32	2.20	6 (21%)	38,44,47	2.95	12 (31%)
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	21,30,33	2.03	3 (14%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.03	9 (27%)
54	PSU	2w	32	54	18,21,22	1.33	2 (11%)	21,30,33	1.95	3 (14%)
1	5MC	1A	1962	1,58	19,22,23	1.81	3 (15%)	26,32,35	1.17	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.14	2 (7%)
57	G7M	2y	46	57	23,26,27	1.66	3 (13%)	34,39,42	2.01	4 (11%)
55	5MU	1x	54	55	19,22,23	1.41	4 (21%)	27,32,35	2.00	6 (22%)
1	5MC	2A	1962	1,58	19,22,23	1.75	3 (15%)	26,32,35	1.11	2 (7%)
56	FME	2z	1	56	8,9,10	0.99	0	8,9,11	1.25	1 (12%)
1	PSU	1A	1917	1	18,21,22	1.43	3 (16%)	21,30,33	1.98	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MC	1x	32	55	19,22,23	1.62	3 (15%)	26,32,35	1.23	3 (11%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.07	9 (27%)
1	OMC	2A	1920	1	19,22,23	0.81	0	25,31,34	0.93	0
57	4SU	2y	8	57	18,21,22	1.72	4 (22%)	25,30,33	2.16	5 (20%)
32	G7M	1a	527	32	23,26,27	1.49	4 (17%)	34,39,42	1.65	5 (14%)
32	M2G	2a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.85	5 (15%)
32	G7M	2a	527	32,58	23,26,27	1.48	3 (13%)	34,39,42	1.65	5 (14%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)
55	8AN	1x	76	55,58	21,24,25	1.45	3 (14%)	26,35,38	2.68	11 (42%)
32	5MC	2a	1407	32	19,22,23	1.57	3 (15%)	26,32,35	1.13	2 (7%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	27,32,35	2.18	6 (22%)
57	PSU	2y	55	57	18,21,22	1.36	2 (11%)	21,30,33	2.00	4 (19%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.12	9 (27%)
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	1.94	4 (19%)
54	G7M	1w	46	54	23,26,27	1.54	3 (13%)	34,39,42	1.67	4 (11%)
1	OMG	2A	2251	55,1,58	23,26,27	1.20	2 (8%)	32,38,41	2.00	8 (25%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.10	5 (23%)
57	PSU	1y	55	57	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
43	0TD	2l	92	43	8,9,10	4.55	1 (12%)	6,11,13	4.56	3 (50%)
32	5MC	1a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.28	4 (15%)
54	5MU	1w	54	54	19,22,23	1.32	5 (26%)	27,32,35	1.99	6 (22%)
1	PSU	1A	1911	1	18,21,22	1.41	2 (11%)	21,30,33	2.15	4 (19%)
32	UR3	2a	1498	32	19,22,23	1.08	1 (5%)	26,32,35	1.73	4 (15%)
32	M2G	1a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.85	6 (18%)
32	5MC	2a	1404	32	19,22,23	1.64	3 (15%)	26,32,35	1.13	2 (7%)
57	PSU	2y	39	57	18,21,22	1.30	2 (11%)	21,30,33	2.23	4 (19%)
55	PSU	1x	55	55	18,21,22	1.42	2 (11%)	21,30,33	2.05	3 (14%)
54	4SU	2w	8	54	18,21,22	1.77	4 (22%)	25,30,33	2.42	5 (20%)
54	PSU	1w	39	54	18,21,22	1.33	2 (11%)	21,30,33	1.99	4 (19%)
56	FME	1z	1	56	8,9,10	0.96	0	8,9,11	1.14	1 (12%)
1	2MA	2A	2503	1,58	22,25,26	1.48	4 (18%)	32,37,40	2.36	8 (25%)
57	PSU	1y	32	57	18,21,22	1.38	2 (11%)	21,30,33	1.96	4 (19%)
57	5MU	2y	54	57	19,22,23	1.53	4 (21%)	27,32,35	2.21	6 (22%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.04	2 (8%)
32	5MC	1a	967	32	19,22,23	1.56	3 (15%)	26,32,35	1.15	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	G7M	2w	46	54	23,26,27	1.44	3 (13%)	34,39,42	1.72	5 (14%)
32	5MC	2a	1400	32	19,22,23	1.76	3 (15%)	26,32,35	1.19	3 (11%)
54	5MU	2w	54	54	19,22,23	1.32	4 (21%)	27,32,35	1.86	6 (22%)
1	PSU	1A	2605	1,58	18,21,22	1.38	2 (11%)	21,30,33	2.26	5 (23%)
32	UR3	1a	1498	32	19,22,23	0.96	0	26,32,35	1.75	3 (11%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	21,30,33	1.82	3 (14%)
57	PSU	2y	32	57	18,21,22	1.39	2 (11%)	21,30,33	1.87	4 (19%)
1	OMU	1A	2552	1,58	19,22,23	1.23	2 (10%)	25,31,34	1.91	5 (20%)
32	2MG	1a	1207	32	23,26,27	1.31	3 (13%)	33,38,41	2.04	5 (15%)
32	5MC	1a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.06	2 (7%)
54	4SU	1w	8	54,58	18,21,22	1.87	5 (27%)	25,30,33	1.90	5 (20%)
1	OMG	1A	2251	55,1,58	23,26,27	1.23	3 (13%)	32,38,41	1.97	6 (18%)
57	5MU	1y	54	57	19,22,23	1.43	5 (26%)	27,32,35	1.73	6 (22%)
32	4OC	1a	1402	32	20,23,24	0.73	0	25,32,35	1.10	2 (8%)
1	2MA	1A	2503	1,58	22,25,26	1.50	5 (22%)	32,37,40	2.40	9 (28%)
32	2MG	2a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.14	7 (21%)
55	4SU	2x	8	55,58	18,21,22	2.13	4 (22%)	25,30,33	1.49	5 (20%)
1	5MC	1A	1942	1	19,22,23	1.58	3 (15%)	26,32,35	1.19	3 (11%)
43	0TD	1l	92	43	8,9,10	4.68	1 (12%)	6,11,13	7.87	3 (50%)
57	MIA	2y	37	57	21,24,32	1.61	3 (14%)	30,35,47	2.02	9 (30%)
32	5MC	2a	967	32	19,22,23	1.63	3 (15%)	26,32,35	1.08	2 (7%)
54	MIA	2w	37	54	24,27,32	2.04	5 (20%)	32,39,47	2.52	11 (34%)
1	OMU	2A	2552	1,58	19,22,23	1.19	2 (10%)	25,31,34	1.89	6 (24%)
54	F3N	1w	76	54,1	33,36,37	1.50	4 (12%)	41,51,54	1.77	9 (21%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.13	8 (24%)
57	MIA	1y	37	57	21,24,32	1.61	4 (19%)	30,35,47	2.06	7 (23%)
1	5MC	2A	1942	1	19,22,23	1.71	2 (10%)	26,32,35	1.11	2 (7%)
1	5MU	2A	1915	1	19,22,23	1.43	5 (26%)	27,32,35	2.14	6 (22%)
1	5MU	1A	1939	1,58	19,22,23	1.37	4 (21%)	27,32,35	2.40	6 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	4SU	1y	8	57	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	55,58	-	3/7/25/26	0/3/3/3
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,58	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,58	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	2/7/25/26	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	54,1	-	3/19/37/38	0/4/4/4
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	3/15/33/34	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	1,58	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
57	G7M	2y	46	57	-	4/7/25/26	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,58	-	0/7/25/26	0/2/2/2
56	FME	2z	1	56	-	3/7/9/11	-
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
57	4SU	2y	8	57	-	1/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/7/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	G7M	2a	527	32,58	-	3/7/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	55,58	-	3/7/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
57	PSU	2y	55	57	-	1/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
1	OMG	2A	2251	55,1,58	-	0/9/27/28	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
57	PSU	2y	39	57	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
56	FME	1z	1	56	-	4/7/9/11	-
1	2MA	2A	2503	1,58	-	0/7/25/26	0/3/3/3
57	PSU	1y	32	57	-	1/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	2/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,58	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
57	PSU	2y	32	57	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,58	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54,58	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,1,58	-	1/9/27/28	0/3/3/3
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
1	2MA	1A	2503	1,58	-	1/7/25/26	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
55	4SU	2x	8	55,58	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
57	MIA	2y	37	57	-	1/7/25/34	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
1	OMU	2A	2552	1,58	-	0/9/27/28	0/2/2/2
54	F3N	1w	76	54,1	-	0/19/37/38	0/4/4/4
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
57	MIA	1y	37	57	-	1/7/25/34	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,58	-	0/7/25/26	0/2/2/2

All (246) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.82	1.69	1.82
43	2l	92	0TD	CB-SB	-12.40	1.69	1.82
1	1A	1962	5MC	C5-C4	6.89	1.49	1.44
55	2x	32	5MC	C5-C4	6.75	1.49	1.44
54	1w	37	MIA	C13-C14	6.67	1.52	1.32
54	2w	37	MIA	C2-S10	-6.66	1.70	1.75
1	2A	1962	5MC	C5-C4	6.55	1.49	1.44
32	2a	1400	5MC	C5-C4	6.51	1.49	1.44
1	2A	1942	5MC	C5-C4	6.25	1.48	1.44
32	1a	1404	5MC	C5-C4	6.20	1.48	1.44
32	2a	967	5MC	C5-C4	5.94	1.48	1.44
32	2a	1404	5MC	C5-C4	5.86	1.48	1.44
32	1a	1400	5MC	C5-C4	5.83	1.48	1.44
32	1a	1407	5MC	C5-C4	5.78	1.48	1.44
55	1x	32	5MC	C5-C4	5.66	1.48	1.44
54	1w	37	MIA	C2-S10	-5.64	1.71	1.75
32	1a	967	5MC	C5-C4	5.61	1.48	1.44
32	2a	1407	5MC	C5-C4	5.59	1.48	1.44
1	1A	1942	5MC	C5-C4	5.46	1.48	1.44
55	1x	8	4SU	C4-N3	-5.36	1.32	1.37
57	1y	37	MIA	C5-C4	5.11	1.48	1.39
54	2w	8	4SU	C4-S4	-5.02	1.59	1.68
57	2y	37	MIA	C5-C4	4.98	1.48	1.39
54	1w	76	F3N	CB-CG	-4.97	1.39	1.51
55	2x	8	4SU	C4-N3	-4.97	1.32	1.37
57	2y	46	G7M	C5-N7	-4.93	1.33	1.39
54	1w	37	MIA	C5-C4	4.89	1.47	1.39
54	1w	8	4SU	C4-S4	-4.81	1.60	1.68
54	2w	37	MIA	C5-C4	4.74	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	76	F3N	CB-CG	-4.71	1.40	1.51
54	1w	46	G7M	C5-N7	-4.71	1.33	1.39
57	2y	8	4SU	C4-S4	-4.69	1.60	1.68
57	1y	8	4SU	C4-S4	-4.68	1.60	1.68
55	2x	8	4SU	C4-S4	-4.64	1.60	1.68
55	1x	8	4SU	C4-S4	-4.56	1.60	1.68
32	1a	527	G7M	C5-N7	-4.50	1.34	1.39
1	2A	2503	2MA	C5-C4	4.36	1.46	1.39
32	2a	527	G7M	C5-N7	-4.34	1.34	1.39
1	1A	2503	2MA	C5-C4	4.22	1.46	1.39
57	1y	46	G7M	C5-N7	-4.16	1.34	1.39
54	2w	46	G7M	C5-N7	-4.16	1.34	1.39
57	1y	39	PSU	C6-C5	4.12	1.39	1.35
57	2y	32	PSU	C6-C5	4.07	1.39	1.35
54	1w	55	PSU	C6-C5	4.01	1.39	1.35
57	1y	32	PSU	C6-C5	3.96	1.39	1.35
54	2w	76	F3N	C5-N7	-3.96	1.31	1.39
54	2w	55	PSU	C6-C5	3.87	1.39	1.35
55	1x	8	4SU	C2-N3	-3.85	1.31	1.38
54	1w	76	F3N	C5-N7	-3.83	1.32	1.39
57	2y	46	G7M	C5-C4	3.79	1.47	1.38
55	2x	76	8AN	C5-N7	-3.79	1.32	1.39
57	1y	55	PSU	C6-C5	3.75	1.39	1.35
1	1A	1917	PSU	C6-C5	3.72	1.39	1.35
55	2x	55	PSU	C6-C5	3.71	1.39	1.35
55	1x	76	8AN	C5-N7	-3.69	1.32	1.39
55	1x	55	PSU	C6-C5	3.67	1.39	1.35
57	1y	46	G7M	C5-C4	3.61	1.47	1.38
55	1x	8	4SU	C5-C4	-3.60	1.38	1.42
32	2a	516	PSU	C6-C5	3.59	1.39	1.35
54	2w	32	PSU	C6-C5	3.59	1.39	1.35
1	2A	1917	PSU	C6-C5	3.58	1.39	1.35
54	2w	39	PSU	C6-C5	3.55	1.39	1.35
54	1w	32	PSU	C6-C5	3.52	1.39	1.35
54	1w	8	4SU	C4-N3	-3.50	1.34	1.37
57	2y	39	PSU	C6-C5	3.47	1.39	1.35
55	2x	8	4SU	C2-N3	-3.38	1.32	1.38
1	1A	1911	PSU	C6-C5	3.37	1.39	1.35
1	2A	1911	PSU	C6-C5	3.37	1.39	1.35
57	2y	55	PSU	C6-C5	3.34	1.39	1.35
54	1w	46	G7M	C5-C4	3.34	1.46	1.38
32	1a	527	G7M	C5-C4	3.33	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	516	PSU	C6-C5	3.32	1.39	1.35
55	2x	8	4SU	C5-C4	-3.28	1.38	1.42
32	2a	966	M2G	C5-C4	3.27	1.47	1.38
32	2a	527	G7M	C5-C4	3.27	1.46	1.38
54	2w	46	G7M	C5-C4	3.23	1.46	1.38
32	2a	1207	2MG	C5-C4	3.22	1.47	1.38
57	2y	54	5MU	C2-N1	3.22	1.43	1.38
54	1w	39	PSU	C6-C5	3.22	1.38	1.35
32	1a	966	M2G	C2-N2	3.19	1.41	1.35
32	1a	966	M2G	C5-C4	3.18	1.47	1.38
55	1x	76	8AN	C5-C4	-3.17	1.33	1.39
55	2x	76	8AN	C5-C4	-3.17	1.33	1.39
32	1a	1207	2MG	C5-C4	3.17	1.47	1.38
57	2y	54	5MU	C6-C5	3.13	1.39	1.34
1	1A	2605	PSU	C6-C5	3.11	1.38	1.35
54	2w	76	F3N	C5-C4	-3.06	1.33	1.39
54	1w	76	F3N	C5-C4	-3.06	1.33	1.39
1	2A	2251	OMG	C5-C4	3.01	1.47	1.38
57	2y	37	MIA	C5-C6	3.00	1.49	1.41
54	2w	8	4SU	C4-N3	-2.98	1.34	1.37
1	2A	2605	PSU	C6-C5	2.98	1.38	1.35
57	1y	54	5MU	C6-C5	2.96	1.39	1.34
1	1A	2251	OMG	C5-C4	2.95	1.46	1.38
1	1A	2552	OMU	C4-N3	-2.95	1.33	1.38
54	1w	37	MIA	C5-C6	2.93	1.49	1.41
1	2A	1942	5MC	C6-C5	2.90	1.39	1.34
32	1a	1207	2MG	C6-N1	-2.89	1.33	1.38
1	2A	1915	5MU	C6-C5	2.89	1.39	1.34
55	1x	32	5MC	C6-C5	2.89	1.39	1.34
57	1y	8	4SU	C4-N3	-2.87	1.34	1.37
57	1y	37	MIA	C5-C6	2.86	1.48	1.41
32	2a	1404	5MC	C6-C5	2.85	1.39	1.34
1	1A	1942	5MC	C6-C5	2.84	1.39	1.34
54	2w	37	MIA	C5-C6	2.84	1.48	1.41
54	1w	8	4SU	C5-C4	-2.83	1.39	1.42
57	2y	8	4SU	C4-N3	-2.83	1.34	1.37
32	1a	1404	5MC	C6-C5	2.83	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.83	1.33	1.38
1	1A	1917	PSU	C4-N3	-2.83	1.33	1.38
32	1a	1400	5MC	C6-C5	2.80	1.39	1.34
32	2a	1400	5MC	C6-C5	2.79	1.39	1.34
55	1x	54	5MU	C6-C5	2.79	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2605	PSU	C4-N3	-2.77	1.33	1.38
55	2x	54	5MU	C6-C5	2.76	1.39	1.34
54	1w	39	PSU	C4-N3	-2.72	1.33	1.38
32	1a	1407	5MC	C6-C5	2.71	1.39	1.34
55	2x	32	5MC	C6-C5	2.70	1.39	1.34
57	1y	54	5MU	C4-N3	-2.69	1.33	1.38
57	2y	54	5MU	C4-C5	2.67	1.49	1.44
57	2y	46	G7M	C6-N1	-2.65	1.33	1.38
1	2A	1917	PSU	C4-N3	-2.63	1.33	1.38
32	2a	966	M2G	C2-N2	2.63	1.39	1.35
1	2A	1962	5MC	C6-C5	2.63	1.38	1.34
1	2A	1915	5MU	C2-N1	2.61	1.42	1.38
32	2a	967	5MC	C6-C5	2.61	1.38	1.34
1	1A	1939	5MU	C6-C5	2.60	1.38	1.34
54	1w	37	MIA	C8-N7	2.60	1.36	1.31
1	2A	1911	PSU	C4-N3	-2.60	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.59	1.34	1.38
1	2A	1939	5MU	C4-C5	2.59	1.49	1.44
1	1A	1939	5MU	C4-C5	2.59	1.49	1.44
1	2A	1915	5MU	C4-C5	2.59	1.49	1.44
55	2x	55	PSU	C4-N3	-2.57	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.57	1.34	1.38
55	1x	54	5MU	C4-N3	-2.57	1.34	1.38
32	2a	966	M2G	C6-N1	-2.56	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.56	1.34	1.38
1	2A	1939	5MU	C6-C5	2.55	1.38	1.34
55	1x	54	5MU	C2-N1	2.55	1.42	1.38
1	2A	2552	OMU	C4-N3	-2.54	1.34	1.38
54	2w	54	5MU	C6-C5	2.54	1.38	1.34
54	1w	54	5MU	C6-C5	2.53	1.38	1.34
54	1w	76	F3N	C5-C6	-2.53	1.33	1.41
54	2w	39	PSU	C4-N3	-2.53	1.34	1.38
57	2y	37	MIA	C8-N7	2.53	1.36	1.31
1	2A	1939	5MU	C6-N1	-2.52	1.33	1.38
54	2w	76	F3N	C5-C6	-2.52	1.34	1.41
55	1x	55	PSU	C4-N3	-2.52	1.34	1.38
55	2x	76	8AN	C5-C6	-2.52	1.34	1.41
1	1A	2251	OMG	C5-N7	-2.52	1.34	1.39
54	2w	8	4SU	C5-C4	-2.51	1.39	1.42
55	1x	76	8AN	C5-C6	-2.51	1.34	1.41
1	1A	1915	5MU	C6-C5	2.51	1.38	1.34
54	1w	46	G7M	C6-N1	-2.50	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2503	2MA	C5-N7	-2.50	1.34	1.39
32	1a	516	PSU	C4-N3	-2.50	1.34	1.38
55	2x	54	5MU	C4-N3	-2.49	1.34	1.38
57	2y	8	4SU	C5-C4	-2.48	1.39	1.42
1	1A	2503	2MA	C5-N7	-2.48	1.34	1.39
1	1A	2503	2MA	C5-C6	2.47	1.47	1.41
1	2A	1915	5MU	C4-N3	-2.46	1.34	1.38
57	1y	32	PSU	C4-N3	-2.45	1.34	1.38
32	2a	1407	5MC	C6-C5	2.43	1.38	1.34
32	1a	1404	5MC	C6-N1	-2.42	1.33	1.38
32	2a	1407	5MC	C6-N1	-2.41	1.33	1.38
57	1y	54	5MU	C2-N1	2.40	1.42	1.38
32	2a	1207	2MG	C6-N1	-2.40	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.40	1.33	1.38
1	1A	1962	5MC	C6-C5	2.39	1.38	1.34
1	1A	1915	5MU	C2-N1	2.39	1.42	1.38
1	2A	1939	5MU	C4-N3	-2.39	1.34	1.38
57	1y	8	4SU	C2-N1	2.37	1.42	1.38
1	1A	1942	5MC	C6-N1	-2.37	1.34	1.38
32	2a	1498	UR3	C2-N1	2.37	1.41	1.38
57	1y	8	4SU	C5-C4	-2.35	1.39	1.42
54	1w	54	5MU	C2-N1	2.34	1.42	1.38
1	2A	2503	2MA	C5-C6	2.33	1.47	1.41
54	2w	54	5MU	C4-N3	-2.33	1.34	1.38
57	1y	55	PSU	C4-N3	-2.33	1.34	1.38
57	2y	54	5MU	C4-N3	-2.33	1.34	1.38
55	1x	8	4SU	O2-C2	2.33	1.27	1.23
1	1A	1939	5MU	C6-N1	-2.32	1.34	1.38
57	1y	37	MIA	C8-N7	2.32	1.36	1.31
32	1a	967	5MC	C6-N1	-2.32	1.34	1.38
57	2y	39	PSU	C4-N3	-2.32	1.34	1.38
54	2w	55	PSU	C4-N3	-2.32	1.34	1.38
1	1A	2552	OMU	C5-C4	2.32	1.48	1.43
1	2A	2605	PSU	C4-N3	-2.32	1.34	1.38
1	1A	2503	2MA	C8-N7	2.32	1.36	1.31
55	2x	32	5MC	C6-N1	-2.31	1.34	1.38
55	1x	32	5MC	C6-N1	-2.31	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.31	1.34	1.38
54	1w	54	5MU	C4-N3	-2.30	1.34	1.38
32	1a	967	5MC	C6-C5	2.30	1.38	1.34
55	1x	54	5MU	C4-C5	2.30	1.48	1.44
54	1w	55	PSU	C4-N3	-2.30	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2y	55	PSU	C4-N3	-2.30	1.34	1.38
57	2y	32	PSU	C4-N3	-2.29	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.29	1.34	1.38
54	1w	8	4SU	C2-N1	2.28	1.42	1.38
55	2x	54	5MU	C4-C5	2.28	1.48	1.44
57	1y	46	G7M	C6-N1	-2.27	1.34	1.38
54	1w	32	PSU	C4-N3	-2.27	1.34	1.38
54	1w	37	MIA	C5-N7	-2.26	1.35	1.39
32	2a	527	G7M	C6-N1	-2.26	1.34	1.38
54	2w	37	MIA	C5-N7	-2.26	1.35	1.39
54	2w	32	PSU	C4-N3	-2.25	1.34	1.38
55	2x	54	5MU	C2-N1	2.25	1.42	1.38
1	1A	1962	5MC	C6-N1	-2.25	1.34	1.38
57	1y	39	PSU	C4-N3	-2.24	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.24	1.34	1.38
54	1w	8	4SU	C2-N3	-2.22	1.34	1.38
32	2a	966	M2G	C5-N7	-2.22	1.34	1.39
54	2w	54	5MU	C4-C5	2.21	1.48	1.44
1	2A	2503	2MA	C8-N7	2.21	1.35	1.31
32	2a	967	5MC	C6-N1	-2.21	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.21	1.34	1.38
57	1y	54	5MU	C4-C5	2.20	1.48	1.44
54	2w	54	5MU	C2-N1	2.20	1.41	1.38
32	2a	516	PSU	C4-N3	-2.20	1.34	1.38
57	2y	8	4SU	C2-N1	2.18	1.41	1.38
54	2w	37	MIA	C8-N7	2.16	1.35	1.31
1	2A	2605	PSU	C2-N1	-2.15	1.33	1.36
1	1A	2503	2MA	C8-N9	-2.15	1.33	1.37
32	1a	966	M2G	C6-N1	-2.13	1.34	1.38
1	1A	1915	5MU	C4-C5	2.13	1.48	1.44
32	1a	527	G7M	C6-N1	-2.13	1.34	1.38
1	1A	1917	PSU	C2-N3	-2.13	1.34	1.37
1	2A	2552	OMU	C5-C4	2.12	1.48	1.43
57	1y	37	MIA	C5-N7	-2.12	1.35	1.39
32	1a	1407	5MC	C6-N1	-2.12	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.11	1.34	1.38
57	1y	46	G7M	C5-C6	2.11	1.49	1.43
32	2a	1207	2MG	C5-N7	-2.10	1.34	1.39
32	1a	527	G7M	C5-C6	2.08	1.49	1.43
54	1w	54	5MU	C6-N1	-2.08	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.06	1.34	1.37
32	2a	1404	5MC	C6-N1	-2.06	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	46	G7M	C5-C6	2.05	1.48	1.43
55	2x	54	5MU	C6-N1	-2.03	1.34	1.38
54	2w	8	4SU	C2-N3	-2.03	1.34	1.38
54	1w	54	5MU	C4-C5	2.02	1.48	1.44
32	1a	1207	2MG	C2-N3	2.02	1.35	1.32
57	1y	54	5MU	C6-N1	-2.02	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.01	1.34	1.38

All (443) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-18.80	68.58	102.36
43	2l	92	0TD	CSB-SB-CB	-10.40	83.67	102.36
54	1w	37	MIA	C12-C13-C14	-10.31	108.50	127.01
54	2w	37	MIA	C5-C4-N3	-8.24	118.50	127.18
54	1w	37	MIA	C5-C4-N3	-7.98	118.77	127.18
1	1A	2503	2MA	C5-C4-N3	-7.89	118.87	127.18
1	2A	2503	2MA	C5-C4-N3	-7.88	118.88	127.18
54	2w	8	4SU	C4-N3-C2	-7.47	120.16	127.31
1	1A	2605	PSU	N1-C2-N3	7.19	122.75	115.17
32	1a	1498	UR3	C4-N3-C2	-6.97	118.97	124.58
55	1x	76	8AN	O4'-C1'-N9	6.85	121.25	108.09
32	2a	1207	2MG	C2-N3-C4	6.77	120.47	112.00
32	2a	1498	UR3	C4-N3-C2	-6.76	119.14	124.58
1	1A	1911	PSU	N1-C2-N3	6.74	122.28	115.17
1	2A	2503	2MA	N3-C4-N9	6.72	135.51	126.99
57	2y	39	PSU	N1-C2-N3	6.71	122.25	115.17
1	1A	2503	2MA	N3-C4-N9	6.69	135.48	126.99
54	2w	37	MIA	N3-C4-N9	6.69	135.47	126.99
32	1a	1207	2MG	C2-N3-C4	6.63	120.30	112.00
57	2y	46	G7M	N9-C4-N3	6.62	139.19	125.95
1	2A	1911	PSU	N1-C2-N3	6.56	122.08	115.17
1	2A	1917	PSU	N1-C2-N3	6.39	121.91	115.17
54	2w	8	4SU	C5-C4-N3	6.34	120.65	114.75
55	1x	55	PSU	N1-C2-N3	6.34	121.86	115.17
54	1w	39	PSU	N1-C2-N3	6.30	121.82	115.17
54	2w	55	PSU	N1-C2-N3	6.27	121.78	115.17
57	2y	8	4SU	C4-N3-C2	-6.25	121.32	127.31
32	2a	966	M2G	C5-C4-N3	-6.23	118.47	128.39
57	1y	39	PSU	N1-C2-N3	6.22	121.73	115.17
54	1w	32	PSU	N1-C2-N3	6.17	121.68	115.17
57	1y	37	MIA	C5-C4-N3	-6.14	118.27	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	55	PSU	N1-C2-N3	6.13	121.63	115.17
57	1y	55	PSU	N1-C2-N3	6.10	121.61	115.17
32	2a	516	PSU	N1-C2-N3	6.08	121.58	115.17
1	1A	2251	OMG	C5-C4-N3	-6.06	118.75	128.39
1	1A	1917	PSU	N1-C2-N3	6.01	121.51	115.17
57	2y	55	PSU	N1-C2-N3	5.95	121.44	115.17
32	2a	1207	2MG	C5-C4-N3	-5.94	118.93	128.39
54	2w	32	PSU	N1-C2-N3	5.94	121.43	115.17
57	2y	46	G7M	C5-C4-N3	-5.93	116.95	128.15
54	1w	55	PSU	N1-C2-N3	5.90	121.39	115.17
54	1w	37	MIA	N3-C4-N9	5.83	134.40	126.99
1	1A	2552	OMU	N3-C2-N1	5.83	122.48	114.89
1	1A	1939	5MU	C4-N3-C2	-5.80	119.74	127.34
32	1a	516	PSU	N1-C2-N3	5.79	121.28	115.17
55	1x	76	8AN	N1-C2-N3	-5.78	119.83	128.58
55	2x	76	8AN	N1-C2-N3	-5.76	119.86	128.58
57	1y	32	PSU	N1-C2-N3	5.76	121.24	115.17
1	2A	2251	OMG	C5-C4-N3	-5.74	119.25	128.39
32	1a	966	M2G	C5-C4-N3	-5.73	119.27	128.39
54	1w	76	F3N	N1-C2-N3	-5.71	119.93	128.58
54	2w	76	F3N	N1-C2-N3	-5.71	119.94	128.58
54	2w	39	PSU	N1-C2-N3	5.71	121.19	115.17
57	1y	46	G7M	N9-C4-N3	5.70	137.34	125.95
1	2A	1939	5MU	C4-N3-C2	-5.68	119.89	127.34
57	2y	32	PSU	N1-C2-N3	5.66	121.14	115.17
57	2y	54	5MU	N3-C2-N1	5.62	122.20	114.89
1	2A	2605	PSU	N1-C2-N3	5.60	121.07	115.17
57	2y	37	MIA	C5-C4-N3	-5.60	119.01	126.72
32	1a	1207	2MG	C5-C4-N3	-5.51	119.62	128.39
57	1y	8	4SU	C4-N3-C2	-5.48	122.06	127.31
57	1y	46	G7M	C5-C4-N3	-5.36	118.02	128.15
57	2y	54	5MU	C4-N3-C2	-5.36	120.31	127.34
1	1A	1939	5MU	O4-C4-C5	-5.34	118.81	124.92
55	2x	54	5MU	N3-C2-N1	5.34	121.84	114.89
54	1w	46	G7M	N9-C4-N3	5.33	136.62	125.95
54	1w	8	4SU	C5-C4-N3	5.33	119.71	114.75
1	1A	1915	5MU	C4-N3-C2	-5.30	120.39	127.34
55	2x	54	5MU	C4-N3-C2	-5.30	120.40	127.34
57	1y	8	4SU	C5-C4-N3	5.29	119.67	114.75
32	1a	1518	MA6	N1-C2-N3	-5.28	120.59	128.58
1	1A	2251	OMG	C2-N3-C4	5.22	121.29	112.30
57	2y	8	4SU	C5-C4-N3	5.22	119.61	114.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1915	5MU	C4-N3-C2	-5.21	120.51	127.34
32	2a	1518	MA6	N1-C2-N3	-5.20	120.71	128.58
32	2a	1519	MA6	N1-C2-N3	-5.19	120.72	128.58
1	1A	1939	5MU	C5-C4-N3	5.17	119.81	115.32
55	1x	76	8AN	C5-C4-N3	-5.16	119.61	126.72
1	2A	1915	5MU	N3-C2-N1	5.14	121.58	114.89
32	1a	527	G7M	N9-C4-N3	5.13	136.21	125.95
32	1a	527	G7M	C5-C4-N3	-5.10	118.51	128.15
54	1w	46	G7M	C5-C4-N3	-5.09	118.53	128.15
57	2y	46	G7M	C2-N3-C4	5.08	121.05	112.30
54	2w	46	G7M	N9-C4-N3	5.08	136.10	125.95
32	2a	527	G7M	N9-C4-N3	5.03	136.01	125.95
54	1w	76	F3N	C5-C4-N3	-5.03	119.79	126.72
55	2x	76	8AN	C5-C4-N3	-5.02	119.80	126.72
32	1a	1519	MA6	N1-C2-N3	-4.98	121.04	128.58
54	2w	46	G7M	C5-C4-N3	-4.97	118.75	128.15
57	1y	37	MIA	N3-C4-N9	4.97	135.62	127.17
1	1A	1915	5MU	N3-C2-N1	4.97	121.36	114.89
54	2w	76	F3N	C5-C4-N3	-4.97	119.88	126.72
54	1w	8	4SU	C4-N3-C2	-4.93	122.59	127.31
32	2a	527	G7M	C5-C4-N3	-4.93	118.83	128.15
1	2A	1939	5MU	N3-C2-N1	4.93	121.31	114.89
55	1x	54	5MU	N3-C2-N1	4.89	121.25	114.89
57	1y	46	G7M	C2-N3-C4	4.88	120.70	112.30
1	2A	1939	5MU	C5-C4-N3	4.86	119.55	115.32
1	2A	2251	OMG	C2-N3-C4	4.83	120.62	112.30
1	1A	1915	5MU	C5-C4-N3	4.83	119.52	115.32
32	2a	966	M2G	N9-C4-N3	4.82	135.59	125.95
57	2y	39	PSU	C4-N3-C2	-4.82	119.74	126.37
55	1x	54	5MU	C4-N3-C2	-4.79	121.06	127.34
32	2a	1518	MA6	C5-C4-N3	-4.76	120.16	126.72
1	1A	2605	PSU	C4-N3-C2	-4.74	119.84	126.37
1	2A	2552	OMU	N3-C2-N1	4.74	121.06	114.89
54	2w	46	G7M	C2-N3-C4	4.71	120.41	112.30
54	1w	37	MIA	C15-C14-C13	-4.71	108.53	122.66
1	1A	1939	5MU	C5-C6-N1	-4.68	118.23	123.31
54	1w	54	5MU	C4-N3-C2	-4.65	121.24	127.34
54	1w	54	5MU	N3-C2-N1	4.64	120.92	114.89
1	1A	1939	5MU	N3-C2-N1	4.63	120.92	114.89
32	2a	527	G7M	C2-N3-C4	4.63	120.27	112.30
1	2A	2552	OMU	C4-N3-C2	-4.62	120.88	126.61
32	1a	966	M2G	C2-N3-C4	4.57	120.97	112.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	54	5MU	O4-C4-C5	-4.57	119.69	124.92
32	1a	527	G7M	C2-N3-C4	4.56	120.16	112.30
1	1A	1911	PSU	O2-C2-N1	-4.54	118.11	122.79
1	2A	1915	5MU	C5-C4-N3	4.52	119.25	115.32
55	1x	8	4SU	C6-C5-C4	-4.38	116.16	119.95
57	2y	54	5MU	C5-C4-N3	4.38	119.13	115.32
54	2w	8	4SU	C5-C4-S4	-4.37	119.31	124.31
55	2x	54	5MU	C5-C4-N3	4.36	119.11	115.32
57	2y	37	MIA	N3-C4-N9	4.36	134.58	127.17
1	1A	2251	OMG	N9-C4-N3	4.36	134.66	125.95
32	2a	1519	MA6	C5-C4-N3	-4.35	120.72	126.72
55	2x	54	5MU	O4-C4-C5	-4.34	119.95	124.92
32	1a	1518	MA6	C2-N1-C6	4.33	122.42	111.83
1	1A	1915	5MU	O4-C4-C5	-4.31	119.98	124.92
32	1a	1519	MA6	C5-C4-N3	-4.31	120.78	126.72
1	2A	1911	PSU	C4-N3-C2	-4.29	120.45	126.37
1	2A	2251	OMG	N9-C4-N3	4.29	134.52	125.95
32	1a	966	M2G	N9-C4-N3	4.28	134.51	125.95
57	1y	54	5MU	N3-C2-N1	4.27	120.45	114.89
55	2x	55	PSU	C4-N3-C2	-4.24	120.53	126.37
57	2y	54	5MU	O4-C4-C5	-4.24	120.07	124.92
54	1w	46	G7M	C2-N3-C4	4.24	119.59	112.30
32	2a	516	PSU	C4-N3-C2	-4.23	120.55	126.37
1	2A	1939	5MU	C5-C6-N1	-4.23	118.72	123.31
54	1w	37	MIA	C6-C5-N7	4.21	137.02	132.43
1	2A	1939	5MU	O4-C4-C5	-4.21	120.11	124.92
32	2a	966	M2G	C2-N3-C4	4.20	120.27	112.51
57	1y	39	PSU	C4-N3-C2	-4.19	120.60	126.37
54	2w	8	4SU	N3-C2-N1	4.19	120.34	114.89
54	2w	54	5MU	C4-N3-C2	-4.18	121.86	127.34
1	1A	2552	OMU	C4-N3-C2	-4.18	121.42	126.61
1	2A	1915	5MU	O4-C4-C5	-4.17	120.14	124.92
54	2w	54	5MU	O4-C4-C5	-4.17	120.15	124.92
54	1w	32	PSU	C4-N3-C2	-4.15	120.65	126.37
57	2y	8	4SU	N3-C2-N1	4.15	120.30	114.89
1	1A	1911	PSU	C4-N3-C2	-4.13	120.68	126.37
32	2a	1518	MA6	C2-N1-C6	4.13	121.92	111.83
1	2A	1939	5MU	O2-C2-N1	-4.13	117.42	122.80
32	2a	1207	2MG	N9-C4-N3	4.13	134.20	125.95
1	1A	2552	OMU	O2-C2-N1	-4.11	117.44	122.80
54	2w	54	5MU	C5-C4-N3	4.11	118.90	115.32
1	2A	1917	PSU	C4-N3-C2	-4.10	120.73	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	54	5MU	C5-C4-N3	4.10	118.89	115.32
54	1w	39	PSU	C4-N3-C2	-4.10	120.73	126.37
57	2y	55	PSU	C4-N3-C2	-4.09	120.74	126.37
54	1w	54	5MU	C5-C4-N3	4.07	118.86	115.32
32	1a	1519	MA6	C2-N1-C6	4.04	121.71	111.83
1	2A	2605	PSU	C4-N3-C2	-4.04	120.81	126.37
32	2a	1519	MA6	C5-N7-C8	4.02	109.77	103.45
32	1a	1207	2MG	N9-C4-N3	4.01	133.98	125.95
55	1x	8	4SU	O2-C2-N1	4.00	128.00	122.80
32	1a	516	PSU	C4-N3-C2	-4.00	120.86	126.37
54	2w	55	PSU	O2-C2-N1	-3.99	118.68	122.79
54	2w	32	PSU	C4-N3-C2	-3.97	120.90	126.37
32	2a	1519	MA6	C2-N1-C6	3.96	121.50	111.83
55	1x	55	PSU	C4-N3-C2	-3.96	120.92	126.37
57	1y	55	PSU	O2-C2-N1	-3.95	118.71	122.79
54	2w	54	5MU	N3-C2-N1	3.94	120.02	114.89
32	1a	1519	MA6	C5-N7-C8	3.91	109.59	103.45
32	2a	1519	MA6	C4-C5-N7	-3.89	106.14	110.58
32	2a	1400	5MC	C5-C6-N1	-3.88	119.10	123.31
54	2w	55	PSU	C4-N3-C2	-3.87	121.03	126.37
32	1a	1519	MA6	C4-C5-N7	-3.87	106.16	110.58
32	2a	1518	MA6	C5-N7-C8	3.85	109.50	103.45
55	1x	54	5MU	O4-C4-C5	-3.84	120.52	124.92
57	2y	8	4SU	C5-C4-S4	-3.84	119.92	124.31
57	2y	39	PSU	O2-C2-N1	-3.83	118.84	122.79
57	2y	37	MIA	C4-C5-N7	-3.82	106.21	110.58
57	1y	37	MIA	C2-N3-C4	3.82	121.16	111.83
1	1A	1917	PSU	C4-N3-C2	-3.81	121.12	126.37
1	2A	2605	PSU	O2-C2-N1	-3.80	118.87	122.79
32	1a	1207	2MG	C6-C5-N7	3.80	137.20	130.29
32	2a	1518	MA6	C4-C5-N7	-3.79	106.25	110.58
54	1w	37	MIA	C4-C5-N7	-3.79	106.25	110.58
32	2a	516	PSU	O2-C2-N1	-3.78	118.89	122.79
57	1y	32	PSU	C4-N3-C2	-3.78	121.16	126.37
54	2w	37	MIA	C11-S10-C2	-3.77	99.42	102.25
32	1a	1518	MA6	C5-N7-C8	3.74	109.33	103.45
55	2x	32	5MC	C5-C6-N1	-3.74	119.25	123.31
57	2y	55	PSU	O2-C2-N1	-3.73	118.94	122.79
32	1a	1518	MA6	C5-C4-N3	-3.72	121.60	126.72
55	1x	55	PSU	O2-C2-N1	-3.71	118.97	122.79
54	1w	32	PSU	O2-C2-N1	-3.68	118.99	122.79
57	2y	32	PSU	C4-N3-C2	-3.68	121.31	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1y	55	PSU	C4-N3-C2	-3.65	121.35	126.37
32	2a	1518	MA6	C2-N3-C4	3.64	120.73	111.83
54	2w	32	PSU	O2-C2-N1	-3.64	119.04	122.79
57	1y	54	5MU	C4-N3-C2	-3.64	122.57	127.34
1	2A	1962	5MC	C5-C6-N1	-3.63	119.37	123.31
54	1w	37	MIA	C2-N3-C4	3.62	121.78	112.29
32	2a	1519	MA6	C2-N3-C4	3.62	120.67	111.83
32	2a	1519	MA6	N9-C8-N7	-3.61	108.82	113.94
1	1A	2605	PSU	O2-C2-N1	-3.60	119.08	122.79
54	1w	55	PSU	C4-N3-C2	-3.56	121.46	126.37
1	2A	1917	PSU	O2-C2-N1	-3.56	119.11	122.79
54	2w	39	PSU	C4-N3-C2	-3.55	121.47	126.37
32	1a	1518	MA6	N9-C8-N7	-3.55	108.89	113.94
32	1a	1400	5MC	C5-C6-N1	-3.55	119.45	123.31
55	1x	32	5MC	C5-C6-N1	-3.55	119.46	123.31
1	2A	1911	PSU	O2-C2-N1	-3.54	119.14	122.79
1	1A	2503	2MA	N6-C6-N1	3.54	121.80	117.03
54	1w	55	PSU	O2-C2-N1	-3.52	119.16	122.79
57	2y	37	MIA	C2-N3-C4	3.52	120.42	111.83
1	1A	2503	2MA	C4-N9-C8	3.49	109.41	105.74
57	1y	32	PSU	O2-C2-N1	-3.49	119.19	122.79
1	2A	2503	2MA	N6-C6-N1	3.48	121.72	117.03
57	1y	37	MIA	N3-C2-N1	-3.48	123.31	128.58
55	2x	76	8AN	N9-C8-N7	-3.48	109.00	113.94
55	2x	8	4SU	C5-C4-N3	3.48	117.98	114.75
54	1w	8	4SU	C5-C4-S4	-3.47	120.34	124.31
32	1a	1518	MA6	C4-C5-N7	-3.45	106.64	110.58
1	2A	2251	OMG	C6-C5-N7	3.45	136.56	130.29
54	1w	76	F3N	N9-C8-N7	-3.44	109.06	113.94
55	2x	54	5MU	C5-C6-N1	-3.44	119.58	123.31
32	1a	1519	MA6	N9-C8-N7	-3.44	109.06	113.94
54	2w	76	F3N	N9-C8-N7	-3.43	109.07	113.94
32	1a	1519	MA6	C2-N3-C4	3.42	120.18	111.83
54	1w	37	MIA	C16-C14-C13	-3.41	112.41	122.66
55	1x	76	8AN	C2-N3-C4	3.40	120.14	111.83
57	1y	8	4SU	C5-C4-S4	-3.40	120.42	124.31
57	1y	39	PSU	O2-C2-N1	-3.39	119.29	122.79
32	1a	1404	5MC	C5-C4-N3	-3.39	118.28	121.75
54	1w	76	F3N	C2-N3-C4	3.39	120.10	111.83
55	2x	76	8AN	C2-N3-C4	3.38	120.09	111.83
54	2w	37	MIA	C4-C5-N7	-3.38	106.72	110.58
54	2w	37	MIA	C2-N3-C4	3.38	121.15	112.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1942	5MC	C5-C6-N1	-3.38	119.64	123.31
1	1A	1939	5MU	O2-C2-N1	-3.37	118.41	122.80
54	2w	76	F3N	C2-N3-C4	3.36	120.04	111.83
32	2a	1407	5MC	C5-C6-N1	-3.36	119.67	123.31
54	2w	37	MIA	C12-N6-C6	-3.35	119.74	122.85
55	1x	76	8AN	N9-C8-N7	-3.34	109.19	113.94
32	1a	966	M2G	C6-C5-N7	3.34	136.37	130.29
32	2a	1518	MA6	N9-C8-N7	-3.34	109.20	113.94
32	1a	516	PSU	O2-C2-N1	-3.31	119.38	122.79
57	1y	54	5MU	C5-C4-N3	3.31	118.20	115.32
1	2A	2552	OMU	O2-C2-N1	-3.30	118.50	122.80
1	1A	2503	2MA	C4-C5-N7	-3.29	106.82	110.58
1	2A	2503	2MA	C4-N9-C8	3.29	109.19	105.74
32	1a	1518	MA6	C2-N3-C4	3.29	119.86	111.83
55	1x	54	5MU	C5-C6-N1	-3.28	119.75	123.31
57	1y	54	5MU	O4-C4-C5	-3.28	121.17	124.92
57	1y	37	MIA	C4-C5-N7	-3.27	106.85	110.58
32	2a	1207	2MG	C6-C5-N7	3.27	136.23	130.29
57	1y	8	4SU	N3-C2-N1	3.26	119.13	114.89
1	1A	1942	5MC	C5-C6-N1	-3.25	119.78	123.31
55	2x	76	8AN	C4'-O4'-C1'	-3.25	102.30	109.47
55	1x	32	5MC	C5-C4-N3	-3.25	118.43	121.75
1	1A	2251	OMG	C6-C5-N7	3.24	136.18	130.29
1	1A	1917	PSU	O2-C2-N1	-3.23	119.46	122.79
1	2A	1915	5MU	C5-C6-N1	-3.22	119.81	123.31
57	2y	37	MIA	N3-C2-N1	-3.22	123.71	128.58
1	2A	2503	2MA	C4-C5-N7	-3.21	106.91	110.58
32	1a	1407	5MC	C5-C6-N1	-3.19	119.85	123.31
43	1l	92	0TD	OD2-CG-CB	3.18	120.03	113.15
55	2x	8	4SU	C6-C5-C4	-3.18	117.20	119.95
55	1x	76	8AN	C4'-O4'-C1'	-3.17	102.46	109.47
55	2x	8	4SU	C1'-N1-C2	3.14	123.22	117.59
1	1A	1962	5MC	C5-C6-N1	-3.13	119.91	123.31
55	1x	8	4SU	C5-C4-N3	3.12	117.65	114.75
1	1A	1915	5MU	C5-C6-N1	-3.12	119.93	123.31
43	2l	92	0TD	OD2-CG-CB	3.10	119.84	113.15
1	2A	2552	OMU	C5-C4-N3	3.08	119.12	114.80
32	1a	1498	UR3	C5-C4-N3	3.08	119.10	115.04
32	2a	1404	5MC	C5-C6-N1	-3.07	119.97	123.31
54	1w	76	F3N	C5-N7-C8	3.06	108.26	103.45
32	2a	967	5MC	C5-C6-N1	-3.06	119.99	123.31
57	2y	32	PSU	O2-C2-N1	-3.04	119.65	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1498	UR3	C5-C4-N3	3.04	119.04	115.04
54	2w	76	F3N	C5-N7-C8	3.03	108.22	103.45
1	2A	2552	OMU	O4-C4-C5	-3.02	119.95	125.16
55	2x	76	8AN	C5-N7-C8	3.01	108.18	103.45
32	1a	1404	5MC	C5-C6-N1	-3.01	120.05	123.31
54	1w	8	4SU	N3-C2-N1	2.99	118.79	114.89
57	2y	54	5MU	C5-C6-N1	-2.99	120.06	123.31
55	1x	76	8AN	C5-N7-C8	2.96	108.11	103.45
32	2a	1518	MA6	N3-C4-N9	2.96	132.19	127.17
1	1A	1942	5MC	C5-C4-N3	-2.93	118.76	121.75
1	2A	2503	2MA	C2-N1-C6	2.91	122.57	118.10
1	1A	1962	5MC	C5-C4-N3	-2.90	118.78	121.75
32	2a	1404	5MC	C5-C4-N3	-2.90	118.78	121.75
54	2w	37	MIA	C6-C5-N7	2.89	135.58	132.43
55	1x	76	8AN	C5-C4-N9	2.89	108.96	105.81
1	1A	2503	2MA	C2-N1-C6	2.89	122.54	118.10
54	1w	37	MIA	N3-C2-N1	-2.89	121.73	127.00
54	1w	39	PSU	O2-C2-N1	-2.88	119.81	122.79
32	2a	1407	5MC	C5-C4-N3	-2.87	118.81	121.75
57	2y	37	MIA	C4-N9-C8	2.85	108.73	105.74
54	1w	37	MIA	C2-N1-C6	2.84	122.93	117.54
32	1a	1400	5MC	C5-C4-N3	-2.82	118.86	121.75
54	2w	39	PSU	O2-C2-N1	-2.81	119.89	122.79
54	2w	76	F3N	C3'-N3'-C	-2.80	118.94	123.20
32	2a	966	M2G	C6-C5-N7	2.80	135.38	130.29
55	2x	54	5MU	O2-C2-N1	-2.79	119.17	122.80
32	1a	1207	2MG	C4-C5-N7	-2.78	106.26	110.67
32	1a	967	5MC	C5-C6-N1	-2.78	120.29	123.31
57	2y	37	MIA	C5-N7-C8	2.76	107.79	103.45
57	1y	32	PSU	C6-C5-C4	-2.76	116.31	118.17
55	2x	55	PSU	O2-C2-N1	-2.74	119.97	122.79
32	2a	1207	2MG	C4-C5-N7	-2.72	106.36	110.67
55	1x	8	4SU	S4-C4-N3	-2.72	117.36	120.20
1	1A	2503	2MA	C5-N7-C8	2.71	107.71	103.45
1	2A	2503	2MA	C5-N7-C8	2.70	107.69	103.45
55	2x	32	5MC	C5-C4-N3	-2.70	118.99	121.75
54	1w	76	F3N	C5-C4-N9	2.70	108.75	105.81
54	2w	46	G7M	O6-C6-C5	-2.69	122.02	128.01
55	2x	76	8AN	C5-C4-N9	2.67	108.72	105.81
54	2w	37	MIA	C4-N9-C8	2.66	108.53	105.74
32	2a	1519	MA6	N3-C4-N9	2.66	131.69	127.17
54	2w	54	5MU	C5-C6-N1	-2.66	120.42	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C5-N7-C8	2.66	107.62	103.45
32	2a	967	5MC	C5-C4-N3	-2.64	119.05	121.75
1	2A	1942	5MC	C5-C4-N3	-2.64	119.05	121.75
55	1x	8	4SU	C1'-N1-C2	2.62	122.31	117.59
54	1w	54	5MU	C5-C6-N1	-2.62	120.47	123.31
54	2w	76	F3N	C5-C4-N9	2.61	108.66	105.81
32	2a	1518	MA6	C4-C5-C6	2.61	118.61	115.91
1	1A	2605	PSU	C5-C6-N1	-2.59	118.54	122.14
32	1a	1519	MA6	N3-C4-N9	2.58	131.56	127.17
54	1w	8	4SU	C1'-N1-C2	2.58	122.22	117.59
55	2x	8	4SU	O2-C2-N1	2.57	126.15	122.80
1	2A	2552	OMU	C2'-C1'-N1	-2.57	109.37	114.24
32	1a	1404	5MC	O2-C2-N3	-2.55	118.31	122.33
1	2A	2251	OMG	CM2-O2'-C2'	-2.55	107.93	114.47
1	2A	2251	OMG	C4-C5-N7	-2.54	106.65	110.67
54	2w	37	MIA	C5-N7-C8	2.53	107.43	103.45
55	2x	76	8AN	N3-C4-N9	2.53	131.48	127.17
57	1y	8	4SU	C1'-N1-C2	2.53	122.14	117.59
54	2w	76	F3N	N3-C4-N9	2.52	131.46	127.17
54	1w	76	F3N	N3-C4-N9	2.52	131.46	127.17
32	1a	1498	UR3	C3U-N3-C4	2.51	121.36	117.87
57	1y	54	5MU	C1'-N1-C2	2.51	122.11	117.59
1	1A	2251	OMG	C4-C5-N7	-2.51	106.69	110.67
32	2a	1400	5MC	C5-C4-N3	-2.51	119.18	121.75
55	1x	76	8AN	N3-C4-N9	2.50	131.43	127.17
32	2a	1402	4OC	C6-C5-C4	2.50	120.01	117.00
1	2A	1939	5MU	C5M-C5-C4	2.49	121.44	118.78
32	1a	1402	4OC	C6-C5-C4	2.49	120.00	117.00
1	1A	2503	2MA	N9-C8-N7	-2.49	110.41	113.94
32	1a	966	M2G	O6-C6-C5	-2.48	119.98	126.53
1	1A	1917	PSU	C6-C5-C4	-2.47	116.50	118.17
55	1x	76	8AN	C6-C5-C4	2.46	120.54	117.18
57	2y	39	PSU	C5-C6-N1	-2.46	118.72	122.14
57	1y	37	MIA	C5-N7-C8	2.44	107.29	103.45
32	1a	1402	4OC	O2-C2-N3	-2.43	118.50	122.33
32	2a	1207	2MG	N1-C2-N2	2.42	119.03	116.56
1	1A	1962	5MC	CM5-C5-C6	-2.42	119.57	122.85
32	2a	1207	2MG	N2-C2-N3	-2.42	117.43	120.51
32	1a	1518	MA6	N3-C4-N9	2.42	131.28	127.17
1	2A	1911	PSU	C5-C6-N1	-2.41	118.79	122.14
32	1a	967	5MC	C1'-N1-C6	-2.40	117.20	121.15
32	1a	966	M2G	C4-C5-N7	-2.40	106.87	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	8	4SU	O2-C2-N1	-2.39	119.68	122.80
32	2a	966	M2G	C4-C5-N7	-2.39	106.88	110.67
1	2A	1915	5MU	O2-C2-N1	-2.37	119.70	122.80
1	1A	1915	5MU	O2-C2-N1	-2.37	119.72	122.80
1	2A	2503	2MA	N9-C8-N7	-2.36	110.58	113.94
1	1A	1920	OMC	O2-C2-N3	-2.34	118.64	122.33
56	2z	1	FME	CB-CA-N	2.31	114.73	110.52
32	1a	967	5MC	C5-C4-N3	-2.30	119.39	121.75
56	1z	1	FME	CA-N-CN	2.30	126.36	122.82
1	1A	2251	OMG	O6-C6-C5	-2.28	120.50	126.53
54	2w	37	MIA	N3-C2-N1	-2.28	122.83	127.00
54	2w	37	MIA	C2-N1-C6	2.28	121.86	117.54
43	1l	92	0TD	OD1-CG-CB	-2.27	117.68	122.44
1	2A	1962	5MC	C5-C4-N3	-2.26	119.44	121.75
54	1w	46	G7M	O6-C6-C5	-2.25	122.98	128.01
55	1x	54	5MU	O2-C2-N1	-2.25	119.87	122.80
55	1x	8	4SU	O2-C2-N3	-2.25	117.34	121.49
57	2y	54	5MU	O2-C2-N3	-2.24	117.35	121.49
55	1x	76	8AN	C4-C5-N7	-2.24	108.02	110.58
32	2a	527	G7M	O6-C6-C5	-2.24	123.01	128.01
32	1a	527	G7M	O6-C6-C5	-2.24	123.02	128.01
54	2w	54	5MU	C5M-C5-C4	2.24	121.17	118.78
43	2l	92	0TD	OD1-CG-CB	-2.22	117.80	122.44
54	1w	37	MIA	C4-N9-C8	2.21	108.06	105.74
54	2w	46	G7M	C5-C6-N1	2.20	116.39	111.84
57	1y	37	MIA	C4-N9-C8	2.20	108.05	105.74
54	1w	76	F3N	C4-C5-N7	-2.20	108.07	110.58
55	2x	76	8AN	C6-C5-C4	2.19	120.17	117.18
1	1A	1942	5MC	O2-C2-N3	-2.18	118.89	122.33
57	2y	55	PSU	C6-C5-C4	-2.18	116.70	118.17
32	2a	1498	UR3	C1'-N1-C2	2.17	120.60	117.04
1	1A	2552	OMU	O4-C4-C5	-2.17	121.42	125.16
1	2A	1917	PSU	C5-C6-N1	-2.17	119.13	122.14
57	2y	37	MIA	N9-C8-N7	-2.17	110.86	113.94
55	2x	76	8AN	C4-C5-N7	-2.16	108.11	110.58
32	1a	1519	MA6	C4-C5-C6	2.16	118.14	115.91
32	1a	1518	MA6	C4-N9-C8	2.16	108.00	105.74
55	2x	55	PSU	C5-C6-N1	-2.15	119.16	122.14
57	2y	46	G7M	O6-C6-C5	-2.15	123.21	128.01
32	2a	527	G7M	C5-C6-N1	2.15	116.28	111.84
32	1a	1404	5MC	CM5-C5-C6	-2.14	119.95	122.85
55	1x	32	5MC	O2-C2-N3	-2.14	118.96	122.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	32	PSU	C6-C5-C4	-2.14	116.73	118.17
55	2x	8	4SU	O2-C2-N3	-2.13	117.55	121.49
54	2w	76	F3N	C4-C5-N7	-2.13	108.14	110.58
1	1A	1920	OMC	C1'-N1-C2	2.13	123.14	118.44
57	1y	46	G7M	O6-C6-C5	-2.12	123.27	128.01
1	1A	1915	5MU	C5M-C5-C4	2.12	121.05	118.78
32	2a	1498	UR3	C3U-N3-C2	2.12	121.03	117.33
54	2w	76	F3N	C6-C5-C4	2.12	120.07	117.18
54	1w	76	F3N	C6-C5-C4	2.11	120.06	117.18
57	2y	37	MIA	C6-C5-N7	2.11	136.15	132.09
55	2x	32	5MC	O2-C2-N3	-2.10	119.02	122.33
1	1A	1911	PSU	C5-C6-N1	-2.09	119.24	122.14
54	1w	39	PSU	C5-C6-N1	-2.09	119.24	122.14
54	1w	54	5MU	O2-C2-N1	-2.09	120.08	122.80
1	2A	2251	OMG	O6-C6-C5	-2.08	121.04	126.53
1	1A	2605	PSU	O2-C2-N3	-2.08	118.17	121.86
32	1a	1407	5MC	C5-C4-N3	-2.07	119.63	121.75
57	2y	8	4SU	O2-C2-N1	-2.07	120.10	122.80
55	1x	8	4SU	C4-N3-C2	2.06	129.29	127.31
57	1y	54	5MU	C5-C6-N1	-2.05	121.09	123.31
1	1A	2503	2MA	C6-C5-N7	2.05	136.03	132.09
1	1A	2552	OMU	C5-C4-N3	2.04	117.66	114.80
55	2x	76	8AN	O2'-C2'-C3'	2.04	116.98	111.61
1	2A	2605	PSU	C5-C6-N1	-2.03	119.32	122.14
57	1y	55	PSU	C6-C5-C4	-2.03	116.81	118.17
57	2y	32	PSU	C6-C5-C4	-2.03	116.81	118.17
1	2A	1911	PSU	O4'-C1'-C2'	2.03	107.95	105.15
1	2A	1939	5MU	C5M-C5-C6	-2.02	120.11	122.85
32	1a	527	G7M	C5-C6-N1	2.02	116.01	111.84
32	2a	1400	5MC	CM5-C5-C6	-2.02	120.12	122.85
54	1w	55	PSU	C6-C5-C4	-2.02	116.81	118.17
57	1y	46	G7M	C5-C6-N1	2.02	116.01	111.84
55	2x	32	5MC	CM5-C5-C6	-2.01	120.13	122.85
1	2A	2251	OMG	C5-C6-N1	2.00	118.35	113.25

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	2251	OMG	C1'-C2'-O2'-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
57	1y	46	G7M	C4'-C5'-O5'-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
57	2y	54	5MU	C3'-C4'-C5'-O5'
57	2y	54	5MU	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12
56	1z	1	FME	O1-CN-N-CA
56	1z	1	FME	N-CA-CB-CG
56	1z	1	FME	C-CA-CB-CG
56	1z	1	FME	O-C-CA-CB
56	2z	1	FME	O1-CN-N-CA
55	1x	76	8AN	C3'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
55	2x	76	8AN	O4'-C4'-C5'-O5'
54	2w	32	PSU	O4'-C4'-C5'-O5'
56	2z	1	FME	CA-CB-CG-SD
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	1x	76	8AN	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
54	2w	32	PSU	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
57	2y	46	G7M	O4'-C4'-C5'-O5'
54	2w	46	G7M	C4'-C5'-O5'-P
57	2y	46	G7M	O4'-C1'-N9-C4
54	2w	76	F3N	N-CA-CB-CG
57	2y	46	G7M	C3'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
57	1y	37	MIA	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
55	1x	76	8AN	C4'-C5'-O5'-P
55	2x	76	8AN	C4'-C5'-O5'-P
54	2w	76	F3N	O4'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	2a	527	G7M	C4'-C5'-O5'-P
57	2y	8	4SU	C4'-C5'-O5'-P
57	1y	32	PSU	O4'-C1'-C5-C4
57	1y	55	PSU	O4'-C1'-C5-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	1w	37	MIA	N6-C12-C13-C14
1	1A	2503	2MA	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
57	2y	46	G7M	O4'-C1'-N9-C8
32	1a	527	G7M	C4'-C5'-O5'-P
57	2y	37	MIA	C3'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
54	2w	76	F3N	C-CA-CB-CG
57	1y	55	PSU	O4'-C1'-C5-C6
57	2y	55	PSU	O4'-C1'-C5-C6
57	1y	46	G7M	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
56	2z	1	FME	N-CA-CB-CG
32	1a	1400	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

40 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1y	8	4SU	3	0
55	2x	76	8AN	1	0
57	1y	39	PSU	1	0
55	1x	8	4SU	1	0
1	2A	1939	5MU	1	0
57	1y	46	G7M	1	0
54	2w	55	PSU	1	0
54	2w	76	F3N	3	0
54	1w	37	MIA	1	0
32	1a	1518	MA6	2	0
57	2y	46	G7M	2	0
56	2z	1	FME	1	0
1	1A	1917	PSU	1	0
32	1a	1519	MA6	2	0
57	2y	8	4SU	1	0
32	2a	966	M2G	1	0
55	2x	55	PSU	1	0
55	1x	76	8AN	1	0
57	2y	55	PSU	5	0
32	2a	1518	MA6	1	0
54	1w	46	G7M	1	0
1	2A	2251	OMG	1	0
57	1y	55	PSU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	2l	92	0TD	1	0
32	2a	1404	5MC	2	0
56	1z	1	FME	2	0
1	2A	2503	2MA	1	0
54	2w	46	G7M	1	0
54	2w	54	5MU	1	0
1	1A	2552	OMU	1	0
1	1A	2251	OMG	1	0
57	1y	54	5MU	2	0
32	1a	1402	4OC	2	0
32	2a	967	5MC	1	0
1	2A	2552	OMU	1	0
54	1w	76	F3N	1	0
32	2a	1519	MA6	1	0
57	1y	37	MIA	2	0
1	2A	1915	5MU	1	0
1	1A	1939	5MU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2739 ligands modelled in this entry, 2737 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	$\# Z > 2$
61	SF4	1d	302	35	0,12,12	-	-	-		
61	SF4	2d	304	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
61	SF4	1d	302	35	-	-	0/6/5/5
61	SF4	2d	304	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.

No monomer is involved in short contacts.

