



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 09:50 AM EDT

PDB ID : 8VTY / pdb_00008vty
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with ciprofloxacin and protein Y at 2.60Å resolution
Authors : Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.
Deposited on : 2024-01-27
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

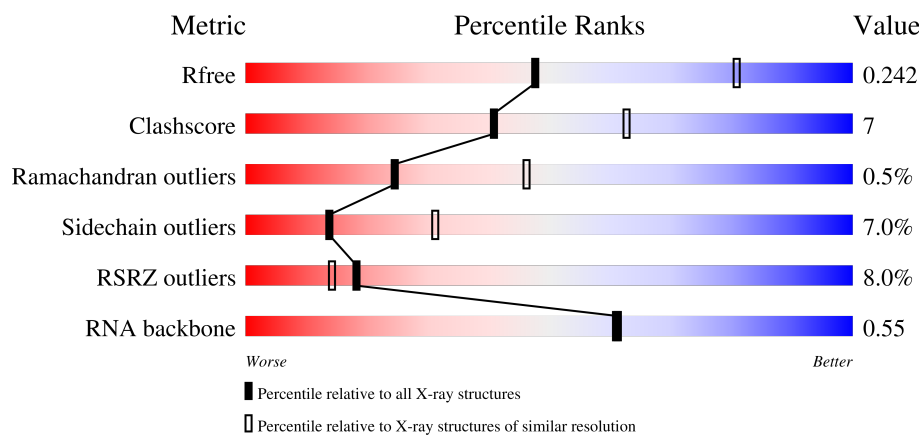
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 69% 25% • •
1	2A	2915	6% 66% 27% 6% •
2	1B	121	2% 80% 18% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	2B	121	5% 59% 37% ..
3	1D	276	% 83% 15% .
3	2D	276	% 83% 13% .
4	1E	206	% 78% 17% ..
4	2E	206	% 76% 19% ..
5	1F	210	% 77% 16% ..
5	2F	210	73% 20% ..
6	1G	182	7% 74% 22% ..
6	2G	182	25% 52% 44% ..
7	1H	180	4% 76% 21% ..
7	2H	180	18% 61% 33% ..
8	1I	148	7% 78% 17% ..
8	2I	148	3% 77% 20% ..
9	1N	140	% 83% 13% .
9	2N	140	2% 78% 21% .
10	1O	122	84% 16%
10	2O	122	84% 16%
11	1P	150	% 81% 17% ..
11	2P	150	% 82% 13% ..
12	1Q	141	87% 11% .
12	2Q	141	4% 82% 16% .
13	1R	118	80% 19% .
13	2R	118	79% 19% .
14	1S	112	% 78% 18% ..
14	2S	112	19% 69% 28% ..

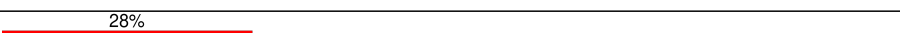
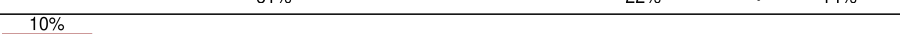
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3641	-	-	-	X
54	MG	1A	3996	-	-	-	X
54	MG	1a	1794	-	-	-	X
54	MG	2A	3190	-	-	-	X
54	MG	2A	3409	-	-	-	X
54	MG	2a	3079	-	-	-	X
54	MG	2a	3160	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 297563 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

Continued on next page...

Continued from previous page...

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

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

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

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1056	Total	Mg	0	0
			1056	1056		
54	1B	29	Total	Mg	0	0
			29	29		
54	1D	18	Total	Mg	0	0
			18	18		
54	1E	9	Total	Mg	0	0
			9	9		
54	1F	19	Total	Mg	0	0
			19	19		
54	1G	4	Total	Mg	0	0
			4	4		
54	1H	3	Total	Mg	0	0
			3	3		
54	1N	5	Total	Mg	0	0
			5	5		
54	1O	1	Total	Mg	0	0
			1	1		
54	1P	6	Total	Mg	0	0
			6	6		
54	1Q	5	Total	Mg	0	0
			5	5		
54	1R	6	Total	Mg	0	0
			6	6		
54	1T	5	Total	Mg	0	0
			5	5		
54	1U	7	Total	Mg	0	0
			7	7		
54	1V	6	Total	Mg	0	0
			6	6		
54	1W	3	Total	Mg	0	0
			3	3		
54	1Z	1	Total	Mg	0	0
			1	1		
54	10	7	Total	Mg	0	0
			7	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	11	5	Total 5	Mg 5	0	0
54	13	4	Total 4	Mg 4	0	0
54	14	1	Total 1	Mg 1	0	0
54	15	8	Total 8	Mg 8	0	0
54	17	7	Total 7	Mg 7	0	0
54	18	3	Total 3	Mg 3	0	0
54	19	2	Total 2	Mg 2	0	0
54	1a	277	Total 277	Mg 277	0	0
54	1b	1	Total 1	Mg 1	0	0
54	1d	5	Total 5	Mg 5	0	0
54	1e	2	Total 2	Mg 2	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1g	3	Total 3	Mg 3	0	0
54	1h	2	Total 2	Mg 2	0	0
54	1i	1	Total 1	Mg 1	0	0
54	1k	1	Total 1	Mg 1	0	0
54	1l	2	Total 2	Mg 2	0	0
54	1m	1	Total 1	Mg 1	0	0
54	1n	3	Total 3	Mg 3	0	0
54	1o	1	Total 1	Mg 1	0	0
54	1t	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

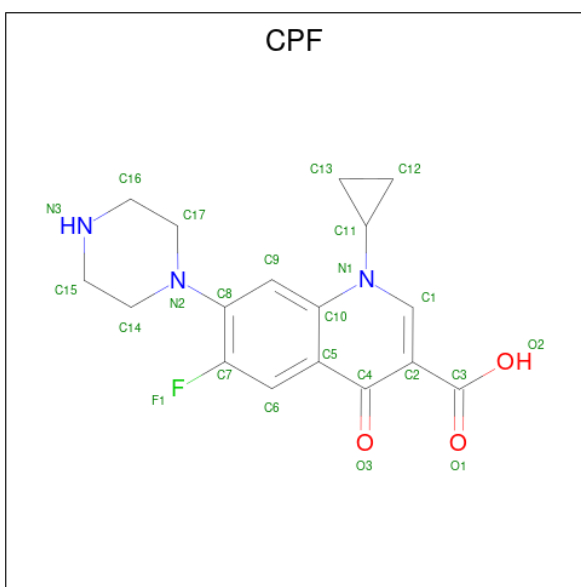
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1y	4	Total 4	Mg 4	0	0
54	2A	741	Total 741	Mg 741	0	0
54	2B	18	Total 18	Mg 18	0	0
54	2D	12	Total 12	Mg 12	0	0
54	2E	7	Total 7	Mg 7	0	0
54	2F	4	Total 4	Mg 4	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2N	1	Total 1	Mg 1	0	0
54	2O	2	Total 2	Mg 2	0	0
54	2Q	3	Total 3	Mg 3	0	0
54	2R	3	Total 3	Mg 3	0	0
54	2T	3	Total 3	Mg 3	0	0
54	2V	3	Total 3	Mg 3	0	0
54	2W	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0
54	2Y	1	Total 1	Mg 1	0	0
54	20	3	Total 3	Mg 3	0	0
54	21	1	Total 1	Mg 1	0	0
54	23	2	Total 2	Mg 2	0	0
54	25	1	Total 1	Mg 1	0	0
54	27	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