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%)	0.21	193 (6%)	24	26	19, 35, 83, 91	0
1	2A	2789/2915 (95%)	0.65	175 (6%)	26	28	31, 52, 81, 93	0
2	1B	120/121 (99%)	0.24	0	100	100	31, 47, 59, 77	0
2	2B	120/121 (99%)	1.01	4 (3%)	49	51	55, 66, 73, 80	0
3	1D	275/276 (99%)	0.74	11 (4%)	42	44	20, 36, 49, 69	0
3	2D	275/276 (99%)	1.40	64 (23%)	2	2	30, 46, 59, 69	0
4	1E	204/206 (99%)	1.01	26 (12%)	8	8	19, 39, 57, 67	0
4	2E	204/206 (99%)	1.26	35 (17%)	4	4	32, 53, 64, 73	0
5	1F	202/210 (96%)	0.96	26 (12%)	7	8	20, 40, 61, 73	0
5	2F	202/210 (96%)	1.59	61 (30%)	1	1	32, 61, 71, 76	0
6	1G	181/182 (99%)	1.29	25 (13%)	6	7	42, 54, 67, 78	0
6	2G	181/182 (99%)	2.12	101 (55%)	0	0	57, 68, 75, 81	0
7	1H	174/180 (96%)	1.43	32 (18%)	3	4	36, 52, 61, 66	0
7	2H	174/180 (96%)	2.39	106 (60%)	0	0	62, 71, 77, 80	0
8	1I	146/148 (98%)	1.88	60 (41%)	0	0	45, 66, 73, 77	0
8	2I	146/148 (98%)	2.66	103 (70%)	0	0	54, 70, 79, 83	0
9	1N	140/140 (100%)	0.81	5 (3%)	46	48	24, 38, 56, 70	0
9	2N	140/140 (100%)	1.52	35 (25%)	2	2	42, 57, 69, 71	0
10	1O	122/122 (100%)	0.91	8 (6%)	24	26	26, 38, 53, 58	0
10	2O	122/122 (100%)	1.32	16 (13%)	7	8	40, 52, 63, 71	0
11	1P	149/150 (99%)	0.91	19 (12%)	7	8	20, 43, 62, 67	0
11	2P	149/150 (99%)	1.61	46 (30%)	1	1	36, 60, 71, 75	0
12	1Q	141/141 (100%)	0.75	6 (4%)	40	41	23, 39, 53, 65	0
12	2Q	141/141 (100%)	1.56	45 (31%)	1	1	38, 57, 65, 70	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%)	0.61	1 (0%) 82 83	25, 35, 44, 54	0
13	2R	118/118 (100%)	1.01	12 (10%) 12 13	38, 49, 57, 61	0
14	1S	110/112 (98%)	1.07	10 (9%) 15 16	36, 47, 59, 62	0
14	2S	110/112 (98%)	1.99	58 (52%) 0 0	54, 63, 70, 73	0
15	1T	131/146 (89%)	1.10	20 (15%) 5 6	31, 42, 63, 73	0
15	2T	131/146 (89%)	1.48	29 (22%) 2 2	47, 55, 67, 73	0
16	1U	116/118 (98%)	0.33	0 100 100	19, 29, 46, 57	0
16	2U	116/118 (98%)	1.36	24 (20%) 2 3	41, 54, 64, 67	0
17	1V	101/101 (100%)	0.61	1 (0%) 79 80	22, 38, 51, 60	0
17	2V	101/101 (100%)	1.75	41 (40%) 0 0	40, 61, 69, 74	0
18	1W	112/113 (99%)	0.61	2 (1%) 67 69	23, 32, 47, 75	0
18	2W	112/113 (99%)	0.94	9 (8%) 18 20	36, 46, 59, 77	0
19	1X	95/96 (98%)	0.78	6 (6%) 26 28	25, 36, 54, 73	0
19	2X	95/96 (98%)	1.61	23 (24%) 2 2	42, 54, 66, 70	0
20	1Y	107/110 (97%)	1.15	12 (11%) 10 11	34, 46, 60, 70	0
20	2Y	107/110 (97%)	1.87	36 (33%) 1 1	52, 64, 71, 77	0
21	1Z	154/206 (74%)	1.62	46 (29%) 1 1	38, 59, 73, 79	0
21	2Z	160/206 (77%)	2.39	105 (65%) 0 0	55, 71, 79, 83	0
22	10	83/85 (97%)	0.64	4 (4%) 35 37	27, 36, 47, 60	0
22	20	83/85 (97%)	1.44	19 (22%) 2 2	40, 54, 61, 71	0
23	11	97/98 (98%)	1.06	10 (10%) 12 13	28, 45, 65, 69	0
23	21	97/98 (98%)	1.79	31 (31%) 1 1	40, 55, 67, 73	0
24	12	70/72 (97%)	0.88	5 (7%) 22 24	35, 44, 57, 67	0
24	22	70/72 (97%)	1.77	26 (37%) 1 1	54, 62, 69, 71	0
25	13	59/60 (98%)	0.55	3 (5%) 33 35	25, 35, 52, 63	0
25	23	59/60 (98%)	1.46	9 (15%) 5 6	48, 55, 69, 72	0
26	14	69/71 (97%)	1.87	24 (34%) 1 1	47, 68, 77, 80	0
26	24	69/71 (97%)	2.44	43 (62%) 0 0	66, 73, 79, 82	0
27	15	59/60 (98%)	0.55	1 (1%) 69 70	21, 33, 51, 64	0
27	25	59/60 (98%)	0.89	3 (5%) 33 35	33, 46, 61, 71	0
28	16	53/54 (98%)	0.74	1 (1%) 66 68	31, 39, 53, 59	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%)	1.41	10 (18%) 3 4	44, 54, 62, 65	0
29	17	48/49 (97%)	0.43	3 (6%) 26 28	18, 27, 51, 57	0
29	27	48/49 (97%)	1.07	8 (16%) 4 5	33, 41, 60, 68	0
30	18	64/65 (98%)	0.56	2 (3%) 51 53	27, 33, 39, 55	0
30	28	64/65 (98%)	1.24	6 (9%) 14 15	40, 50, 54, 59	0
31	19	37/37 (100%)	0.52	0 100 100	28, 36, 49, 51	0
31	29	37/37 (100%)	1.60	10 (27%) 1 1	51, 58, 67, 69	0
32	1a	1488/1521 (97%)	1.06	121 (8%) 18 19	33, 58, 80, 90	0
32	2a	1491/1521 (98%)	1.28	163 (10%) 10 12	45, 67, 81, 91	0
33	1b	231/256 (90%)	2.07	109 (47%) 0 0	57, 68, 75, 81	0
33	2b	231/256 (90%)	2.71	176 (76%) 0 0	63, 72, 77, 83	0
34	1c	206/239 (86%)	1.91	85 (41%) 0 0	47, 61, 69, 75	0
34	2c	206/239 (86%)	2.50	141 (68%) 0 0	63, 71, 76, 81	0
35	1d	208/209 (99%)	1.94	94 (45%) 0 0	48, 59, 67, 72	0
35	2d	208/209 (99%)	2.02	105 (50%) 0 0	53, 65, 72, 79	0
36	1e	148/162 (91%)	1.76	47 (31%) 1 1	45, 56, 64, 70	0
36	2e	148/162 (91%)	2.38	94 (63%) 0 0	57, 66, 72, 78	0
37	1f	100/101 (99%)	1.40	13 (13%) 7 8	49, 58, 66, 68	0
37	2f	100/101 (99%)	1.67	29 (29%) 1 1	51, 61, 66, 69	0
38	1g	155/156 (99%)	1.79	53 (34%) 1 1	54, 62, 73, 78	0
38	2g	155/156 (99%)	2.28	80 (51%) 0 0	64, 70, 77, 80	0
39	1h	137/138 (99%)	1.71	42 (30%) 1 1	48, 59, 65, 69	0
39	2h	137/138 (99%)	2.43	97 (70%) 0 0	57, 67, 71, 75	0
40	1i	127/128 (99%)	2.06	69 (54%) 0 0	47, 66, 72, 76	0
40	2i	127/128 (99%)	2.73	94 (74%) 0 0	62, 72, 77, 79	0
41	1j	97/105 (92%)	2.08	47 (48%) 0 0	49, 65, 73, 79	0
41	2j	96/105 (91%)	2.82	75 (78%) 0 0	63, 73, 77, 79	0
42	1k	114/129 (88%)	1.80	39 (34%) 1 1	44, 61, 70, 75	0
42	2k	114/129 (88%)	2.30	67 (58%) 0 0	51, 65, 70, 74	0
43	1l	121/132 (91%)	1.29	22 (18%) 3 4	37, 47, 59, 62	0
43	2l	121/132 (91%)	1.77	37 (30%) 1 1	50, 58, 66, 69	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.77	43 (34%)	1	1	49, 61, 69, 78	0
44	2m	122/126 (96%)	2.31	70 (57%)	0	0	61, 70, 74, 77	0
45	1n	60/61 (98%)	1.92	24 (40%)	1	0	47, 56, 63, 65	0
45	2n	60/61 (98%)	2.98	52 (86%)	0	0	66, 71, 74, 76	0
46	1o	88/89 (98%)	1.74	29 (32%)	1	1	44, 55, 65, 71	0
46	2o	88/89 (98%)	2.51	64 (72%)	0	0	53, 63, 70, 72	0
47	1p	82/88 (93%)	2.63	60 (73%)	0	0	50, 61, 66, 69	0
47	2p	82/88 (93%)	2.07	44 (53%)	0	0	56, 63, 70, 74	0
48	1q	99/105 (94%)	1.95	41 (41%)	0	0	50, 60, 67, 70	0
48	2q	99/105 (94%)	2.09	52 (52%)	0	0	56, 64, 70, 72	0
49	1r	68/88 (77%)	1.28	8 (11%)	9	10	50, 58, 66, 68	0
49	2r	68/88 (77%)	2.05	35 (51%)	0	0	56, 62, 70, 75	0
50	1s	83/93 (89%)	1.96	36 (43%)	0	0	55, 63, 71, 74	0
50	2s	83/93 (89%)	2.25	48 (57%)	0	0	67, 72, 77, 79	0
51	1t	96/106 (90%)	2.19	50 (52%)	0	0	56, 62, 70, 74	0
51	2t	96/106 (90%)	1.78	37 (38%)	1	0	54, 63, 72, 76	0
52	1u	23/27 (85%)	2.18	13 (56%)	0	0	55, 59, 62, 66	0
52	2u	23/27 (85%)	2.75	20 (86%)	0	0	68, 70, 73, 74	0
53	1v	13/24 (54%)	1.39	4 (30%)	1	1	40, 47, 82, 85	0
53	2v	13/24 (54%)	3.34	10 (76%)	0	0	60, 80, 87, 89	0
54	1w	66/76 (86%)	1.57	18 (27%)	1	1	25, 74, 83, 87	0
54	2w	64/76 (84%)	1.68	18 (28%)	1	1	42, 79, 86, 88	0
55	1x	72/77 (93%)	0.81	4 (5%)	30	32	24, 57, 71, 81	0
55	2x	72/77 (93%)	1.03	3 (4%)	40	42	37, 67, 77, 82	0
56	1z	6/7 (85%)	2.82	3 (50%)	0	0	25, 35, 44, 63	0
56	2z	6/7 (85%)	3.72	3 (50%)	0	0	37, 40, 54, 67	0
57	1y	67/76 (88%)	2.33	47 (70%)	0	0	58, 85, 88, 89	0
57	2y	66/76 (86%)	2.48	50 (75%)	0	0	68, 88, 91, 92	0
All	All	20883/21762 (95%)	1.23	4640 (22%)	2	2	18, 57, 77, 93	0

All (4640) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	8.9
38	1g	81	GLY	7.8
40	2i	14	VAL	7.6
45	1n	2	ALA	7.5
23	1l	2	SER	7.4
38	2g	82	GLY	7.3
33	2b	187	LEU	7.2
1	1A	2115	G	7.1
45	2n	2	ALA	6.9
56	2z	4	SER	6.7
38	2g	83	ALA	6.6
40	2i	102	LEU	6.6
8	2l	100	ALA	6.6
44	2m	123	ALA	6.5
38	2g	80	VAL	6.5
8	2l	107	VAL	6.5
21	1Z	141	VAL	6.4
56	2z	2	THR	6.4
33	1b	7	VAL	6.3
53	2v	22	U	6.2
26	24	50	VAL	6.0
33	2b	165	VAL	6.0
1	2A	2111	C	6.0
44	1m	124	PRO	5.9
34	2c	109	PRO	5.9
47	1p	49	LEU	5.8
1	1A	2114	A	5.8
1	2A	2112	G	5.8
1	1A	2112	G	5.7
1	1A	2113	U	5.7
1	1A	2145	C	5.7
1	2A	2115	G	5.6
41	2j	38	ILE	5.6
44	1m	123	ALA	5.5
51	1t	10	LEU	5.5
23	2l	2	SER	5.5
40	2i	67	GLY	5.5
41	2j	34	VAL	5.5
1	2A	2145	C	5.5
15	1T	131	ALA	5.4
1	1A	2174	C	5.4
34	2c	2	GLY	5.4
56	1z	2	THR	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	74	ILE	5.3
41	2j	40	LEU	5.3
21	2Z	146	ILE	5.3
26	14	56	VAL	5.3
26	14	63	TYR	5.3
26	24	51	ASP	5.2
22	20	84	LEU	5.2
7	2H	19	VAL	5.2
1	2A	2146	C	5.2
36	2e	80	ILE	5.2
1	2A	883	G	5.2
6	2G	139	LEU	5.1
44	2m	122	LYS	5.1
1	2A	2147	G	5.1
35	2d	183	GLY	5.1
49	2r	24	ALA	5.1
1	1A	885	C	5.1
21	2Z	157	LEU	5.1
7	2H	24	VAL	5.1
21	1Z	146	ILE	5.0
7	2H	17	VAL	5.0
34	2c	198	VAL	5.0
41	2j	75	ILE	5.0
38	2g	154	TYR	5.0
45	2n	25	VAL	5.0
38	2g	156	TRP	5.0
7	2H	98	LEU	5.0
33	1b	10	LEU	5.0
34	2c	124	ILE	5.0
1	1A	2178	C	5.0
1	2A	2113	U	5.0
42	1k	89	ALA	5.0
1	2A	2158	A	4.9
1	2A	2125	G	4.9
54	2w	71	G	4.9
51	1t	95	ALA	4.9
21	2Z	149	SER	4.9
38	2g	85	TYR	4.9
39	2h	2	LEU	4.9
50	2s	84	GLY	4.9
33	2b	185	ILE	4.9
43	2l	39	VAL	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	1p	19	ILE	4.9
1	2A	2174	C	4.8
53	2v	21	C	4.8
7	2H	2	SER	4.8
41	2j	44	VAL	4.8
26	24	49	PHE	4.8
51	1t	62	LEU	4.8
1	2A	2143	C	4.8
33	2b	237	ALA	4.8
19	1X	94	GLY	4.8
40	2i	10	ARG	4.8
38	1g	80	VAL	4.8
1	2A	2114	A	4.8
51	1t	103	GLY	4.8
56	1z	4	SER	4.8
42	2k	114	VAL	4.8
1	2A	884	C	4.8
38	1g	83	ALA	4.8
40	2i	126	SER	4.8
1	1A	2116	G	4.8
1	2A	2127	G	4.8
33	1b	230	VAL	4.8
33	2b	7	VAL	4.8
8	2I	96	ASP	4.7
46	2o	3	ILE	4.7
33	2b	17	PHE	4.7
35	1d	120	LEU	4.7
46	2o	69	TYR	4.7
21	2Z	147	GLY	4.7
40	1i	2	GLU	4.7
33	1b	232	PRO	4.7
1	1A	1087	G	4.7
34	2c	77	ILE	4.7
21	2Z	144	LEU	4.7
51	1t	84	LEU	4.7
40	2i	7	THR	4.7
33	2b	80	ILE	4.7
1	2A	2170	A	4.7
42	2k	124	LYS	4.7
26	14	54	GLY	4.7
35	1d	138	TYR	4.7
19	2X	91	ALA	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2104	G	4.6
34	2c	201	TYR	4.6
1	1A	1064	C	4.6
35	1d	194	LEU	4.6
1	2A	2149	G	4.6
46	2o	20	GLY	4.6
46	2o	89	GLY	4.6
33	2b	13	ALA	4.6
54	2w	72	C	4.6
1	2A	2117	A	4.6
50	2s	2	PRO	4.6
42	2k	125	PHE	4.6
38	2g	40	ALA	4.6
39	2h	58	TYR	4.6
38	1g	84	ASN	4.6
8	2I	117	GLU	4.6
8	2I	140	LEU	4.6
21	1Z	105	VAL	4.6
8	2I	109	ILE	4.6
1	2A	2159	G	4.5
26	24	45	GLY	4.5
41	2j	93	GLY	4.5
36	2e	21	ALA	4.5
42	2k	74	ALA	4.5
36	2e	16	THR	4.5
7	2H	52	VAL	4.5
6	1G	48	GLU	4.5
26	24	63	TYR	4.5
42	2k	75	TYR	4.5
7	2H	43	VAL	4.5
36	2e	55	VAL	4.5
8	1I	109	ILE	4.5
44	1m	2	ALA	4.5
6	2G	29	TRP	4.5
21	2Z	150	LEU	4.5
33	1b	187	LEU	4.5
51	1t	13	LEU	4.5
50	2s	45	VAL	4.5
51	1t	55	ILE	4.5
1	1A	1096	A	4.5
15	1T	130	ALA	4.5
1	2A	2155	G	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2175	C	4.5
43	2l	64	TYR	4.4
48	1q	28	PRO	4.4
38	2g	81	GLY	4.4
44	2m	6	GLY	4.4
33	2b	48	MET	4.4
35	1d	111	ALA	4.4
41	2j	32	ALA	4.4
32	1a	1003	G	4.4
41	1j	34	VAL	4.4
1	1A	2189	U	4.4
44	1m	122	LYS	4.4
33	2b	186	ALA	4.4
1	1A	2120	G	4.4
1	2A	2160	G	4.4
33	2b	44	LEU	4.4
38	2g	16	LEU	4.4
43	2l	18	VAL	4.4
1	1A	2117	A	4.4
1	1A	1058	G	4.4
57	2y	19	G	4.4
40	2i	66	ARG	4.4
26	14	67	TYR	4.4
33	2b	33	TYR	4.4
36	2e	76	ILE	4.4
8	2I	119	PRO	4.3
56	2z	3	HIS	4.3
1	1A	2160	G	4.3
1	2A	2101	G	4.3
1	2A	2133	G	4.3
42	2k	25	TYR	4.3
21	2Z	155	LEU	4.3
34	2c	204	LEU	4.3
39	2h	10	LEU	4.3
45	2n	53	LEU	4.3
1	1A	2146	C	4.3
1	1A	2162	G	4.3
32	2a	1030	C	4.3
36	2e	105	VAL	4.3
47	1p	51	VAL	4.3
1	1A	2170	A	4.3
34	2c	53	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	5	ALA	4.3
1	1A	2101	G	4.3
47	2p	82	GLN	4.3
14	2S	35	ILE	4.3
12	2Q	53	ALA	4.3
23	2I	68	PRO	4.3
33	2b	10	LEU	4.3
45	2n	6	LEU	4.3
8	2I	106	GLY	4.3
1	1A	1075	C	4.3
1	2A	885	C	4.3
1	2A	2168	G	4.3
21	2Z	174	VAL	4.2
34	2c	195	VAL	4.2
1	1A	2171	A	4.2
1	2A	2169	A	4.2
5	2F	21	ALA	4.2
40	2i	13	ALA	4.2
8	2I	128	LEU	4.2
33	2b	215	LEU	4.2
21	2Z	166	SER	4.2
38	2g	84	ASN	4.2
47	1p	32	TYR	4.2
50	2s	68	GLY	4.2
26	24	39	CYS	4.2
1	2A	2108	C	4.2
1	2A	2188	C	4.2
33	1b	229	VAL	4.2
39	2h	137	VAL	4.2
32	2a	1031	G	4.2
57	2y	18	G	4.2
53	2v	13	A	4.2
14	2S	55	ALA	4.2
36	1e	132	ALA	4.2
45	2n	10	ALA	4.2
4	1E	195	LEU	4.2
8	2I	121	LYS	4.2
47	1p	78	GLY	4.2
34	2c	39	ILE	4.2
1	1A	2129	C	4.2
1	1A	2803	C	4.2
1	1A	1059	G	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1033	G	4.2
33	2b	161	ALA	4.2
8	2I	114	LEU	4.2
41	2j	88	LEU	4.2
46	2o	31	LEU	4.2
38	1g	82	GLY	4.1
33	2b	162	ILE	4.1
40	2i	63	ILE	4.1
7	2H	44	VAL	4.1
14	2S	46	VAL	4.1
34	2c	76	VAL	4.1
1	1A	1095	A	4.1
33	2b	171	ALA	4.1
42	1k	75	TYR	4.1
47	1p	24	ALA	4.1
5	2F	24	LEU	4.1
6	2G	3	LEU	4.1
6	2G	49	ASP	4.1
1	1A	898	C	4.1
34	2c	173	VAL	4.1
50	1s	9	VAL	4.1
1	1A	2104	G	4.1
8	2I	55	ALA	4.1
45	2n	20	ALA	4.1
34	1c	32	LEU	4.1
45	2n	13	THR	4.1
8	2I	51	ILE	4.1
7	2H	99	VAL	4.1
33	2b	86	GLU	4.1
53	2v	24	A	4.1
1	1A	1068	G	4.1
1	1A	2110	G	4.1
1	1A	2147	G	4.1
1	2A	2120	G	4.1
1	2A	2166	G	4.1
1	2A	2167	U	4.1
34	2c	52	LEU	4.1
53	2v	19	U	4.1
33	2b	28	PHE	4.1
40	2i	5	TYR	4.1
41	2j	11	PHE	4.1
41	2j	42	THR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
18	2W	112	GLY	4.1
39	2h	118	VAL	4.1
40	2i	44	VAL	4.1
1	2A	2138	C	4.1
7	2H	96	ALA	4.0
34	2c	189	ALA	4.0
51	1t	59	ALA	4.0
53	1v	13	A	4.0
1	2A	2162	G	4.0
45	2n	38	GLY	4.0
34	1c	76	VAL	4.0
34	2c	99	VAL	4.0
41	1j	77	PRO	4.0
32	1a	1000	U	4.0
1	2A	896	A	4.0
33	1b	11	LEU	4.0
34	2c	129	ALA	4.0
40	1i	106	ALA	4.0
8	2I	1	MET	4.0
7	2H	36	PRO	4.0
36	2e	70	PRO	4.0
39	2h	97	VAL	4.0
1	2A	2129	C	4.0
1	1A	896	A	4.0
23	2l	54	ALA	4.0
36	2e	104	ALA	4.0
48	2q	76	LEU	4.0
26	14	58	ARG	4.0
45	2n	3	ARG	4.0
1	1A	2133	G	4.0
1	1A	2165	G	4.0
21	2Z	148	ASP	4.0
35	2d	154	ASN	4.0
33	2b	68	ILE	4.0
34	2c	134	ILE	4.0
34	2c	157	ILE	4.0
39	2h	6	ILE	4.0
51	1t	100	ILE	4.0
34	2c	18	TRP	4.0
1	1A	884	C	4.0
1	1A	2128	C	4.0
1	2A	2139	C	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	73	ALA	4.0
8	2I	115	ALA	4.0
19	1X	95	LEU	4.0
33	2b	121	LEU	4.0
47	1p	73	LEU	4.0
46	1o	89	GLY	4.0
54	1w	73	A	4.0
8	2I	99	GLU	4.0
33	2b	70	PHE	4.0
36	2e	84	PHE	4.0
1	2A	2106	G	4.0
33	2b	31	TYR	4.0
38	1g	154	TYR	4.0
33	2b	200	ILE	4.0
44	2m	9	ILE	4.0
33	2b	184	VAL	3.9
33	2b	24	TRP	3.9
43	2l	19	ARG	3.9
44	2m	102	ARG	3.9
34	1c	196	LEU	3.9
40	2i	19	LEU	3.9
8	2I	108	THR	3.9
40	2i	2	GLU	3.9
21	2Z	136	PHE	3.9
26	14	59	PHE	3.9
35	1d	110	PHE	3.9
32	2a	1032	G	3.9
6	1G	146	TYR	3.9
35	2d	5	ILE	3.9
45	2n	21	TYR	3.9
24	22	51	ARG	3.9
33	1b	131	PRO	3.9
1	1A	2108	C	3.9
1	1A	2175	C	3.9
18	1W	112	GLY	3.9
20	2Y	25	GLY	3.9
11	2P	130	PHE	3.9
33	1b	17	PHE	3.9
45	2n	36	PHE	3.9
1	2A	881	G	3.9
7	2H	39	PRO	3.9
33	1b	31	TYR	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	141	VAL	3.9
34	1c	207	VAL	3.9
43	1l	18	VAL	3.9
50	2s	11	VAL	3.9
36	2e	119	LEU	3.9
35	1d	6	GLY	3.9
1	1A	1073	A	3.9
1	2A	2134	A	3.9
32	1a	1001	A	3.9
7	1H	2	SER	3.9
36	2e	101	ILE	3.9
41	2j	77	PRO	3.9
52	2u	23	PRO	3.9
1	1A	2159	G	3.9
32	1a	1033	G	3.9
26	24	32	TYR	3.9
44	2m	87	TYR	3.9
33	2b	174	VAL	3.9
36	1e	82	VAL	3.9
8	2I	38	LEU	3.9
36	2e	71	LEU	3.9
45	2n	15	LYS	3.9
35	2d	130	GLY	3.9
1	1A	2138	C	3.9
1	1A	2161	C	3.9
54	1w	72	C	3.9
36	2e	120	THR	3.9
1	1A	1084	A	3.9
1	1A	2158	A	3.9
1	2A	2119	A	3.9
44	2m	64	TRP	3.9
38	1g	79	ARG	3.9
40	2i	9	ARG	3.9
6	2G	76	SER	3.8
21	2Z	159	PRO	3.8
34	2c	8	ILE	3.8
36	2e	11	ILE	3.8
52	2u	13	ILE	3.8
1	2A	2109	U	3.8
33	1b	9	GLU	3.8
1	2A	2110	G	3.8
1	2A	2154	G	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	48	TYR	3.8
40	2i	62	TYR	3.8
33	2b	230	VAL	3.8
44	1m	53	VAL	3.8
6	2G	127	GLY	3.8
19	2X	95	LEU	3.8
40	1i	50	LEU	3.8
21	2Z	173	ALA	3.8
36	1e	108	ALA	3.8
52	1u	24	ARG	3.8
56	1z	3	HIS	3.8
52	2u	14	TRP	3.8
3	2D	135	PHE	3.8
33	2b	202	PRO	3.8
40	2i	90	PRO	3.8
39	2h	35	ILE	3.8
39	2h	134	ILE	3.8
1	2A	2131	G	3.8
40	2i	36	TYR	3.8
54	1w	70	G	3.8
54	2w	70	G	3.8
4	1E	75	VAL	3.8
44	2m	53	VAL	3.8
7	2H	67	LEU	3.8
20	2Y	90	LEU	3.8
33	2b	228	GLY	3.8
34	2c	171	GLY	3.8
41	2j	71	LEU	3.8
48	1q	6	LEU	3.8
49	2r	57	GLY	3.8
1	1A	2111	C	3.8
1	1A	2143	C	3.8
8	1I	65	ALA	3.8
8	2I	83	ALA	3.8
35	2d	195	ALA	3.8
42	2k	117	ASN	3.8
25	23	60	GLU	3.8
47	1p	80	PHE	3.8
1	1A	1081	U	3.8
1	2A	2118	U	3.8
53	2v	20	U	3.8
34	2c	5	ILE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	129	ILE	3.8
1	1A	2123	G	3.8
1	2A	2123	G	3.8
7	2H	26	VAL	3.8
19	2X	69	TYR	3.8
38	2g	23	VAL	3.8
40	2i	4	TYR	3.8
41	2j	65	LEU	3.8
46	2o	27	VAL	3.8
3	2D	99	ASP	3.8
11	2P	84	ASN	3.8
33	2b	120	ALA	3.8
33	2b	205	ASP	3.8
34	1c	189	ALA	3.8
1	1A	2173	A	3.8
41	2j	91	PRO	3.8
46	2o	75	PRO	3.8
52	1u	23	PRO	3.8
40	2i	37	PHE	3.8
45	2n	61	TRP	3.8
21	2Z	171	ILE	3.8
33	2b	42	ILE	3.8
33	2b	201	ILE	3.8
6	2G	43	LEU	3.8
7	2H	71	LEU	3.8
8	2I	144	VAL	3.8
9	2N	116	LEU	3.8
33	2b	145	LEU	3.8
34	2c	87	LEU	3.8
40	2i	56	LEU	3.8
41	2j	49	VAL	3.8
48	2q	33	GLY	3.8
1	2A	2100	G	3.7
1	2A	2181	G	3.7
45	2n	34	TYR	3.7
47	1p	22	THR	3.7
8	2I	98	ALA	3.7
41	1j	32	ALA	3.7
44	2m	33	ALA	3.7
45	2n	30	ALA	3.7
1	2A	2144	U	3.7
48	2q	99	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	2d	122	ARG	3.7
41	1j	4	ILE	3.7
5	1F	16	GLY	3.7
42	2k	90	GLY	3.7
20	2Y	45	VAL	3.7
1	2A	2802	G	3.7
32	1a	1036	G	3.7
40	2i	125	TYR	3.7
36	2e	75	THR	3.7
4	2E	204	ALA	3.7
7	2H	41	MET	3.7
50	1s	24	ALA	3.7
1	2A	2804	C	3.7
54	2w	73	A	3.7
7	2H	59	ARG	3.7
16	2U	79	PHE	3.7
8	2I	75	LEU	3.7
36	2e	114	GLY	3.7
35	2d	68	TYR	3.7
40	2i	64	THR	3.7
32	1a	1034	G	3.7
46	1o	69	TYR	3.7
35	1d	195	ALA	3.7
57	2y	34	G	3.7
1	1A	1057	A	3.7
32	1a	1035	A	3.7
40	2i	68	GLY	3.7
40	2i	79	LEU	3.7
4	1E	59	VAL	3.7
8	2I	127	VAL	3.7
21	2Z	39	VAL	3.7
21	2Z	126	VAL	3.7
26	14	50	VAL	3.7
33	2b	15	VAL	3.7
33	2b	81	VAL	3.7
38	1g	17	VAL	3.7
41	1j	76	ASN	3.7
47	1p	81	ARG	3.7
52	2u	24	ARG	3.7
8	2I	146	ALA	3.7
34	1c	169	ALA	3.7
47	1p	70	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1063	G	3.7
1	1A	2131	G	3.7
1	2A	882	G	3.7
1	1A	1076	C	3.7
1	1A	1078	U	3.7
1	1A	2109	U	3.7
1	1A	2119	A	3.7
1	1A	2122	U	3.7
43	1l	5	PRO	3.7
1	1A	2169	A	3.7
45	2n	11	LYS	3.7
6	2G	20	ILE	3.6
21	2Z	104	PHE	3.6
41	2j	47	PHE	3.6
5	2F	41	LEU	3.6
34	2c	115	LEU	3.6
36	2e	10	MET	3.6
36	2e	123	LEU	3.6
46	1o	57	LEU	3.6
35	1d	191	ARG	3.6
36	2e	32	VAL	3.6
39	2h	8	ASP	3.6
41	2j	72	VAL	3.6
1	1A	2130	U	3.6
1	2A	2116	G	3.6
1	2A	2121	G	3.6
32	1a	1257	U	3.6
33	2b	236	TYR	3.6
40	1i	88	TYR	3.6
32	2a	1036	G	3.6
32	2a	1117	G	3.6
57	1y	34	G	3.6
1	2A	886	C	3.6
32	2a	1030(D)	A	3.6
32	2a	1038	C	3.6
36	2e	20	GLN	3.6
41	1j	86	MET	3.6
47	1p	1	MET	3.6
33	2b	21	ARG	3.6
40	2i	96	LEU	3.6
46	2o	34	LEU	3.6
48	1q	68	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	1p	48	TRP	3.6
5	2F	183	VAL	3.6
26	24	56	VAL	3.6
34	2c	130	VAL	3.6
39	2h	3	THR	3.6
41	1j	24	VAL	3.6
44	2m	117	VAL	3.6
21	2Z	172	ALA	3.6
43	2l	56	ALA	3.6
45	2n	58	LYS	3.6
8	2I	29	TYR	3.6
33	2b	199	TYR	3.6
38	1g	85	TYR	3.6
43	1l	64	TYR	3.6
32	2a	1002	G	3.6
57	1y	15	G	3.6
1	2A	2107	C	3.6
1	2A	2161	C	3.6
1	2A	2803	C	3.6
8	2I	64	GLU	3.6
7	2H	72	ILE	3.6
15	2T	102	ILE	3.6
20	2Y	5	MET	3.6
33	1b	41	ILE	3.6
35	2d	70	ILE	3.6
39	2h	44	PHE	3.6
11	2P	24	GLY	3.6
4	1E	183	LEU	3.6
39	2h	127	LEU	3.6
17	2V	5	VAL	3.6
1	2A	2150	U	3.6
4	1E	56	PRO	3.6
42	2k	89	ALA	3.6
57	1y	20	U	3.6
14	2S	7	TYR	3.6
1	1A	1093	G	3.6
1	1A	2121	G	3.6
1	2A	2142	C	3.6
1	2A	2148	G	3.6
1	2A	2157	G	3.6
21	2Z	124	ILE	3.6
33	1b	127	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	223	ILE	3.6
44	2m	78	ILE	3.6
33	2b	89	GLY	3.6
33	2b	163	PHE	3.6
34	1c	81	GLY	3.6
24	22	32	LEU	3.6
36	2e	139	LEU	3.6
40	1i	19	LEU	3.6
50	1s	5	LEU	3.6
40	2i	11	LYS	3.6
47	1p	14	ASN	3.6
8	1I	3	VAL	3.6
1	1A	1094	U	3.6
38	2g	71	PRO	3.6
41	2j	37	PRO	3.6
12	2Q	20	ALA	3.6
42	1k	15	ALA	3.6
1	1A	2135	A	3.5
21	2Z	9	TYR	3.5
35	1d	68	TYR	3.5
38	2g	151	TYR	3.5
1	1A	886	C	3.5
32	2a	1030(B)	C	3.5
32	2a	1037	C	3.5
32	2a	1030(A)	G	3.5
7	2H	9	ILE	3.5
33	2b	41	ILE	3.5
40	2i	69	GLY	3.5
40	2i	101	PHE	3.5
47	2p	80	PHE	3.5
49	2r	81	PHE	3.5
3	1D	276	LYS	3.5
33	2b	98	LEU	3.5
35	2d	64	LEU	3.5
50	2s	13	ASP	3.5
7	2H	10	PRO	3.5
21	1Z	139	VAL	3.5
33	2b	170	GLU	3.5
36	1e	96	PRO	3.5
46	1o	19	PRO	3.5
47	1p	79	VAL	3.5
55	2x	47	U	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	1G	50	ALA	3.5
8	2I	94	ALA	3.5
29	27	45	ALA	3.5
5	2F	172	TRP	3.5
33	1b	97	TRP	3.5
40	1i	10	ARG	3.5
1	1A	2790	A	3.5
1	2A	2176	A	3.5
53	1v	12	A	3.5
1	1A	888	C	3.5
1	1A	2136	C	3.5
1	1A	2164	C	3.5
1	2A	2105	C	3.5
1	2A	2182	G	3.5
32	2a	1034	G	3.5
44	2m	120	LYS	3.5
57	2y	57	G	3.5
23	1l	85	LEU	3.5
23	1l	98	LEU	3.5
32	2a	1150	U	3.5
42	2k	31	THR	3.5
8	1I	111	PRO	3.5
48	2q	47	PRO	3.5
21	2Z	139	VAL	3.5
33	2b	112	VAL	3.5
34	2c	70	VAL	3.5
35	2d	8	VAL	3.5
36	2e	41	VAL	3.5
48	2q	35	VAL	3.5
33	1b	237	ALA	3.5
39	1h	138	TRP	3.5
48	2q	100	LYS	3.5
57	1y	35	A	3.5
6	2G	146	TYR	3.5
32	1a	1038	C	3.5
35	1d	5	ILE	3.5
39	2h	100	ILE	3.5
1	1A	2190	G	3.5
57	2y	15	G	3.5
6	1G	139	LEU	3.5
26	24	59	PHE	3.5
33	1b	43	ASP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	43	PHE	3.5
42	1k	98	LEU	3.5
46	2o	66	LEU	3.5
48	1q	31	LEU	3.5
51	1t	36	LEU	3.5
1	1A	1066	U	3.5
1	1A	2144	U	3.5
32	1a	1025	U	3.5
34	2c	151	VAL	3.5
5	1F	146	ALA	3.5
33	2b	34	ALA	3.5
35	2d	164	ALA	3.5
44	2m	75	ALA	3.5
14	2S	93	LYS	3.5
1	2A	2126	A	3.5
53	2v	23	A	3.5
1	2A	1536	C	3.5
8	2I	84	GLY	3.5
32	2a	1149	C	3.5
33	1b	228	GLY	3.5
35	1d	69	GLY	3.5
36	1e	97	GLY	3.5
10	2O	69	ILE	3.5
35	2d	20	TYR	3.5
52	1u	18	TYR	3.5
33	2b	196	LEU	3.5
1	1A	2166	G	3.5
1	2A	1170	G	3.5
1	2A	1533	G	3.5
44	2m	104	ARG	3.5
50	2s	10	PHE	3.5
47	1p	82	GLN	3.5
39	2h	101	PRO	3.4
40	1i	21	PRO	3.4
41	1j	81	THR	3.4
4	2E	34	VAL	3.4
5	2F	6	VAL	3.4
6	2G	15	VAL	3.4
34	2c	68	VAL	3.4
38	2g	36	LYS	3.4
33	1b	120	ALA	3.4
34	2c	149	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	2	ALA	3.4
40	2i	52	ALA	3.4
41	2j	27	ALA	3.4
32	2a	1035	A	3.4
33	2b	97	TRP	3.4
1	1A	2188	C	3.4
6	2G	157	ILE	3.4
41	2j	98	ILE	3.4
50	1s	31	ILE	3.4
3	2D	84	TYR	3.4
5	2F	170	LEU	3.4
6	2G	34	LEU	3.4
11	1P	105	LEU	3.4
1	1A	2207	G	3.4
1	2A	2124	G	3.4
32	1a	1030(A)	G	3.4
39	2h	31	PHE	3.4
57	1y	19	G	3.4
41	2j	41	PRO	3.4
6	2G	149	VAL	3.4
34	1c	194	GLY	3.4
34	2c	190	ARG	3.4
36	2e	27	ARG	3.4
38	2g	4	ARG	3.4
40	1i	8	GLY	3.4
47	1p	75	ARG	3.4
53	2v	14	A	3.4
1	1A	2140	C	3.4
1	2A	2128	C	3.4
19	2X	92	LEU	3.4
26	24	15	ILE	3.4
33	2b	172	ILE	3.4
39	1h	127	LEU	3.4
41	2j	85	LEU	3.4
46	1o	3	ILE	3.4
47	1p	60	LEU	3.4
50	1s	30	LEU	3.4
54	2w	2	C	3.4
50	2s	80	TYR	3.4
57	2y	33	U	3.4
40	2i	18	PHE	3.4
40	2i	59	PHE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	2Y	1	MET	3.4
38	2g	14	PRO	3.4
1	1A	1099	G	3.4
1	1A	2141	G	3.4
32	1a	1002	G	3.4
32	2a	1021	G	3.4
33	2b	190	THR	3.4
44	2m	105	THR	3.4
7	2H	35	VAL	3.4
22	20	63	VAL	3.4
39	2h	79	VAL	3.4
39	2h	95	VAL	3.4
40	2i	109	VAL	3.4
47	1p	53	VAL	3.4
33	2b	123	ALA	3.4
34	2c	160	ALA	3.4
35	2d	147	ALA	3.4
35	1d	150	GLU	3.4
46	2o	88	ARG	3.4
1	1A	1088	A	3.4
46	2o	86	GLY	3.4
53	2v	12	A	3.4
8	2I	28	ASN	3.4
33	1b	39	ILE	3.4
46	2o	85	LEU	3.4
1	2A	894	C	3.4
1	2A	2179	C	3.4
32	2a	1027	C	3.4
7	2H	128	PRO	3.4
21	2Z	88	PHE	3.4
21	2Z	95	PRO	3.4
40	1i	18	PHE	3.4
21	2Z	69	THR	3.4
32	1a	625	G	3.4
32	1a	1032	G	3.4
57	1y	24	G	3.4
6	2G	92	VAL	3.4
7	1H	115	VAL	3.4
9	2N	140	VAL	3.4
33	2b	93	VAL	3.4
36	2e	51	VAL	3.4
42	2k	53	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	2q	57	VAL	3.4
50	1s	67	VAL	3.4
50	2s	67	VAL	3.4
15	2T	131	ALA	3.4
38	1g	4	ARG	3.4
44	2m	69	GLU	3.4
51	1t	12	ALA	3.4
52	2u	15	ARG	3.4
8	2I	13	GLY	3.4
33	2b	22	LYS	3.4
57	1y	38	A	3.4
57	2y	36	A	3.4
8	2I	35	LEU	3.3
1	2A	2122	U	3.3
8	2I	97	ILE	3.3
23	2I	67	ILE	3.3
33	2b	213	LEU	3.3
39	2h	36	LEU	3.3
45	2n	44	LEU	3.3
24	22	1	MET	3.3
1	2A	898	C	3.3
1	2A	2164	C	3.3
21	1Z	136	PHE	3.3
34	1c	23	TYR	3.3
34	2c	29	TYR	3.3
45	2n	37	PHE	3.3
33	1b	107	THR	3.3
14	2S	20	ARG	3.3
26	24	55	ARG	3.3
39	2h	91	ARG	3.3
41	2j	28	ARG	3.3
10	2O	51	ALA	3.3
33	1b	136	VAL	3.3
36	2e	100	VAL	3.3
40	2i	43	ALA	3.3
48	2q	9	VAL	3.3
7	2H	25	LYS	3.3
34	2c	205	GLY	3.3
51	1t	47	GLY	3.3
1	1A	2172	U	3.3
1	2A	2189	U	3.3
8	2I	101	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	121	LEU	3.3
33	2b	51	LEU	3.3
38	2g	12	LEU	3.3
39	1h	112	LEU	3.3
41	2j	16	LEU	3.3
41	2j	6	ILE	3.3
42	2k	21	ILE	3.3
45	1n	42	ILE	3.3
45	2n	7	ILE	3.3
24	22	18	PRO	3.3
38	2g	88	PRO	3.3
57	2y	56	C	3.3
21	2Z	170	THR	3.3
42	2k	126	ARG	3.3
44	1m	49	THR	3.3
40	2i	92	TYR	3.3
1	1A	2182	G	3.3
3	2D	276	LYS	3.3
29	17	48	LYS	3.3
32	1a	1021	G	3.3
35	1d	152	SER	3.3
39	2h	116	LYS	3.3
40	1i	126	SER	3.3
51	1t	38	LYS	3.3
54	1w	71	G	3.3
3	2D	138	VAL	3.3
7	1H	169	VAL	3.3
8	2I	15	VAL	3.3
17	2V	31	ALA	3.3
20	2Y	3	VAL	3.3
34	2c	200	ALA	3.3
40	2i	106	ALA	3.3
46	2o	16	ALA	3.3
31	29	37	GLY	3.3
34	2c	145	GLY	3.3
39	1h	96	GLY	3.3
40	2i	100	GLY	3.3
41	1j	31	GLY	3.3
46	2o	55	GLY	3.3
26	24	65	ASP	3.3
50	1s	12	ASP	3.3
1	1A	1065	U	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2130	U	3.3
5	1F	20	LEU	3.3
5	2F	32	LEU	3.3
14	1S	78	LEU	3.3
36	2e	142	LEU	3.3
39	2h	107	LEU	3.3
46	2o	32	LEU	3.3
47	1p	6	LEU	3.3
47	2p	6	LEU	3.3
34	1c	39	ILE	3.3
46	1o	87	ILE	3.3
3	2D	36	PRO	3.3
1	1A	2105	C	3.3
1	2A	888	C	3.3
1	2A	2137	C	3.3
3	1D	262	ARG	3.3
34	1c	190	ARG	3.3
33	1b	40	HIS	3.3
6	2G	117	PHE	3.3
46	1o	18	PHE	3.3
49	2r	61	LYS	3.3
52	2u	21	TYR	3.3
14	2S	31	SER	3.3
39	2h	115	SER	3.3
1	1A	882	G	3.3
1	2A	2156	G	3.3
7	2H	45	VAL	3.3
8	1I	136	VAL	3.3
8	1I	142	VAL	3.3
9	1N	9	VAL	3.3
21	2Z	86	VAL	3.3
34	1c	151	VAL	3.3
34	2c	75	VAL	3.3
36	1e	69	VAL	3.3
40	2i	41	VAL	3.3
6	2G	24	GLY	3.3
33	1b	203	GLY	3.3
38	2g	34	GLY	3.3
43	2l	95	GLY	3.3
40	2i	105	ASP	3.3
51	1t	9	ASN	3.3
1	1A	1097	U	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1532	U	3.3
3	2D	37	LEU	3.3
19	2X	66	LEU	3.3
33	2b	11	LEU	3.3
51	2t	13	LEU	3.3
6	2G	63	ILE	3.3
35	2d	115	ARG	3.3
39	1h	100	ILE	3.3
39	2h	111	ILE	3.3
42	2k	32	ILE	3.3
42	2k	40	ILE	3.3
48	1q	90	ILE	3.3
26	14	57	GLU	3.3
8	1I	105	HIS	3.3
1	1A	1080	C	3.3
1	1A	2179	C	3.3
51	2t	29	LYS	3.3
47	1p	69	THR	3.3
38	2g	62	PHE	3.3
42	1k	20	TYR	3.3
3	2D	2	ALA	3.2
7	2H	75	ALA	3.2
8	2I	26	ALA	3.2
8	2I	37	VAL	3.3
12	2Q	117	ALA	3.2
35	2d	48	ALA	3.2
36	2e	90	VAL	3.3
38	2g	66	VAL	3.3
44	2m	72	ALA	3.2
45	2n	18	VAL	3.3
1	1A	2168	G	3.2
32	2a	1283	G	3.2
39	2h	9	MET	3.2
57	1y	27	G	3.2
33	2b	72	GLY	3.2
35	1d	2	GLY	3.2
41	2j	36	GLY	3.2
8	2I	20	ASP	3.2
39	2h	15	ASN	3.2
47	1p	18	ARG	3.2
8	2I	68	LEU	3.2
23	2I	85	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	188	LEU	3.2
46	2o	70	LEU	3.2
49	2r	66	LEU	3.2
51	1t	24	LEU	3.2
1	1A	1086	A	3.2
7	2H	175	LYS	3.2
21	2Z	167	PRO	3.2
33	2b	91	PRO	3.2
54	1w	7	A	3.2
1	1A	2137	C	3.2
24	12	70	GLN	3.2
32	1a	63	C	3.2
32	2a	999	C	3.2
32	2a	1116	C	3.2
35	2d	160	GLN	3.2
41	2j	92	THR	3.2
57	2y	4	C	3.2
21	1Z	104	PHE	3.2
36	1e	84	PHE	3.2
45	2n	16	PHE	3.2
21	1Z	166	SER	3.2
7	2H	107	VAL	3.2
8	2I	136	VAL	3.2
33	2b	71	VAL	3.2
34	1c	133	ALA	3.2
34	2c	137	ALA	3.2
39	2h	93	VAL	3.2
51	2t	95	ALA	3.2
7	2H	31	GLY	3.2
8	2I	50	ARG	3.2
8	2I	82	ARG	3.2
14	2S	3	ARG	3.2
21	2Z	22	GLY	3.2
21	2Z	106	GLY	3.2
41	2j	79	ARG	3.2
44	2m	100	GLY	3.2
50	1s	68	GLY	3.2
52	2u	22	ARG	3.2
1	1A	2149	G	3.2
1	2A	2165	G	3.2
1	2A	2186	G	3.2
32	1a	65	U	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	84	U	3.2
32	2a	1127	G	3.2
7	2H	105	LEU	3.2
33	2b	154	LEU	3.2
37	2f	45	LEU	3.2
40	2i	99	LEU	3.2
1	1A	1046	A	3.2
8	2I	132	PRO	3.2
20	2Y	38	ILE	3.2
33	1b	201	ILE	3.2
34	2c	118	GLN	3.2
44	2m	101	GLN	3.2
34	1c	95	THR	3.2
46	2o	4	THR	3.2
32	1a	999	C	3.2
5	2F	15	SER	3.2
36	2e	125	SER	3.2
6	2G	12	TYR	3.2
39	2h	94	TYR	3.2
46	2o	65	ARG	3.2
5	2F	207	GLY	3.2
9	2N	9	VAL	3.2
15	2T	130	ALA	3.2
21	2Z	96	VAL	3.2
33	2b	136	VAL	3.2
46	2o	11	VAL	3.2
48	1q	88	TYR	3.2
48	2q	95	TYR	3.2
40	2i	57	GLY	3.2
52	2u	4	GLY	3.2
1	1A	2150	U	3.2
6	2G	97	ASP	3.2
1	1A	2181	G	3.2
32	2a	1202	G	3.2
21	2Z	41	LEU	3.2
35	1d	7	PRO	3.2
7	1H	4	ILE	3.2
24	22	70	GLN	3.2
32	1a	1041	A	3.2
33	2b	45	GLN	3.2
34	2c	37	GLN	3.2
36	2e	89	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	73	THR	3.2
1	1A	897	C	3.2
33	2b	101	MET	3.2
15	2T	115	ARG	3.2
33	2b	122	PHE	3.2
45	1n	57	ARG	3.2
46	1o	88	ARG	3.2
47	1p	12	LYS	3.2
7	2H	37	VAL	3.2
8	1I	19	VAL	3.2
8	2I	18	VAL	3.2
12	2Q	28	ALA	3.2
17	2V	72	VAL	3.2
33	2b	66	GLY	3.2
33	2b	77	ALA	3.2
33	2b	229	VAL	3.2
34	2c	106	VAL	3.2
40	1i	46	ALA	3.2
42	1k	92	GLU	3.2
35	1d	106	TYR	3.2
41	1j	44	VAL	3.2
44	2m	119	GLY	3.2
5	2F	162	LEU	3.2
6	2G	53	LEU	3.2
6	2G	172	LEU	3.2
7	2H	7	LEU	3.2
11	1P	147	LEU	3.2
20	1Y	67	LEU	3.2
21	1Z	150	LEU	3.2
21	2Z	125	LEU	3.2
34	2c	73	PRO	3.2
38	1g	12	LEU	3.2
39	2h	57	PRO	3.2
43	2l	60	LEU	3.2
44	2m	66	LEU	3.2
1	1A	1089	G	3.2
32	2a	1026	G	3.2
6	2G	144	ILE	3.2
8	2I	138	ILE	3.2
34	2c	14	ILE	3.2
37	1f	25	ILE	3.2
47	1p	4	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2D	262	ARG	3.1
41	1j	79	ARG	3.1
57	2y	61	C	3.1
8	2I	102	SER	3.1
33	2b	57	PHE	3.1
35	1d	75	PHE	3.1
35	1d	149	ALA	3.1
38	1g	37	ASN	3.1
38	2g	152	ALA	3.1
45	1n	5	ALA	3.1
42	1k	14	VAL	3.1
42	2k	36	ASP	3.1
43	1l	43	VAL	3.1
47	2p	13	HIS	3.1
49	2r	73	ALA	3.1
5	1F	11	VAL	3.1
7	2H	114	VAL	3.1
39	2h	19	VAL	3.1
48	1q	77	VAL	3.1
34	2c	193	TYR	3.1
36	2e	60	TYR	3.1
7	2H	33	LEU	3.1
7	2H	88	LEU	3.1
8	2I	32	PRO	3.1
10	1O	91	LEU	3.1
33	1b	202	PRO	3.1
33	2b	142	LEU	3.1
41	2j	8	LEU	3.1
45	1n	44	LEU	3.1
50	2s	71	LEU	3.1
33	1b	24	TRP	3.1
1	1A	1062	G	3.1
32	1a	1001(A)	G	3.1
1	2A	2173	A	3.1
39	2h	86	ILE	3.1
57	2y	14	A	3.1
47	1p	43	LYS	3.1
1	2A	2103	C	3.1
1	2A	2163	C	3.1
38	2g	98	SER	3.1
48	1q	79	SER	3.1
57	2y	2	C	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	152	PHE	3.1
41	2j	68	HIS	3.1
1	1A	271(K)	U	3.1
7	2H	100	GLY	3.1
11	2P	28	GLY	3.1
26	14	64	GLY	3.1
33	1b	13	ALA	3.1
33	2b	207	ALA	3.1
36	2e	17	ALA	3.1
6	2G	37	VAL	3.1
7	2H	49	VAL	3.1
38	2g	75	VAL	3.1
39	2h	103	VAL	3.1
40	1i	26	VAL	3.1
46	2o	60	VAL	3.1
26	24	11	PRO	3.1
35	2d	157	LEU	3.1
41	2j	53	PRO	3.1
46	1o	31	LEU	3.1
7	2H	6	ARG	3.1
8	2I	71	ILE	3.1
21	1Z	137	ILE	3.1
35	1d	126	ILE	3.1
35	2d	146	ILE	3.1
39	2h	83	ILE	3.1
41	2j	23	ILE	3.1
47	1p	59	TRP	3.1
43	2l	21	LYS	3.1
44	1m	4	ILE	3.1
1	1A	229	A	3.1
32	2a	1250	A	3.1
48	2q	82	MET	3.1
47	1p	45	THR	3.1
1	2A	2183	C	3.1
32	2a	1019	C	3.1
47	2p	16	HIS	3.1
34	2c	128	PHE	3.1
1	2A	271(K)	U	3.1
7	2H	66	GLY	3.1
33	1b	220	ASP	3.1
34	2c	3	ASN	3.1
42	2k	49	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	1I	115	ALA	3.1
8	1I	146	ALA	3.1
34	2c	100	ALA	3.1
38	2g	107	ALA	3.1
6	2G	28	VAL	3.1
8	2I	145	VAL	3.1
21	2Z	58	VAL	3.1
36	2e	69	VAL	3.1
38	2g	91	VAL	3.1
40	1i	14	VAL	3.1
43	2l	55	VAL	3.1
6	2G	111	LEU	3.1
7	2H	55	PRO	3.1
7	1H	132	ARG	3.1
7	2H	60	ARG	3.1
23	1l	82	LEU	3.1
23	2l	82	LEU	3.1
33	2b	118	LEU	3.1
35	1d	108	LEU	3.1
35	2d	29	PRO	3.1
35	2d	135	LEU	3.1
41	2j	39	PRO	3.1
8	2I	89	TYR	3.1
37	2f	59	TYR	3.1
46	1o	17	ARG	3.1
20	1Y	1	MET	3.1
33	2b	39	ILE	3.1
40	2i	74	ILE	3.1
42	1k	95	ILE	3.1
32	1a	1286	A	3.1
57	1y	58	A	3.1
1	1A	1091	G	3.1
1	1A	2127	G	3.1
32	2a	630	G	3.1
21	2Z	121	HIS	3.1
1	1A	2794	C	3.1
57	1y	56	C	3.1
3	2D	139	GLY	3.1
7	2H	22	GLY	3.1
15	1T	37	GLY	3.1
21	2Z	154	ASP	3.1
21	2Z	160	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	26	20	ASN	3.1
38	2g	33	ASP	3.1
44	2m	106	ASN	3.1
5	1F	130	ALA	3.1
7	1H	175	LYS	3.1
7	2H	133	VAL	3.1
7	2H	169	VAL	3.1
8	2I	92	VAL	3.1
9	2N	11	PRO	3.1
20	2Y	42	VAL	3.1
23	21	49	VAL	3.1
33	1b	234	PRO	3.1
33	2b	144	ARG	3.1
41	1j	80	LYS	3.1
51	1t	74	LYS	3.1
17	2V	94	LEU	3.1
35	1d	188	LEU	3.1
36	2e	12	LEU	3.1
47	2p	49	LEU	3.1
51	2t	99	LEU	3.1
9	2N	1	MET	3.1
33	2b	92	TYR	3.0
21	1Z	2	GLU	3.0
20	2Y	44	ILE	3.0
33	1b	211	ILE	3.0
33	2b	182	ILE	3.0
38	2g	120	ILE	3.0
1	1A	890	A	3.0
34	1c	191	THR	3.0
45	2n	22	THR	3.0
50	2s	77	THR	3.0
14	2S	34	HIS	3.0
21	2Z	151	HIS	3.0
38	1g	156	TRP	3.0
47	2p	48	TRP	3.0
46	2o	24	SER	3.0
32	1a	1532	U	3.0
34	2c	170	GLN	3.0
5	2F	129	PHE	3.0
20	2Y	89	PHE	3.0
32	2a	1249	C	3.0
36	2e	44	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	1y	75	C	3.0
7	2H	51	ARG	3.0
8	2I	103	ARG	3.0
29	27	47	ARG	3.0
33	1b	22	LYS	3.0
35	2d	3	ARG	3.0
33	1b	218	ALA	3.0
36	2e	146	ALA	3.0
38	2g	65	ALA	3.0
40	1i	84	ALA	3.0
33	2b	131	PRO	3.0
33	2b	167	PRO	3.0
50	2s	76	PRO	3.0
7	2H	64	LEU	3.0
8	1I	12	LEU	3.0
8	1I	35	LEU	3.0
15	2T	66	VAL	3.0
15	2T	70	VAL	3.0
33	1b	44	LEU	3.0
34	2c	33	LEU	3.0
35	2d	120	LEU	3.0
37	1f	21	LEU	3.0
37	2f	21	LEU	3.0
39	1h	2	LEU	3.0
39	2h	39	LEU	3.0
46	1o	43	LEU	3.0
48	2q	31	LEU	3.0