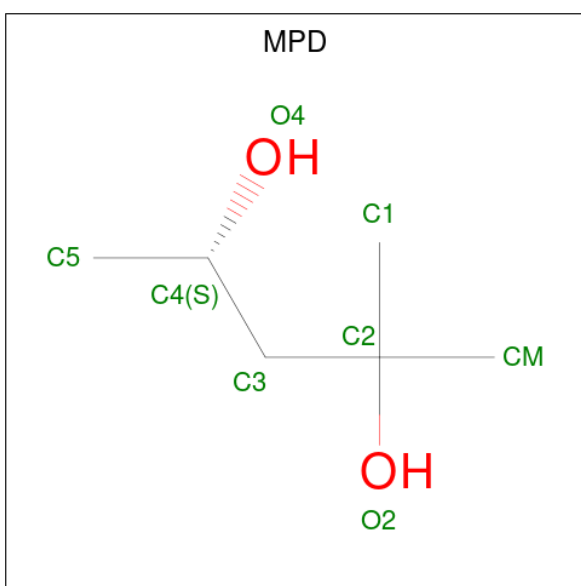
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	28	2	Total 2	Mg 2	0	0
54	2a	195	Total 195	Mg 195	0	0
54	2d	1	Total 1	Mg 1	0	0
54	2e	1	Total 1	Mg 1	0	0
54	2f	2	Total 2	Mg 2	0	0
54	2j	1	Total 1	Mg 1	0	0
54	2k	1	Total 1	Mg 1	0	0
54	2n	1	Total 1	Mg 1	0	0
54	2o	1	Total 1	Mg 1	0	0
54	2p	1	Total 1	Mg 1	0	0
54	2r	1	Total 1	Mg 1	0	0
54	2t	1	Total 1	Mg 1	0	0

- Molecule 55 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDR OQUINOLINE-3-CARBOXYLIC ACID (CCD ID: CPF) (formula: C₁₇H₁₈FN₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	1A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
55	2A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



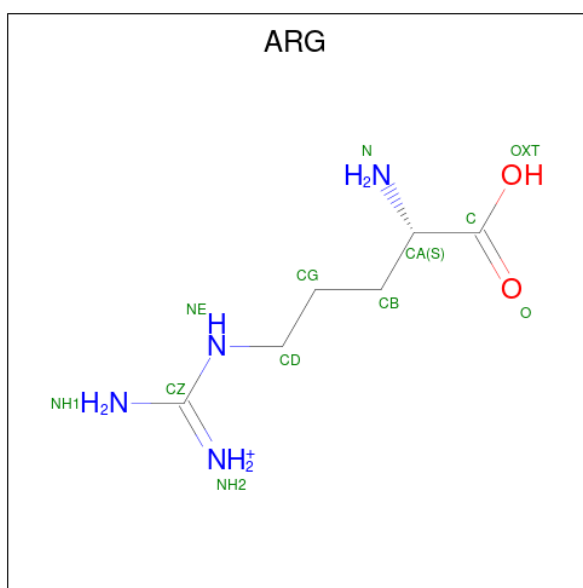
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	1A	1	Total	C	O	0	0
			8	6	2		
56	1O	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	18	1	Total	C	O	0	0
			8	6	2		
56	1a	1	Total	C	O	0	0
			8	6	2		
56	2A	1	Total	C	O	0	0
			8	6	2		
56	2A	1	Total	C	O	0	0
			8	6	2		
56	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 57 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1B	1	Total	C	N	O	0	0
			12	6	4	2		
57	1F	1	Total	C	N	O	0	0
			12	6	4	2		

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

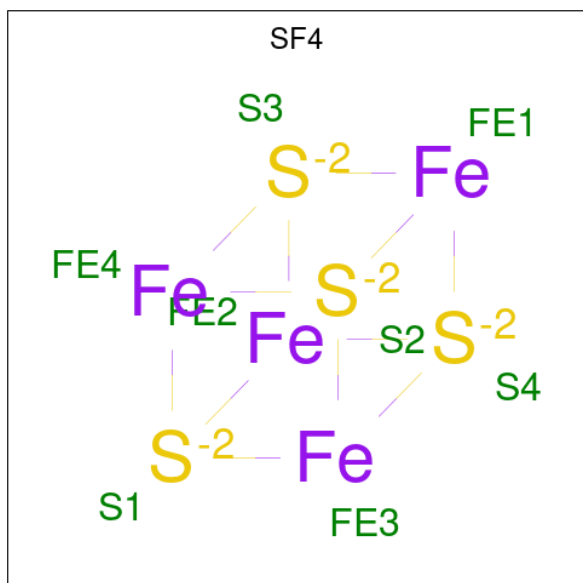
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

Continued on next page...

Continued from previous page...

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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3927	Total	O	0	0
			3927	3927		
60	1B	89	Total	O	0	0
			89	89		
60	1D	110	Total	O	0	0
			110	110		
60	1E	72	Total	O	0	0
			72	72		
60	1F	67	Total	O	0	0
			67	67		
60	1G	16	Total	O	0	0
			16	16		
60	1H	14	Total	O	0	0
			14	14		
60	1I	5	Total	O	0	0
			5	5		
60	1N	52	Total	O	0	0
			52	52		
60	1O	25	Total	O	0	0
			25	25		
60	1P	65	Total	O	0	0
			65	65		
60	1Q	41	Total	O	0	0
			41	41		
60	1R	32	Total	O	0	0
			32	32		
60	1S	8	Total	O	0	0
			8	8		
60	1T	36	Total	O	0	0
			36	36		
60	1U	43	Total	O	0	0
			43	43		
60	1V	36	Total	O	0	0
			36	36		
60	1W	28	Total	O	0	0
			28	28		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1X	26	Total 26	O 26	0	0
60	1Y	17	Total 17	O 17	0	0
60	1Z	11	Total 11	O 11	0	0
60	10	25	Total 25	O 25	0	0
60	11	28	Total 28	O 28	0	0
60	12	13	Total 13	O 13	0	0
60	13	25	Total 25	O 25	0	0
60	14	3	Total 3	O 3	0	0
60	15	28	Total 28	O 28	0	0
60	16	20	Total 20	O 20	0	0
60	17	13	Total 13	O 13	0	0
60	18	28	Total 28	O 28	0	0
60	19	8	Total 8	O 8	0	0
60	1a	496	Total 496	O 496	0	0
60	1b	1	Total 1	O 1	0	0
60	1c	1	Total 1	O 1	0	0
60	1d	9	Total 9	O 9	0	0
60	1e	10	Total 10	O 10	0	0
60	1f	1	Total 1	O 1	0	0
60	1h	1	Total 1	O 1	0	0
60	1j	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1k	1	Total 1	O 1	0	0
60	1l	4	Total 4	O 4	0	0
60	1o	4	Total 4	O 4	0	0
60	1p	1	Total 1	O 1	0	0
60	1y	5	Total 5	O 5	0	0
60	2A	2249	Total 2249	O 2249	0	0
60	2B	42	Total 42	O 42	0	0
60	2D	47	Total 47	O 47	0	0
60	2E	28	Total 28	O 28	0	0
60	2F	23	Total 23	O 23	0	0
60	2G	4	Total 4	O 4	0	0
60	2H	1	Total 1	O 1	0	0
60	2N	6	Total 6	O 6	0	0
60	2O	15	Total 15	O 15	0	0
60	2P	21	Total 21	O 21	0	0
60	2Q	18	Total 18	O 18	0	0
60	2R	22	Total 22	O 22	0	0
60	2S	2	Total 2	O 2	0	0
60	2T	12	Total 12	O 12	0	0
60	2U	16	Total 16	O 16	0	0
60	2V	8	Total 8	O 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2W	19	Total 19	O 19	0	0
60	2X	8	Total 8	O 8	0	0
60	2Y	4	Total 4	O 4	0	0
60	2Z	8	Total 8	O 8	0	0
60	20	10	Total 10	O 10	0	0
60	21	17	Total 17	O 17	0	0
60	22	2	Total 2	O 2	0	0
60	23	2	Total 2	O 2	0	0
60	25	7	Total 7	O 7	0	0
60	26	6	Total 6	O 6	0	0
60	27	9	Total 9	O 9	0	0
60	28	15	Total 15	O 15	0	0
60	2a	404	Total 404	O 404	0	0
60	2d	3	Total 3	O 3	0	0
60	2e	3	Total 3	O 3	0	0
60	2f	3	Total 3	O 3	0	0
60	2j	2	Total 2	O 2	0	0
60	2l	5	Total 5	O 5	0	0
60	2o	2	Total 2	O 2	0	0
60	2p	1	Total 1	O 1	0	0
60	2q	1	Total 1	O 1	0	0

Continued on next page...

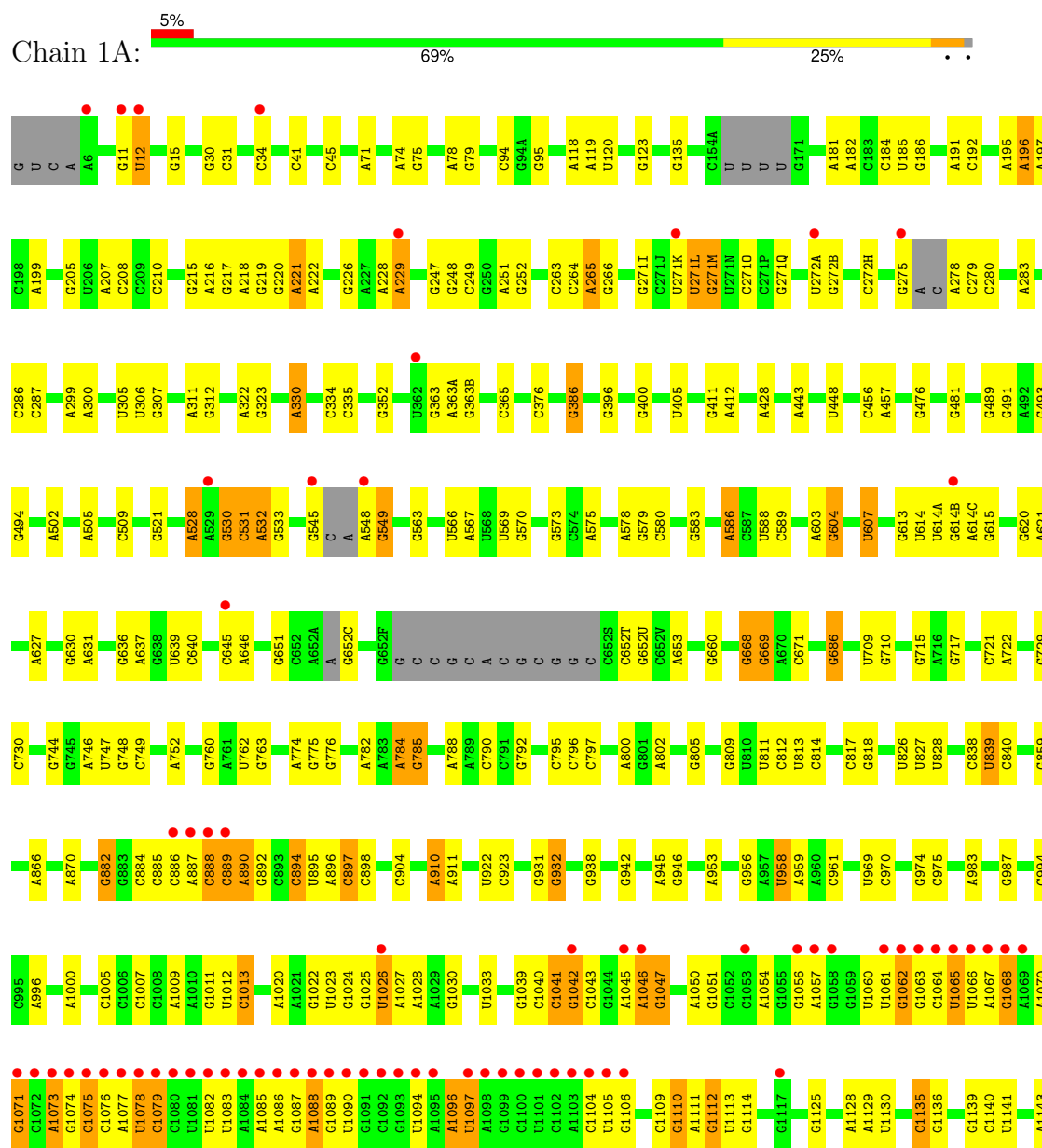
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2r	3	Total 3	O 3	0	0
60	2t	3	Total 3	O 3	0	0
60	2u	1	Total 1	O 1	0	0
60	2y	1	Total 1	O 1	0	0