48	2q	74	LEU	3.0
49	2r	37	VAL	3.0
21	2Z	145	GLU	3.0
26	24	30	GLU	3.0
6	2G	114	ILE	3.0
36	2e	118	ILE	3.0
39	2h	109	ILE	3.0
44	1m	39	ILE	3.0
50	2s	31	ILE	3.0
1	1A	1070	A	3.0
6	2G	145	THR	3.0
17	2V	32	THR	3.0
32	2a	1531	A	3.0
40	2i	103	THR	3.0
57	1y	36	A	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
57	2y	35	A	3.0
1	1A	2100	G	3.0
1	2A	892	G	3.0
1	2A	2141	G	3.0
57	2y	1	G	3.0
21	2Z	129	SER	3.0
46	2o	52	SER	3.0
48	1q	97	SER	3.0
48	2q	12	SER	3.0
6	2G	16	ARG	3.0
19	2X	68	ARG	3.0
50	2s	32	LYS	3.0
1	1A	2183	C	3.0
1	2A	652(T)	C	3.0
24	12	37	PHE	3.0
32	2a	1018	C	3.0
36	2e	6	PHE	3.0
36	2e	45	PHE	3.0
41	2j	63	PHE	3.0
3	2D	130	ALA	3.0
6	2G	2	PRO	3.0
12	2Q	50	ALA	3.0
36	1e	138	ALA	3.0
42	2k	68	ALA	3.0
44	2m	5	ALA	3.0
46	2o	58	MET	3.0
5	2F	157	VAL	3.0
6	2G	120	LEU	3.0
22	20	30	VAL	3.0
26	24	33	VAL	3.0
33	1b	59	GLU	3.0
45	1n	25	VAL	3.0
48	1q	98	LEU	3.0
49	2r	39	VAL	3.0
7	2H	83	TYR	3.0
33	1b	236	TYR	3.0
41	2j	82	ILE	3.0
51	2t	41	ILE	3.0
1	2A	878	A	3.0
1	2A	1445	A	3.0
1	2A	1847	A	3.0
1	2A	2135	A	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	2u	17	THR	3.0
57	2y	26	A	3.0
35	2d	116	GLN	3.0
8	2I	27	ARG	3.0
20	2Y	54	LYS	3.0
23	2I	50	ARG	3.0
40	2i	70	LYS	3.0
41	2j	5	ARG	3.0
42	1k	51	LYS	3.0
43	2l	13	LYS	3.0
47	2p	12	LYS	3.0
1	1A	1060	U	3.0
1	1A	1175	U	3.0
1	1A	2167	U	3.0
34	2c	154	SER	3.0
38	2g	77	SER	3.0
4	2E	115	GLY	3.0
5	1F	61	GLY	3.0
36	2e	23	GLY	3.0
41	2j	78	ASN	3.0
42	2k	42	TRP	3.0
46	1o	86	GLY	3.0
46	2o	61	GLY	3.0
50	1s	13	ASP	3.0
1	1A	1072	C	3.0
1	1A	2142	C	3.0
1	2A	1509	C	3.0
1	2A	2136	C	3.0
1	2A	2896	C	3.0
19	2X	1	MET	3.0
40	1i	59	PHE	3.0
46	2o	18	PHE	3.0
34	2c	133	ALA	3.0
38	2g	2	ALA	3.0
39	2h	28	ALA	3.0
39	2h	110	ALA	3.0
40	1i	13	ALA	3.0
41	2j	64	GLU	3.0
47	2p	70	ALA	3.0
51	1t	94	ALA	3.0
16	2U	90	VAL	3.0
34	2c	43	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	9	VAL	3.0
38	2g	69	VAL	3.0
40	1i	85	LEU	3.0
41	2j	90	LEU	3.0
42	1k	30	VAL	3.0
42	2k	98	LEU	3.0
48	1q	5	VAL	3.0
6	2G	101	ILE	3.0
26	24	31	ILE	3.0
38	1g	27	ILE	3.0
11	2P	79	ARG	3.0
33	2b	107	THR	3.0
1	1A	2801(A)	A	3.0
1	2A	901	A	3.0
32	2a	1257	U	3.0
57	1y	51	U	3.0
34	2c	49	SER	3.0
35	2d	152	SER	3.0
7	2H	57	ASP	3.0
12	2Q	15	GLY	3.0
35	2d	23	GLY	3.0
40	2i	75	ASP	3.0
44	1m	77	ASN	3.0
47	1p	68	ASP	3.0
1	1A	2148	G	3.0
1	2A	11	G	3.0
1	2A	2318	G	3.0
32	1a	630	G	3.0
32	1a	1023	G	3.0
41	2j	86	MET	3.0
9	2N	51	PHE	2.9
33	1b	125	PRO	3.0
34	1c	109	PRO	3.0
34	2c	10	PHE	2.9
36	1e	45	PHE	2.9
43	2l	5	PRO	3.0
47	1p	15	PRO	3.0
20	2Y	105	ALA	2.9
36	2e	30	ALA	2.9
47	1p	56	ALA	2.9
6	1G	82	LEU	2.9
8	1I	123	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	102	LEU	2.9
34	2c	12	LEU	2.9
39	1h	10	LEU	2.9
40	2i	50	LEU	2.9
50	1s	71	LEU	2.9
51	2t	10	LEU	2.9
4	1E	21	VAL	2.9
14	2S	28	VAL	2.9
21	1Z	58	VAL	2.9
21	2Z	128	VAL	2.9
23	21	30	VAL	2.9
34	2c	116	VAL	2.9
35	1d	88	VAL	2.9
38	2g	17	VAL	2.9
38	2g	153	HIS	2.9
39	1h	95	VAL	2.9
40	1i	17	VAL	2.9
43	2l	43	VAL	2.9
48	1q	35	VAL	2.9
50	2s	41	VAL	2.9
29	27	48	LYS	2.9
46	2o	84	LYS	2.9
51	1t	81	LYS	2.9
35	2d	42	GLN	2.9
35	2d	168	ARG	2.9
40	2i	20	ARG	2.9
42	2k	120	ARG	2.9
51	1t	83	ARG	2.9
7	2H	121	ILE	2.9
7	2H	136	ILE	2.9
19	2X	89	ILE	2.9
21	2Z	137	ILE	2.9
26	24	5	ILE	2.9
30	28	16	ILE	2.9
33	1b	223	ILE	2.9
39	1h	45	ILE	2.9
26	14	52	THR	2.9
40	1i	7	THR	2.9
1	1A	887	A	2.9
1	1A	1082	U	2.9
26	24	67	TYR	2.9
32	2a	1004	A	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	59	TYR	2.9
34	1c	62	ASP	2.9
37	1f	83	ASP	2.9
39	2h	131	GLY	2.9
51	2t	47	GLY	2.9
33	2b	26	PRO	2.9
40	1i	49	PRO	2.9
1	2A	889	C	2.9
1	2A	2177	C	2.9
32	1a	1028	C	2.9
32	2a	980	C	2.9
6	1G	3	LEU	2.9
11	2P	105	LEU	2.9
33	1b	213	LEU	2.9
37	2f	30	LEU	2.9
42	1k	74	ALA	2.9
47	2p	77	ALA	2.9
33	2b	16	HIS	2.9
51	2t	24	LEU	2.9
7	2H	50	VAL	2.9
7	2H	76	VAL	2.9
11	2P	76	LYS	2.9
16	2U	8	VAL	2.9
19	2X	12	VAL	2.9
23	2I	4	VAL	2.9
34	2c	207	VAL	2.9
40	2i	65	VAL	2.9
42	2k	14	VAL	2.9
43	1l	23	LYS	2.9
43	2l	24	VAL	2.9
43	2l	46	LYS	2.9
45	2n	35	ARG	2.9
48	2q	73	VAL	2.9
35	2d	74	GLN	2.9
26	24	22	ILE	2.9
45	2n	42	ILE	2.9
48	1q	36	ILE	2.9
49	2r	65	ILE	2.9
32	1a	197	A	2.9
32	2a	1447	A	2.9
57	2y	31	A	2.9
20	2Y	55	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	8	TYR	2.9
22	20	68	GLU	2.9
23	21	71	TYR	2.9
33	1b	134	GLU	2.9
3	2D	110	GLY	2.9
6	2G	79	ASN	2.9
33	1b	37	ASN	2.9
48	2q	97	SER	2.9
34	1c	51	GLY	2.9
11	1P	122	PRO	2.9
33	1b	167	PRO	2.9
46	2o	19	PRO	2.9
1	1A	2893	G	2.9
1	2A	1171	G	2.9
7	2H	61	HIS	2.9
18	1W	111	HIS	2.9
1	1A	889	C	2.9
5	2F	176	LEU	2.9
6	2G	141	PHE	2.9
6	2G	180	PHE	2.9
20	2Y	21	LYS	2.9
13	2R	29	LEU	2.9
14	2S	54	LEU	2.9
24	22	44	LEU	2.9
33	1b	102	LEU	2.9
33	1b	118	LEU	2.9
33	2b	55	PHE	2.9
33	2b	133	LYS	2.9
7	2H	54	ARG	2.9
8	2I	12	LEU	2.9
8	2I	53	ALA	2.9
33	2b	173	ALA	2.9
35	1d	155	LEU	2.9
38	1g	43	PHE	2.9
42	2k	23	ALA	2.9
43	1l	10	LEU	2.9
43	1l	52	LEU	2.9
44	1m	28	ALA	2.9
54	1w	1	G	2.9
57	1y	57	G	2.9
11	2P	148	LEU	2.9
39	1h	30	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	1h	84	ARG	2.9
47	1p	74	LEU	2.9
7	2H	79	VAL	2.9
12	2Q	106	VAL	2.9
15	1T	28	VAL	2.9
29	27	46	VAL	2.9
34	2c	138	VAL	2.9
38	1g	9	VAL	2.9
40	1i	41	VAL	2.9
47	1p	21	VAL	2.9
34	1c	124	ILE	2.9
46	2o	87	ILE	2.9
47	1p	36	ILE	2.9
34	2c	191	THR	2.9
46	1o	22	THR	2.9
33	2b	90	MET	2.9
32	1a	1030(D)	A	2.9
32	1a	1447	A	2.9
53	1v	14	A	2.9
8	2I	11	ASN	2.9
8	2I	74	ASN	2.9
14	2S	92	TYR	2.9
34	1c	13	GLY	2.9
34	1c	193	TYR	2.9
34	2c	158	GLY	2.9
23	2I	78	LYS	2.9
35	1d	169	LYS	2.9
43	2I	31	PRO	2.9
21	1Z	131	ARG	2.9
34	2c	6	HIS	2.9
45	2n	12	ARG	2.9
5	1F	141	ALA	2.9
5	2F	181	LEU	2.9
8	2I	6	LEU	2.9
11	2P	91	PHE	2.9
19	2X	84	ALA	2.9
24	22	60	LEU	2.9
33	2b	135	GLN	2.9
33	2b	225	ALA	2.9
35	1d	19	LEU	2.9
35	2d	21	LEU	2.9
40	1i	45	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	1m	56	LEU	2.9
1	1A	1056	G	2.9
1	1A	2154	G	2.9
32	2a	470	C	2.9
57	1y	70	G	2.9
57	2y	22	G	2.9
6	2G	160	VAL	2.9
21	1Z	165	VAL	2.9
21	2Z	27	VAL	2.9
35	2d	140	VAL	2.9
40	2i	108	VAL	2.9
41	1j	72	VAL	2.9
46	1o	60	VAL	2.9
47	1p	20	VAL	2.9
33	2b	12	GLU	2.9
1	1A	2132	U	2.9
33	2b	108	ILE	2.9
34	2c	152	ILE	2.9
39	1h	80	ILE	2.9
32	2a	1251	A	2.8
41	2j	35	SER	2.8
44	1m	121	LYS	2.8
6	1G	2	PRO	2.8
26	14	32	TYR	2.8
35	1d	207	TYR	2.8
35	2d	123	HIS	2.8
38	2g	78	ARG	2.8
40	1i	58	HIS	2.8
41	2j	62	HIS	2.8
42	2k	35	PRO	2.8
44	1m	21	TYR	2.8
45	1n	3	ARG	2.8
45	2n	26	ARG	2.8
38	2g	11	GLN	2.8
8	1I	128	LEU	2.8
14	2S	4	LEU	2.8
22	10	84	LEU	2.8
24	22	61	LEU	2.8
33	2b	69	LEU	2.8
41	1j	90	LEU	2.8
44	2m	70	LEU	2.8
6	2G	23	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	2Q	104	PHE	2.8
34	2c	50	ALA	2.8
40	2i	82	ALA	2.8
42	2k	72	ALA	2.8
44	1m	30	ALA	2.8
32	1a	225	C	2.8
32	1a	1030(B)	C	2.8
32	1a	1042	G	2.8
57	2y	49	C	2.8
3	2D	173	VAL	2.8
4	2E	150	VAL	2.8
8	1I	127	VAL	2.8
17	2V	58	VAL	2.8
19	2X	43	VAL	2.8
21	2Z	74	VAL	2.8
23	21	53	VAL	2.8
25	23	59	VAL	2.8
33	1b	15	VAL	2.8
21	1Z	69	THR	2.8
33	2b	222	ILE	2.8
34	1c	14	ILE	2.8
34	2c	84	ILE	2.8
44	2m	43	THR	2.8
46	2o	82	ILE	2.8
50	1s	33	THR	2.8
50	2s	62	ILE	2.8
41	2j	14	LYS	2.8
1	2A	1509(A)	A	2.8
7	1H	166	GLY	2.8
9	2N	61	ARG	2.8
12	2Q	19	GLY	2.8
17	2V	54	GLY	2.8
20	2Y	80	GLY	2.8
33	1b	36	ARG	2.8
34	2c	172	ARG	2.8
45	2n	60	SER	2.8
52	2u	16	GLY	2.8
7	2H	21	PRO	2.8
33	2b	125	PRO	2.8
33	2b	234	PRO	2.8
40	1i	90	PRO	2.8
40	2i	98	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	184	TYR	2.8
35	2d	27	TYR	2.8
35	2d	38	TYR	2.8
38	1g	151	TYR	2.8
40	2i	114	TYR	2.8
4	2E	52	LEU	2.8
7	2H	103	LEU	2.8
11	1P	148	LEU	2.8
23	2l	73	LEU	2.8
39	2h	63	LEU	2.8
46	1o	39	LEU	2.8
21	2Z	164	ALA	2.8
33	1b	225	ALA	2.8
35	2d	75	PHE	2.8
40	2i	45	ALA	2.8
42	2k	65	ALA	2.8
1	1A	1509	C	2.8
1	2A	2185	C	2.8
39	2h	136	GLU	2.8
57	2y	75	C	2.8
1	1A	1055	G	2.8
1	2A	879	G	2.8
1	2A	2793	G	2.8
3	2D	113	VAL	2.8
9	2N	5	VAL	2.8
34	1c	66	VAL	2.8
35	1d	17	VAL	2.8
38	1g	73	MET	2.8
42	2k	47	VAL	2.8
45	1n	56	VAL	2.8
48	1q	11	VAL	2.8
1	1A	1026	U	2.8
1	1A	2118	U	2.8
35	1d	173	TRP	2.8
43	1l	21	LYS	2.8
6	2G	52	ILE	2.8
9	2N	73	THR	2.8
9	2N	85	ILE	2.8
12	1Q	59	ARG	2.8
12	2Q	6	ARG	2.8
15	2T	111	ARG	2.8
21	2Z	53	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	12	69	ARG	2.8
33	2b	211	ILE	2.8
35	1d	3	ARG	2.8
36	1e	126	ARG	2.8
38	1g	120	ILE	2.8
41	1j	38	ILE	2.8
41	2j	66	ARG	2.8
50	1s	40	ILE	2.8
20	2Y	107	ASP	2.8
19	2X	94	GLY	2.8
33	2b	124	SER	2.8
33	2b	227	GLY	2.8
34	2c	80	GLY	2.8
39	2h	96	GLY	2.8
41	1j	36	GLY	2.8
42	1k	56	GLY	2.8
48	1q	80	GLY	2.8
1	1A	1069	A	2.8
32	1a	1531	A	2.8
8	2I	139	GLN	2.8
35	2d	40	PRO	2.8
8	2I	130	TYR	2.8
42	2k	59	TYR	2.8
52	2u	18	TYR	2.8
21	2Z	91	LEU	2.8
33	2b	149	LEU	2.8
35	1d	21	LEU	2.8
42	2k	66	LEU	2.8
43	2l	10	LEU	2.8
48	2q	43	LEU	2.8
49	1r	85	LEU	2.8
49	2r	76	LEU	2.8
20	1Y	91	GLU	2.8
35	1d	192	GLU	2.8
3	1D	93	ALA	2.8
3	2D	80	ALA	2.8
8	1I	94	ALA	2.8
34	1c	61	ALA	2.8
36	2e	94	ALA	2.8
38	2g	121	ALA	2.8
44	1m	76	ALA	2.8
45	1n	48	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	59	ALA	2.8
47	1p	77	ALA	2.8
6	2G	148	MET	2.8
1	1A	2163	C	2.8
1	2A	2794	C	2.8
32	1a	624	C	2.8
33	2b	75	LYS	2.8
35	1d	181	MET	2.8
8	1I	15	VAL	2.8
32	2a	1125	U	2.8
36	1e	41	VAL	2.8
49	2r	22	VAL	2.8
50	2s	51	VAL	2.8
32	1a	1024	G	2.8
32	2a	755	G	2.8
32	2a	1023	G	2.8
32	2a	1030(C)	G	2.8
33	2b	178	ARG	2.8
34	2c	126	ARG	2.8
39	2h	30	ARG	2.8
47	2p	8	ARG	2.8
52	1u	6	ARG	2.8
54	2w	15	G	2.8
17	2V	99	ILE	2.8
33	1b	182	ILE	2.8
33	2b	168	THR	2.8
36	2e	13	ILE	2.8
36	2e	98	THR	2.8
41	1j	98	ILE	2.8
41	1j	100	THR	2.8
43	2l	7	ILE	2.8
47	1p	67	THR	2.8
21	1Z	148	ASP	2.8
35	2d	161	ASN	2.8
40	1i	91	ASP	2.8
41	2j	17	ASP	2.8
52	1u	14	TRP	2.8
12	1Q	15	GLY	2.8
14	2S	50	SER	2.8
33	2b	216	SER	2.8
36	2e	22	GLY	2.8
41	2j	10	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	31	GLY	2.8
51	1t	37	SER	2.8
1	2A	2171	A	2.8
4	1E	74	PRO	2.8
8	2I	137	PRO	2.8
32	1a	1005	A	2.8
32	2a	1252	A	2.8
33	2b	183	PRO	2.8
46	2o	2	PRO	2.8
51	2t	98	PRO	2.8
53	1v	15	A	2.8
57	2y	21	A	2.8
8	2I	60	GLU	2.8
7	1H	67	LEU	2.8
8	2I	9	LEU	2.8
11	2P	110	TYR	2.8
17	2V	91	TYR	2.8
22	20	59	LEU	2.8
35	2d	19	LEU	2.8
35	2d	94	LEU	2.8
38	2g	38	LEU	2.8
44	2m	23	TYR	2.8
47	1p	17	TYR	2.8
33	2b	8	LYS	2.8
5	2F	166	ALA	2.8
9	2N	124	ALA	2.8
20	2Y	78	ALA	2.8
33	1b	77	ALA	2.8
33	1b	83	MET	2.8
35	2d	18	LYS	2.8
33	2b	62	ALA	2.8
33	2b	88	ALA	2.8
34	2c	187	ALA	2.8
35	1d	164	ALA	2.8
36	1e	10	MET	2.8
37	2f	20	ALA	2.8
38	2g	31	MET	2.8
51	2t	97	ALA	2.8
14	2S	29	PHE	2.8
22	20	69	PHE	2.8
34	2c	203	PHE	2.8
33	2b	111	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	2d	47	ARG	2.8
50	1s	29	ARG	2.8
1	1A	2103	C	2.8
1	2A	2178	C	2.8
1	2A	2180	U	2.8
32	1a	204	U	2.8
6	1G	28	VAL	2.8
7	1H	15	VAL	2.8
7	2H	125	VAL	2.8
8	2I	19	VAL	2.8
11	1P	146	VAL	2.8
12	2Q	27	VAL	2.8
21	2Z	105	VAL	2.8
25	23	58	VAL	2.8
32	1a	1006	C	2.8
35	2d	121	VAL	2.8
40	2i	17	VAL	2.8
40	2i	53	VAL	2.8
42	1k	84	VAL	2.8
1	1A	2106	G	2.7
1	1A	2125	G	2.7
1	2A	2151	G	2.7
32	1a	64	G	2.7
32	1a	1009	G	2.7
32	1a	1030(C)	G	2.7
32	2a	485	G	2.7
6	2G	39	ILE	2.7
18	2W	6	ILE	2.7
33	1b	58	ILE	2.7
37	2f	8	ILE	2.7
41	2j	67	THR	2.7
42	1k	48	ILE	2.7
42	2k	28	THR	2.7
42	2k	41	THR	2.7
42	2k	95	ILE	2.7
44	2m	84	ILE	2.7
46	2o	22	THR	2.7
49	2r	56	THR	2.7
6	2G	41	GLN	2.7
40	2i	91	ASP	2.7
6	2G	42	GLY	2.7
11	2P	109	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	185	GLY	2.7
41	2j	30	SER	2.7
43	1l	63	GLY	2.7
44	2m	68	GLY	2.7
21	1Z	167	PRO	2.7
25	23	2	PRO	2.7
39	2h	135	CYS	2.7
47	2p	66	PRO	2.7
1	2A	887	A	2.7
53	2v	15	A	2.7
57	2y	7	A	2.7
48	2q	87	LYS	2.7
5	2F	196	LEU	2.7
12	2Q	7	MET	2.7
34	2c	196	LEU	2.7
38	2g	22	LEU	2.7
38	2g	101	LEU	2.7
39	2h	112	LEU	2.7
44	1m	90	LEU	2.7
3	2D	190	TYR	2.7
3	2D	272	ALA	2.7
7	2H	165	ALA	2.7
8	1I	63	ALA	2.7
14	2S	36	TYR	2.7
21	1Z	99	TYR	2.7
38	2g	44	TYR	2.7
39	2h	37	ARG	2.7
39	2h	92	ARG	2.7
47	1p	38	TYR	2.7
1	2A	1026	U	2.7
38	2g	26	PHE	2.7
1	2A	897	C	2.7
8	2I	3	VAL	2.7
8	2I	133	HIS	2.7
32	1a	1037	C	2.7
36	1e	51	VAL	2.7
39	2h	26	VAL	2.7
40	2i	28	VAL	2.7
45	1n	33	VAL	2.7
47	2p	2	VAL	2.7
57	2y	48	C	2.7
38	2g	86	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	103	THR	2.7
1	1A	883	G	2.7
1	1A	892	G	2.7
1	1A	1176	G	2.7
1	2A	2190	G	2.7
26	24	14	ILE	2.7
6	2G	85	GLY	2.7
7	2H	14	GLY	2.7
7	2H	91	GLY	2.7
23	11	55	GLY	2.7
32	1a	1031	G	2.7
48	2q	90	ILE	2.7
34	2c	74	GLY	2.7
48	2q	80	GLY	2.7
51	2t	96	GLY	2.7
52	2u	11	GLY	2.7
57	2y	5	G	2.7
8	1I	143	SER	2.7
42	2k	43	SER	2.7
51	1t	11	SER	2.7
4	2E	56	PRO	2.7
29	27	44	PRO	2.7
35	1d	136	PRO	2.7
21	2Z	94	GLU	2.7
1	1A	2176	A	2.7
1	2A	2208	A	2.7
23	21	81	LYS	2.7
32	1a	171	A	2.7
32	2a	1146	A	2.7
34	2c	135	LYS	2.7
36	2e	92	LYS	2.7
8	1I	77	LEU	2.7
16	2U	83	LEU	2.7
17	2V	18	LEU	2.7
23	11	94	LEU	2.7
33	2b	61	LEU	2.7
34	1c	47	LEU	2.7
35	2d	155	LEU	2.7
38	1g	101	LEU	2.7
40	2i	47	LEU	2.7
48	2q	22	LEU	2.7
49	1r	31	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	1I	126	TYR	2.7
36	2e	132	ALA	2.7
36	2e	133	TYR	2.7
39	1h	16	ALA	2.7
40	2i	15	ALA	2.7
40	2i	88	TYR	2.7
41	1j	27	ALA	2.7
41	2j	26	ALA	2.7
44	2m	21	TYR	2.7
47	1p	16	HIS	2.7
33	1b	55	PHE	2.7
3	2D	166	GLN	2.7
1	1A	652(S)	C	2.7
1	1A	2107	C	2.7
9	2N	98	VAL	2.7
39	2h	129	VAL	2.7
46	2o	9	GLN	2.7
47	2p	79	VAL	2.7
48	2q	93	GLN	2.7
51	1t	18	GLN	2.7
32	1a	1029	C	2.7
32	2a	1277	C	2.7
54	1w	4	C	2.7
57	1y	13	C	2.7
57	2y	62	C	2.7
6	2G	123	ASN	2.7
26	24	27	THR	2.7
33	2b	193	ASP	2.7
35	1d	154	ASN	2.7
36	1e	135	THR	2.7
50	2s	63	THR	2.7
4	1E	50	GLY	2.7
5	2F	28	ILE	2.7
10	1O	47	ILE	2.7
12	2Q	131	ILE	2.7
34	1c	57	ILE	2.7
34	1c	158	GLY	2.7
39	2h	45	ILE	2.7
43	2l	100	ILE	2.7
44	1m	22	ILE	2.7
48	2q	65	ILE	2.7
1	2A	2805	G	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2893	G	2.7
3	2D	22	SER	2.7
33	1b	192	SER	2.7
33	2b	27	LYS	2.7
40	2i	49	PRO	2.7
41	1j	30	SER	2.7
49	2r	21	LYS	2.7
57	1y	18	G	2.7
57	1y	52	G	2.7
57	1y	69	G	2.7
1	1A	1098	A	2.7
5	1F	17	ARG	2.7
33	2b	217	ARG	2.7
35	2d	181	MET	2.7
40	2i	120	ARG	2.7
45	2n	43	CYS	2.7
34	2c	178	LEU	2.7
35	2d	78	LEU	2.7
36	1e	91	LEU	2.7
40	1i	47	LEU	2.7
45	2n	39	LEU	2.7
46	1o	32	LEU	2.7
50	2s	16	LEU	2.7
4	1E	204	ALA	2.7
5	1F	111	ALA	2.7
15	1T	116	ALA	2.7
20	2Y	16	ALA	2.7
21	2Z	51	ALA	2.7
29	17	45	ALA	2.7
32	1a	90	U	2.7
32	2a	1219	U	2.7
40	2i	76	ALA	2.7
40	2i	119	ALA	2.7
44	2m	18	ALA	2.7
47	2p	24	ALA	2.7
49	2r	20	ALA	2.7
16	2U	104	GLN	2.7
40	1i	5	TYR	2.7
41	1j	33	GLN	2.7
47	2p	76	GLN	2.7
12	2Q	29	PHE	2.7
1	2A	277	C	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	1F	6	VAL	2.7
7	2H	141	VAL	2.7
12	2Q	109	VAL	2.7
14	2S	69	VAL	2.7
15	2T	49	VAL	2.7
28	26	52	VAL	2.7
9	2N	84	LYS	2.7
32	1a	620	C	2.7
34	2c	45	LYS	2.7
34	2c	62	ASP	2.7
36	2e	115	VAL	2.7
37	1f	13	ASN	2.7
40	1i	53	VAL	2.7
40	2i	26	VAL	2.7
50	2s	19	VAL	2.7
35	1d	179	GLU	2.7
44	1m	120	LYS	2.7
44	2m	37	THR	2.7
44	2m	121	LYS	2.7
47	2p	69	THR	2.7
48	1q	20	THR	2.7
51	2t	74	LYS	2.7
4	2E	77	ILE	2.7
6	2G	44	GLY	2.7
33	2b	18	GLY	2.7
34	1c	182	ILE	2.7
35	1d	87	GLY	2.7
39	2h	80	ILE	2.7
42	1k	49	GLY	2.7
42	1k	76	GLY	2.7
42	2k	29	ILE	2.7
48	1q	33	GLY	2.7
51	2t	63	ILE	2.7
7	1H	117	PRO	2.7
21	1Z	149	SER	2.7
23	21	38	SER	2.7
41	2j	19	SER	2.7
49	2r	80	PRO	2.7
50	2s	59	PRO	2.7
1	1A	2186	G	2.7
21	1Z	1	MET	2.7
32	1a	1026	G	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1024	G	2.7
34	2c	142	MET	2.7
54	2w	5	G	2.7
57	2y	29	G	2.7
1	2A	528	A	2.7
32	2a	1001	A	2.7
4	2E	5	LEU	2.7
8	1I	9	LEU	2.7
21	1Z	125	LEU	2.7
21	2Z	102	LEU	2.7
23	2I	94	LEU	2.7
34	1c	43	LEU	2.7
35	1d	11	LEU	2.7
41	1j	88	LEU	2.7
42	2k	103	LEU	2.7
44	1m	81	LEU	2.7
50	2s	30	LEU	2.7
33	2b	140	HIS	2.6
48	1q	45	HIS	2.6
51	1t	16	HIS	2.6
1	2A	895	U	2.6
4	2E	46	ALA	2.6
8	2I	65	ALA	2.6
11	1P	141	ALA	2.6
11	2P	120	ALA	2.6
33	1b	95	GLN	2.6
34	2c	71	ALA	2.6
36	2e	86	ALA	2.6
40	1i	61	ALA	2.6
45	2n	48	ALA	2.6
6	2G	182	LYS	2.6
35	2d	4	TYR	2.6
36	1e	28	PHE	2.6
40	1i	101	PHE	2.6
40	1i	125	TYR	2.6
11	2P	83	VAL	2.6
15	2T	104	ASN	2.6
19	2X	83	VAL	2.6
34	2c	141	VAL	2.6
35	1d	102	ASP	2.6
44	2m	60	VAL	2.6
1	1A	1092	C	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2185	C	2.6
1	2A	2140	C	2.6
4	1E	77	ILE	2.6
4	2E	29	GLY	2.6
32	2a	1039	C	2.6
32	2a	1128	C	2.6
41	2j	15	THR	2.6
41	2j	81	THR	2.6
34	2c	41	GLY	2.6
37	2f	25	ILE	2.6
38	1g	132	GLY	2.6
40	1i	80	GLY	2.6
40	2i	6	GLY	2.6
47	2p	10	GLY	2.6
50	1s	26	GLY	2.6
52	2u	2	GLY	2.6
54	1w	2	C	2.6
7	1H	126	PRO	2.6
7	2H	29	PRO	2.6
8	1I	79	ILE	2.6
10	2O	19	ILE	2.6
12	2Q	10	ARG	2.6
15	2T	93	ARG	2.6
20	2Y	53	PRO	2.6
21	1Z	171	ILE	2.6
24	22	50	ILE	2.6
21	1Z	66	SER	2.6
21	2Z	15	PRO	2.6
39	2h	104	ARG	2.6
40	2i	81	ILE	2.6
44	1m	102	ARG	2.6
44	2m	4	ILE	2.6
45	2n	45	ARG	2.6
50	2s	78	ARG	2.6
21	2Z	153	SER	2.6
26	24	66	SER	2.6
15	2T	1	MET	2.6
29	27	1	MET	2.6
32	2a	1154	G	2.6
1	1A	1077	A	2.6
1	1A	1177	A	2.6
57	1y	21	A	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	2F	123	LEU	2.6
11	2P	106	LEU	2.6
21	2Z	85	HIS	2.6
22	20	21	LEU	2.6
36	2e	53	LEU	2.6
37	1f	14	LEU	2.6
38	2g	124	LEU	2.6
39	1h	133	LEU	2.6
39	2h	133	LEU	2.6
41	2j	13	HIS	2.6
46	1o	81	LEU	2.6
1	1A	1083	U	2.6
1	1A	2102	U	2.6
5	2F	199	TRP	2.6
32	1a	1040	U	2.6
50	2s	34	TRP	2.6
57	1y	59	U	2.6
41	2j	99	LYS	2.6
5	2F	128	ALA	2.6
11	2P	127	ALA	2.6
14	2S	105	ALA	2.6
20	2Y	48	ALA	2.6
36	2e	113	ALA	2.6
40	2i	84	ALA	2.6
47	2p	7	ALA	2.6
23	21	83	GLU	2.6
36	2e	50	GLU	2.6
48	1q	78	GLU	2.6
21	2Z	89	PHE	2.6
5	1F	18	ARG	2.6
11	2P	80	TYR	2.6
33	1b	189	ASP	2.6
50	1s	10	PHE	2.6
12	2Q	59	ARG	2.6
24	22	69	ARG	2.6
36	2e	107	ARG	2.6
51	2t	86	ARG	2.6
3	2D	18	VAL	2.6
7	2H	115	VAL	2.6
3	2D	114	GLY	2.6
8	2I	129	THR	2.6
34	1c	106	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	120	VAL	2.6
35	1d	203	VAL	2.6
35	2d	105	VAL	2.6
36	2e	67	VAL	2.6
40	2i	86	VAL	2.6
41	2j	100	THR	2.6
44	1m	117	VAL	2.6
14	2S	60	GLY	2.6
36	1e	114	GLY	2.6
39	2h	43	GLY	2.6
49	2r	48	GLY	2.6
50	2s	79	THR	2.6
1	1A	1079	C	2.6
1	2A	271(J)	C	2.6
7	2H	4	ILE	2.6
8	1I	132	PRO	2.6
32	1a	1027	C	2.6
32	2a	1369	C	2.6
35	1d	29	PRO	2.6
38	1g	50	ILE	2.6
46	2o	12	ILE	2.6
46	2o	36	ILE	2.6
47	1p	41	PRO	2.6
1	1A	878	A	2.6
1	1A	879	G	2.6
1	1A	881	G	2.6
1	1A	2124	G	2.6
8	2I	44	LEU	2.6
12	2Q	2	LEU	2.6
17	2V	95	LEU	2.6
21	2Z	70	LEU	2.6
24	22	21	LEU	2.6
32	1a	617	G	2.6
33	2b	155	LEU	2.6
34	1c	12	LEU	2.6
34	2c	162	GLN	2.6
35	1d	58	LEU	2.6
37	1f	19	LEU	2.6
43	2l	9	GLN	2.6
44	2m	48	LEU	2.6
45	1n	53	LEU	2.6
47	2p	60	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
55	1x	46	G	2.6
57	2y	6	G	2.6
20	1Y	54	LYS	2.6
48	1q	17	LYS	2.6
44	2m	58	GLU	2.6
3	2D	153	ALA	2.6
5	2F	177	ALA	2.6
14	2S	79	ALA	2.6
33	2b	177	ALA	2.6
34	2c	65	ALA	2.6
36	2e	95	ALA	2.6
38	2g	25	ALA	2.6
38	2g	134	ALA	2.6
39	1h	7	ALA	2.6
42	2k	60	ALA	2.6
47	2p	64	ALA	2.6
51	1t	32	ALA	2.6
51	2t	32	ALA	2.6
7	1H	130	ARG	2.6
18	2W	92	ARG	2.6
33	2b	23	ARG	2.6
40	2i	104	ARG	2.6
6	2G	121	ASN	2.6
21	2Z	132	ASN	2.6
34	2c	36	ASP	2.6
41	2j	58	ASP	2.6
46	2o	37	ASN	2.6
6	2G	80	PHE	2.6
7	2H	123	PHE	2.6
21	2Z	44	PHE	2.6
35	2d	185	PHE	2.6
45	1n	16	PHE	2.6
6	2G	142	PRO	2.6
7	1H	14	GLY	2.6
7	2H	113	VAL	2.6
8	2I	111	PRO	2.6
9	1N	140	VAL	2.6
11	1P	93	GLY	2.6
15	2T	10	VAL	2.6
17	2V	37	VAL	2.6
21	2Z	26	GLY	2.6
21	2Z	71	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
23	21	74	VAL	2.6
28	26	48	VAL	2.6
33	2b	83	MET	2.6
34	1c	2	GLY	2.6
34	1c	116	VAL	2.6
34	1c	120	VAL	2.6
34	2c	7	PRO	2.6
35	1d	140	VAL	2.6
35	2d	128	VAL	2.6
36	2e	61	TYR	2.6
38	2g	105	VAL	2.6
39	2h	20	TYR	2.6
39	2h	62	TYR	2.6
39	2h	74	PRO	2.6
39	2h	89	PRO	2.6
39	2h	130	GLY	2.6
42	1k	105	VAL	2.6
43	2l	6	THR	2.6
47	1p	39	TYR	2.6
49	2r	69	THR	2.6
52	1u	8	THR	2.6
5	1F	13	SER	2.6
5	1F	28	ILE	2.6
11	2P	114	ILE	2.6
31	29	17	ILE	2.6
32	1a	221	C	2.6
32	1a	1019	C	2.6
32	1a	1039	C	2.6
32	2a	1203	C	2.6
40	2i	71	SER	2.6
41	1j	74	ILE	2.6
41	1j	75	ILE	2.6
43	1l	7	ILE	2.6
48	2q	39	SER	2.6
50	2s	49	ILE	2.6
57	2y	68	C	2.6
57	2y	74	C	2.6
41	1j	56	HIS	2.6
7	2H	62	LYS	2.6
26	14	60	GLN	2.6
34	2c	123	GLN	2.6
1	1A	548	A	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1054	A	2.6
6	2G	82	LEU	2.6
6	2G	176	LEU	2.6
7	1H	98	LEU	2.6
8	1I	68	LEU	2.6
15	1T	114	LEU	2.6
15	2T	82	LEU	2.6
24	22	3	LEU	2.6
24	22	10	LEU	2.6
32	1a	152	A	2.6
33	2b	115	LEU	2.6
34	1c	204	LEU	2.6
34	2c	34	LEU	2.6
34	2c	47	LEU	2.6
34	2c	188	LEU	2.6
37	2f	79	LEU	2.6
40	1i	102	LEU	2.6
40	2i	40	LEU	2.6
1	1A	2157	G	2.6
1	1A	2802	G	2.6
1	1A	2805	G	2.6
1	2A	271(M)	G	2.6
1	2A	2132	U	2.6
1	2A	2833	G	2.6
32	2a	1182	G	2.6
55	2x	46	G	2.6
15	1T	115	ARG	2.6
21	2Z	122	ARG	2.6
38	2g	79	ARG	2.6
41	1j	28	ARG	2.6
42	1k	126	ARG	2.6
48	2q	70	ARG	2.6
52	2u	9	ARG	2.6
14	1S	79	ALA	2.6
15	2T	94	ALA	2.6
36	1e	113	ALA	2.6
38	2g	147	ALA	2.6
44	1m	107	ALA	2.6
47	2p	59	TRP	2.6
14	2S	61	ASN	2.6
24	22	65	ASN	2.6
38	2g	148	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	2F	14	PRO	2.6
5	2F	175	THR	2.6
7	2H	117	PRO	2.6
33	1b	103	THR	2.6
33	2b	67	THR	2.6
34	2c	13	GLY	2.6
35	2d	2	GLY	2.6
36	2e	85	GLY	2.6
34	1c	68	VAL	2.6
35	2d	112	VAL	2.6
41	1j	37	PRO	2.6
42	2k	39	PRO	2.6
42	2k	87	THR	2.6
42	2k	102	GLY	2.6
45	2n	14	PRO	2.6
46	2o	25	THR	2.6
51	1t	69	GLY	2.6
52	1u	2	GLY	2.6
47	1p	62	VAL	2.6
48	1q	21	VAL	2.6
50	2s	58	VAL	2.6
5	2F	82	ILE	2.6
7	1H	83	TYR	2.6
7	2H	89	ILE	2.6
8	2I	88	ILE	2.6
10	2O	77	ILE	2.6
17	2V	4	ILE	2.6
33	1b	33	TYR	2.6
33	1b	42	ILE	2.6
34	2c	57	ILE	2.6
35	2d	138	TYR	2.6
35	2d	175	SER	2.6
39	1h	134	ILE	2.6
48	1q	66	SER	2.6
50	1s	52	TYR	2.6
8	2I	141	LYS	2.6
9	2N	83	LYS	2.6
38	2g	136	LYS	2.6
40	1i	112	LYS	2.6
47	1p	35	LYS	2.6
34	2c	107	GLN	2.5
4	1E	73	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	1I	72	LEU	2.5
33	1b	129	GLU	2.5
33	2b	129	GLU	2.5
32	1a	344	A	2.5
32	2a	4	U	2.5
33	2b	221	LEU	2.5
42	2k	63	LEU	2.5
44	2m	90	LEU	2.5
46	2o	67	LEU	2.5
57	2y	73	A	2.5
6	2G	51	ARG	2.5
6	2G	115	ARG	2.5
15	1T	108	ARG	2.5
34	2c	38	ARG	2.5
44	2m	88	ARG	2.5
1	1A	2187	G	2.5
1	2A	2184	G	2.5
32	1a	102	G	2.5
32	2a	971	G	2.5
57	1y	53	G	2.5
5	2F	143	ALA	2.5
17	2V	59	ALA	2.5
20	2Y	79	CYS	2.5
21	2Z	21	ALA	2.5
33	1b	85	ALA	2.5
33	2b	29	ALA	2.5
38	1g	145	ALA	2.5
40	2i	94	ALA	2.5
42	1k	23	ALA	2.5
42	2k	119	CYS	2.5
46	2o	30	ALA	2.5
49	1r	24	ALA	2.5
36	1e	73	ASN	2.5
36	2e	5	ASP	2.5
43	2l	8	ASN	2.5
8	1I	80	PRO	2.5
10	2O	119	PRO	2.5
13	2R	7	GLY	2.5
33	1b	99	GLY	2.5
33	2b	232	PRO	2.5
34	1c	171	GLY	2.5
40	1i	103	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	1j	10	GLY	2.5
36	2e	28	PHE	2.5
41	1j	11	PHE	2.5
41	1j	87	THR	2.5
42	2k	76	GLY	2.5
23	1l	60	PHE	2.5
26	24	42	PHE	2.5
3	2D	98	VAL	2.5
10	1O	121	VAL	2.5
12	2Q	22	LYS	2.5
14	2S	49	VAL	2.5
20	2Y	39	VAL	2.5
21	1Z	126	VAL	2.5
40	2i	127	LYS	2.5
41	2j	24	VAL	2.5
43	1l	36	VAL	2.5
44	1m	74	VAL	2.5
44	2m	25	ILE	2.5
44	2m	92	HIS	2.5
45	2n	49	HIS	2.5
46	2o	29	VAL	2.5
48	2q	37	LYS	2.5
48	2q	52	LYS	2.5
48	2q	56	VAL	2.5
50	2s	38	SER	2.5
51	2t	88	VAL	2.5
14	1S	82	ILE	2.5
16	2U	88	ILE	2.5
21	1Z	53	ILE	2.5
23	2l	58	ILE	2.5
24	22	57	ILE	2.5
51	1t	33	ILE	2.5
52	1u	13	ILE	2.5
1	1A	1100	C	2.5
11	1P	70	GLN	2.5
34	2c	23	TYR	2.5
35	1d	4	TYR	2.5
42	1k	25	TYR	2.5
42	2k	50	TYR	2.5
47	1p	65	GLN	2.5
24	22	66	GLU	2.5
1	2A	2172	U	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	2T	112	ARG	2.5
24	12	51	ARG	2.5
33	2b	36	ARG	2.5
34	2c	83	ARG	2.5
38	1g	6	ARG	2.5
45	2n	57	ARG	2.5
4	2E	195	LEU	2.5
11	2P	147	LEU	2.5
42	1k	103	LEU	2.5
50	2s	15	LEU	2.5
51	1t	72	LEU	2.5
32	2a	968	A	2.5
54	2w	14	A	2.5
32	2a	79	G	2.5
32	2a	1001(A)	G	2.5
32	2a	1017	G	2.5
57	2y	70	G	2.5
5	1F	21	ALA	2.5
13	2R	62	ALA	2.5
14	2S	37	ALA	2.5
20	1Y	107	ASP	2.5
26	24	18	CYS	2.5
33	1b	34	ALA	2.5
8	1I	124	GLY	2.5
14	2S	57	LYS	2.5
17	2V	50	PRO	2.5
20	2Y	32	PRO	2.5
26	24	54	GLY	2.5
34	2c	51	GLY	2.5
36	1e	46	GLY	2.5
40	2i	72	GLY	2.5
39	2h	120	THR	2.5
41	2j	48	THR	2.5
33	1b	70	PHE	2.5
39	2h	138	TRP	2.5
47	1p	9	PHE	2.5
3	2D	185	VAL	2.5
5	2F	173	VAL	2.5
8	2I	54	GLN	2.5
19	2X	81	VAL	2.5
34	2c	20	SER	2.5
34	2c	55	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	1d	121	VAL	2.5
43	2l	90	VAL	2.5
44	2m	7	VAL	2.5
3	2D	75	ILE	2.5
8	2I	4	ILE	2.5
9	2N	16	ILE	2.5
12	2Q	47	ILE	2.5
19	2X	8	ILE	2.5
47	1p	33	ILE	2.5
2	2B	4	C	2.5
8	2I	85	GLU	2.5
20	1Y	55	TYR	2.5
21	2Z	29	TYR	2.5
21	2Z	38	TYR	2.5
22	20	26	TYR	2.5
32	1a	1008	C	2.5
32	1a	1030	C	2.5
32	2a	456	C	2.5
33	2b	114	ARG	2.5
33	2b	148	TYR	2.5
33	2b	175	ARG	2.5
35	2d	106	TYR	2.5
39	2h	22	GLU	2.5
45	2n	23	ARG	2.5
45	2n	29	ARG	2.5
45	2n	31	ARG	2.5
47	2p	38	TYR	2.5
48	2q	91	ARG	2.5
52	1u	15	ARG	2.5
57	1y	3	C	2.5
57	1y	43	C	2.5
57	1y	48	C	2.5
57	2y	25	C	2.5
32	1a	841	U	2.5
32	2a	204	U	2.5
32	2a	1159	U	2.5
8	2I	5	LEU	2.5
36	1e	31	LEU	2.5
40	1i	56	LEU	2.5
48	1q	76	LEU	2.5
1	2A	2801(A)	A	2.5
32	2a	1092	A	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2w	31	A	2.5
57	1y	64	A	2.5
57	2y	9	A	2.5
11	2P	1	MET	2.5
6	2G	47	LYS	2.5
6	2G	56	ALA	2.5
10	1O	103	ALA	2.5
13	2R	69	ASP	2.5
20	2Y	81	LYS	2.5
32	2a	80	G	2.5
32	2a	587	G	2.5
33	2b	25	ASN	2.5
33	2b	79	ASP	2.5
34	1c	71	ALA	2.5
36	1e	21	ALA	2.5
38	1g	28	ASN	2.5
39	1h	28	ALA	2.5
39	1h	126	LYS	2.5
44	2m	76	ALA	2.5
48	1q	100	LYS	2.5
57	1y	63	G	2.5
7	2H	126	PRO	2.5
11	2P	73	GLY	2.5
33	2b	14	GLY	2.5
33	2b	159	PRO	2.5
34	1c	78	GLY	2.5
35	2d	167	GLY	2.5
35	2d	171	GLY	2.5
36	2e	49	PRO	2.5
39	2h	76	PRO	2.5
43	1l	29	GLY	2.5
45	2n	27	CYS	2.5
47	1p	66	PRO	2.5
4	2E	48	GLN	2.5
33	1b	73	THR	2.5
44	1m	37	THR	2.5
4	2E	15	PHE	2.5
26	14	49	PHE	2.5
33	1b	122	PHE	2.5
34	2c	112	SER	2.5
34	2c	186	PHE	2.5
4	2E	33	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	38	VAL	2.5
7	1H	17	VAL	2.5
7	1H	89	ILE	2.5
10	1O	69	ILE	2.5
12	2Q	16	ARG	2.5
20	1Y	39	VAL	2.5
21	2Z	56	VAL	2.5
21	2Z	161	VAL	2.5
34	1c	22	TRP	2.5
36	2e	109	ILE	2.5
39	2h	84	ARG	2.5
42	1k	80	VAL	2.5
42	1k	96	ARG	2.5
42	2k	30	VAL	2.5
42	2k	105	VAL	2.5
44	2m	67	GLU	2.5
26	14	15	ILE	2.5
40	1i	74	ILE	2.5
44	2m	39	ILE	2.5
48	2q	11	VAL	2.5
48	2q	21	VAL	2.5
48	2q	68	ARG	2.5
1	1A	34	C	2.5
1	1A	645	C	2.5
1	1A	2180	U	2.5
1	2A	2102	U	2.5
21	2Z	99	TYR	2.5
54	2w	4	C	2.5
54	2w	68	C	2.5
32	2a	1025	U	2.5
5	1F	125	LEU	2.5
6	2G	94	LEU	2.5
8	2I	30	LEU	2.5
11	2P	6	LEU	2.5
11	2P	138	LEU	2.5
16	2U	74	LEU	2.5
26	14	9	LEU	2.5
34	1c	115	LEU	2.5
36	2e	110	LEU	2.5
36	2e	151	LEU	2.5
1	1A	1085	A	2.5
1	1A	1103	A	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	1472	A	2.5
9	2N	2	LYS	2.5
14	2S	19	LYS	2.5
50	2s	70	LYS	2.5
52	2u	20	LYS	2.5
15	1T	107	ASP	2.5
17	2V	26	ASP	2.5
3	2D	156	ALA	2.5
5	2F	118	ALA	2.5
7	2H	65	HIS	2.5
7	2H	145	ALA	2.5
25	23	21	ALA	2.5
33	1b	16	HIS	2.5
33	2b	19	HIS	2.5
34	2c	146	ALA	2.5
46	2o	80	ALA	2.5
47	1p	64	ALA	2.5
50	2s	50	ALA	2.5
1	2A	2152	G	2.5
11	2P	78	PRO	2.5
25	13	2	PRO	2.5
25	23	45	GLY	2.5
33	2b	151	GLY	2.5
34	1c	80	GLY	2.5
34	2c	148	GLY	2.5
34	2c	185	GLY	2.5
35	2d	172	PRO	2.5
36	2e	93	PRO	2.5
39	2h	117	GLY	2.5
40	1i	69	GLY	2.5
40	2i	73	GLN	2.5
50	1s	8	GLY	2.5
54	1w	44	G	2.5
57	1y	22	G	2.5
6	2G	118	ARG	2.4
12	1Q	6	ARG	2.4
26	14	55	ARG	2.4
33	1b	23	ARG	2.4
33	2b	47	THR	2.4
34	2c	90	GLU	2.4
34	2c	165	THR	2.4
36	2e	24	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	3	ARG	2.4
39	2h	17	THR	2.4
44	1m	105	THR	2.4
46	2o	72	ARG	2.4
51	1t	86	ARG	2.4
51	1t	89	ARG	2.4
3	2D	51	VAL	2.4
5	2F	139	PHE	2.4
21	1Z	52	SER	2.4
39	1h	115	SER	2.4
43	2l	66	VAL	2.4
46	2o	15	PHE	2.4
51	2t	70	SER	2.4
7	2H	92	ILE	2.4
14	1S	46	VAL	2.4
16	2U	63	VAL	2.4
25	23	56	VAL	2.4
31	29	16	VAL	2.4
34	1c	153	VAL	2.4
35	1d	8	VAL	2.4
35	1d	112	VAL	2.4
35	1d	158	ILE	2.4
35	2d	126	ILE	2.4
35	2d	198	VAL	2.4
37	2f	91	VAL	2.4
38	2g	49	ILE	2.4
39	1h	53	VAL	2.4
1	2A	405	U	2.4
32	2a	1254	C	2.4
54	2w	3	C	2.4
3	1D	155	LEU	2.4
4	2E	63	LEU	2.4
7	1H	105	LEU	2.4
7	2H	87	LEU	2.4
8	1I	101	LEU	2.4
8	2I	116	LEU	2.4
12	2Q	26	TYR	2.4
15	2T	14	TYR	2.4
16	2U	60	LEU	2.4
16	2U	95	LEU	2.4
22	20	62	LEU	2.4
33	1b	98	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	1d	54	TYR	2.4
35	2d	108	LEU	2.4
35	2d	176	LEU	2.4
38	2g	104	LEU	2.4
44	1m	70	LEU	2.4
8	2I	95	LYS	2.4
32	2a	1157	A	2.4
3	2D	66	ASP	2.4
3	2D	71	ASP	2.4
5	1F	23	ASP	2.4
5	2F	169	ASN	2.4
21	2Z	32	HIS	2.4
33	2b	60	ASP	2.4
46	2o	13	GLN	2.4
46	2o	62	GLN	2.4
3	2D	29	PRO	2.4
6	2G	151	ALA	2.4
8	1I	83	ALA	2.4
12	2Q	44	ALA	2.4
12	2Q	49	ALA	2.4
8	1I	48	GLU	2.4
17	2V	36	PRO	2.4
21	1Z	169	GLU	2.4
22	10	82	ARG	2.4
36	2e	54	ALA	2.4
34	2c	122	GLU	2.4
34	2c	127	ARG	2.4
38	2g	108	ALA	2.4
40	1i	39	GLY	2.4
40	1i	57	GLY	2.4
40	1i	66	ARG	2.4
42	2k	113	PRO	2.4
43	2l	14	GLY	2.4
44	2m	113	PRO	2.4
45	1n	59	ALA	2.4
45	2n	51	GLY	2.4
45	2n	54	PRO	2.4
47	2p	18	ARG	2.4
48	2q	30	PRO	2.4
49	2r	60	ALA	2.4
40	2i	8	GLY	2.4
1	1A	545	G	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2156	G	2.4
1	2A	2191	G	2.4
8	2I	86	THR	2.4
32	1a	447	G	2.4
36	2e	144	THR	2.4
57	2y	10	G	2.4
7	2H	155	SER	2.4
8	1I	91	SER	2.4
15	2T	67	SER	2.4
39	2h	29	SER	2.4
41	1j	35	SER	2.4
5	2F	154	VAL	2.4
7	2H	15	VAL	2.4
14	2S	65	VAL	2.4
17	2V	61	VAL	2.4
18	2W	85	VAL	2.4
20	2Y	85	VAL	2.4
23	2I	70	VAL	2.4
33	2b	208	ILE	2.4
34	1c	157	ILE	2.4
34	2c	86	VAL	2.4
35	2d	158	ILE	2.4
37	2f	60	PHE	2.4
41	2j	96	ILE	2.4
42	1k	21	ILE	2.4
48	1q	73	VAL	2.4
50	2s	60	VAL	2.4
1	1A	895	U	2.4
21	2Z	156	LYS	2.4
33	2b	147	LYS	2.4
36	2e	47	LYS	2.4
14	2S	80	LEU	2.4
15	2T	105	LEU	2.4
28	26	11	LEU	2.4
32	2a	1145	C	2.4
33	1b	63	MET	2.4
3	2D	147	LEU	2.4
4	1E	52	LEU	2.4
8	2I	31	LEU	2.4
8	2I	77	LEU	2.4
33	2b	138	LEU	2.4
34	1c	34	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
37	1f	45	LEU	2.4
38	1g	99	LEU	2.4
49	1r	76	LEU	2.4
21	2Z	3	TYR	2.4
38	1g	18	TYR	2.4
39	1h	20	TYR	2.4
39	1h	48	TYR	2.4
46	2o	78	TYR	2.4
2	2B	120	A	2.4
32	2a	653	A	2.4
32	2a	1261	A	2.4
32	2a	1286	A	2.4
54	1w	14	A	2.4
7	2H	3	ARG	2.4
35	2d	45	GLN	2.4
37	2f	84	ASN	2.4
40	2i	83	ARG	2.4
44	1m	106	ASN	2.4
44	2m	3	ARG	2.4
47	2p	42	ARG	2.4
21	2Z	11	GLU	2.4
48	2q	78	GLU	2.4
5	1F	14	PRO	2.4
6	2G	179	PRO	2.4
9	2N	132	ALA	2.4
26	24	29	PRO	2.4
12	2Q	108	GLY	2.4
14	2S	22	GLY	2.4
21	1Z	12	GLY	2.4
24	22	13	ALA	2.4
34	1c	50	ALA	2.4
34	1c	114	PRO	2.4
34	2c	81	GLY	2.4
35	2d	117	ALA	2.4
39	2h	16	ALA	2.4
42	1k	60	ALA	2.4
44	2m	10	PRO	2.4
44	2m	51	ALA	2.4
44	2m	118	ALA	2.4
51	1t	44	ALA	2.4
8	1I	93	THR	2.4
8	2I	93	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	63	THR	2.4
20	2Y	12	THR	2.4
27	25	29	THR	2.4
34	2c	15	THR	2.4
39	2h	24	THR	2.4
1	2A	2207	G	2.4
7	2H	38	SER	2.4
7	2H	56	SER	2.4
21	2Z	142	SER	2.4
32	1a	61	G	2.4
32	1a	78	G	2.4
32	1a	631	G	2.4
32	2a	933	G	2.4
32	2a	1131	G	2.4
57	1y	5	G	2.4
6	1G	159	VAL	2.4
6	2G	102	PHE	2.4
10	1O	99	PHE	2.4
11	2P	2	LYS	2.4
4	1E	47	VAL	2.4
7	1H	19	VAL	2.4
12	2Q	58	PHE	2.4
12	2Q	127	ILE	2.4
14	2S	98	VAL	2.4
16	2U	57	PHE	2.4
36	2e	88	LYS	2.4
35	1d	133	VAL	2.4
38	1g	42	ILE	2.4
40	2i	33	PHE	2.4
41	2j	54	PHE	2.4
42	2k	122	LYS	2.4
46	1o	82	ILE	2.4
46	2o	5	LYS	2.4
21	1Z	39	VAL	2.4
32	2a	1040	U	2.4
33	1b	81	VAL	2.4
47	2p	51	VAL	2.4
49	2r	86	VAL	2.4
54	1w	45	U	2.4
55	1x	47	U	2.4
57	1y	47	U	2.4
33	1b	48	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1532	C	2.4
4	1E	63	LEU	2.4
8	1I	30	LEU	2.4
11	2P	85	LEU	2.4
11	2P	88	LEU	2.4
13	2R	65	LEU	2.4
17	2V	62	LEU	2.4
21	2Z	59	LEU	2.4
32	1a	613	C	2.4
33	1b	154	LEU	2.4
34	1c	94	LEU	2.4
35	2d	11	LEU	2.4
35	2d	196	LEU	2.4
37	2f	19	LEU	2.4
41	1j	85	LEU	2.4
47	2p	73	LEU	2.4
49	2r	51	LEU	2.4
50	1s	20	LEU	2.4
51	1t	43	LEU	2.4
57	1y	25	C	2.4
34	1c	167	TRP	2.4
42	1k	42	TRP	2.4
5	2F	7	TYR	2.4
6	2G	58	GLN	2.4
6	2G	136	ARG	2.4
9	2N	74	ARG	2.4
11	2P	81	GLN	2.4
17	2V	12	TYR	2.4
29	27	41	ARG	2.4
30	28	46	ARG	2.4
33	2b	78	GLN	2.4
36	1e	60	TYR	2.4
37	1f	16	GLN	2.4
51	2t	8	ARG	2.4
52	2u	7	ARG	2.4
4	1E	89	ASP	2.4
14	2S	75	GLU	2.4
21	1Z	119	GLU	2.4
32	1a	101	A	2.4
33	2b	37	ASN	2.4
35	2d	24	GLU	2.4
38	2g	28	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	140	ASP	2.4
47	2p	68	ASP	2.4
51	2t	26	ASN	2.4
57	1y	14	A	2.4
11	2P	122	PRO	2.4
26	24	41	PRO	2.4
50	1s	59	PRO	2.4
14	2S	72	ALA	2.4
14	2S	90	GLY	2.4
21	1Z	51	ALA	2.4
33	1b	18	GLY	2.4
33	2b	85	ALA	2.4
35	1d	171	GLY	2.4
36	1e	85	GLY	2.4
40	2i	46	ALA	2.4
45	2n	55	GLY	2.4
51	2t	52	ALA	2.4
6	2G	93	THR	2.4
7	2H	106	THR	2.4
12	2Q	63	LYS	2.4
14	2S	33	LYS	2.4
14	2S	44	LYS	2.4
36	2e	9	LYS	2.4
37	2f	92	LYS	2.4
42	1k	57	THR	2.4
45	1n	17	LYS	2.4
47	1p	44	THR	2.4
34	2c	144	SER	2.4
1	1A	271(M)	G	2.4
1	1A	1173	G	2.4
1	1A	2184	G	2.4
1	2A	271(N)	U	2.4
1	2A	1112	G	2.4
1	2A	2153	G	2.4
1	2A	2319	G	2.4
3	2D	125	ILE	2.4
3	2D	174	ILE	2.4
5	2F	206	ILE	2.4
7	1H	113	VAL	2.4
7	1H	148	ILE	2.4
8	1I	71	ILE	2.4
12	2Q	1	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	79	G	2.4
32	1a	216	G	2.4
32	1a	485	G	2.4
32	1a	998	G	2.4
32	1a	1020	U	2.4
12	2Q	132	VAL	2.4
16	2U	105	VAL	2.4
18	2W	95	ILE	2.4
21	1Z	124	ILE	2.4
33	1b	28	PHE	2.4
34	1c	141	VAL	2.4
35	2d	33	MET	2.4
35	2d	165	MET	2.4
36	1e	6	PHE	2.4
36	2e	136	MET	2.4
37	2f	89	MET	2.4
44	1m	25	ILE	2.4
44	2m	98	VAL	2.4
46	2o	59	MET	2.4
48	1q	19	VAL	2.4
48	1q	23	VAL	2.4
48	1q	56	VAL	2.4
48	2q	85	VAL	2.4
50	2s	9	VAL	2.4
51	2t	100	ILE	2.4
5	2F	156	LEU	2.4
6	2G	19	LEU	2.4
8	1I	47	LEU	2.4
13	2R	44	LEU	2.4
14	2S	58	LEU	2.4
24	22	64	LEU	2.4
33	1b	215	LEU	2.4
33	1b	221	LEU	2.4
35	1d	202	LEU	2.4
36	2e	112	LEU	2.4
51	2t	91	LEU	2.4
7	2H	111	HIS	2.4
22	20	82	ARG	2.4
24	22	55	ARG	2.4
33	2b	209	ARG	2.4
36	2e	126	ARG	2.4
38	2g	6	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	1o	64	ARG	2.4
46	2o	17	ARG	2.4
46	2o	54	ARG	2.4
50	2s	14	HIS	2.4
9	2N	8	GLN	2.4
12	2Q	113	GLN	2.4
32	1a	479	C	2.4
32	2a	225	C	2.4
36	1e	20	GLN	2.4
54	2w	67	C	2.4
57	1y	74	C	2.4
5	2F	56	GLU	2.4
35	1d	163	GLU	2.4
35	2d	163	GLU	2.4
48	2q	86	GLU	2.4
28	26	39	TYR	2.3
36	1e	61	TYR	2.3
46	1o	21	ASP	2.3
50	2s	52	TYR	2.3
1	2A	652(B)	A	2.3
32	1a	149	A	2.3
32	1a	228	A	2.3
32	2a	872	A	2.3
32	2a	1151	A	2.3
32	2a	1324	A	2.3
21	1Z	95	PRO	2.3
34	1c	174	PRO	2.3
35	2d	136	PRO	2.3
38	1g	58	PRO	2.3
43	2l	45	PRO	2.3
6	2G	73	ALA	2.3
7	2H	85	LYS	2.3
11	1P	44	GLY	2.3
11	2P	22	GLY	2.3
14	2S	76	LYS	2.3
17	2V	42	GLY	2.3
17	2V	65	GLY	2.3
11	1P	120	ALA	2.3
20	1Y	36	ALA	2.3
33	1b	8	LYS	2.3
34	1c	92	ALA	2.3
35	1d	151	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2k	15	ALA	2.3
44	2m	31	LYS	2.3
51	2t	103	GLY	2.3
38	2g	39	ALA	2.3
9	2N	63	THR	2.3
40	2i	27	THR	2.3
1	1A	405	U	2.3
1	1A	1101	U	2.3
1	2A	272(A)	U	2.3
1	2A	2897	U	2.3
38	2g	89	MET	2.3
48	1q	15	MET	2.3
1	2A	652(U)	G	2.3
3	2D	34	VAL	2.3
5	1F	132	VAL	2.3
5	1F	157	VAL	2.3
5	2F	163	VAL	2.3
5	2F	193	VAL	2.3
6	2G	140	ILE	2.3
6	2G	178	PHE	2.3
7	2H	11	VAL	2.3
8	1I	97	ILE	2.3
8	1I	107	VAL	2.3
8	1I	145	VAL	2.3
8	2I	120	ILE	2.3
14	2S	85	VAL	2.3
17	2V	51	VAL	2.3
21	2Z	100	VAL	2.3
22	20	45	PHE	2.3
32	1a	70	G	2.3
32	1a	392	G	2.3
32	1a	493	G	2.3
32	2a	1156	G	2.3
33	1b	174	VAL	2.3
33	2b	32	ILE	2.3
35	1d	67	ILE	2.3
35	1d	104	VAL	2.3
37	2f	90	VAL	2.3
40	1i	28	VAL	2.3
40	1i	77	ILE	2.3
40	1i	86	VAL	2.3
41	2j	50	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	2r	70	ILE	2.3
7	1H	101	ARG	2.3
11	1P	77	ARG	2.3
14	2S	9	ARG	2.3
33	1b	30	ARG	2.3
39	2h	18	ARG	2.3
41	1j	29	ARG	2.3
41	2j	43	ARG	2.3
46	2o	68	ARG	2.3
50	2s	57	HIS	2.3
5	1F	192	LEU	2.3
5	2F	33	LEU	2.3
21	2Z	163	LEU	2.3
33	1b	180	LEU	2.3
34	1c	136	GLN	2.3
36	1e	12	LEU	2.3
38	1g	16	LEU	2.3
35	1d	72	GLU	2.3
35	2d	156	GLU	2.3
39	2h	70	GLN	2.3
44	2m	19	LEU	2.3
45	1n	47	LEU	2.3
43	2l	65	GLU	2.3
46	1o	28	GLN	2.3
51	1t	20	LEU	2.3
51	2t	20	LEU	2.3
21	1Z	168	GLU	2.3
33	1b	52	GLU	2.3
40	2i	12	GLU	2.3
32	1a	163	C	2.3
32	2a	224	C	2.3
38	2g	37	ASN	2.3
41	2j	76	ASN	2.3
1	1A	2134	A	2.3
4	1E	98	PRO	2.3
6	1G	55	LYS	2.3
7	2H	118	PRO	2.3
8	2I	134	PRO	2.3
9	2N	44	PRO	2.3
32	1a	162	A	2.3
32	1a	622	A	2.3
32	2a	1005	A	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	114	PRO	2.3
35	1d	20	TYR	2.3
40	1i	4	TYR	2.3
40	1i	36	TYR	2.3
3	2D	170	GLY	2.3
6	1G	129	GLY	2.3
7	1H	108	GLY	2.3
11	2P	116	GLY	2.3
17	2V	101	GLY	2.3
21	1Z	147	GLY	2.3
47	2p	30	GLY	2.3
3	2D	77	ALA	2.3
6	1G	56	ALA	2.3
16	2U	42	ALA	2.3
19	1X	91	ALA	2.3
33	2b	188	ALA	2.3
34	2c	61	ALA	2.3
35	1d	32	ALA	2.3
36	2e	134	ALA	2.3
36	2e	138	ALA	2.3
37	2f	99	ALA	2.3
38	1g	65	ALA	2.3
39	1h	124	ALA	2.3
40	1i	52	ALA	2.3
49	1r	20	ALA	2.3
49	1r	60	ALA	2.3
7	2H	68	THR	2.3
8	1I	86	THR	2.3
47	2p	45	THR	2.3
50	1s	48	THR	2.3
1	1A	12	U	2.3
17	2V	56	SER	2.3
32	2a	863	U	2.3
35	1d	91	SER	2.3
42	2k	101	SER	2.3
54	2w	45	U	2.3
6	2G	128	ARG	2.3
6	2G	181	ARG	2.3
21	2Z	131	ARG	2.3
33	2b	137	ARG	2.3
34	2c	132	ARG	2.3
6	1G	140	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	2V	96	ILE	2.3
33	1b	32	ILE	2.3
35	2d	67	ILE	2.3
46	1o	12	ILE	2.3
43	1l	11	VAL	2.3
44	1m	17	VAL	2.3
46	1o	11	VAL	2.3
46	2o	46	HIS	2.3
47	2p	36	ILE	2.3
7	2H	104	GLU	2.3
11	1P	101	VAL	2.3
13	2R	117	VAL	2.3
15	1T	34	VAL	2.3
15	2T	101	PHE	2.3
20	2Y	7	VAL	2.3
21	2Z	168	GLU	2.3
26	14	35	VAL	2.3
36	2e	82	VAL	2.3
38	2g	87	VAL	2.3
39	2h	123	GLU	2.3
47	1p	2	VAL	2.3
48	2q	5	VAL	2.3
49	2r	43	PHE	2.3
1	2A	10	G	2.3
3	1D	37	LEU	2.3
5	2F	101	LEU	2.3
5	2F	148	LEU	2.3
5	2F	192	LEU	2.3
13	1R	54	LEU	2.3
14	2S	110	LEU	2.3
16	2U	109	LEU	2.3
26	14	36	CYS	2.3
32	1a	66	G	2.3
32	1a	200	G	2.3
32	2a	1385	G	2.3
35	1d	64	LEU	2.3
39	1h	135	CYS	2.3
44	2m	96	LEU	2.3
45	1n	6	LEU	2.3
45	1n	43	CYS	2.3
45	2n	24	CYS	2.3
48	1q	53	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	2r	26	LEU	2.3
50	2s	5	LEU	2.3
57	2y	63	G	2.3
21	2Z	75	ASN	2.3
24	12	15	LYS	2.3
32	2a	1029	C	2.3
34	1c	181	ASN	2.3
35	1d	22	LYS	2.3
46	1o	48	LYS	2.3
49	2r	49	LYS	2.3
57	2y	40	C	2.3
3	2D	178	PRO	2.3
8	1I	137	PRO	2.3
36	2e	106	PRO	2.3
39	2h	72	PRO	2.3
45	1n	54	PRO	2.3
4	2E	10	GLY	2.3
5	2F	142	TRP	2.3
6	2G	25	TYR	2.3
6	2G	100	TRP	2.3
11	1P	143	GLY	2.3
19	2X	24	GLY	2.3
32	2a	532	A	2.3
32	2a	996	A	2.3
28	26	42	TRP	2.3
30	18	64	TYR	2.3
40	1i	72	GLY	2.3
42	1k	90	GLY	2.3
50	1s	54	GLY	2.3
50	2s	61	TYR	2.3
51	2t	101	GLY	2.3
6	2G	50	ALA	2.3
8	1I	53	ALA	2.3
14	1S	37	ALA	2.3
21	2Z	7	ALA	2.3
26	24	1	MET	2.3
36	1e	95	ALA	2.3
44	1m	5	ALA	2.3
47	1p	7	ALA	2.3
47	2p	56	ALA	2.3
8	2I	76	THR	2.3
12	2Q	110	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	63	THR	2.3
52	2u	8	THR	2.3
6	2G	113	ARG	2.3
14	2S	53	SER	2.3
19	1X	68	ARG	2.3
20	2Y	17	SER	2.3
23	2I	26	ARG	2.3
23	2I	86	SER	2.3
35	1d	137	SER	2.3
39	2h	113	SER	2.3
41	2j	59	SER	2.3
42	2k	44	SER	2.3
50	1s	38	SER	2.3
51	1t	80	ARG	2.3
17	2V	64	HIS	2.3
39	2h	81	HIS	2.3
4	2E	73	GLU	2.3
6	2G	48	GLU	2.3
21	2Z	50	GLN	2.3
33	2b	76	GLN	2.3
36	2e	149	GLU	2.3
41	2j	33	GLN	2.3
8	1I	4	ILE	2.3
21	2Z	57	ILE	2.3
31	29	10	ILE	2.3
33	2b	127	ILE	2.3
51	2t	33	ILE	2.3
3	2D	269	PHE	2.3
5	2F	114	VAL	2.3
8	2I	142	VAL	2.3
14	2S	12	PHE	2.3
33	2b	197	VAL	2.3
34	1c	198	VAL	2.3
36	1e	26	PHE	2.3
48	2q	19	VAL	2.3
48	2q	77	VAL	2.3
5	2F	12	LEU	2.3
6	2G	133	LEU	2.3
1	2A	1039	G	2.3
1	2A	2206	G	2.3
8	2I	2	LYS	2.3
21	1Z	155	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	42	LEU	2.3
35	2d	22	LYS	2.3
36	1e	43	LEU	2.3
36	1e	119	LEU	2.3
38	1g	36	LYS	2.3
45	2n	50	LYS	2.3
47	1p	3	LYS	2.3
48	1q	89	LEU	2.3
48	2q	84	LEU	2.3
51	1t	53	LEU	2.3
54	2w	19	G	2.3
57	2y	44	G	2.3
34	2c	181	ASN	2.3
39	1h	54	ASP	2.3
41	2j	69	ASN	2.3
42	1k	36	ASP	2.3
32	1a	153	C	2.3
6	2G	32	PRO	2.3
9	2N	111	PRO	2.3
35	2d	39	PRO	2.3
43	1l	31	PRO	2.3
16	2U	73	GLY	2.3
21	2Z	64	GLY	2.3
32	2a	978	A	2.3
32	2a	1248	A	2.3
40	1i	6	GLY	2.3
42	2k	118	GLY	2.3
44	1m	119	GLY	2.3
49	2r	77	GLY	2.3
50	1s	84	GLY	2.3
51	1t	101	GLY	2.3
57	2y	58	A	2.3
7	1H	3	ARG	2.3
7	2H	102	ALA	2.3
8	1I	26	ALA	2.3
9	2N	13	TRP	2.3
21	2Z	19	ARG	2.3
25	13	55	ARG	2.3
29	17	23	ARG	2.3
33	1b	130	ARG	2.3
34	2c	140	ARG	2.3
35	2d	73	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	1i	62	TYR	2.3
47	2p	17	TYR	2.3
48	2q	42	TYR	2.3
48	2q	51	TYR	2.3
48	2q	75	ARG	2.3
49	2r	34	TYR	2.3
36	1e	48	ALA	2.3
37	1f	29	ALA	2.3
42	2k	61	ALA	2.3
50	2s	3	ARG	2.3
1	2A	2098	U	2.3
6	2G	161	THR	2.3
7	1H	122	THR	2.3
32	1a	626	U	2.3
32	2a	950	U	2.3
7	2H	63	SER	2.3
11	2P	35	HIS	2.3
35	2d	125	HIS	2.3
42	2k	116	HIS	2.3
43	2l	22	SER	2.3
41	1j	83	GLU	2.3
51	2t	16	HIS	2.3
6	2G	138	GLN	2.3
11	2P	68	GLN	2.3
12	2Q	141	GLN	2.3
26	24	47	GLN	2.3
42	2k	13	GLN	2.3
3	1D	275	LYS	2.3
3	2D	271	ILE	2.3
8	1I	138	ILE	2.3
21	1Z	133	ILE	2.3
42	2k	48	ILE	2.3
4	2E	21	VAL	2.3
4	2E	196	VAL	2.3
5	1F	162	LEU	2.2
5	2F	105	VAL	2.3
6	1G	149	VAL	2.3
6	1G	176	LEU	2.2
6	2G	5	VAL	2.3
6	2G	107	LEU	2.2
8	1I	44	LEU	2.2
8	2I	21	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	2I	123	LEU	2.2
9	2N	23	LEU	2.2
9	2N	52	VAL	2.3
9	2N	138	LEU	2.2
11	2P	112	LEU	2.2
14	2S	14	VAL	2.3
14	2S	32	LEU	2.2
15	2T	99	LEU	2.2
17	2V	38	LEU	2.2
23	1I	51	VAL	2.3
31	29	7	VAL	2.3
34	1c	178	LEU	2.2
34	2c	153	VAL	2.3
35	1d	101	LEU	2.2
35	1d	128	VAL	2.3
35	1d	186	LEU	2.2
37	1f	60	PHE	2.2
38	1g	69	VAL	2.3
39	1h	93	VAL	2.3
42	2k	109	VAL	2.3
44	2m	56	LEU	2.2
44	2m	74	VAL	2.3
47	2p	20	VAL	2.3
47	2p	62	VAL	2.3
48	1q	9	VAL	2.3
50	1s	19	VAL	2.3
1	1A	171	G	2.2
1	1A	2792	G	2.2
3	1D	203	ASN	2.2
6	1G	123	ASN	2.2
8	1I	20	ASP	2.2
32	1a	69	G	2.2
32	1a	138	G	2.2
32	1a	148	G	2.2
32	1a	406	G	2.2
32	1a	481	G	2.2
32	2a	1009	G	2.2
32	2a	1353	G	2.2
34	2c	56	ASP	2.2
34	2c	102	ASN	2.2
35	2d	134	ASP	2.2
41	1j	78	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2k	26	ASN	2.2
43	2l	112	ASP	2.2
1	1A	2804	C	2.2
3	2D	137	PRO	2.2
11	1P	145	PRO	2.2
32	1a	174	C	2.2
32	2a	443	C	2.2
32	2a	1066	C	2.2
32	2a	1260	C	2.2
47	2p	41	PRO	2.2
54	1w	67	C	2.2
57	1y	49	C	2.2
3	2D	47	GLY	2.2
6	2G	155	MET	2.2
7	2H	28	GLY	2.2
8	1I	106	GLY	2.2
11	2P	82	GLY	2.2
16	2U	82	GLY	2.2
23	2I	61	ARG	2.2
33	1b	209	ARG	2.2
33	2b	53	ARG	2.2
34	2c	9	GLY	2.2
35	1d	33	MET	2.2
35	1d	41	GLY	2.2
35	2d	10	ARG	2.2
36	1e	15	ARG	2.2
37	1f	89	MET	2.2
40	2i	115	GLY	2.2
41	1j	52	GLY	2.2
44	2m	29	ARG	2.2
45	2n	19	ARG	2.2
47	1p	30	GLY	2.2
50	2s	72	GLY	2.2
1	1A	899	A	2.2
1	1A	2126	A	2.2
32	1a	160	A	2.2
32	2a	1016	A	2.2
57	2y	23	A	2.2
57	2y	38	A	2.2
3	2D	81	ALA	2.2
4	1E	68	ALA	2.2
6	2G	163	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2D	259	THR	2.2
8	2I	126	TYR	2.2
15	2T	100	TYR	2.2
19	2X	22	ALA	2.2
24	22	12	GLU	2.2
26	24	25	TYR	2.2
26	24	52	THR	2.2
33	1b	148	TYR	2.2
33	2b	113	HIS	2.2
37	2f	53	ALA	2.2
39	2h	99	GLU	2.2
40	1i	76	ALA	2.2
41	1j	18	ALA	2.2
43	2l	68	ALA	2.2
44	1m	59	TYR	2.2
45	1n	20	ALA	2.2
45	1n	30	ALA	2.2
48	2q	88	TYR	2.2
51	2t	78	ALA	2.2
52	1u	21	TYR	2.2
54	1w	20	U	2.2
14	2S	27	SER	2.2
26	24	26	SER	2.2
33	1b	124	SER	2.2
33	2b	95	GLN	2.2
38	1g	77	SER	2.2
45	2n	32	SER	2.2
46	2o	40	SER	2.2
11	2P	137	LYS	2.2
19	2X	2	LYS	2.2
34	2c	4	LYS	2.2
36	2e	121	LYS	2.2
38	2g	29	LYS	2.2
41	2j	80	LYS	2.2
6	1G	88	ILE	2.2
6	2G	88	ILE	2.2
14	2S	18	ILE	2.2
28	16	54	ILE	2.2
40	1i	81	ILE	2.2
42	1k	29	ILE	2.2
50	2s	40	ILE	2.2
3	1D	98	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	1E	23	VAL	2.2
5	2F	11	VAL	2.2
5	2F	20	LEU	2.2
9	2N	26	LEU	2.2
9	2N	112	LEU	2.2
10	2O	98	VAL	2.2
10	2O	102	VAL	2.2
17	2V	25	LEU	2.2
17	2V	57	VAL	2.2
23	11	80	LEU	2.2
24	22	16	LEU	2.2
24	22	24	LEU	2.2
27	15	60	VAL	2.2
27	25	58	LEU	2.2
34	1c	195	VAL	2.2
35	2d	96	LEU	2.2
35	2d	170	VAL	2.2
35	2d	174	LEU	2.2
37	2f	61	LEU	2.2
46	2o	57	LEU	2.2
50	1s	16	LEU	2.2
38	1g	26	PHE	2.2
50	1s	45	VAL	2.2
31	29	12	ASP	2.2
36	2e	73	ASN	2.2
41	2j	89	ASP	2.2
42	1k	117	ASN	2.2
1	1A	1071	G	2.2
1	1A	2793	G	2.2
1	2A	271(I)	G	2.2
4	1E	1	MET	2.2
8	2I	57	ARG	2.2
8	2I	80	PRO	2.2
11	2P	90	ARG	2.2
32	1a	1138	G	2.2
32	2a	1003	G	2.2
32	2a	1370	G	2.2
15	1T	1	MET	2.2
20	2Y	97	ARG	2.2
21	1Z	122	ARG	2.2
21	2Z	62	PRO	2.2
25	23	55	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	1d	37	PRO	2.2
35	1d	40	PRO	2.2
36	2e	152	ARG	2.2
37	2f	2	ARG	2.2
38	1g	78	ARG	2.2
41	1j	46	ARG	2.2
46	2o	38	ARG	2.2
47	1p	28	ARG	2.2
54	1w	15	G	2.2
57	2y	52	G	2.2
1	2A	876	C	2.2
4	1E	88	GLY	2.2
12	2Q	61	GLY	2.2
23	2I	22	GLY	2.2
32	1a	72	C	2.2
32	1a	217	C	2.2
32	2a	1007	C	2.2
32	2a	1363	C	2.2
33	1b	227	GLY	2.2
34	1c	148	GLY	2.2
36	1e	29	GLY	2.2
38	1g	133	GLY	2.2
39	2h	71	GLY	2.2
40	1i	115	GLY	2.2
42	1k	102	GLY	2.2
57	1y	4	C	2.2
57	1y	68	C	2.2
7	2H	32	GLU	2.2
7	2H	124	GLU	2.2
21	2Z	2	GLU	2.2
21	2Z	162	GLU	2.2
26	24	53	GLU	2.2
32	2a	1123	A	2.2
34	1c	122	GLU	2.2
38	2g	8	GLU	2.2
43	1l	16	GLU	2.2
48	2q	45	HIS	2.2
57	1y	23	A	2.2
3	2D	275	LYS	2.2
4	2E	70	ALA	2.2
8	2I	118	LYS	2.2
21	2Z	73	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	202	U	2.2
32	2a	1126	U	2.2
35	1d	82	ALA	2.2
35	1d	117	ALA	2.2
35	2d	82	ALA	2.2
40	1i	43	ALA	2.2
40	2i	55	ALA	2.2
46	2o	8	LYS	2.2
46	2o	10	LYS	2.2
49	2r	71	LYS	2.2
7	2H	70	THR	2.2
8	1I	40	THR	2.2
8	2I	78	THR	2.2
24	22	62	THR	2.2
25	13	40	THR	2.2
43	1l	61	THR	2.2
26	14	66	SER	2.2
43	1l	105	TYR	2.2
45	1n	34	TYR	2.2
3	2D	204	ILE	2.2
7	2H	151	ILE	2.2
15	2T	83	ILE	2.2
16	2U	62	ILE	2.2
26	14	22	ILE	2.2
33	1b	214	ILE	2.2
36	1e	76	ILE	2.2
39	1h	6	ILE	2.2
40	2i	77	ILE	2.2
45	1n	7	ILE	2.2
51	1t	63	ILE	2.2
5	2F	125	LEU	2.2
6	2G	175	LEU	2.2
11	1P	99	LEU	2.2
11	1P	138	LEU	2.2
12	2Q	118	LEU	2.2
13	2R	20	LEU	2.2
13	2R	60	LEU	2.2
14	1S	24	LEU	2.2
24	22	53	LEU	2.2
34	2c	94	LEU	2.2
37	2f	10	LEU	2.2
38	1g	22	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	2o	81	LEU	2.2
3	2D	79	VAL	2.2
3	2D	145	VAL	2.2
5	2F	126	VAL	2.2
21	1Z	161	VAL	2.2
28	26	5	VAL	2.2
34	1c	130	VAL	2.2
35	1d	148	VAL	2.2
19	2X	21	PHE	2.2
45	1n	37	PHE	2.2
4	2E	58	ARG	2.2
11	2P	15	ARG	2.2
26	14	20	ASN	2.2
28	26	32	ASN	2.2
31	29	19	ARG	2.2
34	1c	126	ARG	2.2
35	2d	35	ARG	2.2
38	2g	94	ARG	2.2
39	2h	102	ARG	2.2
40	2i	128	ARG	2.2
44	1m	99	ARG	2.2
48	1q	75	ARG	2.2
4	2E	177	PRO	2.2
7	2H	112	PRO	2.2
8	2I	8	PRO	2.2
18	2W	14	PRO	2.2
26	24	7	PRO	2.2
36	1e	128	PRO	2.2
37	2f	12	PRO	2.2
40	2i	123	PRO	2.2
50	1s	76	PRO	2.2
51	1t	98	PRO	2.2
1	2A	2187	G	2.2
4	2E	50	GLY	2.2
6	1G	42	GLY	2.2
20	2Y	22	GLY	2.2
26	14	4	GLY	2.2
32	2a	853	G	2.2
34	2c	159	GLY	2.2
35	1d	180	GLY	2.2
35	2d	90	GLY	2.2
35	2d	95	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	19	GLY	2.2
39	2h	55	GLY	2.2
40	2i	30	GLY	2.2
44	1m	24	GLY	2.2
54	2w	34	G	2.2
32	2a	596	C	2.2
32	2a	849	C	2.2
36	2e	83	GLU	2.2
48	2q	96	GLU	2.2
5	2F	8	GLN	2.2
9	2N	69	GLN	2.2
33	2b	74	LYS	2.2
51	2t	30	LYS	2.2
57	2y	3	C	2.2
42	1k	78	GLN	2.2
42	2k	93	GLN	2.2
1	1A	1460	A	2.2
1	2A	229	A	2.2
1	2A	1460	A	2.2
32	1a	495	A	2.2
32	2a	1152	A	2.2
32	2a	1180	A	2.2
32	2a	1372	U	2.2
4	2E	162	ALA	2.2
6	2G	61	ALA	2.2
8	1I	55	ALA	2.2
8	2I	46	ALA	2.2
22	20	61	ALA	2.2
34	1c	113	ALA	2.2
37	2f	29	ALA	2.2
42	1k	28	THR	2.2
51	1t	67	ALA	2.2
33	2b	192	SER	2.2
33	2b	235	SER	2.2
8	1I	89	TYR	2.2
39	2h	65	TYR	2.2
47	2p	39	TYR	2.2
48	1q	51	TYR	2.2
30	28	34	TRP	2.2
7	1H	92	ILE	2.2
15	2T	88	ILE	2.2
30	28	58	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2D	263	ARG	2.2
7	1H	23	ARG	2.2
21	1Z	103	ARG	2.2
33	1b	51	LEU	2.2
34	2c	131	ARG	2.2
34	2c	175	LEU	2.2
39	1h	86	ILE	2.2
38	1g	3	ARG	2.2
38	2g	32	ARG	2.2
39	2h	85	ARG	2.2
41	1j	71	LEU	2.2
48	2q	36	ILE	2.2
43	2l	59	ARG	2.2
46	2o	64	ARG	2.2
51	2t	72	LEU	2.2
52	1u	10	ARG	2.2
4	1E	172	VAL	2.2
5	1F	187	VAL	2.2
6	2G	125	PHE	2.2
8	2I	110	ASP	2.2
18	2W	20	VAL	2.2
20	2Y	98	VAL	2.2
21	2Z	90	VAL	2.2
22	20	23	VAL	2.2
23	21	62	VAL	2.2
33	1b	71	VAL	2.2
33	2b	164	VAL	2.2
33	2b	189	ASP	2.2
34	1c	138	VAL	2.2
35	1d	170	VAL	2.2
39	2h	51	VAL	2.2
35	2d	110	PHE	2.2
40	1i	23	ASN	2.2
41	2j	73	ASP	2.2
41	2j	94	VAL	2.2
42	2k	27	ASN	2.2
44	2m	17	VAL	2.2
44	2m	62	ASN	2.2
48	1q	82	MET	2.2
48	2q	94	ASN	2.2
51	1t	88	VAL	2.2
39	2h	67	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	21	PRO	2.2
47	2p	15	PRO	2.2
3	2D	4	LYS	2.2
6	1G	137	GLU	2.2
6	2G	54	GLU	2.2
34	2c	82	GLU	2.2
44	1m	31	LYS	2.2
47	2p	50	LYS	2.2
5	2F	131	GLY	2.2
11	2P	93	GLY	2.2
14	1S	104	GLY	2.2
17	2V	48	GLY	2.2
33	2b	224	GLN	2.2
34	1c	31	HIS	2.2
35	1d	119	GLN	2.2
41	2j	56	HIS	2.2
44	1m	38	GLY	2.2
46	2o	71	GLN	2.2
1	2A	1169	G	2.2
1	2A	1584	C	2.2
1	2A	2099	U	2.2
1	2A	2792	G	2.2
2	2B	109	C	2.2
32	1a	1132	C	2.2
32	2a	217	C	2.2
32	2a	560	U	2.2
32	2a	1028	C	2.2
32	2a	1062	U	2.2
55	1x	1	C	2.2
55	1x	67	C	2.2
55	2x	1	C	2.2
57	1y	33	U	2.2
57	1y	60	U	2.2
57	1y	62	C	2.2
57	2y	11	C	2.2
57	2y	50	U	2.2
1	1A	900	A	2.2
1	2A	1508	A	2.2
32	2a	1275	A	2.2
3	2D	191	ALA	2.2
5	2F	22	ALA	2.2
5	2F	42	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	1I	102	SER	2.2
10	1O	30	ALA	2.2
14	1S	51	ALA	2.2
18	2W	93	ALA	2.2
20	1Y	65	ALA	2.2
26	24	37	SER	2.2
33	1b	123	ALA	2.2
34	1c	15	THR	2.2
34	1c	192	THR	2.2
36	1e	17	ALA	2.2
40	1i	27	THR	2.2
42	2k	57	THR	2.2
50	2s	4	SER	2.2
50	2s	24	ALA	2.2
51	2t	71	THR	2.2
14	2S	13	ARG	2.1
25	23	3	ARG	2.1
26	24	13	ARG	2.1
31	29	4	ARG	2.1
34	2c	11	ARG	2.1
35	1d	122	ARG	2.1
35	1d	187	ARG	2.1
35	2d	13	ARG	2.1
36	1e	27	ARG	2.1
40	1i	9	ARG	2.1
40	1i	114	TYR	2.1
43	2l	12	ARG	2.1
47	1p	42	ARG	2.1
3	1D	75	ILE	2.1
6	2G	62	LEU	2.1
6	2G	103	LEU	2.1
8	1I	51	ILE	2.1
8	1I	140	LEU	2.1
14	2S	82	ILE	2.1
20	2Y	61	ILE	2.1
20	2Y	96	ILE	2.1
26	24	9	LEU	2.1
33	1b	158	LEU	2.1
33	2b	58	ILE	2.1
34	2c	91	LEU	2.1
35	1d	174	LEU	2.1
36	1e	11	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	43	LEU	2.1
39	1h	83	ILE	2.1
40	1i	99	LEU	2.1
42	2k	108	ILE	2.1
43	1l	100	ILE	2.1
46	2o	39	LEU	2.1
6	2G	108	ASN	2.1
7	2H	74	ASN	2.1
8	1I	92	VAL	2.1
8	2I	81	VAL	2.1
9	2N	103	VAL	2.1
15	2T	63	VAL	2.1
17	2V	46	VAL	2.1
19	2X	7	VAL	2.1
21	2Z	165	VAL	2.1
26	24	10	VAL	2.1
26	24	35	VAL	2.1
33	1b	112	VAL	2.1
40	1i	109	VAL	2.1
43	2l	104	VAL	2.1
44	1m	7	VAL	2.1
45	2n	33	VAL	2.1
47	1p	40	ASP	2.1
49	1r	86	VAL	2.1
3	2D	28	GLU	2.1
4	2E	96	PHE	2.1
7	2H	12	PRO	2.1
7	2H	34	GLU	2.1
11	2P	64	LYS	2.1
14	2S	59	LYS	2.1
21	1Z	46	LYS	2.1
23	21	48	LYS	2.1
35	1d	185	PHE	2.1
35	2d	46	LYS	2.1
35	2d	145	GLU	2.1
40	1i	25	LYS	2.1
37	2f	51	PRO	2.1
39	1h	31	PHE	2.1
39	1h	116	LYS	2.1
36	1e	77	PRO	2.1
40	1i	37	PHE	2.1
44	2m	50	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	1q	40	LYS	2.1
9	2N	86	PRO	2.1
10	1O	48	PRO	2.1
33	1b	183	PRO	2.1
48	2q	27	PHE	2.1
22	20	17	GLN	2.1
50	1s	14	HIS	2.1
5	2F	47	GLY	2.1
7	2H	5	GLY	2.1
12	2Q	24	GLY	2.1
33	1b	151	GLY	2.1
34	1c	197	GLY	2.1
39	1h	128	GLY	2.1
40	1i	22	GLY	2.1
41	1j	93	GLY	2.1
52	1u	19	GLY	2.1
1	2A	2895	U	2.1
32	1a	229	U	2.1
32	2a	1065	U	2.1
57	1y	12	U	2.1
1	2A	1181	C	2.1
2	2B	88	C	2.1
20	2Y	102	CYS	2.1
32	1a	199	G	2.1
32	1a	306	G	2.1
32	1a	401	C	2.1
32	1a	618	C	2.1
32	2a	436	C	2.1
32	2a	457	C	2.1
32	2a	612	C	2.1
32	2a	664	G	2.1
32	2a	1057	G	2.1
32	2a	1253	G	2.1
32	2a	1276	G	2.1
32	2a	1356	G	2.1
57	1y	6	G	2.1
57	1y	44	G	2.1
57	2y	13	C	2.1
57	2y	41	C	2.1
1	2A	529	A	2.1
32	2a	1130	A	2.1
32	2a	1179	A	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1280	A	2.1
32	2a	1287	A	2.1
3	2D	19	ALA	2.1
6	2G	165	THR	2.1
13	2R	112	ALA	2.1
23	2I	34	THR	2.1
33	1b	186	ALA	2.1
35	2d	32	ALA	2.1
42	1k	65	ALA	2.1
42	1k	79	SER	2.1
44	2m	49	THR	2.1
46	1o	30	ALA	2.1
50	1s	35	SER	2.1
50	2s	75	ALA	2.1
51	1t	77	ALA	2.1
51	2t	67	ALA	2.1
9	2N	134	ARG	2.1
19	2X	65	ARG	2.1
34	1c	132	ARG	2.1
40	2i	42	ARG	2.1
41	2j	51	ARG	2.1
42	2k	18	ARG	2.1
47	1p	8	ARG	2.1
47	1p	72	ARG	2.1
49	2r	53	ARG	2.1
7	2H	94	TYR	2.1
12	2Q	32	TYR	2.1
16	2U	47	TYR	2.1
19	2X	5	TYR	2.1
20	1Y	20	TYR	2.1
26	24	43	TYR	2.1
39	1h	65	TYR	2.1
33	2b	179	LYS	2.1
34	1c	101	LEU	2.1
36	2e	91	LEU	2.1
37	1f	81	ILE	2.1
38	1g	124	LEU	2.1
38	1g	144	MET	2.1
43	2l	120	TYR	2.1
3	2D	261	LYS	2.1
4	2E	181	LEU	2.1
5	1F	123	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	60	LEU	2.1
8	1I	45	LYS	2.1
13	2R	54	LEU	2.1
14	2S	40	ILE	2.1
21	1Z	157	LEU	2.1
22	20	75	LEU	2.1
23	11	58	ILE	2.1
33	1b	108	ILE	2.1
38	2g	30	ILE	2.1
38	2g	42	ILE	2.1
38	2g	137	LYS	2.1
39	1h	119	LEU	2.1
39	2h	119	LEU	2.1
47	2p	1	MET	2.1
43	1l	46	LYS	2.1
44	1m	9	ILE	2.1
44	1m	96	LEU	2.1
50	1s	44	MET	2.1
50	1s	49	ILE	2.1
51	1t	85	MET	2.1
44	2m	65	LYS	2.1
49	2r	84	LYS	2.1
50	1s	6	LYS	2.1
52	2u	12	LYS	2.1
4	1E	180	ASN	2.1
7	1H	116	GLU	2.1
10	2O	73	ASP	2.1
21	2Z	93	ASP	2.1
34	1c	19	GLU	2.1
34	2c	19	GLU	2.1
35	1d	161	ASN	2.1
36	1e	5	ASP	2.1
39	2h	54	ASP	2.1
40	1i	60	ASP	2.1
46	2o	6	GLU	2.1
3	1D	34	VAL	2.1
4	1E	196	VAL	2.1
4	2E	59	VAL	2.1
4	2E	75	VAL	2.1
6	2G	159	VAL	2.1
7	1H	24	VAL	2.1
9	1N	13	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	2P	27	HIS	2.1
16	2U	49	HIS	2.1
17	2V	79	VAL	2.1
6	1G	80	PHE	2.1
12	2Q	69	PHE	2.1
14	2S	87	PHE	2.1
21	2Z	158	PRO	2.1
33	2b	219	VAL	2.1
34	2c	174	PRO	2.1
35	2d	178	VAL	2.1
36	2e	34	VAL	2.1
38	1g	87	VAL	2.1
39	1h	51	VAL	2.1
36	2e	56	GLN	2.1
38	1g	56	GLN	2.1
39	2h	27	PRO	2.1
50	1s	60	VAL	2.1
47	2p	9	PHE	2.1
49	2r	63	GLN	2.1
14	1S	81	GLY	2.1
17	2V	17	GLY	2.1
26	14	17	GLY	2.1
35	2d	6	GLY	2.1
35	2d	180	GLY	2.1
37	2f	58	GLY	2.1
38	2g	130	GLY	2.1
47	1p	10	GLY	2.1
48	1q	8	GLY	2.1
1	1A	2099	U	2.1
1	2A	12	U	2.1
54	1w	47	U	2.1
32	1a	201	C	2.1
32	1a	381	C	2.1
32	1a	454	C	2.1
32	1a	1149	C	2.1
32	2a	92	C	2.1
32	2a	1384	C	2.1
1	1A	275	G	2.1
1	1A	2629	A	2.1
1	2A	171	G	2.1
1	2A	2751	G	2.1
1	2A	2891	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	1E	76	ARG	2.1
5	1F	158	THR	2.1
9	2N	43	THR	2.1
21	2Z	81	ARG	2.1
34	2c	21	ARG	2.1
37	2f	3	ARG	2.1
38	2g	143	ARG	2.1
45	2n	40	CYS	2.1
26	14	27	THR	2.1
29	27	24	THR	2.1
32	1a	220	G	2.1
32	1a	380	G	2.1
32	2a	983	A	2.1
32	2a	987	G	2.1
32	2a	1184	G	2.1
32	2a	1190	G	2.1
52	2u	6	ARG	2.1
9	1N	27	ALA	2.1
11	2P	103	ALA	2.1
15	2T	97	ALA	2.1
33	1b	173	ALA	2.1
33	1b	233	SER	2.1
33	2b	218	ALA	2.1
35	1d	48	ALA	2.1
38	1g	25	ALA	2.1
38	1g	98	SER	2.1
57	1y	26	A	2.1
57	2y	27	G	2.1
57	2y	30	G	2.1
38	2g	145	ALA	2.1
39	2h	7	ALA	2.1
46	1o	16	ALA	2.1
51	2t	94	ALA	2.1
8	2I	69	LYS	2.1
21	2Z	1	MET	2.1
38	1g	31	MET	2.1
39	2h	98	LYS	2.1
51	2t	34	LYS	2.1
3	2D	24	ILE	2.1
4	1E	55	ASN	2.1
5	2F	9	ILE	2.1
6	1G	90	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	90	LEU	2.1
8	1I	6	LEU	2.1
15	1T	82	LEU	2.1
21	1Z	24	LEU	2.1
21	2Z	61	LEU	2.1
33	2b	143	GLU	2.1
33	2b	158	LEU	2.1
35	2d	194	LEU	2.1
36	1e	53	LEU	2.1
39	1h	36	LEU	2.1
39	2h	42	GLU	2.1
40	1i	79	LEU	2.1
49	2r	79	LEU	2.1
51	2t	53	LEU	2.1
9	2N	72	TYR	2.1
33	2b	220	ASP	2.1
34	2c	17	ASP	2.1
35	1d	190	ASP	2.1
36	2e	127	ASN	2.1
38	2g	45	ASP	2.1
42	2k	20	TYR	2.1
51	1t	64	ASP	2.1
3	2D	164	GLN	2.1
21	1Z	151	HIS	2.1
36	2e	78	HIS	2.1
40	1i	3	GLN	2.1
47	1p	13	HIS	2.1
48	2q	16	GLN	2.1
50	2s	83	HIS	2.1
3	2D	193	VAL	2.1
9	2N	126	PRO	2.1
10	2O	57	VAL	2.1
11	1P	95	VAL	2.1
11	2P	8	PRO	2.1
11	2P	146	VAL	2.1
21	2Z	83	PRO	2.1
22	20	79	VAL	2.1
27	25	57	VAL	2.1
30	28	23	VAL	2.1
33	1b	219	VAL	2.1
35	2d	17	VAL	2.1
36	1e	93	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	135	VAL	2.1
39	1h	61	VAL	2.1
39	1h	97	VAL	2.1
39	2h	53	VAL	2.1
39	2h	61	VAL	2.1
42	2k	82	VAL	2.1
48	1q	57	VAL	2.1
50	1s	11	VAL	2.1
12	1Q	58	PHE	2.1
15	1T	76	PHE	2.1
15	2T	76	PHE	2.1
48	1q	27	PHE	2.1
5	1F	207	GLY	2.1
7	1H	5	GLY	2.1
7	2H	48	GLY	2.1
21	2Z	143	GLY	2.1
34	2c	155	GLY	2.1
35	1d	109	GLY	2.1
38	2g	55	GLY	2.1
42	2k	56	GLY	2.1
43	2l	88	GLY	2.1
32	2a	1020	U	2.1
32	2a	1086	U	2.1
6	2G	21	ARG	2.1
7	2H	69	ARG	2.1
8	2I	61	ARG	2.1
28	26	50	ARG	2.1
31	29	9	ARG	2.1
34	1c	179	ARG	2.1
34	2c	40	ARG	2.1
35	2d	141	ARG	2.1
35	2d	209	ARG	2.1
36	2e	25	ARG	2.1
44	2m	71	ARG	2.1
1	1A	2177	C	2.1
1	2A	645	C	2.1
21	2Z	66	SER	2.1
30	28	19	SER	2.1
32	1a	67	C	2.1
32	2a	1114	C	2.1
32	2a	1129	C	2.1
35	2d	28	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	2d	113	SER	2.1
48	2q	62	SER	2.1
52	1u	17	THR	2.1
54	1w	68	C	2.1
57	1y	72	C	2.1
1	1A	1067	A	2.1
1	1A	1174	A	2.1
1	1A	1042	G	2.1
8	2I	63	ALA	2.1
14	2S	6	ALA	2.1
15	1T	127	ALA	2.1
16	2U	46	ALA	2.1
17	2V	19	LYS	2.1
21	2Z	46	LYS	2.1
23	2I	3	LYS	2.1
32	2a	663	A	2.1
32	2a	1041	A	2.1
32	2a	1191	A	2.1
32	1a	606	G	2.1
32	2a	588	G	2.1
32	2a	1222	G	2.1
33	2b	106	LYS	2.1
34	2c	180	ALA	2.1
38	1g	150	ALA	2.1
38	2g	7	ALA	2.1
40	1i	94	ALA	2.1
44	2m	107	ALA	2.1
48	2q	44	ALA	2.1
51	1t	76	ALA	2.1
51	2t	49	ALA	2.1
57	1y	9	A	2.1
54	1w	6	G	2.1
54	2w	44	G	2.1
57	2y	69	G	2.1
57	2y	71	G	2.1
11	1P	119	GLU	2.1
15	1T	128	GLU	2.1
33	2b	52	GLU	2.1
38	1g	90	GLU	2.1
39	1h	99	GLU	2.1
3	2D	111	LEU	2.1
6	2G	26	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	106	LEU	2.1
8	2I	72	LEU	2.1
12	2Q	123	HIS	2.1
14	1S	4	LEU	2.1
15	1T	6	LEU	2.1
16	2U	72	HIS	2.1
21	1Z	102	LEU	2.1
18	2W	60	ASN	2.1
21	1Z	63	ASP	2.1
21	2Z	140	ASP	2.1
31	29	20	HIS	2.1
33	1b	196	LEU	2.1
34	1c	69	HIS	2.1
35	1d	135	LEU	2.1
35	1d	157	LEU	2.1
36	2e	72	GLN	2.1
39	1h	59	LEU	2.1
40	2i	58	HIS	2.1
41	1j	40	LEU	2.1
12	2Q	64	ILE	2.1
33	1b	200	ILE	2.1
37	2f	52	ILE	2.1
37	2f	57	GLN	2.1
39	2h	38	ILE	2.1
40	2i	23	ASN	2.1
42	1k	13	GLN	2.1
42	2k	62	GLN	2.1
52	2u	5	ASP	2.1
5	2F	171	PRO	2.1
7	1H	118	PRO	2.1
10	2O	32	TYR	2.1
12	2Q	99	PRO	2.1
21	2Z	101	PRO	2.1
50	1s	80	TYR	2.1
6	2G	31	VAL	2.1
10	2O	10	VAL	2.1
17	2V	22	VAL	2.1
19	1X	54	VAL	2.1
19	2X	51	VAL	2.1
20	1Y	3	VAL	2.1
23	21	51	VAL	2.1
33	1b	165	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	70	VAL	2.1
37	2f	9	VAL	2.1
38	1g	141	VAL	2.1
43	1l	96	VAL	2.1
44	1m	54	VAL	2.1
3	2D	167	GLY	2.1
3	2D	197	GLY	2.1
5	2F	147	GLY	2.1
6	1G	117	PHE	2.1
11	2P	104	GLY	2.1
12	2Q	65	PHE	2.1
17	2V	75	PHE	2.1
20	1Y	59	GLY	2.1
33	1b	163	PHE	2.1
33	2b	181	PHE	2.1
34	1c	128	PHE	2.1
39	2h	106	GLY	2.1
50	2s	26	GLY	2.1
50	2s	82	GLY	2.1
1	2A	877	U	2.1
3	1D	70	TRP	2.1
14	2S	17	ARG	2.1
14	2S	30	ARG	2.1
15	1T	129	ARG	2.1
30	18	46	ARG	2.1
33	1b	217	ARG	2.1
35	2d	36	ARG	2.1
35	2d	132	ARG	2.1
36	2e	150	ARG	2.1
37	1f	46	ARG	2.1
38	2g	155	ARG	2.1
42	2k	54	ARG	2.1
43	2l	41	ARG	2.1
46	1o	65	ARG	2.1
46	2o	35	ARG	2.1
46	2o	79	ARG	2.1
47	2p	81	ARG	2.1
57	2y	51	U	2.1
3	2D	38	LYS	2.0
6	1G	182	LYS	2.0
39	2h	56	LYS	2.0
40	2i	118	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	1n	50	LYS	2.0
50	2s	7	LYS	2.0
7	2H	129	THR	2.0
8	1I	42	SER	2.0
12	2Q	129	THR	2.0
1	1A	1507	A	2.0
1	2A	2198	A	2.0
4	2E	114	ALA	2.0
5	1F	26	ALA	2.0
6	2G	59	GLU	2.0
6	2G	110	ALA	2.0
7	2H	156	ALA	2.0
9	1N	102	ALA	2.0
10	2O	112	MET	2.0
32	1a	40	C	2.0
32	1a	165	C	2.0
12	2Q	107	ALA	2.0
15	2T	116	ALA	2.0
16	2U	67	ALA	2.0
21	1Z	164	ALA	2.0
32	1a	373	A	2.0
32	2a	1147	C	2.0
32	2a	1161	C	2.0
32	2a	1208	C	2.0
34	1c	112	SER	2.0
35	1d	99	SER	2.0
40	1i	64	THR	2.0
57	1y	67	C	2.0
33	1b	12	GLU	2.0
33	2b	50	GLU	2.0
34	2c	161	GLU	2.0
36	2e	58	ALA	2.0
40	1i	122	ALA	2.0
43	2l	37	CYS	2.0
44	1m	72	ALA	2.0
1	1A	274	G	2.0
1	1A	1074	G	2.0
1	1A	2191	G	2.0
32	1a	77	G	2.0
32	1a	129(A)	G	2.0
32	1a	473	G	2.0
32	2a	874	G	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1072	G	2.0
32	2a	1124	G	2.0
32	2a	1160	G	2.0
32	2a	1224	G	2.0
33	2b	40	HIS	2.0
34	1c	118	GLN	2.0
48	1q	26	GLN	2.0
8	1I	74	ASN	2.0
14	2S	56	LEU	2.0
21	2Z	76	LEU	2.0
22	10	75	LEU	2.0
22	20	71	ASP	2.0
34	2c	98	ASN	2.0
35	1d	162	LEU	2.0
35	2d	144	ASP	2.0
39	1h	39	LEU	2.0
39	2h	4	ASP	2.0
40	2i	32	ASP	2.0
44	2m	81	LEU	2.0
46	1o	70	LEU	2.0
49	1r	58	LEU	2.0
50	1s	15	LEU	2.0
51	1t	99	LEU	2.0
51	2t	62	LEU	2.0
3	2D	82	ILE	2.0
39	2h	13	ILE	2.0
41	1j	50	ILE	2.0
48	1q	60	ILE	2.0
35	1d	197	PRO	2.0
19	1X	69	TYR	2.0
4	2E	72	VAL	2.0
4	2E	188	VAL	2.0
5	2F	165	ARG	2.0
6	1G	31	VAL	2.0
7	2H	42	ARG	2.0
7	2H	97	ARG	2.0
13	2R	68	ARG	2.0
14	2S	10	ARG	2.0
15	1T	70	VAL	2.0
20	2Y	30	VAL	2.0
22	20	67	VAL	2.0
26	24	48	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	164	VAL	2.0
33	2b	87	ARG	2.0
33	2b	130	ARG	2.0
33	2b	226	ARG	2.0
34	2c	59	ARG	2.0
35	1d	25	ARG	2.0
35	2d	148	VAL	2.0
37	2f	65	VAL	2.0
40	2i	93	ARG	2.0
43	1l	19	ARG	2.0
44	1m	98	VAL	2.0
45	2n	56	VAL	2.0
47	2p	72	ARG	2.0
51	1t	8	ARG	2.0
51	1t	15	ARG	2.0
51	1t	17	ARG	2.0
1	2A	271(L)	U	2.0
3	2D	55	GLY	2.0
8	1I	90	GLY	2.0
10	2O	27	GLY	2.0
10	2O	50	GLY	2.0
10	2O	74	GLY	2.0
12	2Q	30	GLY	2.0
15	2T	56	GLY	2.0
10	2O	79	PHE	2.0
32	2a	5	U	2.0
34	2c	197	GLY	2.0
46	1o	20	GLY	2.0
41	1j	54	PHE	2.0
11	2P	113	LYS	2.0
22	20	49	LYS	2.0
24	22	54	LYS	2.0
33	2b	139	LYS	2.0
35	2d	169	LYS	2.0
45	2n	4	LYS	2.0
3	2D	70	TRP	2.0
4	2E	90	THR	2.0
4	2E	201	THR	2.0
5	2F	48	THR	2.0
7	1H	134	SER	2.0
12	1Q	139	GLU	2.0
14	2S	64	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	2T	128	GLU	2.0
17	2V	1	MET	2.0
21	2Z	43	GLU	2.0
22	10	43	THR	2.0
24	22	4	SER	2.0
34	1c	49	SER	2.0
36	2e	81	GLU	2.0
39	1h	120	THR	2.0
41	1j	64	GLU	2.0
42	1k	87	THR	2.0
46	2o	14	GLU	2.0
51	1t	61	SER	2.0
51	1t	70	SER	2.0
1	1A	2139	C	2.0
1	1A	2896	C	2.0
1	2A	6	A	2.0
1	2A	271(G)	C	2.0
5	2F	115	ALA	2.0
8	2I	59	ALA	2.0
17	2V	3	ALA	2.0
32	1a	219	C	2.0
32	1a	1044	A	2.0
32	2a	1043	C	2.0
32	2a	1097	C	2.0
32	2a	1107	C	2.0
32	2a	1109	C	2.0
32	2a	1183	A	2.0
32	2a	1225	A	2.0
33	1b	62	ALA	2.0
34	1c	65	ALA	2.0
34	2c	168	ALA	2.0
36	1e	86	ALA	2.0
38	2g	150	ALA	2.0
41	1j	20	ALA	2.0
54	1w	23	A	2.0
54	2w	25	C	2.0
12	1Q	113	GLN	2.0
35	1d	45	GLN	2.0
41	2j	84	GLN	2.0
1	2A	880	G	2.0
3	2D	182	LEU	2.0
5	2F	133	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	1G	147	ASP	2.0
11	2P	99	LEU	2.0
14	2S	78	LEU	2.0
17	2V	20	LEU	2.0
21	2Z	67	LEU	2.0
23	21	80	LEU	2.0
28	26	36	LEU	2.0
32	1a	42	G	2.0
32	1a	610	G	2.0
32	1a	627	G	2.0
32	1a	1131	G	2.0
32	2a	953	G	2.0
32	2a	1058	G	2.0
32	2a	1084	G	2.0
32	2a	1094	G	2.0
32	2a	1164	G	2.0
34	1c	36	ASP	2.0
34	1c	175	LEU	2.0
35	1d	196	LEU	2.0
36	1e	112	LEU	2.0
36	1e	127	ASN	2.0
38	1g	59	LEU	2.0
39	2h	121	ASP	2.0
42	1k	63	LEU	2.0
44	1m	48	LEU	2.0
44	2m	34	LEU	2.0
48	2q	98	LEU	2.0
49	2r	85	LEU	2.0
4	1E	58	ARG	2.0
4	2E	82	ARG	2.0
4	2E	176	ILE	2.0
6	2G	112	PRO	2.0
15	1T	112	ARG	2.0
15	1T	121	ILE	2.0
16	2U	50	ARG	2.0
16	2U	65	ILE	2.0
17	2V	83	ARG	2.0
20	2Y	74	PRO	2.0
21	2Z	80	ARG	2.0
26	24	61	ARG	2.0
33	1b	56	ARG	2.0
34	1c	77	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	127	ARG	2.0
35	1d	70	ILE	2.0
35	2d	118	ARG	2.0
41	1j	5	ARG	2.0
41	1j	43	ARG	2.0
44	2m	91	ARG	2.0
47	2p	33	ILE	2.0
49	2r	50	ILE	2.0
49	2r	55	ARG	2.0
49	2r	64	ARG	2.0
51	1t	25	ARG	2.0
11	1P	137	LYS	2.0
17	1V	44	LYS	2.0
26	24	69	LYS	2.0
34	1c	72	LYS	2.0
35	1d	18	LYS	2.0
39	2h	21	LYS	2.0
43	1l	126	LYS	2.0
43	2l	23	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	4SU	2y	8	20/21	0.32	0.22	87,92,105,113	0
57	5MU	2y	54	21/22	0.50	0.21	74,87,96,109	0
57	MIA	2y	37	22/30	0.56	0.21	79,86,93,107	0
57	G7M	1y	46	24/25	0.56	0.20	78,83,88,95	0
57	4SU	1y	8	20/21	0.57	0.19	81,87,95,100	0
57	G7M	2y	46	24/25	0.61	0.17	83,86,90,104	0
57	PSU	1y	55	20/21	0.61	0.18	77,83,88,96	0
57	PSU	1y	32	20/21	0.64	0.20	75,80,91,93	0
54	G7M	2w	46	24/25	0.64	0.18	72,80,92,108	0
57	PSU	2y	55	20/21	0.65	0.18	82,86,91,100	0
57	MIA	1y	37	22/30	0.65	0.21	73,81,92,101	0
57	PSU	1y	39	20/21	0.66	0.20	75,83,86,93	0
57	PSU	2y	39	20/21	0.69	0.18	77,82,90,94	0
57	PSU	2y	32	20/21	0.70	0.19	78,85,93,95	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	5MU	1y	54	21/22	0.71	0.17	77,81,87,99	0
54	G7M	1w	46	24/25	0.73	0.17	65,73,89,111	0
56	FME	1z	1	10/11	0.76	0.24	51,62,66,67	0
54	4SU	1w	8	20/21	0.84	0.15	71,75,83,85	0
54	4SU	2w	8	20/21	0.85	0.14	74,79,91,92	0
54	PSU	2w	32	20/21	0.85	0.16	60,71,78,79	0
54	MIA	2w	37	25/30	0.85	0.18	61,67,79,99	0
32	M2G	2a	966	25/26	0.86	0.18	52,60,71,77	0