3 Residue-property plots

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

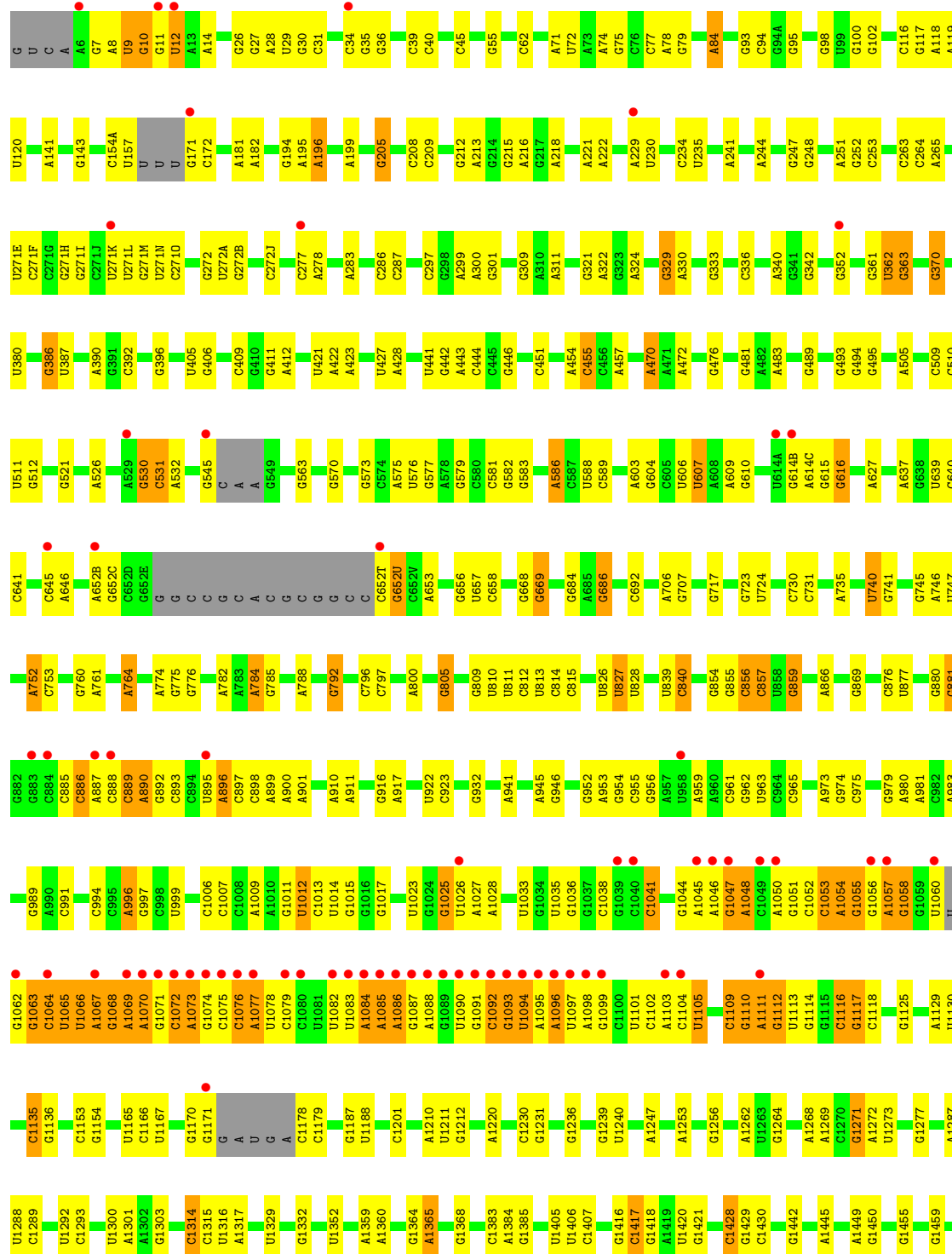
• Molecule 1: 23S Ribosomal RNA



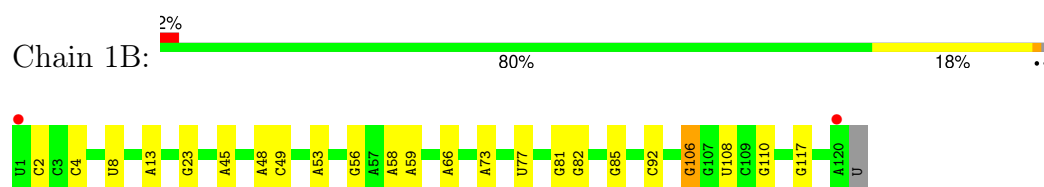
G2694	G2653	A2425	G2304	C2177	G2116	C1999	A1876	G1746	A1566	A1445	U1300	C1152
U2554	U2554	A2426	A2305	C2178	A2117	A2014	A1877	C1754	A1569	G1448	A1301	G1164
G2557	G2557	G2427	A2306	U2179	U2118	A2019	G1878	A1755	A1570	G1449	G1303	U1165
C2558	C2558	G2428	G2308	G2182	G2120	A2020	A1889	G1756	G1450	A1571	C1315	C1166
U2563	U2563	G2429	A2309	G2183	G2121	G2021	G1899	A1762	U1578	U1452	C1320	G1170
A2564	A2564	A2430	A2310	G2184	U2122	U2022	A1900	G1763	A1579	U1453	A1321	G1171
G2565	G2565	U2431	A2312	C2185	G2123	G2023	G1906	G1764	A1580	G1455	G1332	G1173
G2567	G2567	A2435	G2313	C2186	G2125	G2024	U1911	C1765	C1581	G1459	G1333	A1174
A2572	A2572	G2439	G2314	G2187	A2126	A2030	U1912	U1766	C1582	A1460	G1334	U1175
C2573	C2573	C2440	G2315	C2188	G2127	A2031	A1913	C1767	C1584	G1465	U1340	G1176
G2576	G2576	C2441	G2316	U2189	C2128	G2032	A1914	U1768	A1586	C1467	C1345	A1177
U2579	U2579	C2442	G2319	G2191	U2130	A2033	U1915	A1773	A1587	U1466	U1346	C1178
G2586	G2586	G2443	A2320	G2192	U2132	G2039	A1916	U1778	C1588	G1470	C1345	C1187
A2590	A2590	G2444	G2325	G2193	G2133	C2043	U1917	U1779	C1589	A1471	U1352	U1188
C2591	C2591	G2445	G2326	A2198	A2134	G2049	A1918	A1780	G1593	G1482	G1356	G1203
G2592	G2592	G2446	A2327	A2199	A2135	C2055	A1919	C1781	G1594	G1487	U1357	G1203
A2602	A2602	A2447	G2328	G2206	C2136	G2056	G1921	U1782	A1608	A1486	A1359	A1210
G2603	G2603	G2448	A2329	A2207	C2138	G2066	G1922	C1783	A1609	G1487	A1360	U1211
U2604	U2604	A2450	G2330	U2218	C2139	G2069	G1929	A1784	A1610	C1493	G1364	A1220
U2605	U2605	A2453	G2331	U2219	C2140	U2074	U1931	A1785	A1614	G1500	A1365	G1239
G2608	G2608	C2464	G2334	G2224	G2141	U2075	A1932	A1786	A1641	C1506	G1371	U1240
U2609	U2609	A2465	A2335	A2225	C2142	U2086	A1933	C1790	G1642	A1507	U1372	G1250
C2610	C2610	G2468	A2336	C2226	U2144	G2087	G1934	A1791	C1647	A1508	C1251	C1251
G2612	G2612	A2469	G2345	U2232	C2145	U2096	G1935	G1795	G1648	C1509	G1380	A1253
U2617	U2617	G2470	A2346	G2238	C2146	G2097	A1936	U1796	C1649	A1509A	G1381	G1256
G2618	G2618	A2476	G2347	G2239	G2147	U2098	A1937	C1797	G1647	G1510	G1382	G1256
A2629	A2629	C2498	U2348	G2243	U2148	U2099	A1938	U1798	C1647	G1511	A1384	G1280
G2630	G2630	G2499	G2349	U2244	G2149	G2100	U1939	G1799	G1647	C1512	G1385	C1261
A2639	A2639	U2502	C2350	G2244	U2150	C2103	C1942	C1800	G1647	U1518	U1394	A1268
C2646	C2646	A2503	G2364	G2251	G2153	G2104	A1982	G1801	G1553	G1519	A1395	A1269
U2647	U2647	G2504	A2377	C2258	G2154	G2105	U1955	A1816	A1668	G1520	U1405	C1270
G2648	G2648	U2505	A2378	G2259	G2155	G2106	U1956	G1817	C1670	A1528A	U1406	G1271
U2649	U2649	G2506	G2381	A2268	A2158	C2107	C1957	C1826	U1688	G1532	G1416	A1287
U2650	U2650	G2507	G2382	G2271	G2159	U2099	G1962	A1829	G1696	G1537	C1417	U1288
C2651	C2651	A2518	G2383	G2277	C2161	G2100	U1963	A1829	U1688	U1420	U1273	C1289
A2654	A2654	G2520	A2385	A2278	G2162	G2104	G1964	A1829	G1696	G1537	G1421	C1290
U2681	U2681	G2526	G2389	G2279	C2163	G2105	C1967	A1829	G1696	G1537	G1421	C1290
G2682	G2682	U2529	U2390	C2283	G2165	G2106	G1968	A1829	G1696	G1537	G1421	C1290
U2683	U2683	G2535	A2393	A2286	G2166	G2107	A1969	A1829	G1696	G1537	G1421	C1290
G2687	G2687	A2536	C2404	A2287	U2167	C2108	A1970	A1829	G1696	G1537	G1421	C1290
U2688	U2688	G2537	G2405	A2288	A2169	U2109	A1971	A1829	G1696	G1537	G1421	C1290
G2689	G2689	U2548	U2406	G2289	A2170	G2110	A1972	A1829	G1696	G1537	G1421	C1290
C2690	C2690	G2549	U2406	G2290	A2171	G2111	A1972	A1829	G1696	G1537	G1421	C1290
U2691	U2691	U2550	U2406	G2291	U2172	G2112	G1992	A1829	G1696	G1537	G1421	C1290
C2692	C2692	G2551	C2417	C2292	A2173	G2113	U1993	A1829	G1696	G1537	G1421	C1290
A2693	A2693	U2552	A2422	U2296	C2174	A2114	C1996	A1829	G1696	G1537	G1421	C1290
U2694	U2694	U2552	A2422	U2296	A2175	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2695	U2695	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2696	U2696	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2697	U2697	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2698	U2698	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2699	U2699	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2700	U2700	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2701	U2701	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2702	U2702	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2703	U2703	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2704	U2704	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2705	U2705	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2706	U2706	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2707	U2707	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2708	U2708	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2709	U2709	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2710	U2710	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2711	U2711	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2712	U2712	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2713	U2713	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2714	U2714	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2715	U2715	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2716	U2716	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2717	U2717	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2718	U2718	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2719	U2719	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2720	U2720	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2721	U2721	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2722	U2722	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2723	U2723	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2724	U2724	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2725	U2725	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2726	U2726	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2727	U2727	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2728	U2728	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2729	U2729	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2730	U2730	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2731	U2731	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2732	U2732	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2733	U2733	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2734	U2734	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2735	U2735	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2736	U2736	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2737	U2737	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2738	U2738	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2739	U2739	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2740	U2740	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2741	U2741	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2742	U2742	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2743	U2743	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2744	U2744	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2745	U2745	U2552	A2422	U2296	A2176	G2115	G1997	A1829	G1696	G1537	G1421	C1290
U2746	U2746	U2552	A2422	U2296	A2176	G2115	G1997	A18				