32	2MG	2a	1207	24/25	0.87	0.14	64,72,75,76	0
56	FME	2z	1	10/11	0.87	0.24	59,67,73,76	0
54	PSU	1w	32	20/21	0.88	0.16	49,57,68,70	0
54	PSU	1w	55	20/21	0.88	0.13	50,66,71,73	0
43	0TD	2l	92	10/11	0.89	0.14	48,53,61,66	0
55	4SU	2x	8	20/21	0.89	0.13	60,67,72,76	0
55	5MU	2x	54	21/22	0.89	0.14	67,72,77,80	0
54	PSU	2w	55	20/21	0.89	0.11	70,74,77,82	0
55	5MU	1x	54	21/22	0.89	0.15	58,63,71,76	0
32	2MG	1a	1207	24/25	0.89	0.14	50,55,58,69	0
1	5MU	2A	1915	21/22	0.90	0.13	51,60,63,66	0
32	5MC	2a	967	21/22	0.90	0.15	58,61,66,69	0
55	PSU	1x	55	20/21	0.91	0.13	51,58,69,74	0
32	5MC	2a	1400	21/22	0.91	0.15	54,59,65,69	0
54	5MU	2w	54	21/22	0.91	0.12	64,70,73,78	0
55	PSU	2x	55	20/21	0.91	0.12	61,66,72,80	0
32	4OC	2a	1402	22/23	0.91	0.13	48,52,56,57	0
54	MIA	1w	37	29/30	0.91	0.17	38,46,64,78	0
1	PSU	2A	1917	20/21	0.91	0.11	51,56,66,70	0
32	UR3	2a	1498	21/22	0.92	0.14	48,51,55,58	0
43	0TD	1l	92	10/11	0.92	0.12	40,46,48,56	0
55	4SU	1x	8	20/21	0.92	0.12	53,59,66,67	0
32	PSU	2a	516	20/21	0.92	0.12	57,63,67,73	0
55	5MC	1x	32	21/22	0.92	0.15	41,46,52,60	0
32	5MC	2a	1404	21/22	0.92	0.13	45,52,55,57	0
54	PSU	2w	39	20/21	0.92	0.11	62,70,75,76	0
1	PSU	2A	1911	20/21	0.93	0.11	50,57,60,64	0
32	MA6	2a	1518	24/25	0.93	0.13	46,55,60,62	0
32	G7M	2a	527	24/25	0.93	0.12	49,56,62,71	0
32	PSU	1a	516	20/21	0.93	0.12	44,48,52,53	0
55	5MC	2x	32	21/22	0.93	0.13	57,60,66,72	0
1	5MU	1A	1915	21/22	0.93	0.11	33,44,48,50	0
32	5MC	2a	1407	21/22	0.93	0.12	40,47,51,60	0
32	MA6	2a	1519	24/25	0.94	0.14	41,55,60,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	1w	39	20/21	0.94	0.12	41,57,62,65	0
32	4OC	1a	1402	22/23	0.94	0.11	33,40,44,46	0
32	5MC	1a	1407	21/22	0.94	0.12	29,36,42,44	0
32	MA6	1a	1519	24/25	0.94	0.13	35,39,45,53	0
54	5MU	1w	54	21/22	0.94	0.11	50,57,62,66	0
1	PSU	1A	1911	20/21	0.94	0.10	37,43,47,49	0
1	5MC	2A	1962	21/22	0.94	0.12	36,43,49,58	0
32	M2G	1a	966	25/26	0.94	0.12	41,48,51,52	0
1	5MC	1A	1942	21/22	0.94	0.11	28,37,47,51	0
32	5MC	1a	1400	21/22	0.94	0.12	37,40,44,46	0
32	MA6	1a	1518	24/25	0.95	0.11	31,40,43,44	0
1	PSU	1A	1917	20/21	0.95	0.10	36,42,48,52	0
1	OMC	2A	1920	21/22	0.95	0.10	44,53,56,57	0
1	5MC	2A	1942	21/22	0.95	0.11	40,51,54,57	0
32	5MC	1a	967	21/22	0.95	0.11	43,51,56,57	0
1	OMU	2A	2552	21/22	0.95	0.11	31,41,45,49	0
55	8AN	2x	76	22/23	0.95	0.11	29,37,40,47	0
1	PSU	2A	2605	20/21	0.95	0.10	30,36,40,45	0
32	5MC	1a	1404	21/22	0.95	0.12	32,38,41,45	0
32	G7M	1a	527	24/25	0.95	0.10	35,41,47,54	0
55	8AN	1x	76	22/23	0.96	0.10	22,26,32,39	0
32	UR3	1a	1498	21/22	0.96	0.09	32,39,40,44	0
1	5MU	1A	1939	21/22	0.96	0.08	21,25,29,30	0
1	OMC	1A	1920	21/22	0.96	0.09	33,40,45,49	0
54	F3N	2w	76	33/34	0.96	0.10	23,37,41,41	0
1	OMG	2A	2251	24/25	0.96	0.11	34,38,41,43	0
1	OMU	1A	2552	21/22	0.96	0.09	20,25,30,30	0
1	2MA	2A	2503	23/24	0.97	0.09	25,33,39,41	0
1	5MU	2A	1939	21/22	0.97	0.09	30,36,39,42	0
54	F3N	1w	76	33/34	0.97	0.09	16,23,26,28	0
1	PSU	1A	2605	20/21	0.97	0.08	19,26,30,32	0
1	2MA	1A	2503	23/24	0.97	0.08	16,21,27,27	0
1	5MC	1A	1962	21/22	0.97	0.09	25,31,37,40	0
1	OMG	1A	2251	24/25	0.98	0.07	18,25,29,32	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	1A	3409	1/1	0.36	0.32	73,73,73,73	0
58	MG	2a	1805	1/1	0.43	0.27	70,70,70,70	0
58	MG	2A	3160	1/1	0.50	0.27	66,66,66,66	0
58	MG	2A	3787	1/1	0.52	0.22	57,57,57,57	0
58	MG	2v	103	1/1	0.53	0.36	79,79,79,79	0
58	MG	20	101	1/1	0.54	0.37	69,69,69,69	0
58	MG	2w	103	1/1	0.55	0.21	74,74,74,74	0
58	MG	2a	1672	1/1	0.56	0.27	69,69,69,69	0
58	MG	2a	1712	1/1	0.57	0.31	75,75,75,75	0
58	MG	2A	3469	1/1	0.57	0.29	75,75,75,75	0
58	MG	1a	1742	1/1	0.58	0.47	80,80,80,80	0
58	MG	2a	1634	1/1	0.59	0.32	58,58,58,58	0
58	MG	1A	3976	1/1	0.59	0.17	65,65,65,65	0
58	MG	1Y	203	1/1	0.60	0.19	67,67,67,67	0
58	MG	1A	3439	1/1	0.60	0.20	66,66,66,66	0
58	MG	1A	4026	1/1	0.61	0.22	58,58,58,58	0
58	MG	2a	1784	1/1	0.61	0.23	67,67,67,67	0
58	MG	2A	3253	1/1	0.61	0.25	74,74,74,74	0
58	MG	2A	3307	1/1	0.61	0.27	65,65,65,65	0
58	MG	1O	201	1/1	0.61	0.33	65,65,65,65	0
58	MG	1A	3295	1/1	0.62	0.20	67,67,67,67	0
58	MG	2D	307	1/1	0.62	0.26	67,67,67,67	0
58	MG	2a	1702	1/1	0.62	0.21	68,68,68,68	0
58	MG	2A	3670	1/1	0.62	0.22	66,66,66,66	0
58	MG	1A	3721	1/1	0.63	0.32	66,66,66,66	0
58	MG	1A	3325	1/1	0.63	0.28	50,50,50,50	0
58	MG	1A	3559	1/1	0.63	0.27	72,72,72,72	0
58	MG	2a	1724	1/1	0.63	0.33	75,75,75,75	0
58	MG	2B	215	1/1	0.64	0.30	68,68,68,68	0
58	MG	1A	3568	1/1	0.64	0.21	59,59,59,59	0
58	MG	2n	101	1/1	0.64	0.44	77,77,77,77	0
58	MG	2a	1635	1/1	0.64	0.20	64,64,64,64	0
58	MG	2a	1640	1/1	0.64	0.37	74,74,74,74	0
58	MG	2a	1661	1/1	0.65	0.26	65,65,65,65	0
58	MG	2A	3750	1/1	0.65	0.23	60,60,60,60	0
58	MG	1A	3740	1/1	0.65	0.12	51,51,51,51	0
58	MG	1A	3705	1/1	0.65	0.33	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
58	MG	2A	3289	1/1	0.65	0.25	58,58,58,58	0
58	MG	1a	1694	1/1	0.65	0.29	71,71,71,71	0
58	MG	2A	3374	1/1	0.65	0.18	66,66,66,66	0
58	MG	1a	1717	1/1	0.65	0.28	59,59,59,59	0
58	MG	2a	1637	1/1	0.65	0.24	78,78,78,78	0
58	MG	1A	3537	1/1	0.65	0.33	64,64,64,64	0
58	MG	2A	3837	1/1	0.66	0.27	72,72,72,72	0
58	MG	1A	3453	1/1	0.66	0.19	67,67,67,67	0
58	MG	1A	4035	1/1	0.66	0.20	53,53,53,53	0
58	MG	1A	3603	1/1	0.66	0.28	66,66,66,66	0
58	MG	2A	3432	1/1	0.66	0.27	70,70,70,70	0
58	MG	1w	103	1/1	0.66	0.28	72,72,72,72	0
58	MG	2A	3156	1/1	0.66	0.43	70,70,70,70	0
58	MG	1A	3519	1/1	0.66	0.20	70,70,70,70	0
58	MG	1a	1615	1/1	0.66	0.23	58,58,58,58	0
58	MG	2A	3193	1/1	0.67	0.23	64,64,64,64	0
58	MG	1a	1642	1/1	0.67	0.24	55,55,55,55	0
58	MG	2A	3777	1/1	0.67	0.23	61,61,61,61	0
58	MG	2A	3272	1/1	0.67	0.28	70,70,70,70	0
58	MG	1a	1803	1/1	0.67	0.17	72,72,72,72	0
58	MG	1A	3728	1/1	0.67	0.28	70,70,70,70	0
58	MG	1a	1704	1/1	0.67	0.24	66,66,66,66	0
58	MG	1a	1639	1/1	0.67	0.24	65,65,65,65	0
58	MG	2A	3458	1/1	0.67	0.21	69,69,69,69	0
58	MG	2A	3179	1/1	0.67	0.22	62,62,62,62	0
58	MG	2A	3481	1/1	0.67	0.28	66,66,66,66	0
58	MG	2A	3144	1/1	0.68	0.19	66,66,66,66	0
58	MG	2A	3407	1/1	0.68	0.16	51,51,51,51	0
58	MG	1B	228	1/1	0.68	0.22	63,63,63,63	0
58	MG	1A	3852	1/1	0.68	0.18	46,46,46,46	0
58	MG	2a	1820	1/1	0.68	0.25	68,68,68,68	0
58	MG	2A	3274	1/1	0.68	0.16	62,62,62,62	0
58	MG	2A	3165	1/1	0.68	0.30	60,60,60,60	0
58	MG	2A	3096	1/1	0.68	0.28	66,66,66,66	0
58	MG	2A	3321	1/1	0.69	0.19	70,70,70,70	0
58	MG	1a	1690	1/1	0.69	0.25	60,60,60,60	0
58	MG	1A	3482	1/1	0.69	0.24	74,74,74,74	0
58	MG	2A	3781	1/1	0.69	0.23	51,51,51,51	0
58	MG	1A	3687	1/1	0.69	0.15	66,66,66,66	0
58	MG	2A	3280	1/1	0.69	0.22	58,58,58,58	0
58	MG	1a	1708	1/1	0.69	0.32	63,63,63,63	0
58	MG	1A	4066	1/1	0.69	0.18	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
58	MG	2A	3197	1/1	0.70	0.23	67,67,67,67	0
58	MG	1a	1737	1/1	0.70	0.19	71,71,71,71	0
58	MG	1A	3102	1/1	0.70	0.20	63,63,63,63	0
58	MG	1B	236	1/1	0.70	0.21	73,73,73,73	0
58	MG	1A	3946	1/1	0.70	0.13	71,71,71,71	0
58	MG	2A	3801	1/1	0.70	0.20	49,49,49,49	0
58	MG	2A	3047	1/1	0.70	0.20	66,66,66,66	0
58	MG	1B	224	1/1	0.70	0.26	61,61,61,61	0
58	MG	2a	1696	1/1	0.70	0.26	69,69,69,69	0
58	MG	1A	3264	1/1	0.71	0.14	53,53,53,53	0
58	MG	2A	3695	1/1	0.71	0.21	63,63,63,63	0
58	MG	2A	3720	1/1	0.71	0.29	67,67,67,67	0
58	MG	2a	1644	1/1	0.71	0.34	67,67,67,67	0
58	MG	2A	3327	1/1	0.71	0.20	72,72,72,72	0
58	MG	2A	3345	1/1	0.71	0.20	57,57,57,57	0
58	MG	2A	3258	1/1	0.71	0.26	61,61,61,61	0
58	MG	2A	3389	1/1	0.71	0.18	69,69,69,69	0
58	MG	1A	3369	1/1	0.71	0.23	49,49,49,49	0
58	MG	1x	108	1/1	0.71	0.18	30,30,30,30	0
58	MG	1a	1621	1/1	0.71	0.23	58,58,58,58	0
58	MG	2a	1804	1/1	0.71	0.22	64,64,64,64	0
58	MG	2A	3214	1/1	0.71	0.28	57,57,57,57	0
58	MG	2A	3238	1/1	0.71	0.25	60,60,60,60	0
58	MG	2a	1605	1/1	0.71	0.21	69,69,69,69	0
58	MG	2a	1630	1/1	0.71	0.28	71,71,71,71	0
58	MG	2A	3610	1/1	0.71	0.21	62,62,62,62	0
58	MG	2a	1700	1/1	0.72	0.29	80,80,80,80	0
58	MG	1A	3956	1/1	0.72	0.26	45,45,45,45	0
58	MG	1A	3207	1/1	0.72	0.18	69,69,69,69	0
58	MG	2B	216	1/1	0.72	0.19	65,65,65,65	0
58	MG	2a	1638	1/1	0.72	0.36	68,68,68,68	0
58	MG	1F	304	1/1	0.72	0.27	63,63,63,63	0
58	MG	2a	1642	1/1	0.72	0.20	62,62,62,62	0
58	MG	2V	202	1/1	0.72	0.25	68,68,68,68	0
58	MG	2A	3293	1/1	0.72	0.23	68,68,68,68	0
58	MG	1a	1626	1/1	0.72	0.29	64,64,64,64	0
58	MG	1A	3406	1/1	0.72	0.24	44,44,44,44	0
58	MG	1A	3695	1/1	0.73	0.16	35,35,35,35	0
58	MG	1A	4019	1/1	0.73	0.21	64,64,64,64	0
58	MG	2A	3733	1/1	0.73	0.28	72,72,72,72	0
58	MG	1A	3771	1/1	0.73	0.18	40,40,40,40	0
58	MG	2A	3388	1/1	0.73	0.24	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3335	1/1	0.73	0.24	57,57,57,57	0
58	MG	1A	3542	1/1	0.73	0.16	60,60,60,60	0
58	MG	2A	3418	1/1	0.73	0.32	67,67,67,67	0
58	MG	2A	3826	1/1	0.73	0.24	61,61,61,61	0
58	MG	2A	3178	1/1	0.73	0.21	60,60,60,60	0
58	MG	1x	105	1/1	0.73	0.17	62,62,62,62	0
58	MG	2a	1704	1/1	0.73	0.27	59,59,59,59	0
58	MG	2a	1709	1/1	0.73	0.20	69,69,69,69	0
58	MG	1A	4087	1/1	0.73	0.23	78,78,78,78	0
58	MG	2A	3296	1/1	0.73	0.38	40,40,40,40	0
58	MG	2a	1725	1/1	0.73	0.24	66,66,66,66	0
58	MG	2a	1782	1/1	0.73	0.28	68,68,68,68	0
58	MG	2E	301	1/1	0.73	0.17	56,56,56,56	0
58	MG	2a	1795	1/1	0.73	0.26	64,64,64,64	0
58	MG	2F	301	1/1	0.73	0.19	65,65,65,65	0
58	MG	2A	3037	1/1	0.73	0.26	62,62,62,62	0
58	MG	2a	1807	1/1	0.73	0.20	70,70,70,70	0
58	MG	2A	3648	1/1	0.73	0.13	68,68,68,68	0
58	MG	2A	3657	1/1	0.73	0.21	61,61,61,61	0
58	MG	1A	3535	1/1	0.73	0.15	52,52,52,52	0
58	MG	2A	3690	1/1	0.73	0.20	75,75,75,75	0
58	MG	2A	3153	1/1	0.74	0.18	57,57,57,57	0
58	MG	2a	1649	1/1	0.74	0.35	74,74,74,74	0
58	MG	1A	4015	1/1	0.74	0.17	71,71,71,71	0
58	MG	1A	4075	1/1	0.74	0.23	53,53,53,53	0
58	MG	2a	1681	1/1	0.74	0.26	67,67,67,67	0
58	MG	2B	211	1/1	0.74	0.22	69,69,69,69	0
58	MG	1A	3719	1/1	0.74	0.25	64,64,64,64	0
58	MG	2A	3175	1/1	0.74	0.26	59,59,59,59	0
58	MG	2A	3596	1/1	0.74	0.14	39,39,39,39	0
58	MG	1a	1808	1/1	0.74	0.33	78,78,78,78	0
58	MG	18	106	1/1	0.74	0.23	55,55,55,55	0
58	MG	2Q	202	1/1	0.74	0.18	58,58,58,58	0
58	MG	2R	203	1/1	0.74	0.23	65,65,65,65	0
58	MG	2a	1748	1/1	0.74	0.23	63,63,63,63	0
58	MG	1a	1697	1/1	0.74	0.23	66,66,66,66	0
58	MG	1A	3333	1/1	0.74	0.17	45,45,45,45	0
58	MG	2A	3335	1/1	0.74	0.31	73,73,73,73	0
58	MG	2A	3203	1/1	0.74	0.27	70,70,70,70	0
58	MG	2A	3352	1/1	0.74	0.17	65,65,65,65	0
58	MG	2A	3355	1/1	0.74	0.19	62,62,62,62	0
58	MG	2a	1808	1/1	0.74	0.20	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
58	MG	1A	3204	1/1	0.74	0.21	58,58,58,58	0
58	MG	1a	1712	1/1	0.74	0.22	61,61,61,61	0
58	MG	1A	4061	1/1	0.74	0.16	48,48,48,48	0
58	MG	1a	1734	1/1	0.74	0.22	69,69,69,69	0
58	MG	2a	1749	1/1	0.75	0.22	77,77,77,77	0
58	MG	2a	1750	1/1	0.75	0.12	83,83,83,83	0
58	MG	2E	302	1/1	0.75	0.29	71,71,71,71	0
58	MG	2a	1695	1/1	0.75	0.14	51,51,51,51	0
58	MG	1a	1788	1/1	0.75	0.18	76,76,76,76	0
58	MG	2a	1803	1/1	0.75	0.14	52,52,52,52	0
58	MG	1A	3270	1/1	0.75	0.22	64,64,64,64	0
58	MG	1a	1681	1/1	0.75	0.20	53,53,53,53	0
58	MG	2A	3640	1/1	0.75	0.35	59,59,59,59	0
58	MG	2A	3783	1/1	0.75	0.22	73,73,73,73	0
58	MG	2B	220	1/1	0.75	0.21	69,69,69,69	0
58	MG	2d	303	1/1	0.75	0.30	68,68,68,68	0
58	MG	2a	1650	1/1	0.75	0.22	63,63,63,63	0
58	MG	2A	3116	1/1	0.75	0.21	53,53,53,53	0
58	MG	2A	3730	1/1	0.75	0.19	70,70,70,70	0
58	MG	1a	1628	1/1	0.76	0.23	59,59,59,59	0
58	MG	1A	3128	1/1	0.76	0.14	53,53,53,53	0
58	MG	2a	1698	1/1	0.76	0.32	70,70,70,70	0
58	MG	2A	3189	1/1	0.76	0.26	64,64,64,64	0
58	MG	2A	3334	1/1	0.76	0.23	67,67,67,67	0
58	MG	2A	3678	1/1	0.76	0.23	57,57,57,57	0
58	MG	1x	109	1/1	0.76	0.17	60,60,60,60	0
58	MG	1x	110	1/1	0.76	0.20	62,62,62,62	0
58	MG	2a	1721	1/1	0.76	0.17	70,70,70,70	0
58	MG	1A	3410	1/1	0.76	0.19	64,64,64,64	0
58	MG	2A	3211	1/1	0.76	0.17	58,58,58,58	0
58	MG	1A	3669	1/1	0.76	0.14	47,47,47,47	0
58	MG	2a	1611	1/1	0.76	0.21	66,66,66,66	0
58	MG	1A	3347	1/1	0.76	0.23	58,58,58,58	0
58	MG	2A	3759	1/1	0.76	0.19	68,68,68,68	0
58	MG	1a	1757	1/1	0.76	0.24	60,60,60,60	0
58	MG	2a	1793	1/1	0.76	0.21	75,75,75,75	0
58	MG	1a	1607	1/1	0.76	0.16	62,62,62,62	0
58	MG	1A	3190	1/1	0.76	0.13	43,43,43,43	0
58	MG	1A	3284	1/1	0.76	0.18	52,52,52,52	0
58	MG	2A	3788	1/1	0.76	0.19	60,60,60,60	0
58	MG	2A	3278	1/1	0.76	0.18	66,66,66,66	0
58	MG	1n	101	1/1	0.76	0.27	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
58	MG	2a	1810	1/1	0.76	0.30	79,79,79,79	0
58	MG	2a	1811	1/1	0.76	0.17	57,57,57,57	0
58	MG	2A	3475	1/1	0.76	0.22	52,52,52,52	0
58	MG	1w	101	1/1	0.76	0.32	66,66,66,66	0
58	MG	2a	1665	1/1	0.76	0.28	63,63,63,63	0
58	MG	2A	3166	1/1	0.76	0.25	60,60,60,60	0
58	MG	1A	3869	1/1	0.76	0.19	63,63,63,63	0
58	MG	1A	3342	1/1	0.77	0.22	57,57,57,57	0
58	MG	2A	3683	1/1	0.77	0.17	68,68,68,68	0
58	MG	1a	1623	1/1	0.77	0.19	56,56,56,56	0
58	MG	1a	1711	1/1	0.77	0.20	50,50,50,50	0
58	MG	2A	3377	1/1	0.77	0.28	70,70,70,70	0
58	MG	1A	3488	1/1	0.77	0.20	62,62,62,62	0
58	MG	2a	1720	1/1	0.77	0.18	60,60,60,60	0
58	MG	1A	4090	1/1	0.77	0.18	59,59,59,59	0
58	MG	1Z	302	1/1	0.77	0.18	57,57,57,57	0
58	MG	2a	1602	1/1	0.77	0.23	67,67,67,67	0
58	MG	2A	3754	1/1	0.77	0.24	48,48,48,48	0
58	MG	1Z	303	1/1	0.77	0.15	58,58,58,58	0
58	MG	2a	1617	1/1	0.77	0.15	60,60,60,60	0
58	MG	2a	1774	1/1	0.77	0.15	49,49,49,49	0
58	MG	2a	1779	1/1	0.77	0.23	59,59,59,59	0
58	MG	1a	1680	1/1	0.77	0.22	65,65,65,65	0
58	MG	10	107	1/1	0.77	0.26	67,67,67,67	0
58	MG	2A	3298	1/1	0.77	0.22	62,62,62,62	0
58	MG	2A	3784	1/1	0.77	0.18	61,61,61,61	0
58	MG	1a	1758	1/1	0.77	0.14	67,67,67,67	0
58	MG	2A	3115	1/1	0.77	0.27	69,69,69,69	0
58	MG	2A	3554	1/1	0.77	0.20	44,44,44,44	0
58	MG	2A	3803	1/1	0.77	0.17	56,56,56,56	0
58	MG	2A	3324	1/1	0.77	0.17	60,60,60,60	0
58	MG	2A	3325	1/1	0.77	0.18	67,67,67,67	0
58	MG	2B	203	1/1	0.77	0.18	72,72,72,72	0
58	MG	1A	3442	1/1	0.77	0.42	54,54,54,54	0
58	MG	1A	3989	1/1	0.77	0.12	38,38,38,38	0
58	MG	1A	3353	1/1	0.77	0.17	56,56,56,56	0
58	MG	2A	3242	1/1	0.77	0.20	57,57,57,57	0
58	MG	2D	302	1/1	0.77	0.21	56,56,56,56	0
58	MG	1a	1665	1/1	0.78	0.26	60,60,60,60	0
58	MG	1A	3139	1/1	0.78	0.22	53,53,53,53	0
58	MG	2A	3128	1/1	0.78	0.14	51,51,51,51	0
58	MG	2A	3672	1/1	0.78	0.23	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3871	1/1	0.78	0.18	52,52,52,52	0
58	MG	1a	1688	1/1	0.78	0.23	61,61,61,61	0
58	MG	1A	3887	1/1	0.78	0.23	57,57,57,57	0
58	MG	2A	3262	1/1	0.78	0.32	60,60,60,60	0
58	MG	2F	306	1/1	0.78	0.26	59,59,59,59	0
58	MG	1A	3245	1/1	0.78	0.28	56,56,56,56	0
58	MG	1A	3560	1/1	0.78	0.28	63,63,63,63	0
58	MG	2T	201	1/1	0.78	0.17	55,55,55,55	0
58	MG	2T	203	1/1	0.78	0.15	62,62,62,62	0
58	MG	2a	1731	1/1	0.78	0.35	64,64,64,64	0
58	MG	1A	4099	1/1	0.78	0.22	50,50,50,50	0
58	MG	2A	3735	1/1	0.78	0.24	62,62,62,62	0
58	MG	2a	1601	1/1	0.78	0.15	69,69,69,69	0
58	MG	2A	3174	1/1	0.78	0.21	63,63,63,63	0
58	MG	2a	1604	1/1	0.78	0.30	71,71,71,71	0
58	MG	2A	3286	1/1	0.78	0.23	65,65,65,65	0
58	MG	1A	3494	1/1	0.78	0.30	57,57,57,57	0
58	MG	1A	3263	1/1	0.78	0.22	57,57,57,57	0
58	MG	2A	3778	1/1	0.78	0.22	58,58,58,58	0
58	MG	2A	3439	1/1	0.78	0.31	74,74,74,74	0
58	MG	1A	3668	1/1	0.78	0.15	56,56,56,56	0
58	MG	1A	3124	1/1	0.78	0.20	40,40,40,40	0
58	MG	2A	3300	1/1	0.78	0.24	69,69,69,69	0
58	MG	1a	1630	1/1	0.78	0.21	59,59,59,59	0
58	MG	2A	3500	1/1	0.78	0.24	68,68,68,68	0
58	MG	2A	3531	1/1	0.78	0.19	65,65,65,65	0
58	MG	2A	3813	1/1	0.78	0.17	45,45,45,45	0
58	MG	2A	3308	1/1	0.78	0.19	45,45,45,45	0
58	MG	2j	201	1/1	0.78	0.20	59,59,59,59	0
58	MG	2A	3309	1/1	0.78	0.15	52,52,52,52	0
58	MG	1A	3846	1/1	0.78	0.38	71,71,71,71	0
58	MG	1A	3074	1/1	0.78	0.21	59,59,59,59	0
58	MG	2x	105	1/1	0.78	0.28	63,63,63,63	0
58	MG	2A	3747	1/1	0.79	0.17	68,68,68,68	0
58	MG	2A	3198	1/1	0.79	0.15	51,51,51,51	0
58	MG	2R	204	1/1	0.79	0.22	65,65,65,65	0
58	MG	1a	1775	1/1	0.79	0.16	70,70,70,70	0
58	MG	2A	3453	1/1	0.79	0.30	70,70,70,70	0
58	MG	2a	1719	1/1	0.79	0.21	68,68,68,68	0
58	MG	1A	3942	1/1	0.79	0.14	67,67,67,67	0
58	MG	1A	3344	1/1	0.79	0.28	64,64,64,64	0
58	MG	2A	3310	1/1	0.79	0.14	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
58	MG	2A	3782	1/1	0.79	0.17	62,62,62,62	0
58	MG	2A	3318	1/1	0.79	0.17	66,66,66,66	0
58	MG	1A	3250	1/1	0.79	0.12	57,57,57,57	0
58	MG	2a	1608	1/1	0.79	0.24	67,67,67,67	0
58	MG	2A	3322	1/1	0.79	0.21	73,73,73,73	0
58	MG	1A	3314	1/1	0.79	0.18	52,52,52,52	0
58	MG	2a	1776	1/1	0.79	0.29	67,67,67,67	0
58	MG	1A	3423	1/1	0.79	0.16	59,59,59,59	0
58	MG	1a	1660	1/1	0.79	0.16	52,52,52,52	0
58	MG	2A	3329	1/1	0.79	0.18	59,59,59,59	0
58	MG	2A	3332	1/1	0.79	0.22	56,56,56,56	0
58	MG	2A	3655	1/1	0.79	0.13	65,65,65,65	0
58	MG	2A	3259	1/1	0.79	0.32	68,68,68,68	0
58	MG	2B	206	1/1	0.79	0.28	64,64,64,64	0
58	MG	1A	3996	1/1	0.79	0.15	47,47,47,47	0
58	MG	1a	1671	1/1	0.79	0.37	73,73,73,73	0
58	MG	1A	3356	1/1	0.79	0.23	59,59,59,59	0
58	MG	2a	1651	1/1	0.79	0.16	71,71,71,71	0
58	MG	2a	1652	1/1	0.79	0.16	72,72,72,72	0
58	MG	1A	3709	1/1	0.79	0.24	54,54,54,54	0
58	MG	2A	3021	1/1	0.79	0.24	69,69,69,69	0
58	MG	2A	3029	1/1	0.79	0.15	53,53,53,53	0
58	MG	1A	3595	1/1	0.79	0.27	63,63,63,63	0
58	MG	2A	3041	1/1	0.79	0.26	54,54,54,54	0
58	MG	1A	3343	1/1	0.79	0.16	56,56,56,56	0
58	MG	2x	102	1/1	0.79	0.24	64,64,64,64	0
58	MG	2A	3053	1/1	0.79	0.18	63,63,63,63	0
58	MG	2A	3291	1/1	0.80	0.25	61,61,61,61	0
58	MG	1A	3167	1/1	0.80	0.23	45,45,45,45	0
58	MG	1a	1769	1/1	0.80	0.15	62,62,62,62	0
58	MG	1a	1622	1/1	0.80	0.22	61,61,61,61	0
58	MG	2A	3201	1/1	0.80	0.30	67,67,67,67	0
58	MG	2A	3740	1/1	0.80	0.17	47,47,47,47	0
58	MG	2A	3419	1/1	0.80	0.19	55,55,55,55	0
58	MG	1A	3495	1/1	0.80	0.12	56,56,56,56	0
58	MG	2A	3207	1/1	0.80	0.25	58,58,58,58	0
58	MG	1A	3838	1/1	0.80	0.19	80,80,80,80	0
58	MG	2A	3212	1/1	0.80	0.18	66,66,66,66	0
58	MG	2a	1735	1/1	0.80	0.18	57,57,57,57	0
58	MG	2a	1739	1/1	0.80	0.18	51,51,51,51	0
58	MG	2a	1603	1/1	0.80	0.29	58,58,58,58	0
58	MG	1A	3413	1/1	0.80	0.18	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
58	MG	1b	301	1/1	0.80	0.14	75,75,75,75	0
58	MG	1A	3520	1/1	0.80	0.14	55,55,55,55	0
58	MG	1A	3300	1/1	0.80	0.31	62,62,62,62	0
58	MG	1l	104	1/1	0.80	0.13	44,44,44,44	0
58	MG	2A	3541	1/1	0.80	0.16	45,45,45,45	0
58	MG	1a	1643	1/1	0.80	0.16	56,56,56,56	0
58	MG	2A	3575	1/1	0.80	0.14	43,43,43,43	0
58	MG	2a	1794	1/1	0.80	0.15	68,68,68,68	0
58	MG	2A	3580	1/1	0.80	0.24	62,62,62,62	0
58	MG	2A	3328	1/1	0.80	0.16	68,68,68,68	0
58	MG	1A	3163	1/1	0.80	0.13	47,47,47,47	0
58	MG	2A	3612	1/1	0.80	0.20	53,53,53,53	0
58	MG	2A	3846	1/1	0.80	0.13	49,49,49,49	0
58	MG	2B	202	1/1	0.80	0.18	59,59,59,59	0
58	MG	2A	3636	1/1	0.80	0.18	48,48,48,48	0
58	MG	1A	3615	1/1	0.80	0.13	31,31,31,31	0
58	MG	1a	1670	1/1	0.80	0.17	62,62,62,62	0
58	MG	1x	111	1/1	0.80	0.20	60,60,60,60	0
58	MG	1a	1741	1/1	0.80	0.24	68,68,68,68	0
58	MG	2A	3281	1/1	0.80	0.21	60,60,60,60	0
58	MG	2q	201	1/1	0.80	0.18	60,60,60,60	0
58	MG	2q	202	1/1	0.80	0.17	71,71,71,71	0
58	MG	1A	3541	1/1	0.80	0.17	48,48,48,48	0
58	MG	2A	3356	1/1	0.80	0.18	58,58,58,58	0
58	MG	2A	3368	1/1	0.80	0.25	68,68,68,68	0
58	MG	1a	1619	1/1	0.80	0.24	50,50,50,50	0
58	MG	2A	3471	1/1	0.81	0.13	50,50,50,50	0
58	MG	2A	3313	1/1	0.81	0.26	50,50,50,50	0
58	MG	1A	3431	1/1	0.81	0.16	38,38,38,38	0
58	MG	2A	3484	1/1	0.81	0.25	66,66,66,66	0
58	MG	1A	3600	1/1	0.81	0.22	61,61,61,61	0
58	MG	1a	1802	1/1	0.81	0.24	69,69,69,69	0
58	MG	2A	3106	1/1	0.81	0.15	56,56,56,56	0
58	MG	2a	1680	1/1	0.81	0.19	58,58,58,58	0
58	MG	2A	3235	1/1	0.81	0.14	54,54,54,54	0
58	MG	1A	3471	1/1	0.81	0.16	59,59,59,59	0
58	MG	10	108	1/1	0.81	0.18	64,64,64,64	0
58	MG	2A	3587	1/1	0.81	0.14	62,62,62,62	0
58	MG	2A	3244	1/1	0.81	0.19	60,60,60,60	0
58	MG	2A	3609	1/1	0.81	0.17	38,38,38,38	0
58	MG	1A	3252	1/1	0.81	0.18	67,67,67,67	0
58	MG	2A	3137	1/1	0.81	0.22	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
58	MG	2B	212	1/1	0.81	0.22	61,61,61,61	0
58	MG	2B	214	1/1	0.81	0.15	56,56,56,56	0
58	MG	2A	3617	1/1	0.81	0.21	60,60,60,60	0
58	MG	14	101	1/1	0.81	0.14	64,64,64,64	0
58	MG	16	101	1/1	0.81	0.15	56,56,56,56	0
58	MG	2A	3644	1/1	0.81	0.26	63,63,63,63	0
58	MG	1A	3486	1/1	0.81	0.20	58,58,58,58	0
58	MG	1x	102	1/1	0.81	0.32	70,70,70,70	0
58	MG	1x	104	1/1	0.81	0.14	60,60,60,60	0
58	MG	1A	3529	1/1	0.81	0.17	58,58,58,58	0
58	MG	1a	1669	1/1	0.81	0.17	56,56,56,56	0
58	MG	1A	3305	1/1	0.81	0.31	52,52,52,52	0
58	MG	2A	3382	1/1	0.81	0.14	50,50,50,50	0
58	MG	2A	3689	1/1	0.81	0.25	74,74,74,74	0
58	MG	1A	4058	1/1	0.81	0.12	48,48,48,48	0
58	MG	2A	3692	1/1	0.81	0.12	55,55,55,55	0
58	MG	2a	1783	1/1	0.81	0.26	69,69,69,69	0
58	MG	1A	3947	1/1	0.81	0.28	69,69,69,69	0
58	MG	2A	3697	1/1	0.81	0.25	71,71,71,71	0
58	MG	2A	3702	1/1	0.81	0.12	41,41,41,41	0
58	MG	2A	3712	1/1	0.81	0.20	66,66,66,66	0
58	MG	2A	3406	1/1	0.81	0.23	61,61,61,61	0
58	MG	2A	3186	1/1	0.81	0.24	58,58,58,58	0
58	MG	2A	3409	1/1	0.81	0.19	62,62,62,62	0
58	MG	2A	3413	1/1	0.81	0.29	60,60,60,60	0
58	MG	2A	3015	1/1	0.81	0.21	62,62,62,62	0
58	MG	1A	3592	1/1	0.81	0.26	66,66,66,66	0
58	MG	2a	1620	1/1	0.81	0.18	74,74,74,74	0
58	MG	2a	1816	1/1	0.81	0.26	65,65,65,65	0
58	MG	2A	3748	1/1	0.81	0.20	54,54,54,54	0
58	MG	2A	3423	1/1	0.81	0.20	58,58,58,58	0
58	MG	2A	3194	1/1	0.81	0.13	53,53,53,53	0
58	MG	2l	203	1/1	0.81	0.10	57,57,57,57	0
58	MG	1a	1686	1/1	0.81	0.26	59,59,59,59	0
58	MG	1a	1761	1/1	0.81	0.19	68,68,68,68	0
58	MG	1a	1687	1/1	0.81	0.30	53,53,53,53	0
58	MG	2q	203	1/1	0.81	0.17	70,70,70,70	0
58	MG	2a	1641	1/1	0.81	0.17	50,50,50,50	0
58	MG	2A	3779	1/1	0.81	0.19	54,54,54,54	0
58	MG	2A	3042	1/1	0.81	0.15	51,51,51,51	0
58	MG	2a	1647	1/1	0.81	0.19	69,69,69,69	0
58	MG	2a	1654	1/1	0.82	0.18	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
58	MG	2a	1660	1/1	0.82	0.18	65,65,65,65	0
58	MG	2A	3001	1/1	0.82	0.29	62,62,62,62	0
58	MG	1a	1720	1/1	0.82	0.25	66,66,66,66	0
58	MG	2A	3571	1/1	0.82	0.19	56,56,56,56	0
58	MG	2a	1677	1/1	0.82	0.14	56,56,56,56	0
58	MG	1A	3714	1/1	0.82	0.17	50,50,50,50	0
58	MG	1A	3027	1/1	0.82	0.14	63,63,63,63	0
58	MG	1a	1656	1/1	0.82	0.21	64,64,64,64	0
58	MG	2A	3209	1/1	0.82	0.28	62,62,62,62	0
58	MG	1A	3944	1/1	0.82	0.12	33,33,33,33	0
58	MG	1A	3034	1/1	0.82	0.16	32,32,32,32	0
58	MG	1A	3299	1/1	0.82	0.23	49,49,49,49	0
58	MG	2A	3615	1/1	0.82	0.22	63,63,63,63	0
58	MG	2A	3225	1/1	0.82	0.15	64,64,64,64	0
58	MG	2A	3336	1/1	0.82	0.20	49,49,49,49	0
58	MG	2A	3340	1/1	0.82	0.14	66,66,66,66	0
58	MG	2A	3234	1/1	0.82	0.16	63,63,63,63	0
58	MG	1A	3222	1/1	0.82	0.28	54,54,54,54	0
58	MG	2A	3650	1/1	0.82	0.14	61,61,61,61	0
58	MG	2A	3071	1/1	0.82	0.22	59,59,59,59	0
58	MG	2A	3088	1/1	0.82	0.20	48,48,48,48	0
58	MG	2A	3669	1/1	0.82	0.17	58,58,58,58	0
58	MG	1a	1764	1/1	0.82	0.18	59,59,59,59	0
58	MG	2P	201	1/1	0.82	0.20	58,58,58,58	0
58	MG	2A	3371	1/1	0.82	0.23	61,61,61,61	0
58	MG	1A	3456	1/1	0.82	0.17	62,62,62,62	0
58	MG	2a	1768	1/1	0.82	0.17	69,69,69,69	0
58	MG	2A	3255	1/1	0.82	0.19	60,60,60,60	0
58	MG	2a	1775	1/1	0.82	0.24	62,62,62,62	0
58	MG	2A	3687	1/1	0.82	0.20	68,68,68,68	0
58	MG	2A	3108	1/1	0.82	0.30	64,64,64,64	0
58	MG	2A	3384	1/1	0.82	0.19	68,68,68,68	0
58	MG	1a	1679	1/1	0.82	0.18	62,62,62,62	0
58	MG	17	105	1/1	0.82	0.17	52,52,52,52	0
58	MG	2a	1786	1/1	0.82	0.16	67,67,67,67	0
58	MG	2a	1788	1/1	0.82	0.16	66,66,66,66	0
58	MG	2a	1790	1/1	0.82	0.17	60,60,60,60	0
58	MG	2A	3395	1/1	0.82	0.20	52,52,52,52	0
58	MG	1a	1795	1/1	0.82	0.21	65,65,65,65	0
58	MG	1a	1800	1/1	0.82	0.21	68,68,68,68	0
58	MG	2A	3408	1/1	0.82	0.17	56,56,56,56	0
58	MG	1A	3985	1/1	0.82	0.14	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
58	MG	1a	1682	1/1	0.82	0.18	71,71,71,71	0
58	MG	1a	1602	1/1	0.82	0.19	64,64,64,64	0
58	MG	1B	206	1/1	0.82	0.21	47,47,47,47	0
58	MG	1B	223	1/1	0.82	0.20	65,65,65,65	0
58	MG	1a	1689	1/1	0.82	0.27	55,55,55,55	0
58	MG	2A	3168	1/1	0.82	0.13	52,52,52,52	0
58	MG	2a	1817	1/1	0.82	0.13	65,65,65,65	0
58	MG	2a	1636	1/1	0.82	0.28	64,64,64,64	0
58	MG	2A	3442	1/1	0.82	0.13	55,55,55,55	0
58	MG	2A	3445	1/1	0.82	0.14	58,58,58,58	0
58	MG	1A	3517	1/1	0.82	0.19	61,61,61,61	0
58	MG	1A	3462	1/1	0.82	0.20	62,62,62,62	0
58	MG	1A	3563	1/1	0.82	0.17	46,46,46,46	0
58	MG	1E	308	1/1	0.82	0.09	28,28,28,28	0
58	MG	1A	4017	1/1	0.82	0.15	46,46,46,46	0
58	MG	1A	3378	1/1	0.82	0.14	39,39,39,39	0
58	MG	1R	204	1/1	0.82	0.25	53,53,53,53	0
58	MG	1A	3522	1/1	0.82	0.15	60,60,60,60	0
58	MG	2A	3196	1/1	0.82	0.21	65,65,65,65	0
58	MG	1A	3571	1/1	0.83	0.28	52,52,52,52	0
58	MG	1E	305	1/1	0.83	0.24	54,54,54,54	0
58	MG	1A	3441	1/1	0.83	0.15	44,44,44,44	0
58	MG	1A	3874	1/1	0.83	0.20	41,41,41,41	0
58	MG	1a	1633	1/1	0.83	0.26	58,58,58,58	0
58	MG	2A	3839	1/1	0.83	0.18	66,66,66,66	0
58	MG	1a	1635	1/1	0.83	0.14	49,49,49,49	0
58	MG	1a	1636	1/1	0.83	0.17	53,53,53,53	0
58	MG	2a	1697	1/1	0.83	0.18	63,63,63,63	0
58	MG	2A	3331	1/1	0.83	0.18	70,70,70,70	0
58	MG	2a	1699	1/1	0.83	0.22	70,70,70,70	0
58	MG	1A	3255	1/1	0.83	0.23	58,58,58,58	0
58	MG	1a	1640	1/1	0.83	0.24	59,59,59,59	0
58	MG	1A	4049	1/1	0.83	0.19	62,62,62,62	0
58	MG	1A	3716	1/1	0.83	0.19	51,51,51,51	0
58	MG	1A	3717	1/1	0.83	0.17	54,54,54,54	0
58	MG	2a	1715	1/1	0.83	0.22	65,65,65,65	0
58	MG	2A	3224	1/1	0.83	0.21	60,60,60,60	0
58	MG	2A	3056	1/1	0.83	0.13	60,60,60,60	0
58	MG	2A	3230	1/1	0.83	0.15	68,68,68,68	0
58	MG	1a	1659	1/1	0.83	0.24	68,68,68,68	0
58	MG	2A	3366	1/1	0.83	0.20	67,67,67,67	0
58	MG	2A	3086	1/1	0.83	0.22	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3450	1/1	0.83	0.32	65,65,65,65	0
58	MG	2a	1736	1/1	0.83	0.26	62,62,62,62	0
58	MG	2A	3665	1/1	0.83	0.23	61,61,61,61	0
58	MG	2A	3667	1/1	0.83	0.11	51,51,51,51	0
58	MG	1A	3168	1/1	0.83	0.12	46,46,46,46	0
58	MG	2A	3099	1/1	0.83	0.23	60,60,60,60	0
58	MG	1A	3385	1/1	0.83	0.21	68,68,68,68	0
58	MG	1A	4089	1/1	0.83	0.18	50,50,50,50	0
58	MG	1a	1786	1/1	0.83	0.12	59,59,59,59	0
58	MG	1A	3633	1/1	0.83	0.14	57,57,57,57	0
58	MG	1a	1678	1/1	0.83	0.24	65,65,65,65	0
58	MG	28	102	1/1	0.83	0.19	61,61,61,61	0
58	MG	2A	3266	1/1	0.83	0.19	67,67,67,67	0
58	MG	2A	3136	1/1	0.83	0.17	50,50,50,50	0
58	MG	1A	3315	1/1	0.83	0.25	59,59,59,59	0
58	MG	2A	3143	1/1	0.83	0.17	51,51,51,51	0
58	MG	1A	4100	1/1	0.83	0.11	41,41,41,41	0
58	MG	1A	3437	1/1	0.83	0.22	56,56,56,56	0
58	MG	2A	3282	1/1	0.83	0.17	70,70,70,70	0
58	MG	1a	1807	1/1	0.83	0.20	56,56,56,56	0
58	MG	18	107	1/1	0.83	0.17	62,62,62,62	0
58	MG	2a	1622	1/1	0.83	0.19	59,59,59,59	0
58	MG	2A	3161	1/1	0.83	0.11	60,60,60,60	0
58	MG	1B	212	1/1	0.83	0.21	58,58,58,58	0
58	MG	2A	3743	1/1	0.83	0.22	59,59,59,59	0
58	MG	1d	301	1/1	0.83	0.26	55,55,55,55	0
58	MG	2A	3446	1/1	0.83	0.25	57,57,57,57	0
58	MG	1B	213	1/1	0.83	0.16	57,57,57,57	0
58	MG	2a	1639	1/1	0.83	0.27	67,67,67,67	0
58	MG	2a	1818	1/1	0.83	0.22	54,54,54,54	0
58	MG	1A	3993	1/1	0.83	0.14	45,45,45,45	0
58	MG	2A	3465	1/1	0.83	0.11	59,59,59,59	0
58	MG	2A	3466	1/1	0.83	0.28	59,59,59,59	0
58	MG	1A	3358	1/1	0.83	0.18	43,43,43,43	0
58	MG	1A	3527	1/1	0.83	0.24	37,37,37,37	0
58	MG	1a	1692	1/1	0.83	0.15	51,51,51,51	0
58	MG	2A	3183	1/1	0.83	0.15	66,66,66,66	0
58	MG	1a	1693	1/1	0.83	0.25	61,61,61,61	0
58	MG	2v	101	1/1	0.83	0.18	58,58,58,58	0
58	MG	2A	3493	1/1	0.83	0.26	61,61,61,61	0
58	MG	1B	231	1/1	0.83	0.20	66,66,66,66	0
58	MG	2a	1658	1/1	0.83	0.21	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
58	MG	2A	3514	1/1	0.83	0.20	54,54,54,54	0
58	MG	2a	1646	1/1	0.84	0.14	66,66,66,66	0
58	MG	1A	3598	1/1	0.84	0.13	48,48,48,48	0
58	MG	1B	225	1/1	0.84	0.19	52,52,52,52	0
58	MG	1a	1637	1/1	0.84	0.19	55,55,55,55	0
58	MG	1A	3401	1/1	0.84	0.20	41,41,41,41	0
58	MG	2A	3275	1/1	0.84	0.15	62,62,62,62	0
58	MG	2A	3758	1/1	0.84	0.16	64,64,64,64	0
58	MG	1A	3487	1/1	0.84	0.11	42,42,42,42	0
58	MG	2A	3774	1/1	0.84	0.20	62,62,62,62	0
58	MG	1A	3738	1/1	0.84	0.23	77,77,77,77	0
58	MG	1D	313	1/1	0.84	0.16	40,40,40,40	0
58	MG	1A	3040	1/1	0.84	0.25	62,62,62,62	0
58	MG	1A	3745	1/1	0.84	0.14	57,57,57,57	0
58	MG	1E	310	1/1	0.84	0.19	62,62,62,62	0
58	MG	2A	3460	1/1	0.84	0.27	62,62,62,62	0
58	MG	2a	1688	1/1	0.84	0.25	65,65,65,65	0
58	MG	2A	3463	1/1	0.84	0.15	52,52,52,52	0
58	MG	1A	4010	1/1	0.84	0.08	36,36,36,36	0
58	MG	1A	3755	1/1	0.84	0.12	61,61,61,61	0
58	MG	2A	3294	1/1	0.84	0.21	65,65,65,65	0
58	MG	1O	204	1/1	0.84	0.14	43,43,43,43	0
58	MG	2A	3807	1/1	0.84	0.11	63,63,63,63	0
58	MG	1Q	206	1/1	0.84	0.16	58,58,58,58	0
58	MG	2A	3820	1/1	0.84	0.12	50,50,50,50	0
58	MG	1A	3770	1/1	0.84	0.10	30,30,30,30	0
58	MG	2A	3301	1/1	0.84	0.15	63,63,63,63	0
58	MG	1W	201	1/1	0.84	0.24	53,53,53,53	0
58	MG	1A	3268	1/1	0.84	0.17	60,60,60,60	0
58	MG	2A	3506	1/1	0.84	0.12	55,55,55,55	0
58	MG	2A	3181	1/1	0.84	0.20	61,61,61,61	0
58	MG	2a	1723	1/1	0.84	0.26	64,64,64,64	0
58	MG	2A	3182	1/1	0.84	0.32	60,60,60,60	0
58	MG	2A	3536	1/1	0.84	0.16	47,47,47,47	0
58	MG	2a	1730	1/1	0.84	0.28	55,55,55,55	0
58	MG	1A	4023	1/1	0.84	0.12	52,52,52,52	0
58	MG	1A	3793	1/1	0.84	0.10	36,36,36,36	0
58	MG	2A	3320	1/1	0.84	0.20	57,57,57,57	0
58	MG	1A	3805	1/1	0.84	0.14	64,64,64,64	0
58	MG	1x	106	1/1	0.84	0.17	54,54,54,54	0
58	MG	1A	3644	1/1	0.84	0.10	36,36,36,36	0
58	MG	2A	3195	1/1	0.84	0.31	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
58	MG	2A	3602	1/1	0.84	0.13	57,57,57,57	0
58	MG	1A	3549	1/1	0.84	0.19	59,59,59,59	0
58	MG	1A	4059	1/1	0.84	0.15	56,56,56,56	0
58	MG	1A	3357	1/1	0.84	0.14	53,53,53,53	0
58	MG	2G	201	1/1	0.84	0.13	62,62,62,62	0
58	MG	2A	3330	1/1	0.84	0.15	59,59,59,59	0
58	MG	1A	3862	1/1	0.84	0.12	47,47,47,47	0
58	MG	1A	3069	1/1	0.84	0.24	61,61,61,61	0
58	MG	1A	4081	1/1	0.84	0.15	56,56,56,56	0
58	MG	1a	1601	1/1	0.84	0.23	56,56,56,56	0
58	MG	1A	4085	1/1	0.84	0.28	69,69,69,69	0
58	MG	2A	3337	1/1	0.84	0.22	57,57,57,57	0
58	MG	1A	3039	1/1	0.84	0.24	35,35,35,35	0
58	MG	1A	3100	1/1	0.84	0.16	61,61,61,61	0
58	MG	2A	3222	1/1	0.84	0.19	58,58,58,58	0
58	MG	1A	3707	1/1	0.84	0.11	30,30,30,30	0
58	MG	1a	1713	1/1	0.84	0.20	71,71,71,71	0
58	MG	2A	3363	1/1	0.84	0.28	61,61,61,61	0
58	MG	1A	4095	1/1	0.84	0.16	57,57,57,57	0
58	MG	2A	3233	1/1	0.84	0.18	63,63,63,63	0
58	MG	2A	3370	1/1	0.84	0.13	57,57,57,57	0
58	MG	2a	1815	1/1	0.84	0.22	61,61,61,61	0
58	MG	2a	1615	1/1	0.84	0.14	57,57,57,57	0
58	MG	2A	3059	1/1	0.84	0.24	51,51,51,51	0
58	MG	1A	3888	1/1	0.84	0.23	43,43,43,43	0
58	MG	2A	3237	1/1	0.84	0.22	70,70,70,70	0
58	MG	2a	1628	1/1	0.84	0.17	65,65,65,65	0
58	MG	1a	1724	1/1	0.84	0.20	50,50,50,50	0
58	MG	2l	202	1/1	0.84	0.18	59,59,59,59	0
58	MG	2A	3240	1/1	0.84	0.16	67,67,67,67	0
58	MG	2A	3385	1/1	0.84	0.15	56,56,56,56	0
58	MG	1A	3929	1/1	0.84	0.11	32,32,32,32	0
58	MG	2A	3705	1/1	0.84	0.17	52,52,52,52	0
58	MG	2A	3243	1/1	0.84	0.18	62,62,62,62	0
58	MG	1a	1625	1/1	0.84	0.23	58,58,58,58	0
58	MG	1A	3469	1/1	0.84	0.13	53,53,53,53	0
58	MG	1A	3588	1/1	0.84	0.11	29,29,29,29	0
58	MG	1A	3435	1/1	0.84	0.12	42,42,42,42	0
58	MG	1A	3297	1/1	0.84	0.29	56,56,56,56	0
58	MG	2A	3482	1/1	0.85	0.15	56,56,56,56	0
58	MG	1B	215	1/1	0.85	0.12	63,63,63,63	0
58	MG	1a	1663	1/1	0.85	0.13	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
58	MG	2A	3498	1/1	0.85	0.33	65,65,65,65	0
58	MG	1a	1664	1/1	0.85	0.13	50,50,50,50	0
58	MG	2A	3082	1/1	0.85	0.18	51,51,51,51	0
58	MG	2a	1670	1/1	0.85	0.16	56,56,56,56	0
58	MG	2A	3791	1/1	0.85	0.17	52,52,52,52	0
58	MG	2a	1674	1/1	0.85	0.34	68,68,68,68	0
58	MG	2A	3508	1/1	0.85	0.18	38,38,38,38	0
58	MG	2a	1678	1/1	0.85	0.17	59,59,59,59	0
58	MG	15	107	1/1	0.85	0.11	54,54,54,54	0
58	MG	1a	1666	1/1	0.85	0.21	63,63,63,63	0
58	MG	2A	3223	1/1	0.85	0.32	66,66,66,66	0
58	MG	2A	3091	1/1	0.85	0.15	58,58,58,58	0
58	MG	2A	3822	1/1	0.85	0.12	63,63,63,63	0
58	MG	1A	3940	1/1	0.85	0.12	43,43,43,43	0
58	MG	2A	3229	1/1	0.85	0.20	41,41,41,41	0
58	MG	1A	4031	1/1	0.85	0.14	49,49,49,49	0
58	MG	2A	3842	1/1	0.85	0.15	49,49,49,49	0
58	MG	2A	3100	1/1	0.85	0.16	58,58,58,58	0
58	MG	1A	3631	1/1	0.85	0.22	61,61,61,61	0
58	MG	2a	1708	1/1	0.85	0.18	60,60,60,60	0
58	MG	2A	3594	1/1	0.85	0.16	61,61,61,61	0
58	MG	1a	1676	1/1	0.85	0.23	58,58,58,58	0
58	MG	2A	3601	1/1	0.85	0.21	58,58,58,58	0
58	MG	2A	3114	1/1	0.85	0.23	56,56,56,56	0
58	MG	1A	3801	1/1	0.85	0.14	31,31,31,31	0
58	MG	2A	3349	1/1	0.85	0.21	61,61,61,61	0
58	MG	1A	3020	1/1	0.85	0.18	46,46,46,46	0
58	MG	2A	3353	1/1	0.85	0.12	71,71,71,71	0
58	MG	2A	3123	1/1	0.85	0.17	59,59,59,59	0
58	MG	1A	3814	1/1	0.85	0.17	38,38,38,38	0
58	MG	1D	303	1/1	0.85	0.33	58,58,58,58	0
58	MG	2A	3252	1/1	0.85	0.13	61,61,61,61	0
58	MG	1A	3582	1/1	0.85	0.12	57,57,57,57	0
58	MG	2A	3141	1/1	0.85	0.18	58,58,58,58	0
58	MG	2a	1740	1/1	0.85	0.25	63,63,63,63	0
58	MG	2A	3257	1/1	0.85	0.33	69,69,69,69	0
58	MG	1a	1810	1/1	0.85	0.17	55,55,55,55	0
58	MG	1A	3974	1/1	0.85	0.12	72,72,72,72	0
58	MG	2a	1753	1/1	0.85	0.25	77,77,77,77	0
58	MG	2A	3261	1/1	0.85	0.16	57,57,57,57	0
58	MG	2a	1773	1/1	0.85	0.10	50,50,50,50	0
58	MG	1A	4074	1/1	0.85	0.18	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3975	1/1	0.85	0.12	56,56,56,56	0
58	MG	2A	3268	1/1	0.85	0.15	51,51,51,51	0
58	MG	1A	3096	1/1	0.85	0.11	40,40,40,40	0
58	MG	1I	201	1/1	0.85	0.13	55,55,55,55	0
58	MG	25	103	1/1	0.85	0.18	65,65,65,65	0
58	MG	2A	3162	1/1	0.85	0.14	58,58,58,58	0
58	MG	1A	3480	1/1	0.85	0.16	36,36,36,36	0
58	MG	1a	1627	1/1	0.85	0.12	52,52,52,52	0
58	MG	1A	3671	1/1	0.85	0.12	33,33,33,33	0
58	MG	1A	3395	1/1	0.85	0.21	51,51,51,51	0
58	MG	1A	3691	1/1	0.85	0.19	65,65,65,65	0
58	MG	1V	204	1/1	0.85	0.20	54,54,54,54	0
58	MG	2a	1800	1/1	0.85	0.29	57,57,57,57	0
58	MG	1A	4094	1/1	0.85	0.21	52,52,52,52	0
58	MG	2a	1612	1/1	0.85	0.15	59,59,59,59	0
58	MG	2A	3709	1/1	0.85	0.19	55,55,55,55	0
58	MG	2a	1806	1/1	0.85	0.21	68,68,68,68	0
58	MG	2A	3430	1/1	0.85	0.22	54,54,54,54	0
58	MG	2a	1619	1/1	0.85	0.16	61,61,61,61	0
58	MG	2a	1809	1/1	0.85	0.16	47,47,47,47	0
58	MG	2A	3714	1/1	0.85	0.16	53,53,53,53	0
58	MG	1A	3311	1/1	0.85	0.13	63,63,63,63	0
58	MG	2A	3722	1/1	0.85	0.22	68,68,68,68	0
58	MG	1A	4011	1/1	0.85	0.15	44,44,44,44	0
58	MG	2a	1631	1/1	0.85	0.17	64,64,64,64	0
58	MG	1A	3884	1/1	0.85	0.10	57,57,57,57	0
58	MG	2A	3016	1/1	0.85	0.23	51,51,51,51	0
58	MG	1a	1718	1/1	0.85	0.21	66,66,66,66	0
58	MG	2e	201	1/1	0.85	0.15	71,71,71,71	0
58	MG	1Z	304	1/1	0.85	0.17	58,58,58,58	0
58	MG	2k	201	1/1	0.85	0.13	58,58,58,58	0
58	MG	2A	3744	1/1	0.85	0.17	61,61,61,61	0
58	MG	2A	3456	1/1	0.85	0.19	54,54,54,54	0
58	MG	1A	3239	1/1	0.85	0.14	29,29,29,29	0
58	MG	2A	3038	1/1	0.85	0.24	54,54,54,54	0
58	MG	2A	3040	1/1	0.85	0.19	64,64,64,64	0
58	MG	1a	1646	1/1	0.85	0.11	42,42,42,42	0
58	MG	2A	3311	1/1	0.85	0.19	59,59,59,59	0
58	MG	1a	1654	1/1	0.85	0.20	53,53,53,53	0
58	MG	2A	3315	1/1	0.85	0.23	68,68,68,68	0
58	MG	1A	3436	1/1	0.85	0.23	56,56,56,56	0
58	MG	2x	104	1/1	0.85	0.22	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3352	1/1	0.85	0.18	62,62,62,62	0
58	MG	2A	3603	1/1	0.86	0.14	67,67,67,67	0
58	MG	2A	3836	1/1	0.86	0.11	48,48,48,48	0
58	MG	2A	3604	1/1	0.86	0.12	41,41,41,41	0
58	MG	1A	3360	1/1	0.86	0.21	52,52,52,52	0
58	MG	1A	3237	1/1	0.86	0.11	39,39,39,39	0
58	MG	2a	1683	1/1	0.86	0.24	57,57,57,57	0
58	MG	1Q	208	1/1	0.86	0.21	42,42,42,42	0
58	MG	2a	1691	1/1	0.86	0.17	50,50,50,50	0
58	MG	2A	3851	1/1	0.86	0.16	61,61,61,61	0
58	MG	1A	3104	1/1	0.86	0.19	32,32,32,32	0
58	MG	1a	1638	1/1	0.86	0.24	62,62,62,62	0
58	MG	2B	204	1/1	0.86	0.14	72,72,72,72	0
58	MG	1S	203	1/1	0.86	0.12	62,62,62,62	0
58	MG	2B	207	1/1	0.86	0.12	60,60,60,60	0
58	MG	1A	3121	1/1	0.86	0.13	39,39,39,39	0
58	MG	1A	3607	1/1	0.86	0.19	46,46,46,46	0
58	MG	1A	3479	1/1	0.86	0.24	49,49,49,49	0
58	MG	1A	3432	1/1	0.86	0.20	62,62,62,62	0
58	MG	1a	1647	1/1	0.86	0.16	58,58,58,58	0
58	MG	2a	1713	1/1	0.86	0.12	43,43,43,43	0
58	MG	1A	3248	1/1	0.86	0.13	56,56,56,56	0
58	MG	2A	3410	1/1	0.86	0.18	57,57,57,57	0
58	MG	1A	3639	1/1	0.86	0.13	55,55,55,55	0
58	MG	1A	3398	1/1	0.86	0.13	29,29,29,29	0
58	MG	2A	3079	1/1	0.86	0.16	59,59,59,59	0
58	MG	1A	3653	1/1	0.86	0.09	29,29,29,29	0
58	MG	1a	1662	1/1	0.86	0.18	55,55,55,55	0
58	MG	2a	1729	1/1	0.86	0.21	61,61,61,61	0
58	MG	1A	3060	1/1	0.86	0.13	48,48,48,48	0
58	MG	1A	3403	1/1	0.86	0.14	40,40,40,40	0
58	MG	2A	3092	1/1	0.86	0.18	70,70,70,70	0
58	MG	15	102	1/1	0.86	0.16	44,44,44,44	0
58	MG	2A	3218	1/1	0.86	0.19	51,51,51,51	0
58	MG	2A	3694	1/1	0.86	0.12	30,30,30,30	0
58	MG	2a	1744	1/1	0.86	0.13	81,81,81,81	0
58	MG	1A	3006	1/1	0.86	0.26	66,66,66,66	0
58	MG	2A	3454	1/1	0.86	0.18	47,47,47,47	0
58	MG	1a	1667	1/1	0.86	0.27	68,68,68,68	0
58	MG	1A	3407	1/1	0.86	0.17	37,37,37,37	0
58	MG	1A	3817	1/1	0.86	0.14	59,59,59,59	0
58	MG	2a	1772	1/1	0.86	0.16	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3228	1/1	0.86	0.20	52,52,52,52	0
58	MG	2A	3113	1/1	0.86	0.17	50,50,50,50	0
58	MG	2A	3717	1/1	0.86	0.14	64,64,64,64	0
58	MG	1A	3819	1/1	0.86	0.17	63,63,63,63	0
58	MG	2A	3326	1/1	0.86	0.28	66,66,66,66	0
58	MG	2a	1607	1/1	0.86	0.18	56,56,56,56	0
58	MG	2A	3726	1/1	0.86	0.13	39,39,39,39	0
58	MG	2a	1609	1/1	0.86	0.19	64,64,64,64	0
58	MG	2A	3727	1/1	0.86	0.14	63,63,63,63	0
58	MG	1A	3821	1/1	0.86	0.12	54,54,54,54	0
58	MG	1A	3689	1/1	0.86	0.12	40,40,40,40	0
58	MG	2a	1616	1/1	0.86	0.27	58,58,58,58	0
58	MG	1A	3502	1/1	0.86	0.11	51,51,51,51	0
58	MG	2A	3236	1/1	0.86	0.25	62,62,62,62	0
58	MG	2A	3742	1/1	0.86	0.11	38,38,38,38	0
58	MG	1a	1606	1/1	0.86	0.27	52,52,52,52	0
58	MG	2a	1624	1/1	0.86	0.14	60,60,60,60	0
58	MG	2A	3135	1/1	0.86	0.21	50,50,50,50	0
58	MG	2a	1629	1/1	0.86	0.14	52,52,52,52	0
58	MG	2A	3495	1/1	0.86	0.21	64,64,64,64	0
58	MG	1A	3581	1/1	0.86	0.21	32,32,32,32	0
58	MG	1l	202	1/1	0.86	0.10	58,58,58,58	0
58	MG	1a	1611	1/1	0.86	0.11	52,52,52,52	0
58	MG	1A	3854	1/1	0.86	0.14	51,51,51,51	0
58	MG	2A	3510	1/1	0.86	0.15	63,63,63,63	0
58	MG	2A	3247	1/1	0.86	0.20	60,60,60,60	0
58	MG	2A	3521	1/1	0.86	0.12	40,40,40,40	0
58	MG	2A	3527	1/1	0.86	0.09	29,29,29,29	0
58	MG	1A	3696	1/1	0.86	0.11	27,27,27,27	0
58	MG	2d	301	1/1	0.86	0.17	51,51,51,51	0
58	MG	1A	3408	1/1	0.86	0.23	56,56,56,56	0
58	MG	2a	1643	1/1	0.86	0.16	61,61,61,61	0
58	MG	2A	3540	1/1	0.86	0.12	48,48,48,48	0
58	MG	2A	3351	1/1	0.86	0.16	54,54,54,54	0
58	MG	1A	4038	1/1	0.86	0.10	48,48,48,48	0
58	MG	2A	3561	1/1	0.86	0.13	59,59,59,59	0
58	MG	1A	4041	1/1	0.86	0.17	41,41,41,41	0
58	MG	1A	3584	1/1	0.86	0.17	40,40,40,40	0
58	MG	2A	3799	1/1	0.86	0.09	34,34,34,34	0
58	MG	1A	3452	1/1	0.86	0.12	48,48,48,48	0
58	MG	1G	202	1/1	0.86	0.21	63,63,63,63	0
58	MG	2v	102	1/1	0.86	0.34	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1696	1/1	0.86	0.38	56,56,56,56	0
58	MG	1A	3711	1/1	0.86	0.12	35,35,35,35	0
58	MG	2A	3815	1/1	0.86	0.11	44,44,44,44	0
58	MG	1A	3313	1/1	0.86	0.13	45,45,45,45	0
58	MG	2A	3269	1/1	0.86	0.13	47,47,47,47	0
58	MG	1A	3848	1/1	0.87	0.11	61,61,61,61	0
58	MG	2A	3200	1/1	0.87	0.28	71,71,71,71	0
58	MG	1A	3427	1/1	0.87	0.13	50,50,50,50	0
58	MG	2A	3677	1/1	0.87	0.20	68,68,68,68	0
58	MG	1A	3367	1/1	0.87	0.16	42,42,42,42	0
58	MG	1A	3698	1/1	0.87	0.17	67,67,67,67	0
58	MG	2A	3685	1/1	0.87	0.22	59,59,59,59	0
58	MG	1A	3702	1/1	0.87	0.09	33,33,33,33	0
58	MG	2A	3210	1/1	0.87	0.21	55,55,55,55	0
58	MG	1a	1674	1/1	0.87	0.23	55,55,55,55	0
58	MG	2A	3364	1/1	0.87	0.15	59,59,59,59	0
58	MG	1A	3149	1/1	0.87	0.18	32,32,32,32	0
58	MG	1A	3180	1/1	0.87	0.21	48,48,48,48	0
58	MG	1A	4077	1/1	0.87	0.12	30,30,30,30	0
58	MG	11	105	1/1	0.87	0.12	63,63,63,63	0
58	MG	2a	1648	1/1	0.87	0.22	61,61,61,61	0
58	MG	2A	3003	1/1	0.87	0.32	56,56,56,56	0
58	MG	12	101	1/1	0.87	0.14	50,50,50,50	0
58	MG	2A	3378	1/1	0.87	0.11	55,55,55,55	0
58	MG	2A	3380	1/1	0.87	0.14	53,53,53,53	0
58	MG	2a	1653	1/1	0.87	0.15	55,55,55,55	0
58	MG	2A	3381	1/1	0.87	0.12	57,57,57,57	0
58	MG	13	104	1/1	0.87	0.13	48,48,48,48	0
58	MG	1a	1684	1/1	0.87	0.20	67,67,67,67	0
58	MG	1A	3883	1/1	0.87	0.14	36,36,36,36	0
58	MG	1A	3489	1/1	0.87	0.17	45,45,45,45	0
58	MG	1A	3181	1/1	0.87	0.10	54,54,54,54	0
58	MG	1A	3309	1/1	0.87	0.22	57,57,57,57	0
58	MG	2A	3403	1/1	0.87	0.16	46,46,46,46	0
58	MG	1A	3184	1/1	0.87	0.18	38,38,38,38	0
58	MG	1A	3594	1/1	0.87	0.29	59,59,59,59	0
58	MG	1A	3350	1/1	0.87	0.24	59,59,59,59	0
58	MG	1A	3351	1/1	0.87	0.20	59,59,59,59	0
58	MG	2A	3239	1/1	0.87	0.27	68,68,68,68	0
58	MG	1a	1695	1/1	0.87	0.19	55,55,55,55	0
58	MG	2A	3414	1/1	0.87	0.31	64,64,64,64	0
58	MG	1A	3726	1/1	0.87	0.14	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3060	1/1	0.87	0.17	62,62,62,62	0
58	MG	2A	3062	1/1	0.87	0.23	59,59,59,59	0
58	MG	2A	3245	1/1	0.87	0.18	49,49,49,49	0
58	MG	2A	3063	1/1	0.87	0.15	60,60,60,60	0
58	MG	2A	3064	1/1	0.87	0.21	63,63,63,63	0
58	MG	1a	1603	1/1	0.87	0.13	53,53,53,53	0
58	MG	2A	3077	1/1	0.87	0.12	47,47,47,47	0
58	MG	2a	1707	1/1	0.87	0.23	66,66,66,66	0
58	MG	1a	1699	1/1	0.87	0.20	48,48,48,48	0
58	MG	2A	3448	1/1	0.87	0.16	68,68,68,68	0
58	MG	1A	3404	1/1	0.87	0.19	54,54,54,54	0
58	MG	1B	208	1/1	0.87	0.14	60,60,60,60	0
58	MG	1a	1709	1/1	0.87	0.19	56,56,56,56	0
58	MG	1A	3129	1/1	0.87	0.13	37,37,37,37	0
58	MG	2A	3263	1/1	0.87	0.17	66,66,66,66	0
58	MG	1A	3962	1/1	0.87	0.10	58,58,58,58	0
58	MG	2A	3267	1/1	0.87	0.14	64,64,64,64	0
58	MG	1A	3524	1/1	0.87	0.13	47,47,47,47	0
58	MG	1B	216	1/1	0.87	0.14	65,65,65,65	0
58	MG	2a	1726	1/1	0.87	0.16	57,57,57,57	0
58	MG	2A	3470	1/1	0.87	0.20	54,54,54,54	0
58	MG	1A	3744	1/1	0.87	0.14	47,47,47,47	0
58	MG	1A	3195	1/1	0.87	0.14	38,38,38,38	0
58	MG	2A	3480	1/1	0.87	0.10	45,45,45,45	0
58	MG	2A	3107	1/1	0.87	0.28	62,62,62,62	0
58	MG	1A	3984	1/1	0.87	0.12	23,23,23,23	0
58	MG	1a	1728	1/1	0.87	0.10	64,64,64,64	0
58	MG	2a	1742	1/1	0.87	0.11	55,55,55,55	0
58	MG	1a	1729	1/1	0.87	0.12	55,55,55,55	0
58	MG	1B	227	1/1	0.87	0.14	46,46,46,46	0
58	MG	1A	3752	1/1	0.87	0.12	55,55,55,55	0
58	MG	1A	3354	1/1	0.87	0.19	59,59,59,59	0
58	MG	1A	3287	1/1	0.87	0.14	53,53,53,53	0
58	MG	2a	1759	1/1	0.87	0.15	63,63,63,63	0
58	MG	1a	1747	1/1	0.87	0.21	66,66,66,66	0
58	MG	2B	205	1/1	0.87	0.13	59,59,59,59	0
58	MG	1A	3536	1/1	0.87	0.26	55,55,55,55	0
58	MG	2A	3512	1/1	0.87	0.20	50,50,50,50	0
58	MG	2B	208	1/1	0.87	0.18	55,55,55,55	0
58	MG	1A	4009	1/1	0.87	0.08	40,40,40,40	0
58	MG	2a	1778	1/1	0.87	0.15	67,67,67,67	0
58	MG	2A	3518	1/1	0.87	0.16	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
58	MG	1A	3772	1/1	0.87	0.11	29,29,29,29	0
58	MG	1A	3776	1/1	0.87	0.11	60,60,60,60	0
58	MG	2A	3528	1/1	0.87	0.20	63,63,63,63	0
58	MG	1A	3323	1/1	0.87	0.11	38,38,38,38	0
58	MG	2A	3146	1/1	0.87	0.14	52,52,52,52	0
58	MG	1a	1771	1/1	0.87	0.13	45,45,45,45	0
58	MG	1E	311	1/1	0.87	0.16	43,43,43,43	0
58	MG	2A	3551	1/1	0.87	0.10	65,65,65,65	0
58	MG	1a	1776	1/1	0.87	0.14	43,43,43,43	0
58	MG	2a	1799	1/1	0.87	0.21	62,62,62,62	0
58	MG	1a	1784	1/1	0.87	0.10	52,52,52,52	0
58	MG	2A	3567	1/1	0.87	0.14	49,49,49,49	0
58	MG	2A	3570	1/1	0.87	0.16	67,67,67,67	0
58	MG	1E	312	1/1	0.87	0.13	50,50,50,50	0
58	MG	1A	3035	1/1	0.87	0.18	44,44,44,44	0
58	MG	2A	3577	1/1	0.87	0.21	73,73,73,73	0
58	MG	1A	3655	1/1	0.87	0.15	65,65,65,65	0
58	MG	1G	204	1/1	0.87	0.12	59,59,59,59	0
58	MG	1A	4020	1/1	0.87	0.09	52,52,52,52	0
58	MG	1a	1652	1/1	0.87	0.23	61,61,61,61	0
58	MG	2A	3323	1/1	0.87	0.22	66,66,66,66	0
58	MG	1a	1806	1/1	0.87	0.10	54,54,54,54	0
58	MG	1A	3472	1/1	0.87	0.14	51,51,51,51	0
58	MG	1A	3544	1/1	0.87	0.29	64,64,64,64	0
58	MG	2A	3608	1/1	0.87	0.12	34,34,34,34	0
58	MG	1A	3548	1/1	0.87	0.16	64,64,64,64	0
58	MG	1Q	207	1/1	0.87	0.21	58,58,58,58	0
58	MG	2a	1606	1/1	0.87	0.24	59,59,59,59	0
58	MG	1A	4034	1/1	0.87	0.16	42,42,42,42	0
58	MG	2A	3187	1/1	0.87	0.18	59,59,59,59	0
58	MG	1e	201	1/1	0.87	0.10	63,63,63,63	0
58	MG	2A	3192	1/1	0.87	0.18	48,48,48,48	0
58	MG	2A	3637	1/1	0.87	0.15	46,46,46,46	0
58	MG	2A	3333	1/1	0.87	0.36	50,50,50,50	0
58	MG	2A	3641	1/1	0.87	0.14	57,57,57,57	0
58	MG	1f	202	1/1	0.87	0.27	60,60,60,60	0
58	MG	2a	1618	1/1	0.87	0.27	73,73,73,73	0
58	MG	1A	3476	1/1	0.87	0.16	58,58,58,58	0
58	MG	1A	3415	1/1	0.87	0.19	69,69,69,69	0
58	MG	2v	104	1/1	0.87	0.15	62,62,62,62	0
58	MG	1t	201	1/1	0.87	0.11	49,49,49,49	0
58	MG	1A	3206	1/1	0.87	0.17	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3343	1/1	0.87	0.14	63,63,63,63	0
58	MG	2A	3344	1/1	0.87	0.24	62,62,62,62	0
58	MG	1a	1691	1/1	0.88	0.23	49,49,49,49	0
58	MG	2A	3751	1/1	0.88	0.16	56,56,56,56	0
58	MG	1A	3370	1/1	0.88	0.15	49,49,49,49	0
58	MG	1A	3813	1/1	0.88	0.13	56,56,56,56	0
58	MG	1A	3419	1/1	0.88	0.15	49,49,49,49	0
58	MG	2A	3770	1/1	0.88	0.13	60,60,60,60	0
58	MG	2a	1655	1/1	0.88	0.20	56,56,56,56	0
58	MG	2A	3314	1/1	0.88	0.21	70,70,70,70	0
58	MG	2A	3494	1/1	0.88	0.26	58,58,58,58	0
58	MG	1a	1609	1/1	0.88	0.15	57,57,57,57	0
58	MG	2A	3497	1/1	0.88	0.18	46,46,46,46	0
58	MG	2a	1666	1/1	0.88	0.23	58,58,58,58	0
58	MG	2A	3190	1/1	0.88	0.10	49,49,49,49	0
58	MG	1A	3135	1/1	0.88	0.12	53,53,53,53	0
58	MG	1A	3597	1/1	0.88	0.12	45,45,45,45	0
58	MG	1A	4007	1/1	0.88	0.12	33,33,33,33	0
58	MG	2A	3014	1/1	0.88	0.17	38,38,38,38	0
58	MG	1A	3382	1/1	0.88	0.15	48,48,48,48	0
58	MG	1a	1706	1/1	0.88	0.28	63,63,63,63	0
58	MG	2a	1682	1/1	0.88	0.26	60,60,60,60	0
58	MG	2A	3793	1/1	0.88	0.11	46,46,46,46	0
58	MG	2a	1685	1/1	0.88	0.24	54,54,54,54	0
58	MG	1B	235	1/1	0.88	0.14	70,70,70,70	0
58	MG	2A	3199	1/1	0.88	0.14	47,47,47,47	0
58	MG	1A	3823	1/1	0.88	0.10	39,39,39,39	0
58	MG	1A	3227	1/1	0.88	0.12	24,24,24,24	0
58	MG	1A	3840	1/1	0.88	0.07	37,37,37,37	0
58	MG	2A	3206	1/1	0.88	0.21	53,53,53,53	0
58	MG	1A	3843	1/1	0.88	0.15	58,58,58,58	0
58	MG	2A	3208	1/1	0.88	0.18	60,60,60,60	0
58	MG	2A	3550	1/1	0.88	0.17	51,51,51,51	0
58	MG	2A	3833	1/1	0.88	0.12	52,52,52,52	0
58	MG	1A	4018	1/1	0.88	0.12	49,49,49,49	0
58	MG	1A	3231	1/1	0.88	0.16	40,40,40,40	0
58	MG	2A	3838	1/1	0.88	0.17	60,60,60,60	0
58	MG	1A	3158	1/1	0.88	0.12	50,50,50,50	0
58	MG	2A	3048	1/1	0.88	0.14	57,57,57,57	0
58	MG	2A	3050	1/1	0.88	0.18	58,58,58,58	0
58	MG	2a	1716	1/1	0.88	0.27	53,53,53,53	0
58	MG	2A	3847	1/1	0.88	0.13	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
58	MG	1A	3197	1/1	0.88	0.09	36,36,36,36	0
58	MG	1A	3626	1/1	0.88	0.10	26,26,26,26	0
58	MG	2a	1722	1/1	0.88	0.27	58,58,58,58	0
58	MG	1F	306	1/1	0.88	0.07	28,28,28,28	0
58	MG	1A	4027	1/1	0.88	0.10	47,47,47,47	0
58	MG	1a	1735	1/1	0.88	0.25	61,61,61,61	0
58	MG	1A	3308	1/1	0.88	0.35	64,64,64,64	0
58	MG	1A	4033	1/1	0.88	0.10	41,41,41,41	0
58	MG	2A	3600	1/1	0.88	0.14	58,58,58,58	0
58	MG	1A	3724	1/1	0.88	0.21	50,50,50,50	0
58	MG	2A	3232	1/1	0.88	0.17	47,47,47,47	0
58	MG	1a	1746	1/1	0.88	0.10	57,57,57,57	0
58	MG	1A	3438	1/1	0.88	0.14	51,51,51,51	0
58	MG	1a	1752	1/1	0.88	0.21	67,67,67,67	0
58	MG	2B	218	1/1	0.88	0.15	70,70,70,70	0
58	MG	2A	3367	1/1	0.88	0.13	54,54,54,54	0
58	MG	1A	3872	1/1	0.88	0.14	42,42,42,42	0
58	MG	1A	3336	1/1	0.88	0.16	53,53,53,53	0
58	MG	1a	1759	1/1	0.88	0.19	61,61,61,61	0
58	MG	1A	3881	1/1	0.88	0.17	42,42,42,42	0
58	MG	1A	3641	1/1	0.88	0.08	19,19,19,19	0
58	MG	2a	1764	1/1	0.88	0.13	74,74,74,74	0
58	MG	2a	1767	1/1	0.88	0.12	61,61,61,61	0
58	MG	2F	303	1/1	0.88	0.11	58,58,58,58	0
58	MG	2A	3097	1/1	0.88	0.23	55,55,55,55	0
58	MG	1a	1768	1/1	0.88	0.11	62,62,62,62	0
58	MG	1A	3552	1/1	0.88	0.28	49,49,49,49	0
58	MG	2A	3104	1/1	0.88	0.14	58,58,58,58	0
58	MG	1U	206	1/1	0.88	0.15	44,44,44,44	0
58	MG	1A	3885	1/1	0.88	0.13	38,38,38,38	0
58	MG	2A	3651	1/1	0.88	0.14	63,63,63,63	0
58	MG	2A	3652	1/1	0.88	0.12	49,49,49,49	0
58	MG	1A	4062	1/1	0.88	0.12	18,18,18,18	0
58	MG	2A	3110	1/1	0.88	0.16	50,50,50,50	0
58	MG	1a	1779	1/1	0.88	0.14	55,55,55,55	0
58	MG	1Y	201	1/1	0.88	0.14	49,49,49,49	0
58	MG	2A	3405	1/1	0.88	0.13	51,51,51,51	0
58	MG	2a	1791	1/1	0.88	0.17	75,75,75,75	0
58	MG	1A	3405	1/1	0.88	0.13	41,41,41,41	0
58	MG	2A	3260	1/1	0.88	0.12	58,58,58,58	0
58	MG	1A	3340	1/1	0.88	0.12	51,51,51,51	0
58	MG	1a	1789	1/1	0.88	0.11	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
58	MG	1a	1792	1/1	0.88	0.11	79,79,79,79	0
58	MG	2A	3129	1/1	0.88	0.17	41,41,41,41	0
58	MG	2A	3131	1/1	0.88	0.19	72,72,72,72	0
58	MG	1A	3908	1/1	0.88	0.17	51,51,51,51	0
58	MG	1A	3919	1/1	0.88	0.13	34,34,34,34	0
58	MG	2A	3271	1/1	0.88	0.23	60,60,60,60	0
58	MG	2a	1614	1/1	0.88	0.15	58,58,58,58	0
58	MG	2A	3426	1/1	0.88	0.15	50,50,50,50	0
58	MG	1A	3341	1/1	0.88	0.24	39,39,39,39	0
58	MG	1A	3504	1/1	0.88	0.16	48,48,48,48	0
58	MG	2a	1814	1/1	0.88	0.17	52,52,52,52	0
58	MG	2A	3699	1/1	0.88	0.17	57,57,57,57	0
58	MG	1A	3761	1/1	0.88	0.23	51,51,51,51	0
58	MG	1A	3762	1/1	0.88	0.16	49,49,49,49	0
58	MG	2A	3706	1/1	0.88	0.10	49,49,49,49	0
58	MG	2a	1819	1/1	0.88	0.10	56,56,56,56	0
58	MG	1a	1675	1/1	0.88	0.15	44,44,44,44	0
58	MG	2a	1627	1/1	0.88	0.25	66,66,66,66	0
58	MG	1A	3506	1/1	0.88	0.14	49,49,49,49	0
58	MG	13	102	1/1	0.88	0.14	37,37,37,37	0
58	MG	2i	201	1/1	0.88	0.22	61,61,61,61	0
58	MG	2A	3283	1/1	0.88	0.17	62,62,62,62	0
58	MG	2A	3718	1/1	0.88	0.24	62,62,62,62	0
58	MG	1A	3017	1/1	0.88	0.21	59,59,59,59	0
58	MG	2A	3455	1/1	0.88	0.17	59,59,59,59	0
58	MG	2A	3725	1/1	0.88	0.10	54,54,54,54	0
58	MG	1A	3362	1/1	0.88	0.18	61,61,61,61	0
58	MG	1A	3958	1/1	0.88	0.16	43,43,43,43	0
58	MG	1A	3961	1/1	0.88	0.09	41,41,41,41	0
58	MG	1A	3583	1/1	0.88	0.10	29,29,29,29	0
58	MG	1A	3966	1/1	0.88	0.12	51,51,51,51	0
58	MG	1A	3182	1/1	0.88	0.18	72,72,72,72	0
58	MG	2A	3468	1/1	0.88	0.14	56,56,56,56	0
58	MG	2w	102	1/1	0.88	0.12	62,62,62,62	0
58	MG	1A	3795	1/1	0.88	0.12	68,68,68,68	0
58	MG	2w	104	1/1	0.88	0.14	70,70,70,70	0
58	MG	1w	106	1/1	0.88	0.15	71,71,71,71	0
58	MG	1B	214	1/1	0.88	0.11	61,61,61,61	0
58	MG	1A	3142	1/1	0.88	0.12	42,42,42,42	0
58	MG	1A	3518	1/1	0.89	0.23	40,40,40,40	0
58	MG	2A	3654	1/1	0.89	0.16	68,68,68,68	0
58	MG	2a	1621	1/1	0.89	0.31	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
58	MG	1B	211	1/1	0.89	0.12	50,50,50,50	0
58	MG	1A	3076	1/1	0.89	0.09	27,27,27,27	0
58	MG	2a	1626	1/1	0.89	0.20	65,65,65,65	0
58	MG	2A	3659	1/1	0.89	0.13	55,55,55,55	0
58	MG	2A	3660	1/1	0.89	0.14	59,59,59,59	0
58	MG	2A	3379	1/1	0.89	0.24	57,57,57,57	0
58	MG	1a	1613	1/1	0.89	0.09	47,47,47,47	0
58	MG	1A	3804	1/1	0.89	0.09	44,44,44,44	0
58	MG	2a	1633	1/1	0.89	0.23	54,54,54,54	0
58	MG	2A	3061	1/1	0.89	0.16	66,66,66,66	0
58	MG	1a	1727	1/1	0.89	0.11	52,52,52,52	0
58	MG	2A	3676	1/1	0.89	0.09	40,40,40,40	0
58	MG	1A	3585	1/1	0.89	0.10	48,48,48,48	0
58	MG	1A	3809	1/1	0.89	0.10	21,21,21,21	0
58	MG	2A	3070	1/1	0.89	0.13	55,55,55,55	0
58	MG	2A	3394	1/1	0.89	0.20	54,54,54,54	0
58	MG	1A	3329	1/1	0.89	0.16	45,45,45,45	0
58	MG	2A	3688	1/1	0.89	0.10	59,59,59,59	0
58	MG	2A	3397	1/1	0.89	0.23	46,46,46,46	0
58	MG	2A	3074	1/1	0.89	0.13	40,40,40,40	0
58	MG	1B	221	1/1	0.89	0.12	45,45,45,45	0
58	MG	2A	3693	1/1	0.89	0.16	66,66,66,66	0
58	MG	1A	3460	1/1	0.89	0.17	40,40,40,40	0
58	MG	1A	3701	1/1	0.89	0.09	36,36,36,36	0
58	MG	1A	3818	1/1	0.89	0.09	53,53,53,53	0
58	MG	1a	1743	1/1	0.89	0.14	54,54,54,54	0
58	MG	1a	1745	1/1	0.89	0.10	52,52,52,52	0
58	MG	2A	3412	1/1	0.89	0.10	49,49,49,49	0
58	MG	1A	3384	1/1	0.89	0.13	47,47,47,47	0
58	MG	1a	1629	1/1	0.89	0.25	55,55,55,55	0
58	MG	2A	3415	1/1	0.89	0.29	56,56,56,56	0
58	MG	2a	1659	1/1	0.89	0.22	71,71,71,71	0
58	MG	2A	3417	1/1	0.89	0.25	52,52,52,52	0
58	MG	1a	1751	1/1	0.89	0.10	45,45,45,45	0
58	MG	2a	1663	1/1	0.89	0.18	53,53,53,53	0
58	MG	1A	3986	1/1	0.89	0.13	38,38,38,38	0
58	MG	1A	3417	1/1	0.89	0.26	42,42,42,42	0
58	MG	1B	234	1/1	0.89	0.11	41,41,41,41	0
58	MG	2A	3428	1/1	0.89	0.17	51,51,51,51	0
58	MG	1A	3596	1/1	0.89	0.14	54,54,54,54	0
58	MG	2a	1676	1/1	0.89	0.12	57,57,57,57	0
58	MG	1A	3256	1/1	0.89	0.12	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
58	MG	2A	3436	1/1	0.89	0.12	43,43,43,43	0
58	MG	2a	1679	1/1	0.89	0.14	54,54,54,54	0
58	MG	1a	1762	1/1	0.89	0.21	71,71,71,71	0
58	MG	2A	3734	1/1	0.89	0.20	50,50,50,50	0
58	MG	1A	3386	1/1	0.89	0.18	38,38,38,38	0
58	MG	1D	307	1/1	0.89	0.13	42,42,42,42	0
58	MG	1A	3841	1/1	0.89	0.13	51,51,51,51	0
58	MG	2A	3447	1/1	0.89	0.15	48,48,48,48	0
58	MG	1a	1770	1/1	0.89	0.11	62,62,62,62	0
58	MG	2A	3451	1/1	0.89	0.14	40,40,40,40	0
58	MG	2A	3270	1/1	0.89	0.14	58,58,58,58	0
58	MG	1A	3392	1/1	0.89	0.23	37,37,37,37	0
58	MG	2A	3119	1/1	0.89	0.13	55,55,55,55	0
58	MG	2A	3273	1/1	0.89	0.18	73,73,73,73	0
58	MG	1A	3429	1/1	0.89	0.17	62,62,62,62	0
58	MG	1a	1645	1/1	0.89	0.15	55,55,55,55	0
58	MG	2A	3762	1/1	0.89	0.16	66,66,66,66	0
58	MG	2A	3462	1/1	0.89	0.16	53,53,53,53	0
58	MG	1a	1777	1/1	0.89	0.10	50,50,50,50	0
58	MG	2A	3775	1/1	0.89	0.17	54,54,54,54	0
58	MG	2A	3279	1/1	0.89	0.18	49,49,49,49	0
58	MG	1A	3606	1/1	0.89	0.13	54,54,54,54	0
58	MG	2A	3134	1/1	0.89	0.26	57,57,57,57	0
58	MG	1A	3851	1/1	0.89	0.11	44,44,44,44	0
58	MG	1A	3539	1/1	0.89	0.21	50,50,50,50	0
58	MG	1A	3853	1/1	0.89	0.15	55,55,55,55	0
58	MG	2A	3472	1/1	0.89	0.11	56,56,56,56	0
58	MG	2A	3786	1/1	0.89	0.12	70,70,70,70	0
58	MG	1A	3610	1/1	0.89	0.13	51,51,51,51	0
58	MG	2A	3478	1/1	0.89	0.19	54,54,54,54	0
58	MG	1A	3614	1/1	0.89	0.11	54,54,54,54	0
58	MG	1A	3868	1/1	0.89	0.11	44,44,44,44	0
58	MG	1H	201	1/1	0.89	0.15	42,42,42,42	0
58	MG	1A	3301	1/1	0.89	0.20	43,43,43,43	0
58	MG	2A	3488	1/1	0.89	0.17	61,61,61,61	0
58	MG	2A	3804	1/1	0.89	0.12	49,49,49,49	0
58	MG	2A	3155	1/1	0.89	0.09	33,33,33,33	0
58	MG	1N	205	1/1	0.89	0.14	45,45,45,45	0
58	MG	2A	3158	1/1	0.89	0.09	37,37,37,37	0
58	MG	1A	3622	1/1	0.89	0.09	10,10,10,10	0
58	MG	1A	3235	1/1	0.89	0.27	32,32,32,32	0
58	MG	1A	3873	1/1	0.89	0.11	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3827	1/1	0.89	0.09	41,41,41,41	0
58	MG	2A	3504	1/1	0.89	0.12	35,35,35,35	0
58	MG	1A	3107	1/1	0.89	0.11	24,24,24,24	0
58	MG	2a	1755	1/1	0.89	0.08	41,41,41,41	0
58	MG	2A	3507	1/1	0.89	0.11	49,49,49,49	0
58	MG	1A	3402	1/1	0.89	0.14	48,48,48,48	0
58	MG	2a	1765	1/1	0.89	0.14	60,60,60,60	0
58	MG	1A	3635	1/1	0.89	0.08	47,47,47,47	0
58	MG	2A	3511	1/1	0.89	0.11	35,35,35,35	0
58	MG	1a	1672	1/1	0.89	0.10	50,50,50,50	0
58	MG	1A	4042	1/1	0.89	0.10	28,28,28,28	0
58	MG	2A	3177	1/1	0.89	0.15	47,47,47,47	0
58	MG	2A	3519	1/1	0.89	0.11	49,49,49,49	0
58	MG	1A	4044	1/1	0.89	0.15	38,38,38,38	0
58	MG	1A	3747	1/1	0.89	0.10	19,19,19,19	0
58	MG	1A	3166	1/1	0.89	0.09	28,28,28,28	0
58	MG	2A	3530	1/1	0.89	0.09	32,32,32,32	0
58	MG	1A	3359	1/1	0.89	0.15	59,59,59,59	0
58	MG	1A	3493	1/1	0.89	0.14	43,43,43,43	0
58	MG	1w	105	1/1	0.89	0.19	64,64,64,64	0
58	MG	1A	3890	1/1	0.89	0.09	33,33,33,33	0
58	MG	2A	3188	1/1	0.89	0.15	51,51,51,51	0
58	MG	1A	3899	1/1	0.89	0.09	20,20,20,20	0
58	MG	1A	3902	1/1	0.89	0.17	41,41,41,41	0
58	MG	1A	3906	1/1	0.89	0.13	52,52,52,52	0
58	MG	2A	3564	1/1	0.89	0.15	40,40,40,40	0
58	MG	1A	3055	1/1	0.89	0.12	43,43,43,43	0
58	MG	1A	3766	1/1	0.89	0.12	25,25,25,25	0
58	MG	2a	1802	1/1	0.89	0.12	68,68,68,68	0
58	MG	1A	4082	1/1	0.89	0.16	56,56,56,56	0
58	MG	1l	106	1/1	0.89	0.14	51,51,51,51	0
58	MG	2E	308	1/1	0.89	0.13	50,50,50,50	0
58	MG	2E	309	1/1	0.89	0.11	48,48,48,48	0
58	MG	2A	3576	1/1	0.89	0.09	52,52,52,52	0
58	MG	1A	4083	1/1	0.89	0.16	50,50,50,50	0
58	MG	1A	3213	1/1	0.89	0.12	58,58,58,58	0
58	MG	1A	3931	1/1	0.89	0.17	50,50,50,50	0
58	MG	2N	201	1/1	0.89	0.15	51,51,51,51	0
58	MG	2a	1813	1/1	0.89	0.15	54,54,54,54	0
58	MG	2A	3593	1/1	0.89	0.12	50,50,50,50	0
58	MG	2A	3004	1/1	0.89	0.18	45,45,45,45	0
58	MG	2R	202	1/1	0.89	0.18	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3341	1/1	0.89	0.18	54,54,54,54	0
58	MG	2A	3598	1/1	0.89	0.20	50,50,50,50	0
58	MG	2A	3342	1/1	0.89	0.27	63,63,63,63	0
58	MG	2A	3005	1/1	0.89	0.18	54,54,54,54	0
58	MG	1A	3130	1/1	0.89	0.15	57,57,57,57	0
58	MG	2W	201	1/1	0.89	0.20	61,61,61,61	0
58	MG	1A	3448	1/1	0.89	0.17	55,55,55,55	0
58	MG	1A	4092	1/1	0.89	0.25	56,56,56,56	0
58	MG	27	102	1/1	0.89	0.14	52,52,52,52	0
58	MG	2A	3350	1/1	0.89	0.18	68,68,68,68	0
58	MG	2A	3018	1/1	0.89	0.17	64,64,64,64	0
58	MG	1A	3251	1/1	0.89	0.16	59,59,59,59	0
58	MG	2A	3027	1/1	0.89	0.19	58,58,58,58	0
58	MG	1A	3945	1/1	0.89	0.12	30,30,30,30	0
58	MG	1A	4098	1/1	0.89	0.14	56,56,56,56	0
58	MG	2A	3618	1/1	0.89	0.09	45,45,45,45	0
58	MG	2r	101	1/1	0.89	0.15	63,63,63,63	0
58	MG	2A	3623	1/1	0.89	0.16	34,34,34,34	0
58	MG	2A	3358	1/1	0.89	0.11	52,52,52,52	0
58	MG	1a	1705	1/1	0.89	0.16	57,57,57,57	0
58	MG	2A	3216	1/1	0.89	0.16	52,52,52,52	0
58	MG	1A	3784	1/1	0.89	0.15	35,35,35,35	0
58	MG	1A	3178	1/1	0.89	0.17	36,36,36,36	0
58	MG	2A	3645	1/1	0.89	0.28	66,66,66,66	0
58	MG	1B	202	1/1	0.89	0.15	52,52,52,52	0
58	MG	1B	204	1/1	0.89	0.23	59,59,59,59	0
58	MG	1A	3950	1/1	0.89	0.10	57,57,57,57	0
58	MG	1U	202	1/1	0.90	0.22	46,46,46,46	0
58	MG	2A	3461	1/1	0.90	0.08	38,38,38,38	0
58	MG	1A	3618	1/1	0.90	0.13	39,39,39,39	0
58	MG	1A	4051	1/1	0.90	0.19	59,59,59,59	0
58	MG	2A	3715	1/1	0.90	0.12	62,62,62,62	0
58	MG	2A	3167	1/1	0.90	0.15	37,37,37,37	0
58	MG	1A	3467	1/1	0.90	0.11	37,37,37,37	0
58	MG	2A	3171	1/1	0.90	0.24	54,54,54,54	0
58	MG	2A	3721	1/1	0.90	0.12	55,55,55,55	0
58	MG	1A	3088	1/1	0.90	0.13	32,32,32,32	0
58	MG	1x	101	1/1	0.90	0.20	66,66,66,66	0
58	MG	1a	1683	1/1	0.90	0.18	57,57,57,57	0
58	MG	1x	103	1/1	0.90	0.09	53,53,53,53	0
58	MG	2A	3728	1/1	0.90	0.17	49,49,49,49	0
58	MG	1A	3416	1/1	0.90	0.10	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
58	MG	2A	3476	1/1	0.90	0.11	50,50,50,50	0
58	MG	2A	3477	1/1	0.90	0.23	64,64,64,64	0
58	MG	1A	3372	1/1	0.90	0.21	54,54,54,54	0
58	MG	2A	3736	1/1	0.90	0.14	51,51,51,51	0
58	MG	1A	3543	1/1	0.90	0.17	54,54,54,54	0
58	MG	1A	3900	1/1	0.90	0.14	66,66,66,66	0
58	MG	1A	3474	1/1	0.90	0.12	42,42,42,42	0
58	MG	1A	3545	1/1	0.90	0.15	54,54,54,54	0
58	MG	1I	103	1/1	0.90	0.12	41,41,41,41	0
58	MG	2A	3490	1/1	0.90	0.11	56,56,56,56	0
58	MG	2A	3491	1/1	0.90	0.31	59,59,59,59	0
58	MG	1A	3642	1/1	0.90	0.10	49,49,49,49	0
58	MG	1A	3911	1/1	0.90	0.15	49,49,49,49	0
58	MG	1A	3373	1/1	0.90	0.13	47,47,47,47	0
58	MG	1A	3924	1/1	0.90	0.11	64,64,64,64	0
58	MG	2A	3761	1/1	0.90	0.11	44,44,44,44	0
58	MG	1A	3774	1/1	0.90	0.10	30,30,30,30	0
58	MG	1A	3775	1/1	0.90	0.07	22,22,22,22	0
58	MG	1A	3645	1/1	0.90	0.13	56,56,56,56	0
58	MG	1A	4091	1/1	0.90	0.14	44,44,44,44	0
58	MG	1A	3781	1/1	0.90	0.11	45,45,45,45	0
58	MG	1A	3089	1/1	0.90	0.20	40,40,40,40	0
58	MG	1A	3791	1/1	0.90	0.07	52,52,52,52	0
58	MG	1A	4096	1/1	0.90	0.09	40,40,40,40	0
58	MG	1A	3004	1/1	0.90	0.18	36,36,36,36	0
58	MG	1A	3068	1/1	0.90	0.08	27,27,27,27	0
58	MG	2A	3338	1/1	0.90	0.17	59,59,59,59	0
58	MG	2A	3785	1/1	0.90	0.16	65,65,65,65	0
58	MG	2a	1686	1/1	0.90	0.19	56,56,56,56	0
58	MG	1A	3430	1/1	0.90	0.12	59,59,59,59	0
58	MG	1B	201	1/1	0.90	0.16	45,45,45,45	0
58	MG	2A	3522	1/1	0.90	0.16	61,61,61,61	0
58	MG	2A	3790	1/1	0.90	0.14	55,55,55,55	0
58	MG	2A	3525	1/1	0.90	0.12	37,37,37,37	0
58	MG	1a	1605	1/1	0.90	0.11	50,50,50,50	0
58	MG	2A	3797	1/1	0.90	0.12	47,47,47,47	0
58	MG	1A	3952	1/1	0.90	0.09	52,52,52,52	0
58	MG	1A	3953	1/1	0.90	0.13	48,48,48,48	0
58	MG	1A	3955	1/1	0.90	0.09	48,48,48,48	0
58	MG	2A	3532	1/1	0.90	0.18	52,52,52,52	0
58	MG	2A	3535	1/1	0.90	0.21	62,62,62,62	0
58	MG	2A	3348	1/1	0.90	0.13	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
58	MG	2a	1710	1/1	0.90	0.22	59,59,59,59	0
58	MG	2A	3054	1/1	0.90	0.17	63,63,63,63	0
58	MG	1A	3802	1/1	0.90	0.14	24,24,24,24	0
58	MG	2a	1714	1/1	0.90	0.14	59,59,59,59	0
58	MG	2A	3547	1/1	0.90	0.10	46,46,46,46	0
58	MG	2A	3058	1/1	0.90	0.10	38,38,38,38	0
58	MG	1A	3561	1/1	0.90	0.16	38,38,38,38	0
58	MG	1A	3675	1/1	0.90	0.10	39,39,39,39	0
58	MG	1a	1617	1/1	0.90	0.11	41,41,41,41	0
58	MG	1a	1618	1/1	0.90	0.11	53,53,53,53	0
58	MG	2A	3357	1/1	0.90	0.18	54,54,54,54	0
58	MG	1A	3807	1/1	0.90	0.17	46,46,46,46	0
58	MG	1A	3041	1/1	0.90	0.09	33,33,33,33	0
58	MG	2A	3844	1/1	0.90	0.19	59,59,59,59	0
58	MG	1A	3969	1/1	0.90	0.23	53,53,53,53	0
58	MG	1A	3001	1/1	0.90	0.09	34,34,34,34	0
58	MG	2A	3848	1/1	0.90	0.17	59,59,59,59	0
58	MG	1A	3057	1/1	0.90	0.12	44,44,44,44	0
58	MG	1A	3262	1/1	0.90	0.17	68,68,68,68	0
58	MG	2A	3581	1/1	0.90	0.22	58,58,58,58	0
58	MG	2A	3585	1/1	0.90	0.17	59,59,59,59	0
58	MG	1A	3977	1/1	0.90	0.11	43,43,43,43	0
58	MG	1A	3978	1/1	0.90	0.10	65,65,65,65	0
58	MG	1a	1755	1/1	0.90	0.09	42,42,42,42	0
58	MG	2A	3376	1/1	0.90	0.24	57,57,57,57	0
58	MG	2B	210	1/1	0.90	0.18	75,75,75,75	0
58	MG	2a	1751	1/1	0.90	0.12	64,64,64,64	0
58	MG	2a	1752	1/1	0.90	0.15	69,69,69,69	0
58	MG	1A	3118	1/1	0.90	0.11	29,29,29,29	0
58	MG	2A	3599	1/1	0.90	0.15	56,56,56,56	0
58	MG	2a	1758	1/1	0.90	0.10	66,66,66,66	0
58	MG	1A	3312	1/1	0.90	0.10	43,43,43,43	0
58	MG	1A	3700	1/1	0.90	0.09	47,47,47,47	0
58	MG	2A	3093	1/1	0.90	0.13	43,43,43,43	0
58	MG	2a	1766	1/1	0.90	0.10	65,65,65,65	0
58	MG	2A	3095	1/1	0.90	0.24	64,64,64,64	0
58	MG	1A	3233	1/1	0.90	0.20	44,44,44,44	0
58	MG	1A	3824	1/1	0.90	0.10	39,39,39,39	0
58	MG	2D	304	1/1	0.90	0.13	55,55,55,55	0
58	MG	1A	3086	1/1	0.90	0.15	28,28,28,28	0
58	MG	2A	3248	1/1	0.90	0.16	48,48,48,48	0
58	MG	2A	3249	1/1	0.90	0.19	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2E	304	1/1	0.90	0.20	65,65,65,65	0
58	MG	2A	3393	1/1	0.90	0.15	39,39,39,39	0
58	MG	2a	1780	1/1	0.90	0.20	67,67,67,67	0
58	MG	2A	3251	1/1	0.90	0.26	63,63,63,63	0
58	MG	1A	4005	1/1	0.90	0.07	26,26,26,26	0
58	MG	2A	3103	1/1	0.90	0.20	56,56,56,56	0
58	MG	2a	1785	1/1	0.90	0.14	60,60,60,60	0
58	MG	2A	3400	1/1	0.90	0.35	60,60,60,60	0
58	MG	1A	3703	1/1	0.90	0.15	29,29,29,29	0
58	MG	1A	3194	1/1	0.90	0.30	51,51,51,51	0
58	MG	1A	3445	1/1	0.90	0.10	36,36,36,36	0
58	MG	1A	3275	1/1	0.90	0.17	40,40,40,40	0
58	MG	1A	3122	1/1	0.90	0.17	35,35,35,35	0
58	MG	1A	3327	1/1	0.90	0.14	45,45,45,45	0
58	MG	1A	3242	1/1	0.90	0.14	48,48,48,48	0
58	MG	2A	3411	1/1	0.90	0.22	59,59,59,59	0
58	MG	1A	3523	1/1	0.90	0.09	68,68,68,68	0
58	MG	2V	201	1/1	0.90	0.30	45,45,45,45	0
58	MG	2A	3264	1/1	0.90	0.11	54,54,54,54	0
58	MG	1A	3332	1/1	0.90	0.24	55,55,55,55	0
58	MG	2Z	301	1/1	0.90	0.15	68,68,68,68	0
58	MG	1A	4021	1/1	0.90	0.13	51,51,51,51	0
58	MG	2I	101	1/1	0.90	0.27	55,55,55,55	0
58	MG	23	101	1/1	0.90	0.15	63,63,63,63	0
58	MG	23	102	1/1	0.90	0.11	48,48,48,48	0
58	MG	25	102	1/1	0.90	0.10	43,43,43,43	0
58	MG	1a	1658	1/1	0.90	0.20	47,47,47,47	0
58	MG	2A	3125	1/1	0.90	0.18	45,45,45,45	0
58	MG	1A	3601	1/1	0.90	0.25	56,56,56,56	0
58	MG	1A	3863	1/1	0.90	0.23	37,37,37,37	0
58	MG	1a	1797	1/1	0.90	0.10	45,45,45,45	0
58	MG	2A	3427	1/1	0.90	0.24	43,43,43,43	0
58	MG	2A	3671	1/1	0.90	0.22	58,58,58,58	0
58	MG	1A	3866	1/1	0.90	0.17	52,52,52,52	0
58	MG	2A	3675	1/1	0.90	0.27	55,55,55,55	0
58	MG	1A	3458	1/1	0.90	0.25	51,51,51,51	0
58	MG	1A	3528	1/1	0.90	0.13	41,41,41,41	0
58	MG	2f	201	1/1	0.90	0.07	42,42,42,42	0
58	MG	2A	3434	1/1	0.90	0.28	53,53,53,53	0
58	MG	2a	1610	1/1	0.90	0.14	52,52,52,52	0
58	MG	2A	3680	1/1	0.90	0.12	52,52,52,52	0