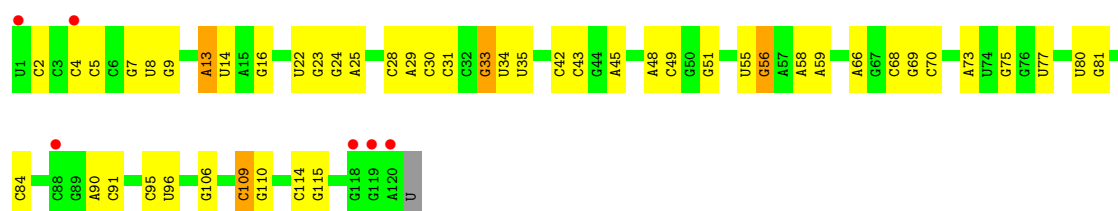
- Molecule 1: 23S Ribosomal RNA



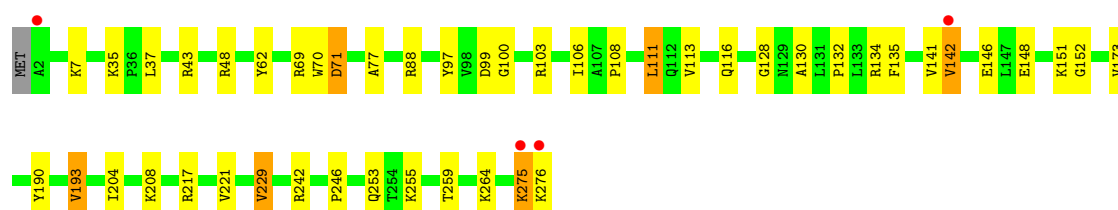
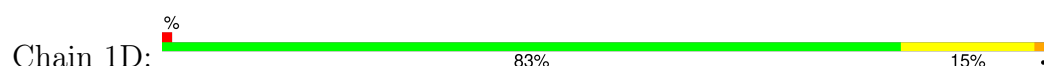




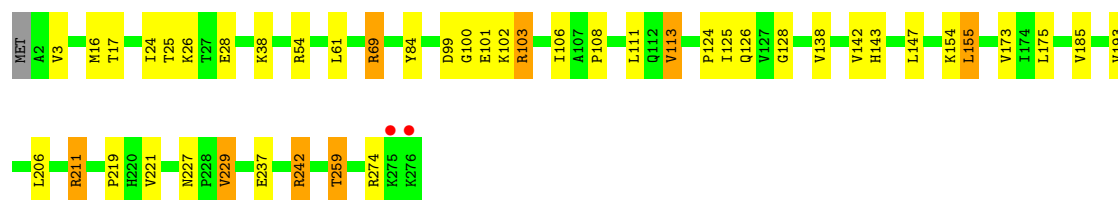
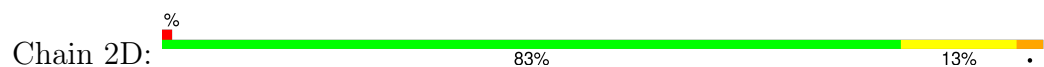
- Molecule 2: 5S Ribosomal RNA



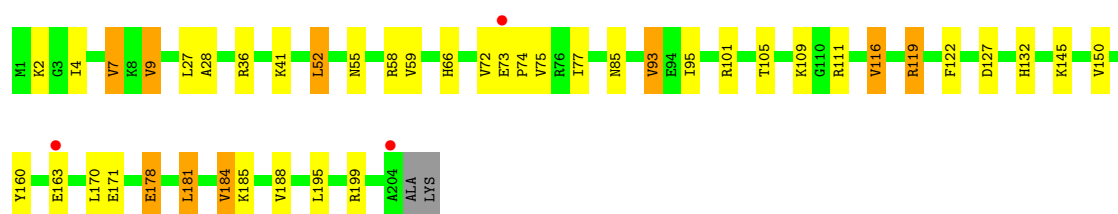
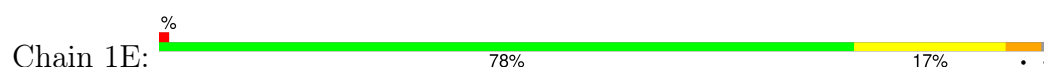
- Molecule 3: 50S ribosomal protein L2



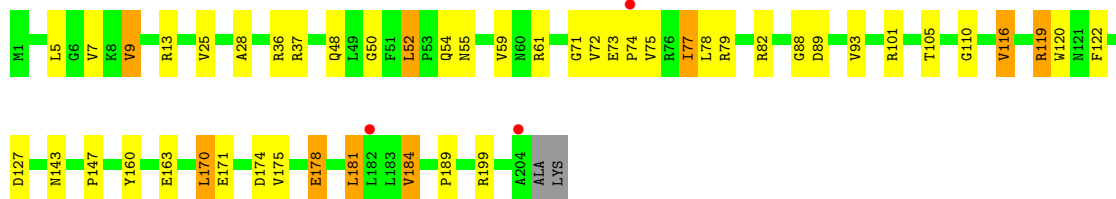
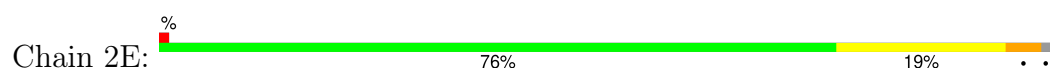
- Molecule 3: 50S ribosomal protein L2



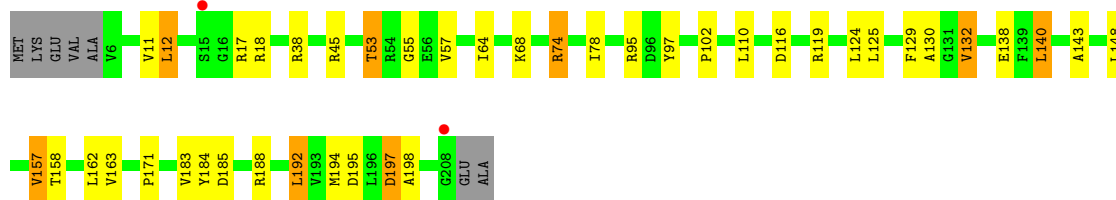
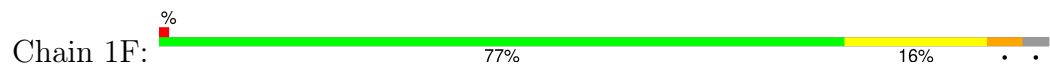
- Molecule 4: 50S ribosomal protein L3



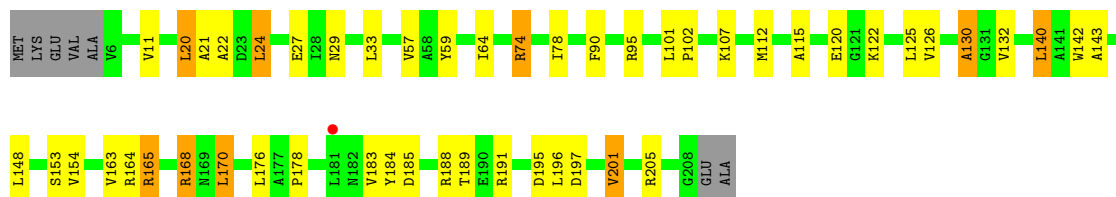
- Molecule 4: 50S ribosomal protein L3



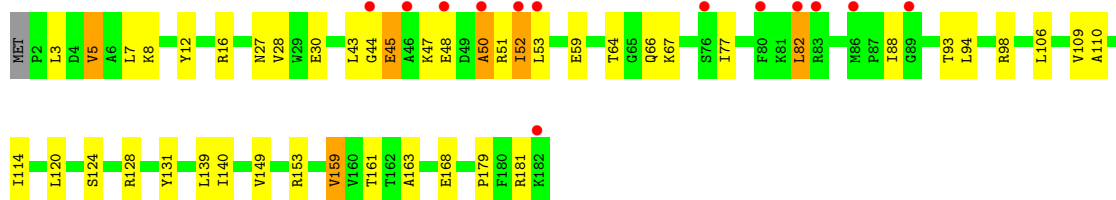
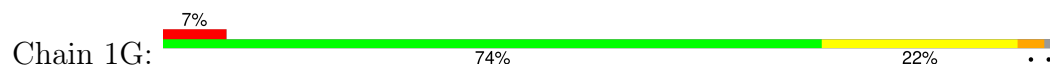
- Molecule 5: 50S ribosomal protein L4



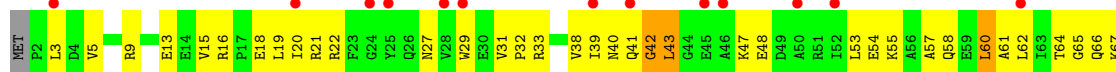
- Molecule 5: 50S ribosomal protein L4

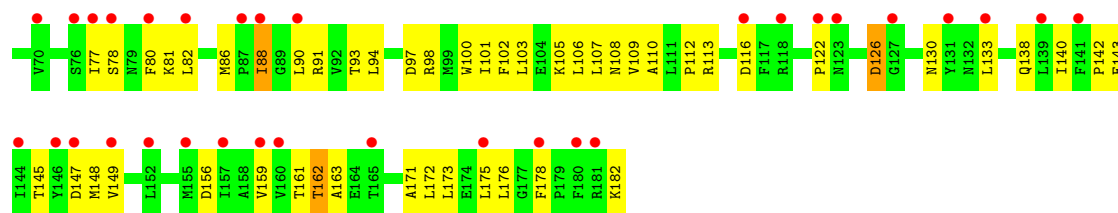


- Molecule 6: 50S ribosomal protein L5

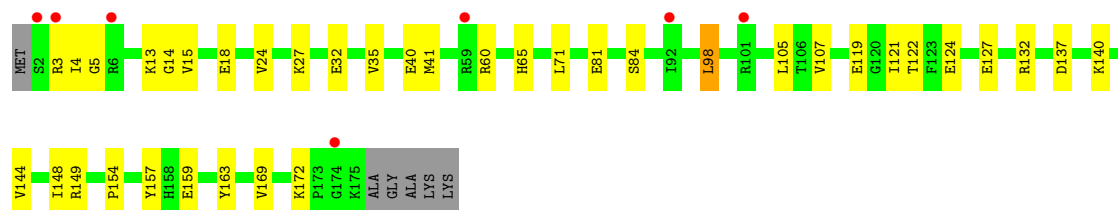
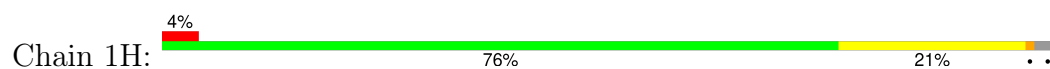