58	MG	2A	3681	1/1	0.90	0.21	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
58	MG	2a	1613	1/1	0.90	0.17	62,62,62,62	0
58	MG	2A	3277	1/1	0.90	0.17	63,63,63,63	0
58	MG	1a	1805	1/1	0.90	0.14	58,58,58,58	0
58	MG	1A	3290	1/1	0.90	0.12	48,48,48,48	0
58	MG	1O	205	1/1	0.90	0.11	54,54,54,54	0
58	MG	1P	203	1/1	0.90	0.19	32,32,32,32	0
58	MG	2t	201	1/1	0.90	0.14	59,59,59,59	0
58	MG	2t	202	1/1	0.90	0.12	48,48,48,48	0
58	MG	1A	3730	1/1	0.90	0.16	59,59,59,59	0
58	MG	1A	3532	1/1	0.90	0.20	55,55,55,55	0
58	MG	2A	3449	1/1	0.90	0.15	39,39,39,39	0
58	MG	2A	3285	1/1	0.90	0.24	56,56,56,56	0
58	MG	2w	101	1/1	0.90	0.24	52,52,52,52	0
58	MG	1A	3461	1/1	0.90	0.37	68,68,68,68	0
58	MG	2a	1625	1/1	0.90	0.16	61,61,61,61	0
58	MG	1R	201	1/1	0.90	0.20	31,31,31,31	0
58	MG	1A	3743	1/1	0.90	0.08	46,46,46,46	0
58	MG	1S	201	1/1	0.90	0.19	38,38,38,38	0
58	MG	1A	3291	1/1	0.90	0.12	52,52,52,52	0
58	MG	1A	3733	1/1	0.91	0.22	68,68,68,68	0
58	MG	2a	1623	1/1	0.91	0.19	55,55,55,55	0
58	MG	1A	3296	1/1	0.91	0.08	41,41,41,41	0
58	MG	1A	3199	1/1	0.91	0.10	36,36,36,36	0
58	MG	1V	207	1/1	0.91	0.14	55,55,55,55	0
58	MG	1A	3742	1/1	0.91	0.14	50,50,50,50	0
58	MG	2A	3241	1/1	0.91	0.12	72,72,72,72	0
58	MG	1A	3447	1/1	0.91	0.15	38,38,38,38	0
58	MG	2A	3052	1/1	0.91	0.12	46,46,46,46	0
58	MG	1Y	202	1/1	0.91	0.13	51,51,51,51	0
58	MG	1A	4054	1/1	0.91	0.10	36,36,36,36	0
58	MG	2A	3055	1/1	0.91	0.33	68,68,68,68	0
58	MG	1A	3400	1/1	0.91	0.10	35,35,35,35	0
58	MG	2A	3429	1/1	0.91	0.15	52,52,52,52	0
58	MG	1A	3896	1/1	0.91	0.10	30,30,30,30	0
58	MG	1a	1700	1/1	0.91	0.13	45,45,45,45	0
58	MG	1a	1702	1/1	0.91	0.10	51,51,51,51	0
58	MG	1A	3201	1/1	0.91	0.10	47,47,47,47	0
58	MG	2A	3438	1/1	0.91	0.13	33,33,33,33	0
58	MG	2A	3254	1/1	0.91	0.12	47,47,47,47	0
58	MG	10	102	1/1	0.91	0.14	45,45,45,45	0
58	MG	1A	3525	1/1	0.91	0.11	43,43,43,43	0
58	MG	2A	3716	1/1	0.91	0.12	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
58	MG	1A	3092	1/1	0.91	0.12	54,54,54,54	0
58	MG	1A	4073	1/1	0.91	0.12	45,45,45,45	0
58	MG	1a	1710	1/1	0.91	0.19	53,53,53,53	0
58	MG	1A	3616	1/1	0.91	0.10	52,52,52,52	0
58	MG	2A	3450	1/1	0.91	0.12	58,58,58,58	0
58	MG	2A	3076	1/1	0.91	0.11	46,46,46,46	0
58	MG	1A	3907	1/1	0.91	0.09	32,32,32,32	0
58	MG	1A	3123	1/1	0.91	0.09	36,36,36,36	0
58	MG	1A	4080	1/1	0.91	0.07	32,32,32,32	0
58	MG	2A	3083	1/1	0.91	0.13	53,53,53,53	0
58	MG	1A	3620	1/1	0.91	0.10	28,28,28,28	0
58	MG	1A	3304	1/1	0.91	0.12	43,43,43,43	0
58	MG	1a	1722	1/1	0.91	0.33	55,55,55,55	0
58	MG	1A	3531	1/1	0.91	0.28	51,51,51,51	0
58	MG	2A	3737	1/1	0.91	0.12	56,56,56,56	0
58	MG	2A	3738	1/1	0.91	0.18	65,65,65,65	0
58	MG	1A	4084	1/1	0.91	0.15	45,45,45,45	0
58	MG	2a	1671	1/1	0.91	0.11	41,41,41,41	0
58	MG	15	104	1/1	0.91	0.15	26,26,26,26	0
58	MG	2a	1673	1/1	0.91	0.16	57,57,57,57	0
58	MG	1A	3629	1/1	0.91	0.11	46,46,46,46	0
58	MG	2a	1675	1/1	0.91	0.14	54,54,54,54	0
58	MG	1A	4086	1/1	0.91	0.14	54,54,54,54	0
58	MG	1A	3094	1/1	0.91	0.15	42,42,42,42	0
58	MG	18	103	1/1	0.91	0.09	35,35,35,35	0
58	MG	1a	1740	1/1	0.91	0.11	40,40,40,40	0
58	MG	18	105	1/1	0.91	0.16	50,50,50,50	0
58	MG	2A	3474	1/1	0.91	0.09	29,29,29,29	0
58	MG	1A	3632	1/1	0.91	0.07	23,23,23,23	0
58	MG	1A	3212	1/1	0.91	0.14	42,42,42,42	0
58	MG	19	101	1/1	0.91	0.16	52,52,52,52	0
58	MG	2A	3284	1/1	0.91	0.18	56,56,56,56	0
58	MG	1A	3634	1/1	0.91	0.07	33,33,33,33	0
58	MG	1A	3050	1/1	0.91	0.17	40,40,40,40	0
58	MG	2a	1694	1/1	0.91	0.20	67,67,67,67	0
58	MG	2A	3287	1/1	0.91	0.19	55,55,55,55	0
58	MG	1A	3097	1/1	0.91	0.08	28,28,28,28	0
58	MG	1A	3463	1/1	0.91	0.23	63,63,63,63	0
58	MG	1A	3465	1/1	0.91	0.21	66,66,66,66	0
58	MG	1A	3078	1/1	0.91	0.09	30,30,30,30	0
58	MG	1A	3265	1/1	0.91	0.23	58,58,58,58	0
58	MG	2a	1701	1/1	0.91	0.13	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
58	MG	2A	3297	1/1	0.91	0.16	63,63,63,63	0
58	MG	2A	3124	1/1	0.91	0.12	65,65,65,65	0
58	MG	2a	1705	1/1	0.91	0.26	65,65,65,65	0
58	MG	1A	3954	1/1	0.91	0.12	53,53,53,53	0
58	MG	1A	4102	1/1	0.91	0.36	55,55,55,55	0
58	MG	1A	3649	1/1	0.91	0.09	64,64,64,64	0
58	MG	2A	3502	1/1	0.91	0.11	53,53,53,53	0
58	MG	2A	3503	1/1	0.91	0.20	53,53,53,53	0
58	MG	1A	3267	1/1	0.91	0.16	45,45,45,45	0
58	MG	1A	3080	1/1	0.91	0.14	51,51,51,51	0
58	MG	1A	3661	1/1	0.91	0.07	43,43,43,43	0
58	MG	1a	1620	1/1	0.91	0.09	38,38,38,38	0
58	MG	1A	3665	1/1	0.91	0.07	24,24,24,24	0
58	MG	2A	3138	1/1	0.91	0.23	53,53,53,53	0
58	MG	1B	210	1/1	0.91	0.15	52,52,52,52	0
58	MG	2A	3317	1/1	0.91	0.15	67,67,67,67	0
58	MG	2A	3517	1/1	0.91	0.15	58,58,58,58	0
58	MG	1A	3547	1/1	0.91	0.15	57,57,57,57	0
58	MG	1A	3968	1/1	0.91	0.11	33,33,33,33	0
58	MG	2A	3821	1/1	0.91	0.12	66,66,66,66	0
58	MG	1A	3473	1/1	0.91	0.10	51,51,51,51	0
58	MG	2A	3147	1/1	0.91	0.23	54,54,54,54	0
58	MG	1a	1781	1/1	0.91	0.11	44,44,44,44	0
58	MG	2A	3154	1/1	0.91	0.07	54,54,54,54	0
58	MG	1A	3971	1/1	0.91	0.14	65,65,65,65	0
58	MG	1A	3361	1/1	0.91	0.19	56,56,56,56	0
58	MG	1A	3475	1/1	0.91	0.14	53,53,53,53	0
58	MG	1A	3556	1/1	0.91	0.17	40,40,40,40	0
58	MG	1a	1631	1/1	0.91	0.23	57,57,57,57	0
58	MG	2A	3843	1/1	0.91	0.14	47,47,47,47	0
58	MG	1A	3558	1/1	0.91	0.12	33,33,33,33	0
58	MG	2A	3164	1/1	0.91	0.26	58,58,58,58	0
58	MG	1a	1634	1/1	0.91	0.21	59,59,59,59	0
58	MG	1a	1798	1/1	0.91	0.09	57,57,57,57	0
58	MG	1A	3320	1/1	0.91	0.20	26,26,26,26	0
58	MG	2B	201	1/1	0.91	0.18	59,59,59,59	0
58	MG	1A	3982	1/1	0.91	0.11	55,55,55,55	0
58	MG	1A	3983	1/1	0.91	0.19	53,53,53,53	0
58	MG	2A	3558	1/1	0.91	0.11	59,59,59,59	0
58	MG	1A	3365	1/1	0.91	0.17	32,32,32,32	0
58	MG	1A	3830	1/1	0.91	0.08	34,34,34,34	0
58	MG	2A	3339	1/1	0.91	0.32	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3420	1/1	0.91	0.21	61,61,61,61	0
58	MG	2a	1771	1/1	0.91	0.10	52,52,52,52	0
58	MG	1A	3839	1/1	0.91	0.11	34,34,34,34	0
58	MG	1A	3992	1/1	0.91	0.10	52,52,52,52	0
58	MG	1A	3269	1/1	0.91	0.27	49,49,49,49	0
58	MG	1A	3324	1/1	0.91	0.21	55,55,55,55	0
58	MG	2A	3578	1/1	0.91	0.11	30,30,30,30	0
58	MG	1A	4001	1/1	0.91	0.10	59,59,59,59	0
58	MG	2A	3184	1/1	0.91	0.24	73,73,73,73	0
58	MG	1A	3138	1/1	0.91	0.10	29,29,29,29	0
58	MG	1l	201	1/1	0.91	0.09	66,66,66,66	0
58	MG	2A	3588	1/1	0.91	0.21	53,53,53,53	0
58	MG	1a	1653	1/1	0.91	0.09	41,41,41,41	0
58	MG	1A	3578	1/1	0.91	0.09	29,29,29,29	0
58	MG	1a	1655	1/1	0.91	0.18	55,55,55,55	0
58	MG	1A	3274	1/1	0.91	0.07	41,41,41,41	0
58	MG	2E	305	1/1	0.91	0.12	35,35,35,35	0
58	MG	1A	3082	1/1	0.91	0.14	34,34,34,34	0
58	MG	1A	3491	1/1	0.91	0.13	43,43,43,43	0
58	MG	1A	3374	1/1	0.91	0.15	40,40,40,40	0
58	MG	2F	302	1/1	0.91	0.10	44,44,44,44	0
58	MG	2a	1796	1/1	0.91	0.12	57,57,57,57	0
58	MG	2A	3361	1/1	0.91	0.10	45,45,45,45	0
58	MG	1A	3710	1/1	0.91	0.09	30,30,30,30	0
58	MG	1A	3858	1/1	0.91	0.07	53,53,53,53	0
58	MG	2A	3365	1/1	0.91	0.14	66,66,66,66	0
58	MG	1G	203	1/1	0.91	0.12	61,61,61,61	0
58	MG	1A	3433	1/1	0.91	0.12	43,43,43,43	0
58	MG	1A	3053	1/1	0.91	0.10	41,41,41,41	0
58	MG	2A	3614	1/1	0.91	0.23	52,52,52,52	0
58	MG	1A	3590	1/1	0.91	0.09	48,48,48,48	0
58	MG	1N	201	1/1	0.91	0.28	47,47,47,47	0
58	MG	2T	202	1/1	0.91	0.21	65,65,65,65	0
58	MG	2A	3373	1/1	0.91	0.10	49,49,49,49	0
58	MG	2A	3205	1/1	0.91	0.30	66,66,66,66	0
58	MG	2A	3632	1/1	0.91	0.11	39,39,39,39	0
58	MG	2A	3633	1/1	0.91	0.10	46,46,46,46	0
58	MG	2Y	201	1/1	0.91	0.20	53,53,53,53	0
58	MG	2A	3635	1/1	0.91	0.14	41,41,41,41	0
58	MG	2A	3375	1/1	0.91	0.17	70,70,70,70	0
58	MG	1A	4022	1/1	0.91	0.11	65,65,65,65	0
58	MG	2A	3639	1/1	0.91	0.13	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
58	MG	1A	3867	1/1	0.91	0.16	38,38,38,38	0
58	MG	25	101	1/1	0.91	0.11	46,46,46,46	0
58	MG	1O	203	1/1	0.91	0.30	57,57,57,57	0
58	MG	1A	4024	1/1	0.91	0.11	46,46,46,46	0
58	MG	1A	3285	1/1	0.91	0.11	43,43,43,43	0
58	MG	2A	3647	1/1	0.91	0.09	49,49,49,49	0
58	MG	1A	3143	1/1	0.91	0.19	51,51,51,51	0
58	MG	1P	206	1/1	0.91	0.09	46,46,46,46	0
58	MG	2A	3383	1/1	0.91	0.18	58,58,58,58	0
58	MG	2A	3213	1/1	0.91	0.26	36,36,36,36	0
58	MG	2A	3653	1/1	0.91	0.13	51,51,51,51	0
58	MG	2A	3006	1/1	0.91	0.17	58,58,58,58	0
58	MG	2A	3009	1/1	0.91	0.18	55,55,55,55	0
58	MG	2A	3011	1/1	0.91	0.08	35,35,35,35	0
58	MG	2A	3219	1/1	0.91	0.18	44,44,44,44	0
58	MG	1A	3012	1/1	0.91	0.08	26,26,26,26	0
58	MG	2A	3662	1/1	0.91	0.10	56,56,56,56	0
58	MG	1A	4032	1/1	0.91	0.09	38,38,38,38	0
58	MG	1A	3508	1/1	0.91	0.08	41,41,41,41	0
58	MG	2A	3017	1/1	0.91	0.14	38,38,38,38	0
58	MG	1A	3514	1/1	0.91	0.27	28,28,28,28	0
58	MG	1R	203	1/1	0.91	0.08	33,33,33,33	0
58	MG	1A	3026	1/1	0.91	0.15	51,51,51,51	0
58	MG	1A	4037	1/1	0.91	0.15	40,40,40,40	0
58	MG	2x	101	1/1	0.91	0.20	44,44,44,44	0
58	MG	2A	3034	1/1	0.91	0.16	52,52,52,52	0
58	MG	1A	3246	1/1	0.91	0.13	48,48,48,48	0
58	MG	1T	202	1/1	0.91	0.15	49,49,49,49	0
58	MG	1A	3530	1/1	0.92	0.24	48,48,48,48	0
58	MG	1A	4002	1/1	0.92	0.11	57,57,57,57	0
58	MG	1A	4003	1/1	0.92	0.07	62,62,62,62	0
58	MG	1B	238	1/1	0.92	0.07	29,29,29,29	0
58	MG	1a	1787	1/1	0.92	0.13	49,49,49,49	0
58	MG	1A	3713	1/1	0.92	0.13	40,40,40,40	0
58	MG	2a	1632	1/1	0.92	0.20	51,51,51,51	0
58	MG	1D	304	1/1	0.92	0.10	43,43,43,43	0
58	MG	1D	306	1/1	0.92	0.11	18,18,18,18	0
58	MG	1A	3193	1/1	0.92	0.22	35,35,35,35	0
58	MG	1A	3715	1/1	0.92	0.11	46,46,46,46	0
58	MG	1A	3083	1/1	0.92	0.17	41,41,41,41	0
58	MG	1E	307	1/1	0.92	0.11	50,50,50,50	0
58	MG	2A	3299	1/1	0.92	0.13	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
58	MG	2A	3149	1/1	0.92	0.11	43,43,43,43	0
58	MG	1a	1801	1/1	0.92	0.31	66,66,66,66	0
58	MG	2A	3304	1/1	0.92	0.12	49,49,49,49	0
58	MG	2A	3306	1/1	0.92	0.08	43,43,43,43	0
58	MG	2A	3483	1/1	0.92	0.11	40,40,40,40	0
58	MG	1A	3048	1/1	0.92	0.10	36,36,36,36	0
58	MG	2A	3739	1/1	0.92	0.09	43,43,43,43	0
58	MG	1E	309	1/1	0.92	0.12	32,32,32,32	0
58	MG	2A	3741	1/1	0.92	0.33	48,48,48,48	0
58	MG	2A	3489	1/1	0.92	0.27	53,53,53,53	0
58	MG	1A	4013	1/1	0.92	0.16	53,53,53,53	0
58	MG	1A	3718	1/1	0.92	0.10	65,65,65,65	0
58	MG	2A	3159	1/1	0.92	0.17	55,55,55,55	0
58	MG	1A	4016	1/1	0.92	0.09	64,64,64,64	0
58	MG	1A	3613	1/1	0.92	0.11	25,25,25,25	0
58	MG	1F	305	1/1	0.92	0.08	30,30,30,30	0
58	MG	2A	3163	1/1	0.92	0.09	54,54,54,54	0
58	MG	1A	3019	1/1	0.92	0.12	34,34,34,34	0
58	MG	1F	307	1/1	0.92	0.08	25,25,25,25	0
58	MG	1F	308	1/1	0.92	0.12	31,31,31,31	0
58	MG	1A	3345	1/1	0.92	0.18	30,30,30,30	0
58	MG	1A	3434	1/1	0.92	0.14	31,31,31,31	0
58	MG	2A	3773	1/1	0.92	0.10	60,60,60,60	0
58	MG	2A	3169	1/1	0.92	0.23	73,73,73,73	0
58	MG	1A	3310	1/1	0.92	0.08	45,45,45,45	0
58	MG	2A	3509	1/1	0.92	0.23	66,66,66,66	0
58	MG	2A	3172	1/1	0.92	0.17	47,47,47,47	0
58	MG	1A	3348	1/1	0.92	0.15	29,29,29,29	0
58	MG	1A	3484	1/1	0.92	0.11	39,39,39,39	0
58	MG	2A	3176	1/1	0.92	0.15	64,64,64,64	0
58	MG	1A	3625	1/1	0.92	0.10	59,59,59,59	0
58	MG	1A	3879	1/1	0.92	0.11	30,30,30,30	0
58	MG	1A	3485	1/1	0.92	0.14	35,35,35,35	0
58	MG	1A	3271	1/1	0.92	0.15	38,38,38,38	0
58	MG	1A	3546	1/1	0.92	0.14	59,59,59,59	0
58	MG	1A	3016	1/1	0.92	0.16	52,52,52,52	0
58	MG	1A	3175	1/1	0.92	0.08	26,26,26,26	0
58	MG	1A	3440	1/1	0.92	0.13	46,46,46,46	0
58	MG	2A	3792	1/1	0.92	0.13	46,46,46,46	0
58	MG	2a	1689	1/1	0.92	0.33	67,67,67,67	0
58	MG	1A	3277	1/1	0.92	0.14	37,37,37,37	0
58	MG	1A	3753	1/1	0.92	0.13	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
58	MG	1A	3898	1/1	0.92	0.04	26,26,26,26	0
58	MG	2A	3800	1/1	0.92	0.09	52,52,52,52	0
58	MG	1A	3555	1/1	0.92	0.13	36,36,36,36	0
58	MG	2A	3802	1/1	0.92	0.13	39,39,39,39	0
58	MG	2A	3191	1/1	0.92	0.09	43,43,43,43	0
58	MG	1A	3760	1/1	0.92	0.10	53,53,53,53	0
58	MG	1A	3176	1/1	0.92	0.10	19,19,19,19	0
58	MG	2A	3810	1/1	0.92	0.08	45,45,45,45	0
58	MG	1A	4050	1/1	0.92	0.09	12,12,12,12	0
58	MG	2A	3814	1/1	0.92	0.12	56,56,56,56	0
58	MG	2a	1706	1/1	0.92	0.22	63,63,63,63	0
58	MG	2A	3548	1/1	0.92	0.09	32,32,32,32	0
58	MG	2A	3002	1/1	0.92	0.14	63,63,63,63	0
58	MG	1A	3904	1/1	0.92	0.08	33,33,33,33	0
58	MG	1A	3905	1/1	0.92	0.08	37,37,37,37	0
58	MG	2a	1711	1/1	0.92	0.31	60,60,60,60	0
58	MG	2A	3824	1/1	0.92	0.12	73,73,73,73	0
58	MG	1A	3444	1/1	0.92	0.16	41,41,41,41	0
58	MG	1A	3643	1/1	0.92	0.12	46,46,46,46	0
58	MG	2A	3828	1/1	0.92	0.12	49,49,49,49	0
58	MG	2A	3007	1/1	0.92	0.14	47,47,47,47	0
58	MG	2a	1717	1/1	0.92	0.30	58,58,58,58	0
58	MG	2a	1718	1/1	0.92	0.10	64,64,64,64	0
58	MG	2A	3834	1/1	0.92	0.10	57,57,57,57	0
58	MG	1A	3316	1/1	0.92	0.09	35,35,35,35	0
58	MG	2A	3202	1/1	0.92	0.11	55,55,55,55	0
58	MG	1A	3909	1/1	0.92	0.17	24,24,24,24	0
58	MG	2A	3572	1/1	0.92	0.19	44,44,44,44	0
58	MG	2A	3204	1/1	0.92	0.14	49,49,49,49	0
58	MG	1A	3498	1/1	0.92	0.08	50,50,50,50	0
58	MG	1A	4072	1/1	0.92	0.09	44,44,44,44	0
58	MG	1A	3501	1/1	0.92	0.09	41,41,41,41	0
58	MG	1A	3921	1/1	0.92	0.16	36,36,36,36	0
58	MG	1A	3177	1/1	0.92	0.11	35,35,35,35	0
58	MG	2a	1732	1/1	0.92	0.28	65,65,65,65	0
58	MG	2a	1733	1/1	0.92	0.24	55,55,55,55	0
58	MG	1A	3926	1/1	0.92	0.10	35,35,35,35	0
58	MG	1A	3002	1/1	0.92	0.12	55,55,55,55	0
58	MG	2a	1738	1/1	0.92	0.22	53,53,53,53	0
58	MG	1A	3656	1/1	0.92	0.15	48,48,48,48	0
58	MG	10	105	1/1	0.92	0.22	58,58,58,58	0
58	MG	1a	1698	1/1	0.92	0.17	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
58	MG	1A	3935	1/1	0.92	0.14	60,60,60,60	0
58	MG	2A	3597	1/1	0.92	0.18	67,67,67,67	0
58	MG	2A	3217	1/1	0.92	0.17	36,36,36,36	0
58	MG	1A	3657	1/1	0.92	0.09	28,28,28,28	0
58	MG	2B	209	1/1	0.92	0.15	58,58,58,58	0
58	MG	1A	3660	1/1	0.92	0.17	45,45,45,45	0
58	MG	1a	1703	1/1	0.92	0.21	49,49,49,49	0
58	MG	2A	3044	1/1	0.92	0.10	49,49,49,49	0
58	MG	1A	3786	1/1	0.92	0.14	48,48,48,48	0
58	MG	1A	3569	1/1	0.92	0.13	30,30,30,30	0
58	MG	2a	1760	1/1	0.92	0.09	74,74,74,74	0
58	MG	2A	3606	1/1	0.92	0.12	56,56,56,56	0
58	MG	2A	3226	1/1	0.92	0.15	49,49,49,49	0
58	MG	1A	3663	1/1	0.92	0.11	35,35,35,35	0
58	MG	1A	3505	1/1	0.92	0.09	46,46,46,46	0
58	MG	1A	3796	1/1	0.92	0.18	60,60,60,60	0
58	MG	2a	1769	1/1	0.92	0.28	68,68,68,68	0
58	MG	1A	3179	1/1	0.92	0.20	53,53,53,53	0
58	MG	1A	3148	1/1	0.92	0.18	42,42,42,42	0
58	MG	2A	3392	1/1	0.92	0.24	52,52,52,52	0
58	MG	1A	3803	1/1	0.92	0.09	39,39,39,39	0
58	MG	15	103	1/1	0.92	0.10	33,33,33,33	0
58	MG	2E	306	1/1	0.92	0.14	51,51,51,51	0
58	MG	2a	1777	1/1	0.92	0.10	53,53,53,53	0
58	MG	1a	1715	1/1	0.92	0.16	34,34,34,34	0
58	MG	1a	1716	1/1	0.92	0.10	29,29,29,29	0
58	MG	2E	310	1/1	0.92	0.19	41,41,41,41	0
58	MG	2a	1781	1/1	0.92	0.24	72,72,72,72	0
58	MG	1A	3512	1/1	0.92	0.13	27,27,27,27	0
58	MG	2A	3402	1/1	0.92	0.11	36,36,36,36	0
58	MG	15	105	1/1	0.92	0.10	30,30,30,30	0
58	MG	2F	304	1/1	0.92	0.14	42,42,42,42	0
58	MG	1a	1719	1/1	0.92	0.36	54,54,54,54	0
58	MG	15	106	1/1	0.92	0.12	50,50,50,50	0
58	MG	2A	3068	1/1	0.92	0.18	51,51,51,51	0
58	MG	2O	201	1/1	0.92	0.18	59,59,59,59	0
58	MG	2A	3642	1/1	0.92	0.20	65,65,65,65	0
58	MG	1A	3672	1/1	0.92	0.09	34,34,34,34	0
58	MG	2Q	203	1/1	0.92	0.23	62,62,62,62	0
58	MG	2R	201	1/1	0.92	0.12	55,55,55,55	0
58	MG	2a	1798	1/1	0.92	0.13	53,53,53,53	0
58	MG	1A	3806	1/1	0.92	0.07	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
58	MG	17	104	1/1	0.92	0.17	49,49,49,49	0
58	MG	1A	3959	1/1	0.92	0.12	55,55,55,55	0
58	MG	18	102	1/1	0.92	0.21	36,36,36,36	0
58	MG	1A	3960	1/1	0.92	0.07	40,40,40,40	0
58	MG	2A	3250	1/1	0.92	0.21	57,57,57,57	0
58	MG	2T	204	1/1	0.92	0.12	51,51,51,51	0
58	MG	1A	3293	1/1	0.92	0.13	32,32,32,32	0
58	MG	2A	3416	1/1	0.92	0.13	56,56,56,56	0
58	MG	1a	1736	1/1	0.92	0.11	48,48,48,48	0
58	MG	1A	3682	1/1	0.92	0.09	27,27,27,27	0
58	MG	1A	3684	1/1	0.92	0.13	53,53,53,53	0
58	MG	2A	3420	1/1	0.92	0.22	49,49,49,49	0
58	MG	2A	3421	1/1	0.92	0.18	53,53,53,53	0
58	MG	2A	3664	1/1	0.92	0.11	49,49,49,49	0
58	MG	2A	3422	1/1	0.92	0.19	63,63,63,63	0
58	MG	1B	203	1/1	0.92	0.10	40,40,40,40	0
58	MG	2A	3424	1/1	0.92	0.15	45,45,45,45	0
58	MG	1A	3217	1/1	0.92	0.15	40,40,40,40	0
58	MG	1B	205	1/1	0.92	0.09	49,49,49,49	0
58	MG	28	101	1/1	0.92	0.13	58,58,58,58	0
58	MG	1A	3816	1/1	0.92	0.12	41,41,41,41	0
58	MG	28	104	1/1	0.92	0.21	55,55,55,55	0
58	MG	1A	3457	1/1	0.92	0.10	49,49,49,49	0
58	MG	1A	3364	1/1	0.92	0.10	41,41,41,41	0
58	MG	1A	3259	1/1	0.92	0.10	38,38,38,38	0
58	MG	1A	3521	1/1	0.92	0.21	68,68,68,68	0
58	MG	2A	3435	1/1	0.92	0.14	55,55,55,55	0
58	MG	1A	3073	1/1	0.92	0.07	12,12,12,12	0
58	MG	1A	3334	1/1	0.92	0.23	55,55,55,55	0
58	MG	2A	3105	1/1	0.92	0.17	43,43,43,43	0
58	MG	1A	3153	1/1	0.92	0.11	39,39,39,39	0
58	MG	1A	3095	1/1	0.92	0.11	52,52,52,52	0
58	MG	1B	220	1/1	0.92	0.13	49,49,49,49	0
58	MG	2A	3109	1/1	0.92	0.15	49,49,49,49	0
58	MG	1A	3338	1/1	0.92	0.18	53,53,53,53	0
58	MG	1A	3599	1/1	0.92	0.09	32,32,32,32	0
58	MG	1A	3706	1/1	0.92	0.10	32,32,32,32	0
58	MG	1A	3842	1/1	0.92	0.13	49,49,49,49	0
58	MG	2A	3276	1/1	0.92	0.17	66,66,66,66	0
58	MG	2A	3698	1/1	0.92	0.14	61,61,61,61	0
58	MG	1B	226	1/1	0.92	0.12	62,62,62,62	0
58	MG	1A	3162	1/1	0.92	0.11	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
58	MG	1a	1772	1/1	0.92	0.14	57,57,57,57	0
58	MG	1A	3428	1/1	0.92	0.11	45,45,45,45	0
58	MG	1A	3602	1/1	0.92	0.33	55,55,55,55	0
58	MG	2x	103	1/1	0.92	0.08	53,53,53,53	0
58	MG	2A	3710	1/1	0.92	0.10	40,40,40,40	0
58	MG	1B	233	1/1	0.92	0.18	59,59,59,59	0
58	MG	2A	3303	1/1	0.93	0.11	56,56,56,56	0
58	MG	1A	3223	1/1	0.93	0.08	37,37,37,37	0
58	MG	2A	3148	1/1	0.93	0.12	36,36,36,36	0
58	MG	1a	1791	1/1	0.93	0.09	59,59,59,59	0
58	MG	2A	3485	1/1	0.93	0.19	53,53,53,53	0
58	MG	1A	3732	1/1	0.93	0.08	42,42,42,42	0
58	MG	1A	3627	1/1	0.93	0.11	29,29,29,29	0
58	MG	1A	3063	1/1	0.93	0.15	41,41,41,41	0
58	MG	1E	301	1/1	0.93	0.12	46,46,46,46	0
58	MG	2A	3312	1/1	0.93	0.14	54,54,54,54	0
58	MG	1A	3739	1/1	0.93	0.09	56,56,56,56	0
58	MG	1A	3337	1/1	0.93	0.22	61,61,61,61	0
58	MG	2A	3496	1/1	0.93	0.27	60,60,60,60	0
58	MG	1A	3229	1/1	0.93	0.09	40,40,40,40	0
58	MG	1A	3339	1/1	0.93	0.29	65,65,65,65	0
58	MG	1A	3230	1/1	0.93	0.17	44,44,44,44	0
58	MG	1A	3880	1/1	0.93	0.14	38,38,38,38	0
58	MG	1A	3288	1/1	0.93	0.08	38,38,38,38	0
58	MG	1A	3289	1/1	0.93	0.15	54,54,54,54	0
58	MG	1a	1648	1/1	0.93	0.16	58,58,58,58	0
58	MG	1a	1650	1/1	0.93	0.11	38,38,38,38	0
58	MG	1A	3064	1/1	0.93	0.20	39,39,39,39	0
58	MG	2a	1656	1/1	0.93	0.08	62,62,62,62	0
58	MG	1A	3105	1/1	0.93	0.14	43,43,43,43	0
58	MG	1e	202	1/1	0.93	0.13	49,49,49,49	0
58	MG	1A	3011	1/1	0.93	0.10	42,42,42,42	0
58	MG	1A	3411	1/1	0.93	0.10	43,43,43,43	0
58	MG	1F	309	1/1	0.93	0.09	37,37,37,37	0
58	MG	2A	3515	1/1	0.93	0.12	39,39,39,39	0
58	MG	1F	311	1/1	0.93	0.15	29,29,29,29	0
58	MG	1n	102	1/1	0.93	0.11	43,43,43,43	0
58	MG	1G	201	1/1	0.93	0.10	40,40,40,40	0
58	MG	1A	3294	1/1	0.93	0.24	47,47,47,47	0
58	MG	1a	1661	1/1	0.93	0.11	58,58,58,58	0
58	MG	1A	3894	1/1	0.93	0.06	42,42,42,42	0
58	MG	1A	4030	1/1	0.93	0.10	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
58	MG	1w	107	1/1	0.93	0.10	35,35,35,35	0
58	MG	2A	3185	1/1	0.93	0.25	49,49,49,49	0
58	MG	1A	3895	1/1	0.93	0.10	23,23,23,23	0
58	MG	2A	3789	1/1	0.93	0.12	67,67,67,67	0
58	MG	1A	3144	1/1	0.93	0.12	37,37,37,37	0
58	MG	1A	3554	1/1	0.93	0.18	29,29,29,29	0
58	MG	1N	203	1/1	0.93	0.11	47,47,47,47	0
58	MG	2A	3539	1/1	0.93	0.07	38,38,38,38	0
58	MG	2A	3794	1/1	0.93	0.13	52,52,52,52	0
58	MG	1A	3768	1/1	0.93	0.07	27,27,27,27	0
58	MG	1A	3183	1/1	0.93	0.10	39,39,39,39	0
58	MG	2A	3543	1/1	0.93	0.07	38,38,38,38	0
58	MG	1A	3241	1/1	0.93	0.10	40,40,40,40	0
58	MG	2a	1693	1/1	0.93	0.15	58,58,58,58	0
58	MG	1A	3418	1/1	0.93	0.21	52,52,52,52	0
58	MG	1A	4039	1/1	0.93	0.09	46,46,46,46	0
58	MG	1A	3659	1/1	0.93	0.13	38,38,38,38	0
58	MG	2A	3805	1/1	0.93	0.09	40,40,40,40	0
58	MG	2A	3552	1/1	0.93	0.11	39,39,39,39	0
58	MG	2A	3553	1/1	0.93	0.11	40,40,40,40	0
58	MG	1A	3110	1/1	0.93	0.18	27,27,27,27	0
58	MG	1Q	204	1/1	0.93	0.07	34,34,34,34	0
58	MG	1A	4043	1/1	0.93	0.12	42,42,42,42	0
58	MG	2A	3817	1/1	0.93	0.17	45,45,45,45	0
58	MG	1A	3186	1/1	0.93	0.12	40,40,40,40	0
58	MG	1A	4046	1/1	0.93	0.07	53,53,53,53	0
58	MG	2A	3568	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	4047	1/1	0.93	0.06	25,25,25,25	0
58	MG	2A	3360	1/1	0.93	0.24	55,55,55,55	0
58	MG	1A	3778	1/1	0.93	0.07	28,28,28,28	0
58	MG	1A	3421	1/1	0.93	0.10	47,47,47,47	0
58	MG	2A	3832	1/1	0.93	0.12	54,54,54,54	0
58	MG	1A	3910	1/1	0.93	0.13	55,55,55,55	0
58	MG	1A	4053	1/1	0.93	0.13	54,54,54,54	0
58	MG	1A	3664	1/1	0.93	0.10	29,29,29,29	0
58	MG	1A	3913	1/1	0.93	0.09	45,45,45,45	0
58	MG	1U	203	1/1	0.93	0.31	40,40,40,40	0
58	MG	2A	3582	1/1	0.93	0.10	52,52,52,52	0
58	MG	2A	3840	1/1	0.93	0.10	54,54,54,54	0
58	MG	2A	3583	1/1	0.93	0.15	46,46,46,46	0
58	MG	1A	3916	1/1	0.93	0.12	32,32,32,32	0
58	MG	1A	3187	1/1	0.93	0.26	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
58	MG	2A	3022	1/1	0.93	0.12	50,50,50,50	0
58	MG	2A	3592	1/1	0.93	0.09	45,45,45,45	0
58	MG	1V	206	1/1	0.93	0.09	43,43,43,43	0
58	MG	2A	3028	1/1	0.93	0.11	38,38,38,38	0
58	MG	2a	1727	1/1	0.93	0.32	47,47,47,47	0
58	MG	2a	1728	1/1	0.93	0.33	69,69,69,69	0
58	MG	1A	3788	1/1	0.93	0.08	59,59,59,59	0
58	MG	2A	3033	1/1	0.93	0.12	37,37,37,37	0
58	MG	1A	4065	1/1	0.93	0.20	58,58,58,58	0
58	MG	1W	202	1/1	0.93	0.10	41,41,41,41	0
58	MG	1A	3922	1/1	0.93	0.13	48,48,48,48	0
58	MG	2a	1734	1/1	0.93	0.39	67,67,67,67	0
58	MG	2A	3039	1/1	0.93	0.27	55,55,55,55	0
58	MG	1A	3355	1/1	0.93	0.10	38,38,38,38	0
58	MG	2a	1737	1/1	0.93	0.38	62,62,62,62	0
58	MG	1A	3925	1/1	0.93	0.07	35,35,35,35	0
58	MG	1A	3117	1/1	0.93	0.23	39,39,39,39	0
58	MG	1A	3927	1/1	0.93	0.09	44,44,44,44	0
58	MG	2a	1741	1/1	0.93	0.20	63,63,63,63	0
58	MG	2A	3227	1/1	0.93	0.16	39,39,39,39	0
58	MG	1A	3492	1/1	0.93	0.10	42,42,42,42	0
58	MG	2a	1746	1/1	0.93	0.11	66,66,66,66	0
58	MG	2a	1747	1/1	0.93	0.15	63,63,63,63	0
58	MG	1A	3014	1/1	0.93	0.08	26,26,26,26	0
58	MG	1A	3932	1/1	0.93	0.07	33,33,33,33	0
58	MG	1A	3797	1/1	0.93	0.14	46,46,46,46	0
58	MG	2B	217	1/1	0.93	0.11	52,52,52,52	0
58	MG	1a	1707	1/1	0.93	0.12	41,41,41,41	0
58	MG	1A	3937	1/1	0.93	0.07	32,32,32,32	0
58	MG	2A	3398	1/1	0.93	0.20	54,54,54,54	0
58	MG	2a	1756	1/1	0.93	0.23	58,58,58,58	0
58	MG	2D	303	1/1	0.93	0.09	43,43,43,43	0
58	MG	2A	3620	1/1	0.93	0.14	51,51,51,51	0
58	MG	2A	3622	1/1	0.93	0.12	56,56,56,56	0
58	MG	2a	1762	1/1	0.93	0.09	67,67,67,67	0
58	MG	10	109	1/1	0.93	0.09	53,53,53,53	0
58	MG	2A	3624	1/1	0.93	0.16	58,58,58,58	0
58	MG	2A	3625	1/1	0.93	0.08	38,38,38,38	0
58	MG	2A	3627	1/1	0.93	0.20	55,55,55,55	0
58	MG	1A	3939	1/1	0.93	0.17	52,52,52,52	0
58	MG	1A	3674	1/1	0.93	0.12	32,32,32,32	0
58	MG	2A	3404	1/1	0.93	0.28	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3156	1/1	0.93	0.23	24,24,24,24	0
58	MG	1A	3677	1/1	0.93	0.09	23,23,23,23	0
58	MG	1A	4088	1/1	0.93	0.12	67,67,67,67	0
58	MG	1A	3042	1/1	0.93	0.17	27,27,27,27	0
58	MG	13	103	1/1	0.93	0.11	56,56,56,56	0
58	MG	1A	3253	1/1	0.93	0.14	48,48,48,48	0
58	MG	1A	3029	1/1	0.93	0.12	30,30,30,30	0
58	MG	1A	3075	1/1	0.93	0.07	19,19,19,19	0
58	MG	1A	3951	1/1	0.93	0.07	54,54,54,54	0
58	MG	2O	202	1/1	0.93	0.14	54,54,54,54	0
58	MG	1A	3808	1/1	0.93	0.07	21,21,21,21	0
58	MG	1A	3690	1/1	0.93	0.06	27,27,27,27	0
58	MG	1A	3503	1/1	0.93	0.09	54,54,54,54	0
58	MG	1A	3257	1/1	0.93	0.10	26,26,26,26	0
58	MG	2A	3080	1/1	0.93	0.12	45,45,45,45	0
58	MG	1A	3815	1/1	0.93	0.08	34,34,34,34	0
58	MG	1A	3164	1/1	0.93	0.13	34,34,34,34	0
58	MG	2A	3656	1/1	0.93	0.14	58,58,58,58	0
58	MG	1A	3202	1/1	0.93	0.14	20,20,20,20	0
58	MG	18	101	1/1	0.93	0.14	51,51,51,51	0
58	MG	2A	3089	1/1	0.93	0.12	40,40,40,40	0
58	MG	2U	201	1/1	0.93	0.18	44,44,44,44	0
58	MG	2a	1797	1/1	0.93	0.15	47,47,47,47	0
58	MG	2A	3090	1/1	0.93	0.11	42,42,42,42	0
58	MG	1A	3059	1/1	0.93	0.11	42,42,42,42	0
58	MG	1A	3510	1/1	0.93	0.17	54,54,54,54	0
58	MG	2a	1801	1/1	0.93	0.17	59,59,59,59	0
58	MG	1A	3318	1/1	0.93	0.12	52,52,52,52	0
58	MG	1A	3371	1/1	0.93	0.16	47,47,47,47	0
58	MG	1a	1744	1/1	0.93	0.12	58,58,58,58	0
58	MG	1A	3967	1/1	0.93	0.11	25,25,25,25	0
58	MG	1B	207	1/1	0.93	0.08	46,46,46,46	0
58	MG	1A	3516	1/1	0.93	0.10	44,44,44,44	0
58	MG	23	103	1/1	0.93	0.07	43,43,43,43	0
58	MG	1a	1748	1/1	0.93	0.19	36,36,36,36	0
58	MG	2A	3437	1/1	0.93	0.11	53,53,53,53	0
58	MG	1B	209	1/1	0.93	0.09	46,46,46,46	0
58	MG	2A	3679	1/1	0.93	0.11	52,52,52,52	0
58	MG	1A	3205	1/1	0.93	0.10	31,31,31,31	0
58	MG	1a	1753	1/1	0.93	0.08	49,49,49,49	0
58	MG	28	103	1/1	0.93	0.20	60,60,60,60	0
58	MG	2A	3682	1/1	0.93	0.17	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3321	1/1	0.93	0.12	50,50,50,50	0
58	MG	1A	3443	1/1	0.93	0.11	31,31,31,31	0
58	MG	1A	3077	1/1	0.93	0.16	45,45,45,45	0
58	MG	1A	3049	1/1	0.93	0.06	19,19,19,19	0
58	MG	1A	3211	1/1	0.93	0.07	39,39,39,39	0
58	MG	1A	3170	1/1	0.93	0.08	39,39,39,39	0
58	MG	1A	3979	1/1	0.93	0.07	59,59,59,59	0
58	MG	2f	202	1/1	0.93	0.22	66,66,66,66	0
58	MG	1a	1765	1/1	0.93	0.09	45,45,45,45	0
58	MG	1a	1767	1/1	0.93	0.10	54,54,54,54	0
58	MG	2j	202	1/1	0.93	0.12	61,61,61,61	0
58	MG	2A	3121	1/1	0.93	0.15	44,44,44,44	0
58	MG	2l	201	1/1	0.93	0.17	66,66,66,66	0
58	MG	2A	3696	1/1	0.93	0.16	59,59,59,59	0
58	MG	1A	3062	1/1	0.93	0.07	41,41,41,41	0
58	MG	1A	3451	1/1	0.93	0.14	54,54,54,54	0
58	MG	1A	3330	1/1	0.93	0.10	43,43,43,43	0
58	MG	1A	3131	1/1	0.93	0.15	44,44,44,44	0
58	MG	1A	3220	1/1	0.93	0.10	41,41,41,41	0
58	MG	2A	3288	1/1	0.93	0.13	52,52,52,52	0
58	MG	1a	1774	1/1	0.93	0.10	56,56,56,56	0
58	MG	2A	3290	1/1	0.93	0.11	47,47,47,47	0
58	MG	1A	3101	1/1	0.93	0.09	40,40,40,40	0
58	MG	1A	3856	1/1	0.93	0.10	20,20,20,20	0
58	MG	1A	3857	1/1	0.93	0.12	44,44,44,44	0
58	MG	2A	3295	1/1	0.93	0.12	46,46,46,46	0
58	MG	1A	3621	1/1	0.93	0.08	27,27,27,27	0
58	MG	1A	3997	1/1	0.93	0.07	10,10,10,10	0
58	MG	1A	3399	1/1	0.93	0.11	46,46,46,46	0
58	MG	1A	3459	1/1	0.93	0.15	56,56,56,56	0
58	MG	1A	3865	1/1	0.93	0.09	47,47,47,47	0
58	MG	2A	3723	1/1	0.93	0.09	53,53,53,53	0
58	MG	1A	4004	1/1	0.93	0.06	31,31,31,31	0
58	MG	2A	3479	1/1	0.93	0.10	52,52,52,52	0
58	MG	2A	3302	1/1	0.93	0.13	58,58,58,58	0
58	MG	1A	3115	1/1	0.94	0.08	40,40,40,40	0
58	MG	1T	201	1/1	0.94	0.18	55,55,55,55	0
58	MG	1A	3003	1/1	0.94	0.12	23,23,23,23	0
58	MG	1A	3844	1/1	0.94	0.09	46,46,46,46	0
58	MG	2A	3745	1/1	0.94	0.14	67,67,67,67	0
58	MG	2A	3746	1/1	0.94	0.09	59,59,59,59	0
58	MG	1A	3507	1/1	0.94	0.08	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
58	MG	2A	3180	1/1	0.94	0.30	67,67,67,67	0
58	MG	1U	204	1/1	0.94	0.11	44,44,44,44	0
58	MG	1A	3847	1/1	0.94	0.08	30,30,30,30	0
58	MG	2A	3753	1/1	0.94	0.13	41,41,41,41	0
58	MG	1U	209	1/1	0.94	0.16	32,32,32,32	0
58	MG	2A	3756	1/1	0.94	0.08	60,60,60,60	0
58	MG	2A	3520	1/1	0.94	0.12	39,39,39,39	0
58	MG	1A	3008	1/1	0.94	0.07	20,20,20,20	0
58	MG	2A	3760	1/1	0.94	0.07	45,45,45,45	0
58	MG	1A	3849	1/1	0.94	0.11	57,57,57,57	0
58	MG	1x	112	1/1	0.94	0.16	58,58,58,58	0
58	MG	2A	3765	1/1	0.94	0.06	45,45,45,45	0
58	MG	2A	3768	1/1	0.94	0.10	63,63,63,63	0
58	MG	2a	1657	1/1	0.94	0.19	59,59,59,59	0
58	MG	2A	3769	1/1	0.94	0.08	36,36,36,36	0
58	MG	1A	3850	1/1	0.94	0.10	45,45,45,45	0
58	MG	1A	3031	1/1	0.94	0.10	25,25,25,25	0
58	MG	1A	3511	1/1	0.94	0.13	28,28,28,28	0
58	MG	2a	1662	1/1	0.94	0.31	54,54,54,54	0
58	MG	1X	103	1/1	0.94	0.09	35,35,35,35	0
58	MG	2a	1664	1/1	0.94	0.07	47,47,47,47	0
58	MG	1X	104	1/1	0.94	0.07	46,46,46,46	0
58	MG	2A	3534	1/1	0.94	0.15	50,50,50,50	0
58	MG	2a	1668	1/1	0.94	0.11	61,61,61,61	0
58	MG	1A	3377	1/1	0.94	0.11	50,50,50,50	0
58	MG	2A	3347	1/1	0.94	0.23	65,65,65,65	0
58	MG	2A	3537	1/1	0.94	0.07	38,38,38,38	0
58	MG	1A	3574	1/1	0.94	0.12	31,31,31,31	0
58	MG	1A	3973	1/1	0.94	0.07	44,44,44,44	0
58	MG	1Y	204	1/1	0.94	0.25	39,39,39,39	0
58	MG	1A	3741	1/1	0.94	0.08	51,51,51,51	0
58	MG	2A	3544	1/1	0.94	0.11	48,48,48,48	0
58	MG	1A	3576	1/1	0.94	0.16	49,49,49,49	0
58	MG	1A	3577	1/1	0.94	0.11	37,37,37,37	0
58	MG	2A	3354	1/1	0.94	0.17	39,39,39,39	0
58	MG	1A	3066	1/1	0.94	0.16	47,47,47,47	0
58	MG	1a	1701	1/1	0.94	0.09	47,47,47,47	0
58	MG	1A	3579	1/1	0.94	0.13	34,34,34,34	0
58	MG	1A	3864	1/1	0.94	0.07	43,43,43,43	0
58	MG	2A	3556	1/1	0.94	0.10	31,31,31,31	0
58	MG	2A	3798	1/1	0.94	0.10	47,47,47,47	0
58	MG	2A	3557	1/1	0.94	0.17	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
58	MG	2A	3026	1/1	0.94	0.14	47,47,47,47	0
58	MG	1A	3464	1/1	0.94	0.08	38,38,38,38	0
58	MG	2A	3563	1/1	0.94	0.09	44,44,44,44	0
58	MG	1A	3749	1/1	0.94	0.09	22,22,22,22	0
58	MG	1I	101	1/1	0.94	0.21	40,40,40,40	0
58	MG	1A	3379	1/1	0.94	0.09	47,47,47,47	0
58	MG	1A	3381	1/1	0.94	0.15	36,36,36,36	0
58	MG	1A	3150	1/1	0.94	0.12	27,27,27,27	0
58	MG	2A	3811	1/1	0.94	0.11	65,65,65,65	0
58	MG	2A	3812	1/1	0.94	0.09	54,54,54,54	0
58	MG	1A	3757	1/1	0.94	0.10	47,47,47,47	0
58	MG	1A	3991	1/1	0.94	0.09	48,48,48,48	0
58	MG	1A	3662	1/1	0.94	0.10	45,45,45,45	0
58	MG	1A	3470	1/1	0.94	0.14	50,50,50,50	0
58	MG	1A	3995	1/1	0.94	0.08	45,45,45,45	0
58	MG	2A	3579	1/1	0.94	0.17	56,56,56,56	0
58	MG	2A	3215	1/1	0.94	0.10	53,53,53,53	0
58	MG	2A	3043	1/1	0.94	0.27	63,63,63,63	0
58	MG	2A	3825	1/1	0.94	0.07	52,52,52,52	0
58	MG	1A	3586	1/1	0.94	0.08	44,44,44,44	0
58	MG	2A	3045	1/1	0.94	0.11	29,29,29,29	0
58	MG	2A	3046	1/1	0.94	0.10	38,38,38,38	0
58	MG	2A	3829	1/1	0.94	0.09	37,37,37,37	0
58	MG	1A	3875	1/1	0.94	0.28	35,35,35,35	0
58	MG	1A	3999	1/1	0.94	0.11	26,26,26,26	0
58	MG	2A	3591	1/1	0.94	0.11	63,63,63,63	0
58	MG	2A	3835	1/1	0.94	0.10	60,60,60,60	0
58	MG	1A	3152	1/1	0.94	0.36	42,42,42,42	0
58	MG	2A	3051	1/1	0.94	0.20	63,63,63,63	0
58	MG	1A	3666	1/1	0.94	0.05	22,22,22,22	0
58	MG	2A	3595	1/1	0.94	0.10	53,53,53,53	0
58	MG	1a	1721	1/1	0.94	0.29	49,49,49,49	0
58	MG	2A	3841	1/1	0.94	0.14	67,67,67,67	0
58	MG	2A	3387	1/1	0.94	0.12	64,64,64,64	0
58	MG	1A	3589	1/1	0.94	0.06	29,29,29,29	0
58	MG	1A	3067	1/1	0.94	0.06	26,26,26,26	0
58	MG	2A	3845	1/1	0.94	0.11	63,63,63,63	0
58	MG	2A	3390	1/1	0.94	0.17	43,43,43,43	0
58	MG	1a	1726	1/1	0.94	0.11	54,54,54,54	0
58	MG	1A	3022	1/1	0.94	0.08	38,38,38,38	0
58	MG	2A	3849	1/1	0.94	0.18	57,57,57,57	0
58	MG	1A	3389	1/1	0.94	0.08	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3390	1/1	0.94	0.09	49,49,49,49	0
58	MG	1a	1733	1/1	0.94	0.08	57,57,57,57	0
58	MG	1A	3216	1/1	0.94	0.11	45,45,45,45	0
58	MG	1A	3393	1/1	0.94	0.18	63,63,63,63	0
58	MG	1A	3892	1/1	0.94	0.08	28,28,28,28	0
58	MG	2A	3067	1/1	0.94	0.11	51,51,51,51	0
58	MG	18	104	1/1	0.94	0.16	41,41,41,41	0
58	MG	1A	3780	1/1	0.94	0.07	57,57,57,57	0
58	MG	1A	3679	1/1	0.94	0.05	23,23,23,23	0
58	MG	2A	3073	1/1	0.94	0.10	38,38,38,38	0
58	MG	2A	3619	1/1	0.94	0.07	39,39,39,39	0
58	MG	1A	3783	1/1	0.94	0.06	24,24,24,24	0
58	MG	2B	213	1/1	0.94	0.27	58,58,58,58	0
58	MG	1A	3680	1/1	0.94	0.16	27,27,27,27	0
58	MG	1A	3394	1/1	0.94	0.09	45,45,45,45	0
58	MG	2A	3078	1/1	0.94	0.08	40,40,40,40	0
58	MG	1A	3481	1/1	0.94	0.17	36,36,36,36	0
58	MG	1A	3286	1/1	0.94	0.12	33,33,33,33	0
58	MG	2A	3081	1/1	0.94	0.10	50,50,50,50	0
58	MG	1a	1604	1/1	0.94	0.08	51,51,51,51	0
58	MG	2A	3634	1/1	0.94	0.12	35,35,35,35	0
58	MG	1A	3483	1/1	0.94	0.14	52,52,52,52	0
58	MG	2A	3085	1/1	0.94	0.10	51,51,51,51	0
58	MG	1D	302	1/1	0.94	0.14	46,46,46,46	0
58	MG	2A	3638	1/1	0.94	0.15	40,40,40,40	0
58	MG	2A	3256	1/1	0.94	0.07	42,42,42,42	0
58	MG	1A	3533	1/1	0.94	0.17	43,43,43,43	0
58	MG	1A	3126	1/1	0.94	0.08	25,25,25,25	0
58	MG	1A	3694	1/1	0.94	0.06	33,33,33,33	0
58	MG	1A	3798	1/1	0.94	0.07	32,32,32,32	0
58	MG	1D	310	1/1	0.94	0.10	49,49,49,49	0
58	MG	2A	3425	1/1	0.94	0.17	47,47,47,47	0