- Molecule 6: 50S ribosomal protein L5

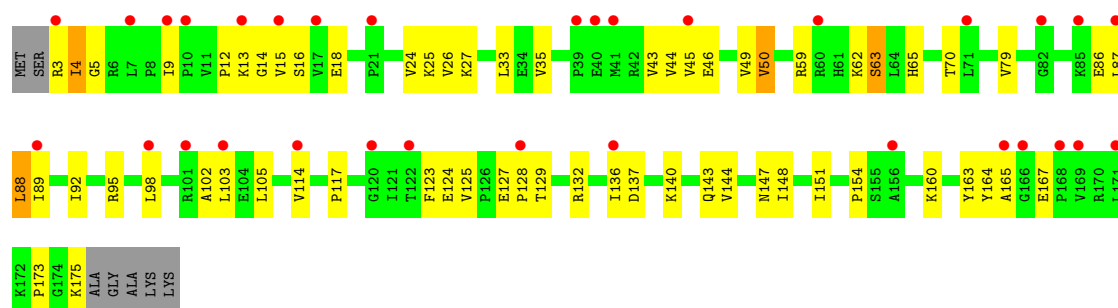




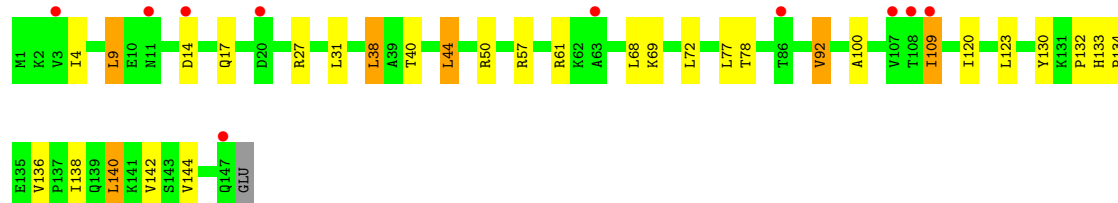
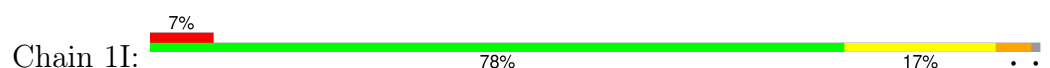
• Molecule 7: 50S ribosomal protein L6



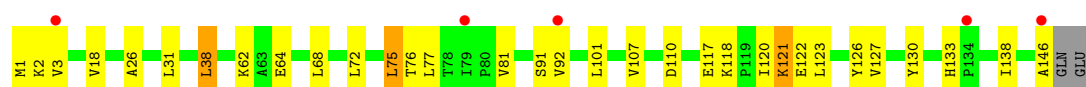
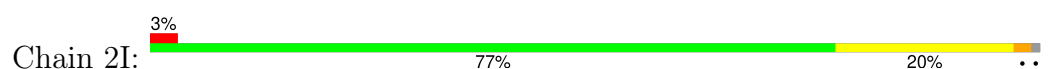
• Molecule 7: 50S ribosomal protein L6



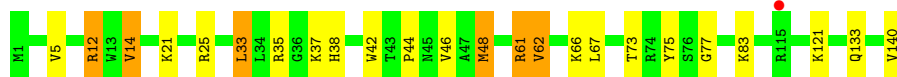
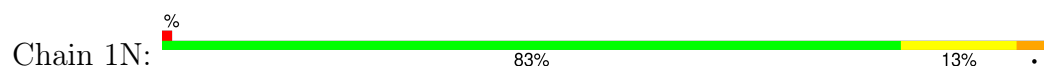
• Molecule 8: 50S ribosomal protein L9



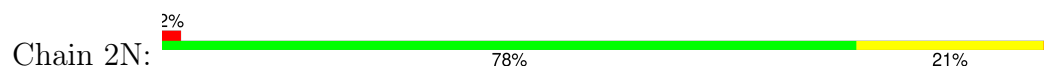
• Molecule 8: 50S ribosomal protein L9



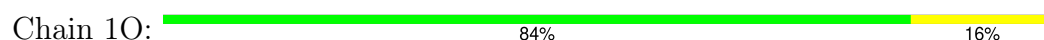
• Molecule 9: 50S ribosomal protein L13



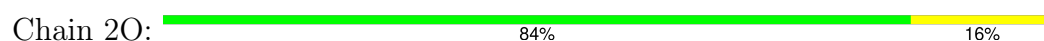
• Molecule 9: 50S ribosomal protein L13



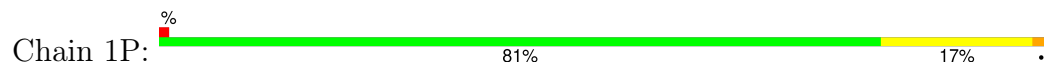
• Molecule 10: 50S ribosomal protein L14



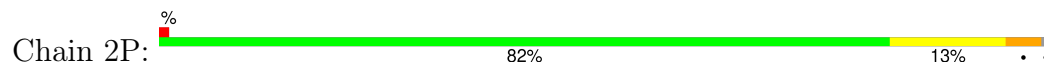
• Molecule 10: 50S ribosomal protein L14



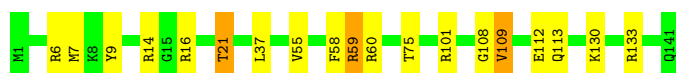
• Molecule 11: 50S ribosomal protein L15



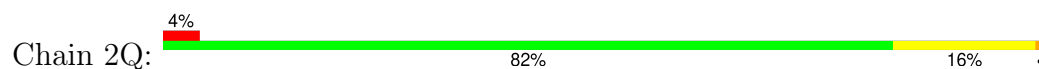
• Molecule 11: 50S ribosomal protein L15



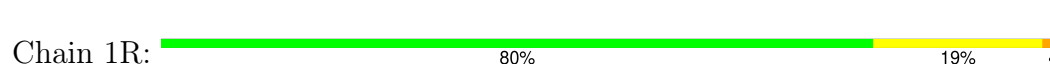
• Molecule 12: 50S ribosomal protein L16



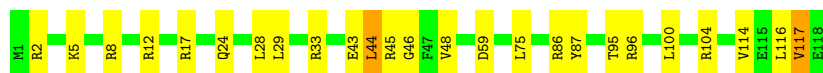
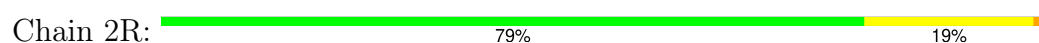
- Molecule 12: 50S ribosomal protein L16



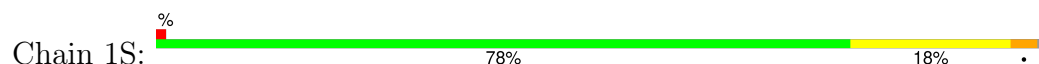
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17



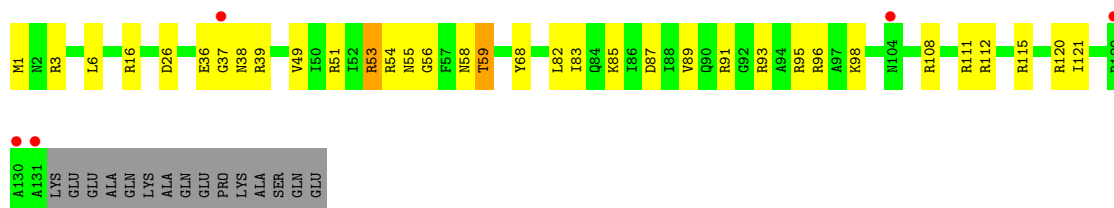
- Molecule 14: 50S ribosomal protein L18