58	MG	1D	312	1/1	0.94	0.17	32,32,32,32	0
58	MG	1A	3604	1/1	0.94	0.10	41,41,41,41	0
58	MG	1A	3605	1/1	0.94	0.26	47,47,47,47	0
58	MG	2A	3265	1/1	0.94	0.10	54,54,54,54	0
58	MG	1E	304	1/1	0.94	0.11	33,33,33,33	0
58	MG	1A	3697	1/1	0.94	0.06	27,27,27,27	0
58	MG	1A	3159	1/1	0.94	0.10	31,31,31,31	0
58	MG	2A	3101	1/1	0.94	0.08	44,44,44,44	0
58	MG	1A	3254	1/1	0.94	0.14	19,19,19,19	0
58	MG	2Q	201	1/1	0.94	0.08	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3056	1/1	0.94	0.08	30,30,30,30	0
58	MG	1A	3611	1/1	0.94	0.11	24,24,24,24	0
58	MG	2A	3661	1/1	0.94	0.14	55,55,55,55	0
58	MG	1A	3540	1/1	0.94	0.09	47,47,47,47	0
58	MG	2a	1789	1/1	0.94	0.17	60,60,60,60	0
58	MG	1A	3923	1/1	0.94	0.09	35,35,35,35	0
58	MG	1A	4040	1/1	0.94	0.12	30,30,30,30	0
58	MG	2a	1792	1/1	0.94	0.16	63,63,63,63	0
58	MG	1A	3704	1/1	0.94	0.07	21,21,21,21	0
58	MG	1A	3810	1/1	0.94	0.08	50,50,50,50	0
58	MG	1A	3103	1/1	0.94	0.11	35,35,35,35	0
58	MG	1A	3326	1/1	0.94	0.11	58,58,58,58	0
58	MG	1a	1780	1/1	0.94	0.13	47,47,47,47	0
58	MG	1A	3292	1/1	0.94	0.14	32,32,32,32	0
58	MG	1F	310	1/1	0.94	0.16	54,54,54,54	0
58	MG	2A	3120	1/1	0.94	0.28	53,53,53,53	0
58	MG	1A	3225	1/1	0.94	0.08	44,44,44,44	0
58	MG	1F	312	1/1	0.94	0.10	42,42,42,42	0
58	MG	1A	4048	1/1	0.94	0.08	54,54,54,54	0
58	MG	1A	3045	1/1	0.94	0.08	34,34,34,34	0
58	MG	1A	3260	1/1	0.94	0.15	51,51,51,51	0
58	MG	1A	3261	1/1	0.94	0.12	48,48,48,48	0
58	MG	1a	1644	1/1	0.94	0.12	41,41,41,41	0
58	MG	2A	3464	1/1	0.94	0.09	37,37,37,37	0
58	MG	1G	205	1/1	0.94	0.17	61,61,61,61	0
58	MG	2A	3292	1/1	0.94	0.10	57,57,57,57	0
58	MG	1A	4052	1/1	0.94	0.07	47,47,47,47	0
58	MG	2a	1812	1/1	0.94	0.13	57,57,57,57	0
58	MG	2A	3691	1/1	0.94	0.09	62,62,62,62	0
58	MG	1a	1799	1/1	0.94	0.12	46,46,46,46	0
58	MG	1A	3820	1/1	0.94	0.09	24,24,24,24	0
58	MG	1A	3624	1/1	0.94	0.07	26,26,26,26	0
58	MG	29	101	1/1	0.94	0.10	61,61,61,61	0
58	MG	1N	202	1/1	0.94	0.10	46,46,46,46	0
58	MG	2A	3473	1/1	0.94	0.06	34,34,34,34	0
58	MG	1A	4055	1/1	0.94	0.13	49,49,49,49	0
58	MG	1A	3941	1/1	0.94	0.09	49,49,49,49	0
58	MG	2d	302	1/1	0.94	0.08	62,62,62,62	0
58	MG	1A	3046	1/1	0.94	0.08	26,26,26,26	0
58	MG	1O	202	1/1	0.94	0.11	42,42,42,42	0
58	MG	1A	3499	1/1	0.94	0.11	33,33,33,33	0
58	MG	1a	1809	1/1	0.94	0.09	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3707	1/1	0.94	0.15	61,61,61,61	0
58	MG	1A	3828	1/1	0.94	0.11	29,29,29,29	0
58	MG	2A	3305	1/1	0.94	0.10	59,59,59,59	0
58	MG	2A	3711	1/1	0.94	0.11	41,41,41,41	0
58	MG	1A	4063	1/1	0.94	0.13	38,38,38,38	0
58	MG	1A	3500	1/1	0.94	0.21	56,56,56,56	0
58	MG	1P	204	1/1	0.94	0.07	29,29,29,29	0
58	MG	2A	3157	1/1	0.94	0.08	45,45,45,45	0
58	MG	1A	3832	1/1	0.94	0.07	46,46,46,46	0
58	MG	1f	201	1/1	0.94	0.12	47,47,47,47	0
58	MG	1A	4071	1/1	0.94	0.06	40,40,40,40	0
58	MG	1Q	205	1/1	0.94	0.13	56,56,56,56	0
58	MG	2A	3492	1/1	0.94	0.11	42,42,42,42	0
58	MG	1A	3834	1/1	0.94	0.18	47,47,47,47	0
58	MG	1m	3001	1/1	0.94	0.07	51,51,51,51	0
58	MG	1A	3091	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3013	1/1	0.94	0.11	23,23,23,23	0
58	MG	2A	3319	1/1	0.94	0.12	51,51,51,51	0
58	MG	1A	3111	1/1	0.94	0.10	36,36,36,36	0
58	MG	1R	202	1/1	0.94	0.17	39,39,39,39	0
58	MG	1A	4076	1/1	0.94	0.10	36,36,36,36	0
58	MG	1w	104	1/1	0.94	0.22	64,64,64,64	0
58	MG	2A	3170	1/1	0.94	0.07	41,41,41,41	0
58	MG	2A	3505	1/1	0.94	0.11	71,71,71,71	0
58	MG	1A	3266	1/1	0.94	0.20	41,41,41,41	0
58	MG	1A	4079	1/1	0.94	0.14	37,37,37,37	0
58	MG	1S	202	1/1	0.94	0.13	49,49,49,49	0
58	MG	1A	3882	1/1	0.95	0.08	28,28,28,28	0
58	MG	2A	3649	1/1	0.95	0.15	41,41,41,41	0
58	MG	1A	3723	1/1	0.95	0.07	36,36,36,36	0
58	MG	1N	204	1/1	0.95	0.08	48,48,48,48	0
58	MG	1A	3084	1/1	0.95	0.19	39,39,39,39	0
58	MG	1A	3725	1/1	0.95	0.07	40,40,40,40	0
58	MG	1A	3047	1/1	0.95	0.05	20,20,20,20	0
58	MG	1A	3557	1/1	0.95	0.16	39,39,39,39	0
58	MG	1A	3889	1/1	0.95	0.07	28,28,28,28	0
58	MG	1A	3079	1/1	0.95	0.09	24,24,24,24	0
58	MG	1A	3990	1/1	0.95	0.09	50,50,50,50	0
58	MG	1A	3731	1/1	0.95	0.10	56,56,56,56	0
58	MG	1a	1749	1/1	0.95	0.12	50,50,50,50	0
58	MG	2a	1692	1/1	0.95	0.22	60,60,60,60	0
58	MG	1P	205	1/1	0.95	0.25	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
58	MG	2A	3663	1/1	0.95	0.07	39,39,39,39	0
58	MG	2A	3852	1/1	0.95	0.17	54,54,54,54	0
58	MG	1A	3188	1/1	0.95	0.12	30,30,30,30	0
58	MG	1Q	201	1/1	0.95	0.21	38,38,38,38	0
58	MG	1A	4093	1/1	0.95	0.11	54,54,54,54	0
58	MG	1A	3478	1/1	0.95	0.09	37,37,37,37	0
58	MG	2A	3486	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3174	1/1	0.95	0.07	27,27,27,27	0
58	MG	1A	3244	1/1	0.95	0.24	62,62,62,62	0
58	MG	2A	3674	1/1	0.95	0.11	57,57,57,57	0
58	MG	1A	3317	1/1	0.95	0.31	54,54,54,54	0
58	MG	1A	3132	1/1	0.95	0.08	33,33,33,33	0
58	MG	1A	3901	1/1	0.95	0.07	35,35,35,35	0
58	MG	1a	1641	1/1	0.95	0.10	51,51,51,51	0
58	MG	1A	3570	1/1	0.95	0.12	50,50,50,50	0
58	MG	1A	3375	1/1	0.95	0.07	38,38,38,38	0
58	MG	2A	3065	1/1	0.95	0.13	52,52,52,52	0
58	MG	1A	3346	1/1	0.95	0.11	35,35,35,35	0
58	MG	1A	3623	1/1	0.95	0.12	37,37,37,37	0
58	MG	1A	3134	1/1	0.95	0.07	32,32,32,32	0
58	MG	1A	3526	1/1	0.95	0.08	42,42,42,42	0
58	MG	1a	1773	1/1	0.95	0.06	38,38,38,38	0
58	MG	1A	3827	1/1	0.95	0.07	20,20,20,20	0
58	MG	1A	3054	1/1	0.95	0.07	45,45,45,45	0
58	MG	2A	3220	1/1	0.95	0.15	44,44,44,44	0
58	MG	2A	3221	1/1	0.95	0.10	34,34,34,34	0
58	MG	1a	1651	1/1	0.95	0.06	43,43,43,43	0
58	MG	1A	3829	1/1	0.95	0.11	39,39,39,39	0
58	MG	1A	3380	1/1	0.95	0.09	25,25,25,25	0
58	MG	1A	3831	1/1	0.95	0.07	39,39,39,39	0
58	MG	2E	307	1/1	0.95	0.06	33,33,33,33	0
58	MG	1A	3349	1/1	0.95	0.07	38,38,38,38	0
58	MG	1a	1782	1/1	0.95	0.06	51,51,51,51	0
58	MG	1V	201	1/1	0.95	0.18	27,27,27,27	0
58	MG	2A	3516	1/1	0.95	0.09	43,43,43,43	0
58	MG	2A	3084	1/1	0.95	0.15	44,44,44,44	0
58	MG	1a	1657	1/1	0.95	0.08	41,41,41,41	0
58	MG	1A	3920	1/1	0.95	0.06	37,37,37,37	0
58	MG	1V	205	1/1	0.95	0.07	34,34,34,34	0
58	MG	1A	3693	1/1	0.95	0.06	30,30,30,30	0
58	MG	2A	3369	1/1	0.95	0.19	58,58,58,58	0
58	MG	2A	3524	1/1	0.95	0.17	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3713	1/1	0.95	0.08	33,33,33,33	0
58	MG	1A	3835	1/1	0.95	0.10	45,45,45,45	0
58	MG	2P	202	1/1	0.95	0.09	64,64,64,64	0
58	MG	1A	3759	1/1	0.95	0.15	29,29,29,29	0
58	MG	1a	1793	1/1	0.95	0.15	58,58,58,58	0
58	MG	2A	3529	1/1	0.95	0.10	43,43,43,43	0
58	MG	2Q	204	1/1	0.95	0.09	42,42,42,42	0
58	MG	1a	1794	1/1	0.95	0.08	60,60,60,60	0
58	MG	1A	3630	1/1	0.95	0.07	43,43,43,43	0
58	MG	1a	1796	1/1	0.95	0.07	39,39,39,39	0
58	MG	1X	101	1/1	0.95	0.05	34,34,34,34	0
58	MG	1B	217	1/1	0.95	0.07	50,50,50,50	0
58	MG	1A	3322	1/1	0.95	0.08	41,41,41,41	0
58	MG	1A	3455	1/1	0.95	0.16	46,46,46,46	0
58	MG	1B	222	1/1	0.95	0.08	37,37,37,37	0
58	MG	2A	3246	1/1	0.95	0.09	53,53,53,53	0
58	MG	2A	3729	1/1	0.95	0.06	60,60,60,60	0
58	MG	2a	1757	1/1	0.95	0.12	46,46,46,46	0
58	MG	1A	3763	1/1	0.95	0.09	27,27,27,27	0
58	MG	1A	3928	1/1	0.95	0.10	55,55,55,55	0
58	MG	1A	3764	1/1	0.95	0.10	43,43,43,43	0
58	MG	1A	3930	1/1	0.95	0.12	41,41,41,41	0
58	MG	1A	3765	1/1	0.95	0.07	36,36,36,36	0
58	MG	1A	3845	1/1	0.95	0.09	39,39,39,39	0
58	MG	1a	1677	1/1	0.95	0.16	58,58,58,58	0
58	MG	2A	3391	1/1	0.95	0.20	59,59,59,59	0
58	MG	10	103	1/1	0.95	0.08	32,32,32,32	0
58	MG	1B	229	1/1	0.95	0.07	41,41,41,41	0
58	MG	1A	3196	1/1	0.95	0.13	30,30,30,30	0
58	MG	1A	3137	1/1	0.95	0.27	33,33,33,33	0
58	MG	2A	3117	1/1	0.95	0.07	53,53,53,53	0
58	MG	2A	3560	1/1	0.95	0.06	34,34,34,34	0
58	MG	1A	3938	1/1	0.95	0.09	39,39,39,39	0
58	MG	2A	3399	1/1	0.95	0.30	51,51,51,51	0
58	MG	1A	3769	1/1	0.95	0.07	34,34,34,34	0
58	MG	2A	3749	1/1	0.95	0.13	49,49,49,49	0
58	MG	2A	3401	1/1	0.95	0.26	50,50,50,50	0
58	MG	11	102	1/1	0.95	0.10	52,52,52,52	0
58	MG	2A	3752	1/1	0.95	0.05	36,36,36,36	0
58	MG	1A	3699	1/1	0.95	0.10	23,23,23,23	0
58	MG	1B	237	1/1	0.95	0.07	40,40,40,40	0
58	MG	1A	3109	1/1	0.95	0.11	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3757	1/1	0.95	0.11	59,59,59,59	0
58	MG	2A	3574	1/1	0.95	0.11	35,35,35,35	0
58	MG	2a	1787	1/1	0.95	0.10	58,58,58,58	0
58	MG	1A	3638	1/1	0.95	0.09	25,25,25,25	0
58	MG	1A	3773	1/1	0.95	0.08	36,36,36,36	0
58	MG	12	102	1/1	0.95	0.08	34,34,34,34	0
58	MG	2A	3133	1/1	0.95	0.08	54,54,54,54	0
58	MG	13	101	1/1	0.95	0.09	33,33,33,33	0
58	MG	2A	3767	1/1	0.95	0.09	52,52,52,52	0
58	MG	1A	3090	1/1	0.95	0.14	43,43,43,43	0
58	MG	1A	3640	1/1	0.95	0.09	33,33,33,33	0
58	MG	1A	3424	1/1	0.95	0.08	30,30,30,30	0
58	MG	1A	3948	1/1	0.95	0.08	56,56,56,56	0
58	MG	2A	3139	1/1	0.95	0.14	40,40,40,40	0
58	MG	15	101	1/1	0.95	0.13	27,27,27,27	0
58	MG	2A	3142	1/1	0.95	0.10	46,46,46,46	0
58	MG	1A	3777	1/1	0.95	0.15	24,24,24,24	0
58	MG	1A	3071	1/1	0.95	0.08	15,15,15,15	0
58	MG	2A	3780	1/1	0.95	0.08	39,39,39,39	0
58	MG	1A	3859	1/1	0.95	0.10	23,23,23,23	0
58	MG	1E	302	1/1	0.95	0.09	36,36,36,36	0
58	MG	1A	3860	1/1	0.95	0.13	21,21,21,21	0
58	MG	1A	3203	1/1	0.95	0.07	29,29,29,29	0
58	MG	2A	3150	1/1	0.95	0.06	52,52,52,52	0
58	MG	2A	3151	1/1	0.95	0.10	57,57,57,57	0
58	MG	1A	3302	1/1	0.95	0.14	34,34,34,34	0
58	MG	1A	3127	1/1	0.95	0.10	35,35,35,35	0
58	MG	1A	3957	1/1	0.95	0.08	58,58,58,58	0
58	MG	1A	4056	1/1	0.95	0.05	31,31,31,31	0
58	MG	1A	3648	1/1	0.95	0.13	47,47,47,47	0
58	MG	1A	3785	1/1	0.95	0.13	53,53,53,53	0
58	MG	2A	3433	1/1	0.95	0.32	57,57,57,57	0
58	MG	1A	3279	1/1	0.95	0.07	34,34,34,34	0
58	MG	2A	3795	1/1	0.95	0.11	41,41,41,41	0
58	MG	1A	3466	1/1	0.95	0.11	41,41,41,41	0
58	MG	1A	3789	1/1	0.95	0.10	46,46,46,46	0
58	MG	2A	3611	1/1	0.95	0.08	53,53,53,53	0
58	MG	1A	3963	1/1	0.95	0.09	30,30,30,30	0
58	MG	1A	3397	1/1	0.95	0.08	26,26,26,26	0
58	MG	2a	1645	1/1	0.95	0.18	57,57,57,57	0
58	MG	1A	4067	1/1	0.95	0.07	19,19,19,19	0
58	MG	2A	3440	1/1	0.95	0.08	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
58	MG	1A	3468	1/1	0.95	0.08	38,38,38,38	0
58	MG	1A	3307	1/1	0.95	0.06	31,31,31,31	0
58	MG	2A	3012	1/1	0.95	0.08	39,39,39,39	0
58	MG	2A	3808	1/1	0.95	0.08	50,50,50,50	0
58	MG	1A	3281	1/1	0.95	0.23	31,31,31,31	0
58	MG	1A	3970	1/1	0.95	0.09	42,42,42,42	0
58	MG	1A	3509	1/1	0.95	0.11	42,42,42,42	0
58	MG	1A	3876	1/1	0.95	0.07	39,39,39,39	0
58	MG	1a	1723	1/1	0.95	0.18	50,50,50,50	0
58	MG	2A	3452	1/1	0.95	0.11	50,50,50,50	0
58	MG	2A	3020	1/1	0.95	0.11	36,36,36,36	0
58	MG	1a	1608	1/1	0.95	0.07	43,43,43,43	0
58	MG	1A	3878	1/1	0.95	0.12	32,32,32,32	0
58	MG	2A	3023	1/1	0.95	0.08	38,38,38,38	0
58	MG	1A	4078	1/1	0.95	0.12	34,34,34,34	0
58	MG	1a	1612	1/1	0.95	0.10	57,57,57,57	0
58	MG	1A	3009	1/1	0.95	0.06	24,24,24,24	0
58	MG	1a	1731	1/1	0.95	0.11	37,37,37,37	0
58	MG	2A	3030	1/1	0.95	0.10	44,44,44,44	0
58	MG	2a	1667	1/1	0.95	0.10	51,51,51,51	0
58	MG	2A	3031	1/1	0.95	0.15	38,38,38,38	0
58	MG	2A	3830	1/1	0.95	0.09	33,33,33,33	0
58	MG	2A	3831	1/1	0.95	0.09	55,55,55,55	0
58	MG	2A	3643	1/1	0.95	0.12	38,38,38,38	0
58	MG	1A	3258	1/1	0.95	0.09	37,37,37,37	0
58	MG	1a	1616	1/1	0.95	0.08	40,40,40,40	0
58	MG	1A	3722	1/1	0.95	0.08	34,34,34,34	0
58	MG	2x	106	1/1	0.95	0.09	51,51,51,51	0
59	K	2A	3443	1/1	0.95	0.07	51,51,51,51	0
60	ZN	24	501	1/1	0.95	0.12	103,103,103,103	0
61	SF4	1d	302	8/8	0.95	0.08	52,54,59,62	0
58	MG	1A	3612	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3553	1/1	0.96	0.07	27,27,27,27	0
58	MG	1A	3683	1/1	0.96	0.06	31,31,31,31	0
58	MG	1U	205	1/1	0.96	0.18	33,33,33,33	0
58	MG	1A	3215	1/1	0.96	0.09	38,38,38,38	0
58	MG	1U	208	1/1	0.96	0.28	29,29,29,29	0
58	MG	2A	3658	1/1	0.96	0.05	32,32,32,32	0
58	MG	2a	1684	1/1	0.96	0.14	49,49,49,49	0
58	MG	2A	3057	1/1	0.96	0.16	40,40,40,40	0
58	MG	1A	3686	1/1	0.96	0.06	27,27,27,27	0
58	MG	1A	3099	1/1	0.96	0.07	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
58	MG	1V	202	1/1	0.96	0.12	37,37,37,37	0
58	MG	2A	3487	1/1	0.96	0.12	27,27,27,27	0
58	MG	1A	3112	1/1	0.96	0.09	29,29,29,29	0
58	MG	1A	4025	1/1	0.96	0.06	34,34,34,34	0
58	MG	2A	3850	1/1	0.96	0.10	46,46,46,46	0
58	MG	2A	3666	1/1	0.96	0.09	36,36,36,36	0
58	MG	1B	219	1/1	0.96	0.07	41,41,41,41	0
58	MG	1A	3391	1/1	0.96	0.23	38,38,38,38	0
58	MG	1A	3319	1/1	0.96	0.09	36,36,36,36	0
58	MG	2A	3066	1/1	0.96	0.08	33,33,33,33	0
58	MG	2A	3346	1/1	0.96	0.13	63,63,63,63	0
58	MG	1A	4028	1/1	0.96	0.04	19,19,19,19	0
58	MG	1A	4029	1/1	0.96	0.07	42,42,42,42	0
58	MG	2a	1703	1/1	0.96	0.07	65,65,65,65	0
58	MG	2A	3069	1/1	0.96	0.07	42,42,42,42	0
58	MG	1X	102	1/1	0.96	0.08	46,46,46,46	0
58	MG	1A	3934	1/1	0.96	0.04	11,11,11,11	0
58	MG	2A	3501	1/1	0.96	0.08	59,59,59,59	0
58	MG	2A	3072	1/1	0.96	0.18	40,40,40,40	0
58	MG	1A	3767	1/1	0.96	0.09	37,37,37,37	0
58	MG	1A	3692	1/1	0.96	0.08	32,32,32,32	0
58	MG	2A	3075	1/1	0.96	0.08	22,22,22,22	0
58	MG	2A	3684	1/1	0.96	0.07	61,61,61,61	0
58	MG	1A	3513	1/1	0.96	0.14	30,30,30,30	0
58	MG	2A	3686	1/1	0.96	0.15	46,46,46,46	0
58	MG	1a	1783	1/1	0.96	0.07	47,47,47,47	0
58	MG	1A	3218	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3515	1/1	0.96	0.07	33,33,33,33	0
58	MG	1Z	301	1/1	0.96	0.14	43,43,43,43	0
58	MG	2A	3362	1/1	0.96	0.20	49,49,49,49	0
58	MG	2D	306	1/1	0.96	0.14	40,40,40,40	0
58	MG	1B	230	1/1	0.96	0.06	40,40,40,40	0
58	MG	1A	4036	1/1	0.96	0.07	29,29,29,29	0
58	MG	1a	1790	1/1	0.96	0.06	45,45,45,45	0
58	MG	1A	3192	1/1	0.96	0.11	27,27,27,27	0
58	MG	1A	3564	1/1	0.96	0.10	53,53,53,53	0
58	MG	1A	3943	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3855	1/1	0.96	0.09	49,49,49,49	0
58	MG	1A	3565	1/1	0.96	0.08	35,35,35,35	0
58	MG	2A	3701	1/1	0.96	0.10	35,35,35,35	0
58	MG	1a	1673	1/1	0.96	0.14	48,48,48,48	0
58	MG	2A	3703	1/1	0.96	0.11	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3372	1/1	0.96	0.15	38,38,38,38	0
58	MG	1A	3146	1/1	0.96	0.18	32,32,32,32	0
58	MG	1A	3147	1/1	0.96	0.07	31,31,31,31	0
58	MG	2A	3526	1/1	0.96	0.04	38,38,38,38	0
58	MG	1A	3224	1/1	0.96	0.08	47,47,47,47	0
58	MG	1A	3010	1/1	0.96	0.06	30,30,30,30	0
58	MG	1D	305	1/1	0.96	0.08	36,36,36,36	0
58	MG	1A	3572	1/1	0.96	0.16	31,31,31,31	0
58	MG	1A	3023	1/1	0.96	0.06	13,13,13,13	0
58	MG	1a	1804	1/1	0.96	0.16	52,52,52,52	0
58	MG	1D	308	1/1	0.96	0.07	28,28,28,28	0
58	MG	2a	1743	1/1	0.96	0.07	56,56,56,56	0
58	MG	2A	3102	1/1	0.96	0.13	50,50,50,50	0
58	MG	2a	1745	1/1	0.96	0.11	70,70,70,70	0
58	MG	1A	3782	1/1	0.96	0.09	32,32,32,32	0
58	MG	2A	3719	1/1	0.96	0.06	43,43,43,43	0
58	MG	1A	3575	1/1	0.96	0.40	34,34,34,34	0
58	MG	2A	3538	1/1	0.96	0.13	47,47,47,47	0
58	MG	1A	3015	1/1	0.96	0.10	32,32,32,32	0
58	MG	2A	3386	1/1	0.96	0.14	43,43,43,43	0
58	MG	1a	1685	1/1	0.96	0.12	33,33,33,33	0
58	MG	1A	3133	1/1	0.96	0.06	38,38,38,38	0
58	MG	2a	1754	1/1	0.96	0.15	59,59,59,59	0
58	MG	1A	3200	1/1	0.96	0.09	31,31,31,31	0
58	MG	2A	3545	1/1	0.96	0.07	46,46,46,46	0
58	MG	1A	3331	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3298	1/1	0.96	0.08	28,28,28,28	0
58	MG	2A	3112	1/1	0.96	0.08	29,29,29,29	0
58	MG	1A	3232	1/1	0.96	0.07	44,44,44,44	0
58	MG	1A	4057	1/1	0.96	0.05	18,18,18,18	0
58	MG	1A	3368	1/1	0.96	0.14	49,49,49,49	0
58	MG	2A	3396	1/1	0.96	0.22	48,48,48,48	0
58	MG	20	102	1/1	0.96	0.08	50,50,50,50	0
58	MG	2A	3555	1/1	0.96	0.05	40,40,40,40	0
58	MG	1A	3005	1/1	0.96	0.07	32,32,32,32	0
58	MG	1A	4060	1/1	0.96	0.08	45,45,45,45	0
58	MG	2A	3118	1/1	0.96	0.09	60,60,60,60	0
58	MG	1A	3154	1/1	0.96	0.12	33,33,33,33	0
58	MG	1F	303	1/1	0.96	0.07	28,28,28,28	0
58	MG	2A	3562	1/1	0.96	0.06	38,38,38,38	0
58	MG	27	101	1/1	0.96	0.11	45,45,45,45	0
58	MG	1A	3964	1/1	0.96	0.06	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
58	MG	17	102	1/1	0.96	0.06	29,29,29,29	0
58	MG	17	103	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3646	1/1	0.96	0.04	22,22,22,22	0
58	MG	2A	3569	1/1	0.96	0.07	42,42,42,42	0
58	MG	2A	3126	1/1	0.96	0.05	40,40,40,40	0
58	MG	2A	3127	1/1	0.96	0.11	44,44,44,44	0
58	MG	1A	3058	1/1	0.96	0.10	22,22,22,22	0
58	MG	1A	3587	1/1	0.96	0.24	43,43,43,43	0
58	MG	1A	3720	1/1	0.96	0.05	13,13,13,13	0
58	MG	1A	3650	1/1	0.96	0.09	25,25,25,25	0
58	MG	1A	3303	1/1	0.96	0.06	22,22,22,22	0
58	MG	1A	3654	1/1	0.96	0.05	27,27,27,27	0
58	MG	1A	3136	1/1	0.96	0.10	21,21,21,21	0
58	MG	1A	3534	1/1	0.96	0.17	51,51,51,51	0
58	MG	1A	3454	1/1	0.96	0.15	39,39,39,39	0
58	MG	1A	3658	1/1	0.96	0.06	37,37,37,37	0
58	MG	2A	3763	1/1	0.96	0.11	41,41,41,41	0
58	MG	1x	107	1/1	0.96	0.05	47,47,47,47	0
58	MG	1A	3729	1/1	0.96	0.07	42,42,42,42	0
58	MG	1A	3812	1/1	0.96	0.18	18,18,18,18	0
58	MG	1A	3891	1/1	0.96	0.14	25,25,25,25	0
58	MG	2A	3145	1/1	0.96	0.12	50,50,50,50	0
58	MG	2A	3771	1/1	0.96	0.08	71,71,71,71	0
58	MG	1a	1714	1/1	0.96	0.18	41,41,41,41	0
58	MG	1A	3043	1/1	0.96	0.12	35,35,35,35	0
58	MG	1A	3051	1/1	0.96	0.09	22,22,22,22	0
58	MG	1A	3496	1/1	0.96	0.10	26,26,26,26	0
58	MG	1A	3497	1/1	0.96	0.10	27,27,27,27	0
58	MG	1A	3987	1/1	0.96	0.12	29,29,29,29	0
58	MG	1a	1610	1/1	0.96	0.10	23,23,23,23	0
58	MG	1A	3735	1/1	0.96	0.10	48,48,48,48	0
58	MG	2A	3431	1/1	0.96	0.26	58,58,58,58	0
58	MG	1A	3243	1/1	0.96	0.12	40,40,40,40	0
58	MG	2A	3008	1/1	0.96	0.06	36,36,36,36	0
58	MG	1A	3052	1/1	0.96	0.09	24,24,24,24	0
58	MG	2A	3010	1/1	0.96	0.06	43,43,43,43	0
58	MG	2A	3605	1/1	0.96	0.10	55,55,55,55	0
58	MG	1a	1614	1/1	0.96	0.06	45,45,45,45	0
58	MG	1A	3208	1/1	0.96	0.07	37,37,37,37	0
58	MG	1A	3185	1/1	0.96	0.20	40,40,40,40	0
58	MG	1A	3994	1/1	0.96	0.06	36,36,36,36	0
58	MG	1A	3278	1/1	0.96	0.06	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1730	1/1	0.96	0.07	39,39,39,39	0
58	MG	2A	3444	1/1	0.96	0.10	25,25,25,25	0
58	MG	1A	3422	1/1	0.96	0.08	44,44,44,44	0
58	MG	1a	1732	1/1	0.96	0.06	40,40,40,40	0
58	MG	1A	3825	1/1	0.96	0.05	20,20,20,20	0
58	MG	1A	3998	1/1	0.96	0.11	19,19,19,19	0
58	MG	1P	207	1/1	0.96	0.12	34,34,34,34	0
58	MG	2A	3621	1/1	0.96	0.07	39,39,39,39	0
58	MG	2A	3025	1/1	0.96	0.10	38,38,38,38	0
58	MG	1A	3826	1/1	0.96	0.08	34,34,34,34	0
58	MG	1a	1624	1/1	0.96	0.15	50,50,50,50	0
58	MG	2A	3173	1/1	0.96	0.09	39,39,39,39	0
58	MG	2A	3626	1/1	0.96	0.09	60,60,60,60	0
58	MG	1a	1738	1/1	0.96	0.14	48,48,48,48	0
58	MG	2A	3809	1/1	0.96	0.07	51,51,51,51	0
58	MG	2A	3628	1/1	0.96	0.08	37,37,37,37	0
58	MG	2A	3629	1/1	0.96	0.15	41,41,41,41	0
58	MG	1a	1739	1/1	0.96	0.10	56,56,56,56	0
58	MG	1A	3670	1/1	0.96	0.07	35,35,35,35	0
58	MG	1A	3247	1/1	0.96	0.13	33,33,33,33	0
58	MG	1A	3036	1/1	0.96	0.08	41,41,41,41	0
58	MG	1A	4101	1/1	0.96	0.09	50,50,50,50	0
58	MG	2A	3819	1/1	0.96	0.06	56,56,56,56	0
58	MG	1A	3426	1/1	0.96	0.08	38,38,38,38	0
58	MG	1A	3912	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3750	1/1	0.96	0.08	16,16,16,16	0
58	MG	1a	1632	1/1	0.96	0.12	24,24,24,24	0
58	MG	1A	3915	1/1	0.96	0.14	34,34,34,34	0
58	MG	1A	3751	1/1	0.96	0.13	50,50,50,50	0
58	MG	1a	1750	1/1	0.96	0.19	52,52,52,52	0
58	MG	1A	3550	1/1	0.96	0.10	33,33,33,33	0
58	MG	2a	1669	1/1	0.96	0.10	35,35,35,35	0
58	MG	1A	3551	1/1	0.96	0.08	32,32,32,32	0
58	MG	2A	3646	1/1	0.96	0.08	47,47,47,47	0
58	MG	1A	3836	1/1	0.96	0.11	56,56,56,56	0
58	MG	1A	3837	1/1	0.96	0.08	50,50,50,50	0
58	MG	1a	1756	1/1	0.96	0.10	45,45,45,45	0
58	MG	2A	3049	1/1	0.96	0.17	58,58,58,58	0
58	MG	1A	3165	1/1	0.96	0.12	30,30,30,30	0
61	SF4	2d	304	8/8	0.96	0.08	61,70,76,84	0
58	MG	1A	3209	1/1	0.97	0.09	40,40,40,40	0
58	MG	1A	3306	1/1	0.97	0.07	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
58	MG	2A	3764	1/1	0.97	0.07	50,50,50,50	0
58	MG	1a	1778	1/1	0.97	0.07	62,62,62,62	0
58	MG	1A	3708	1/1	0.97	0.04	15,15,15,15	0
58	MG	2A	3630	1/1	0.97	0.12	39,39,39,39	0
58	MG	2A	3631	1/1	0.97	0.07	34,34,34,34	0
58	MG	2A	3499	1/1	0.97	0.11	66,66,66,66	0
58	MG	1A	3914	1/1	0.97	0.05	34,34,34,34	0
58	MG	2A	3772	1/1	0.97	0.10	39,39,39,39	0
58	MG	1A	3651	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	3652	1/1	0.97	0.05	22,22,22,22	0
58	MG	1A	3917	1/1	0.97	0.09	34,34,34,34	0
58	MG	2A	3776	1/1	0.97	0.06	66,66,66,66	0
58	MG	1A	3918	1/1	0.97	0.04	28,28,28,28	0
58	MG	1a	1785	1/1	0.97	0.07	59,59,59,59	0
58	MG	1A	3113	1/1	0.97	0.09	28,28,28,28	0
58	MG	1A	3712	1/1	0.97	0.10	38,38,38,38	0
58	MG	1A	3272	1/1	0.97	0.10	46,46,46,46	0
58	MG	1A	3145	1/1	0.97	0.14	27,27,27,27	0
58	MG	1A	3114	1/1	0.97	0.07	28,28,28,28	0
58	MG	1A	4006	1/1	0.97	0.05	27,27,27,27	0
58	MG	1A	3383	1/1	0.97	0.07	43,43,43,43	0
58	MG	2A	3513	1/1	0.97	0.10	23,23,23,23	0
58	MG	1A	3425	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	3214	1/1	0.97	0.08	34,34,34,34	0
58	MG	1A	3061	1/1	0.97	0.09	36,36,36,36	0
58	MG	1A	4012	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3191	1/1	0.97	0.13	30,30,30,30	0
58	MG	1A	4014	1/1	0.97	0.06	59,59,59,59	0
58	MG	1A	3608	1/1	0.97	0.07	26,26,26,26	0
58	MG	1A	3787	1/1	0.97	0.11	28,28,28,28	0
58	MG	1A	3609	1/1	0.97	0.07	34,34,34,34	0
58	MG	2A	3796	1/1	0.97	0.05	36,36,36,36	0
58	MG	2A	3523	1/1	0.97	0.08	36,36,36,36	0
58	MG	1A	3280	1/1	0.97	0.20	37,37,37,37	0
58	MG	1P	201	1/1	0.97	0.18	29,29,29,29	0
58	MG	1A	3790	1/1	0.97	0.05	31,31,31,31	0
58	MG	1A	3116	1/1	0.97	0.15	29,29,29,29	0
58	MG	1A	3282	1/1	0.97	0.09	28,28,28,28	0
58	MG	1A	3861	1/1	0.97	0.05	24,24,24,24	0
58	MG	1A	3794	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3283	1/1	0.97	0.17	35,35,35,35	0
58	MG	1Q	202	1/1	0.97	0.12	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
58	MG	2A	3533	1/1	0.97	0.07	43,43,43,43	0
58	MG	1Q	203	1/1	0.97	0.04	24,24,24,24	0
58	MG	2A	3668	1/1	0.97	0.09	63,63,63,63	0
58	MG	2a	1763	1/1	0.97	0.15	59,59,59,59	0
58	MG	1A	3727	1/1	0.97	0.09	23,23,23,23	0
58	MG	1A	3249	1/1	0.97	0.06	28,28,28,28	0
58	MG	1A	3028	1/1	0.97	0.13	27,27,27,27	0
58	MG	1A	3799	1/1	0.97	0.08	18,18,18,18	0
58	MG	2A	3673	1/1	0.97	0.10	46,46,46,46	0
58	MG	2A	3816	1/1	0.97	0.08	51,51,51,51	0
58	MG	2a	1770	1/1	0.97	0.11	51,51,51,51	0
58	MG	1A	3219	1/1	0.97	0.08	37,37,37,37	0
58	MG	1A	3567	1/1	0.97	0.09	23,23,23,23	0
58	MG	1A	3673	1/1	0.97	0.05	26,26,26,26	0
58	MG	2A	3542	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3396	1/1	0.97	0.10	35,35,35,35	0
58	MG	2A	3087	1/1	0.97	0.10	40,40,40,40	0
58	MG	1A	3949	1/1	0.97	0.04	45,45,45,45	0
58	MG	1B	218	1/1	0.97	0.05	45,45,45,45	0
58	MG	1A	3171	1/1	0.97	0.07	19,19,19,19	0
58	MG	2A	3549	1/1	0.97	0.12	39,39,39,39	0
58	MG	1A	3737	1/1	0.97	0.10	20,20,20,20	0
58	MG	2A	3316	1/1	0.97	0.06	44,44,44,44	0
58	MG	1w	102	1/1	0.97	0.13	46,46,46,46	0
58	MG	1A	3676	1/1	0.97	0.05	43,43,43,43	0
58	MG	1A	3221	1/1	0.97	0.08	33,33,33,33	0
58	MG	1U	201	1/1	0.97	0.06	30,30,30,30	0
58	MG	1A	3877	1/1	0.97	0.20	33,33,33,33	0
58	MG	1A	3172	1/1	0.97	0.14	27,27,27,27	0
58	MG	1a	1725	1/1	0.97	0.14	56,56,56,56	0
58	MG	2A	3559	1/1	0.97	0.06	46,46,46,46	0
58	MG	1A	3085	1/1	0.97	0.15	28,28,28,28	0
58	MG	1A	3811	1/1	0.97	0.04	22,22,22,22	0
58	MG	1A	3120	1/1	0.97	0.07	44,44,44,44	0
58	MG	1U	207	1/1	0.97	0.12	31,31,31,31	0
58	MG	1A	3024	1/1	0.97	0.13	45,45,45,45	0
58	MG	2A	3441	1/1	0.97	0.13	51,51,51,51	0
58	MG	1A	3030	1/1	0.97	0.14	31,31,31,31	0
58	MG	1A	3685	1/1	0.97	0.08	58,58,58,58	0
58	MG	1A	3746	1/1	0.97	0.07	45,45,45,45	0
58	MG	2A	3704	1/1	0.97	0.05	43,43,43,43	0
58	MG	1B	232	1/1	0.97	0.05	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
58	MG	1A	3228	1/1	0.97	0.07	28,28,28,28	0
58	MG	2A	3573	1/1	0.97	0.07	45,45,45,45	0
58	MG	2A	3111	1/1	0.97	0.19	49,49,49,49	0
58	MG	1A	3155	1/1	0.97	0.09	39,39,39,39	0
58	MG	1A	3965	1/1	0.97	0.09	31,31,31,31	0
58	MG	1A	3446	1/1	0.97	0.26	28,28,28,28	0
58	MG	1A	3366	1/1	0.97	0.09	27,27,27,27	0
58	MG	1A	3098	1/1	0.97	0.10	18,18,18,18	0
58	MG	1D	301	1/1	0.97	0.06	32,32,32,32	0
58	MG	1A	3449	1/1	0.97	0.09	42,42,42,42	0
58	MG	2A	3231	1/1	0.97	0.10	54,54,54,54	0
58	MG	1A	3893	1/1	0.97	0.08	47,47,47,47	0
58	MG	1A	3754	1/1	0.97	0.08	37,37,37,37	0
58	MG	2A	3586	1/1	0.97	0.05	58,58,58,58	0
58	MG	1A	3972	1/1	0.97	0.07	53,53,53,53	0
58	MG	2A	3122	1/1	0.97	0.14	39,39,39,39	0
58	MG	2A	3589	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3157	1/1	0.97	0.06	33,33,33,33	0
58	MG	1a	1649	1/1	0.97	0.06	41,41,41,41	0
58	MG	1A	3636	1/1	0.97	0.04	22,22,22,22	0
58	MG	2A	3013	1/1	0.97	0.06	35,35,35,35	0
58	MG	2A	3467	1/1	0.97	0.06	49,49,49,49	0
58	MG	2D	301	1/1	0.97	0.10	34,34,34,34	0
58	MG	1A	3897	1/1	0.97	0.06	25,25,25,25	0
58	MG	2A	3731	1/1	0.97	0.05	48,48,48,48	0
58	MG	1A	3637	1/1	0.97	0.04	27,27,27,27	0
58	MG	2D	305	1/1	0.97	0.09	29,29,29,29	0
58	MG	1D	311	1/1	0.97	0.06	38,38,38,38	0
58	MG	2A	3130	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3072	1/1	0.97	0.28	31,31,31,31	0
58	MG	2a	1687	1/1	0.97	0.10	59,59,59,59	0
58	MG	10	101	1/1	0.97	0.11	37,37,37,37	0
58	MG	2E	303	1/1	0.97	0.13	48,48,48,48	0
58	MG	1A	3538	1/1	0.97	0.09	27,27,27,27	0
58	MG	1A	3125	1/1	0.97	0.14	25,25,25,25	0
58	MG	10	104	1/1	0.97	0.10	41,41,41,41	0
58	MG	1A	3980	1/1	0.97	0.04	40,40,40,40	0
58	MG	10	106	1/1	0.97	0.12	45,45,45,45	0
58	MG	2A	3607	1/1	0.97	0.06	48,48,48,48	0
58	MG	1A	3234	1/1	0.97	0.05	56,56,56,56	0
58	MG	1A	4070	1/1	0.97	0.05	37,37,37,37	0
58	MG	1E	306	1/1	0.97	0.08	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3903	1/1	0.97	0.08	49,49,49,49	0
58	MG	1a	1766	1/1	0.97	0.07	44,44,44,44	0
58	MG	1A	3412	1/1	0.97	0.09	37,37,37,37	0
58	MG	1A	3833	1/1	0.97	0.10	39,39,39,39	0
58	MG	2A	3616	1/1	0.97	0.06	54,54,54,54	0
58	MG	1A	3160	1/1	0.97	0.04	19,19,19,19	0
58	MG	2A	3035	1/1	0.97	0.07	42,42,42,42	0
58	MG	2A	3036	1/1	0.97	0.04	22,22,22,22	0
58	MG	2A	3755	1/1	0.97	0.10	53,53,53,53	0
58	MG	1a	1668	1/1	0.97	0.15	55,55,55,55	0
58	MG	1A	3414	1/1	0.97	0.09	43,43,43,43	0
58	MG	1A	3236	1/1	0.97	0.10	27,27,27,27	0
60	ZN	1Y	205	1/1	0.97	0.05	56,56,56,56	0
60	ZN	14	102	1/1	0.97	0.07	100,100,100,100	0
60	ZN	15	108	1/1	0.97	0.11	41,41,41,41	0
60	ZN	1n	103	1/1	0.97	0.05	51,51,51,51	0
60	ZN	2Y	202	1/1	0.97	0.05	85,85,85,85	0
58	MG	1F	302	1/1	0.97	0.07	30,30,30,30	0
60	ZN	26	501	1/1	0.97	0.06	57,57,57,57	0
60	ZN	2n	102	1/1	0.97	0.05	86,86,86,86	0
58	MG	1A	3065	1/1	0.97	0.19	39,39,39,39	0
58	MG	1A	3025	1/1	0.97	0.07	25,25,25,25	0
58	MG	1A	3007	1/1	0.98	0.05	26,26,26,26	0
58	MG	1A	3328	1/1	0.98	0.07	42,42,42,42	0
58	MG	1A	3119	1/1	0.98	0.05	33,33,33,33	0
58	MG	1U	210	1/1	0.98	0.28	32,32,32,32	0
58	MG	1A	3161	1/1	0.98	0.09	24,24,24,24	0
58	MG	1A	4064	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3238	1/1	0.98	0.07	31,31,31,31	0
58	MG	1A	3198	1/1	0.98	0.12	26,26,26,26	0
58	MG	2A	3546	1/1	0.98	0.07	38,38,38,38	0
58	MG	1A	3748	1/1	0.98	0.06	24,24,24,24	0
58	MG	1A	4068	1/1	0.98	0.07	44,44,44,44	0
58	MG	2A	3132	1/1	0.98	0.12	38,38,38,38	0
58	MG	1A	4069	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3667	1/1	0.98	0.04	20,20,20,20	0
58	MG	2B	219	1/1	0.98	0.14	54,54,54,54	0
58	MG	1W	204	1/1	0.98	0.05	34,34,34,34	0
58	MG	1A	3591	1/1	0.98	0.10	31,31,31,31	0
58	MG	1A	3240	1/1	0.98	0.07	32,32,32,32	0
58	MG	1A	3593	1/1	0.98	0.28	40,40,40,40	0
58	MG	1A	3108	1/1	0.98	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
58	MG	2A	3140	1/1	0.98	0.07	32,32,32,32	0
58	MG	1A	3081	1/1	0.98	0.09	36,36,36,36	0
58	MG	1A	3044	1/1	0.98	0.08	31,31,31,31	0
58	MG	1A	3886	1/1	0.98	0.04	45,45,45,45	0
58	MG	1A	3756	1/1	0.98	0.03	37,37,37,37	0
58	MG	1A	3800	1/1	0.98	0.10	17,17,17,17	0
58	MG	1A	3933	1/1	0.98	0.04	36,36,36,36	0
58	MG	1A	3387	1/1	0.98	0.11	30,30,30,30	0
58	MG	2A	3565	1/1	0.98	0.10	34,34,34,34	0
58	MG	2A	3566	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3981	1/1	0.98	0.07	56,56,56,56	0
58	MG	2A	3724	1/1	0.98	0.14	52,52,52,52	0
58	MG	1A	3758	1/1	0.98	0.07	25,25,25,25	0
58	MG	1A	3388	1/1	0.98	0.08	31,31,31,31	0
58	MG	2A	3019	1/1	0.98	0.04	23,23,23,23	0
58	MG	2A	3152	1/1	0.98	0.10	42,42,42,42	0
58	MG	1A	3070	1/1	0.98	0.08	22,22,22,22	0
58	MG	2F	305	1/1	0.98	0.10	47,47,47,47	0
58	MG	1A	3018	1/1	0.98	0.19	27,27,27,27	0
58	MG	2A	3359	1/1	0.98	0.04	30,30,30,30	0
58	MG	2A	3732	1/1	0.98	0.08	35,35,35,35	0
58	MG	1P	202	1/1	0.98	0.06	27,27,27,27	0
58	MG	1A	3566	1/1	0.98	0.12	28,28,28,28	0
58	MG	2A	3024	1/1	0.98	0.07	44,44,44,44	0
58	MG	1A	3363	1/1	0.98	0.14	31,31,31,31	0
58	MG	2A	3818	1/1	0.98	0.06	32,32,32,32	0
58	MG	1A	3151	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3477	1/1	0.98	0.06	42,42,42,42	0
58	MG	1A	3093	1/1	0.98	0.06	22,22,22,22	0
58	MG	1A	3226	1/1	0.98	0.06	23,23,23,23	0
58	MG	2A	3823	1/1	0.98	0.07	23,23,23,23	0
58	MG	2A	3094	1/1	0.98	0.05	40,40,40,40	0
58	MG	2A	3584	1/1	0.98	0.07	34,34,34,34	0
58	MG	1A	3032	1/1	0.98	0.09	31,31,31,31	0
58	MG	1A	3573	1/1	0.98	0.07	35,35,35,35	0
58	MG	2A	3032	1/1	0.98	0.05	39,39,39,39	0
58	MG	1A	3037	1/1	0.98	0.07	19,19,19,19	0
58	MG	1D	309	1/1	0.98	0.09	33,33,33,33	0
58	MG	2A	3590	1/1	0.98	0.04	34,34,34,34	0
58	MG	1A	3189	1/1	0.98	0.13	34,34,34,34	0
58	MG	1A	4097	1/1	0.98	0.04	41,41,41,41	0
58	MG	2X	3500	1/1	0.98	0.03	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
58	MG	1A	4045	1/1	0.98	0.05	43,43,43,43	0
58	MG	1A	3140	1/1	0.98	0.11	26,26,26,26	0
58	MG	1A	3276	1/1	0.98	0.10	40,40,40,40	0
58	MG	1A	3173	1/1	0.98	0.10	29,29,29,29	0
58	MG	1E	303	1/1	0.98	0.06	28,28,28,28	0
58	MG	1A	4000	1/1	0.98	0.06	33,33,33,33	0
58	MG	1A	3141	1/1	0.98	0.10	13,13,13,13	0
58	MG	2a	1761	1/1	0.98	0.11	48,48,48,48	0
58	MG	1a	1760	1/1	0.98	0.06	48,48,48,48	0
58	MG	1A	3580	1/1	0.98	0.07	28,28,28,28	0
58	MG	1A	3087	1/1	0.98	0.05	32,32,32,32	0
58	MG	1a	1763	1/1	0.98	0.05	37,37,37,37	0
58	MG	2A	3457	1/1	0.98	0.04	19,19,19,19	0
58	MG	1A	3822	1/1	0.98	0.17	24,24,24,24	0
59	K	1A	3562	1/1	0.98	0.10	43,43,43,43	0
58	MG	2A	3459	1/1	0.98	0.16	46,46,46,46	0
58	MG	1A	3617	1/1	0.98	0.13	32,32,32,32	0
58	MG	2A	3766	1/1	0.98	0.06	52,52,52,52	0
58	MG	1A	3106	1/1	0.98	0.07	33,33,33,33	0
60	ZN	16	102	1/1	0.98	0.04	40,40,40,40	0
58	MG	1A	3619	1/1	0.98	0.05	44,44,44,44	0
58	MG	17	101	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	4008	1/1	0.98	0.09	23,23,23,23	0
58	MG	1A	3376	1/1	0.98	0.15	31,31,31,31	0
58	MG	2A	3613	1/1	0.98	0.10	35,35,35,35	0
58	MG	2a	1690	1/1	0.98	0.18	36,36,36,36	0
58	MG	1A	3490	1/1	0.98	0.06	27,27,27,27	0
58	MG	2A	3708	1/1	0.99	0.03	49,49,49,49	0
58	MG	1A	3936	1/1	0.99	0.06	33,33,33,33	0
58	MG	2A	3806	1/1	0.99	0.04	35,35,35,35	0
58	MG	1A	3988	1/1	0.99	0.04	30,30,30,30	0
58	MG	1A	3628	1/1	0.99	0.06	26,26,26,26	0
58	MG	1A	3273	1/1	0.99	0.08	27,27,27,27	0
58	MG	1A	3021	1/1	0.99	0.03	20,20,20,20	0
58	MG	1A	3169	1/1	0.99	0.12	11,11,11,11	0
58	MG	1V	203	1/1	0.99	0.14	25,25,25,25	0
58	MG	1A	3688	1/1	0.99	0.05	18,18,18,18	0
58	MG	2A	3098	1/1	0.99	0.04	26,26,26,26	0
58	MG	1A	3678	1/1	0.99	0.04	27,27,27,27	0
58	MG	1A	3734	1/1	0.99	0.07	39,39,39,39	0
58	MG	1A	3210	1/1	0.99	0.12	28,28,28,28	0
58	MG	1A	3736	1/1	0.99	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
58	MG	1A	3647	1/1	0.99	0.10	17,17,17,17	0
58	MG	1W	203	1/1	0.99	0.07	31,31,31,31	0
58	MG	2A	3700	1/1	0.99	0.09	31,31,31,31	0
60	ZN	19	102	1/1	0.99	0.03	38,38,38,38	0
58	MG	1A	3681	1/1	0.99	0.07	23,23,23,23	0
58	MG	1A	3792	1/1	0.99	0.03	35,35,35,35	0
58	MG	1A	3033	1/1	0.99	0.27	30,30,30,30	0
60	ZN	25	104	1/1	0.99	0.07	59,59,59,59	0
58	MG	1A	3779	1/1	0.99	0.03	37,37,37,37	0
60	ZN	29	102	1/1	0.99	0.03	57,57,57,57	0
58	MG	1A	3870	1/1	0.99	0.02	19,19,19,19	0
58	MG	1F	301	1/1	0.99	0.06	35,35,35,35	0
58	MG	1A	3038	1/1	0.99	0.05	26,26,26,26	0
58	MG	1a	1754	1/1	1.00	0.11	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.