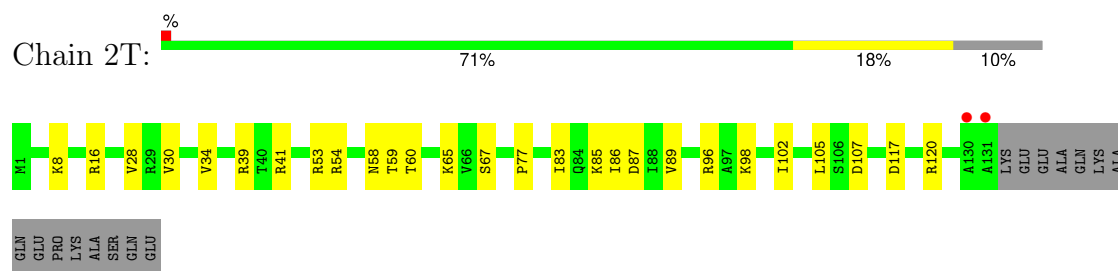
- Molecule 14: 50S ribosomal protein L18



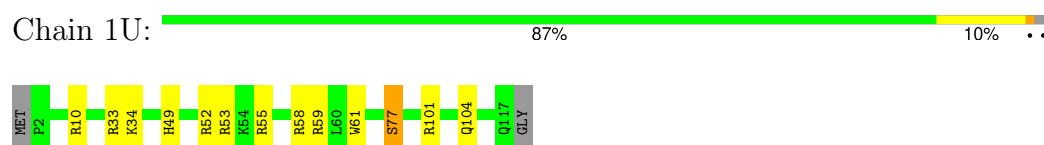
- Molecule 15: 50S ribosomal protein L19



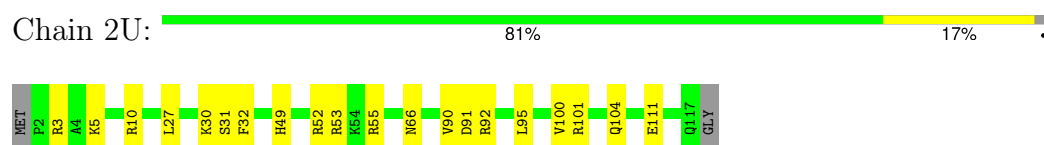
- Molecule 15: 50S ribosomal protein L19



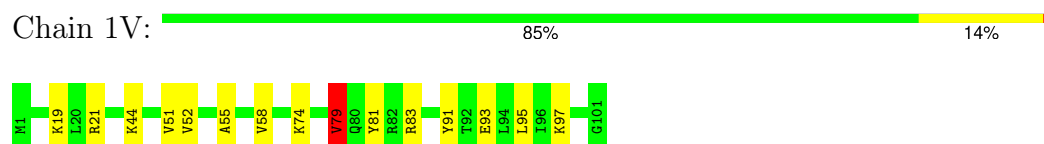
- Molecule 16: 50S ribosomal protein L20



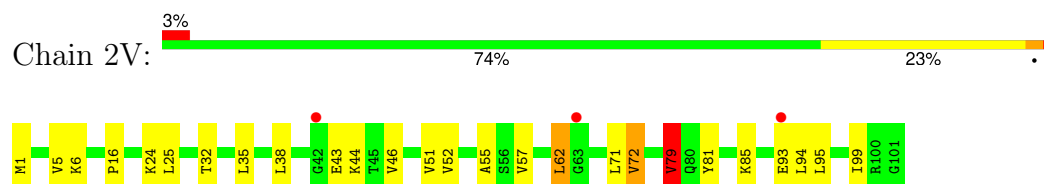
- Molecule 16: 50S ribosomal protein L20



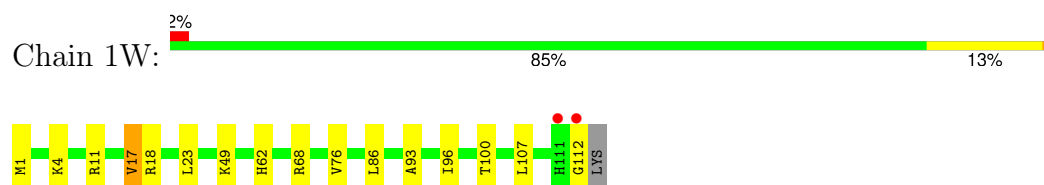
- Molecule 17: 50S ribosomal protein L21



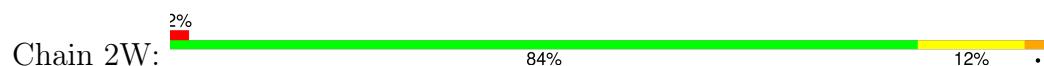
- Molecule 17: 50S ribosomal protein L21

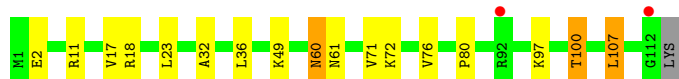


- Molecule 18: 50S ribosomal protein L22

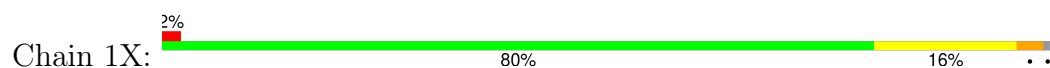


- Molecule 18: 50S ribosomal protein L22

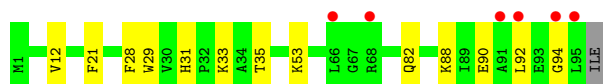
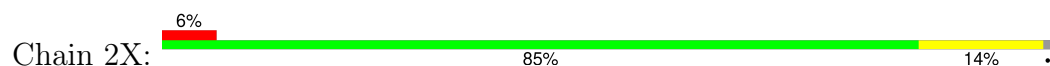




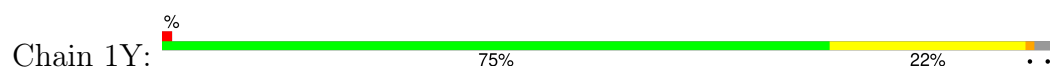
- Molecule 19: 50S ribosomal protein L23



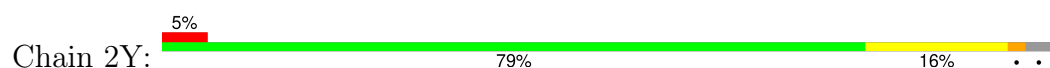
- Molecule 19: 50S ribosomal protein L23



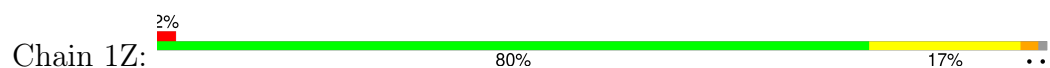
- Molecule 20: 50S ribosomal protein L24



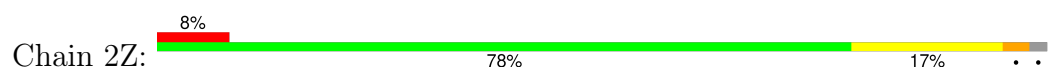
- Molecule 20: 50S ribosomal protein L24

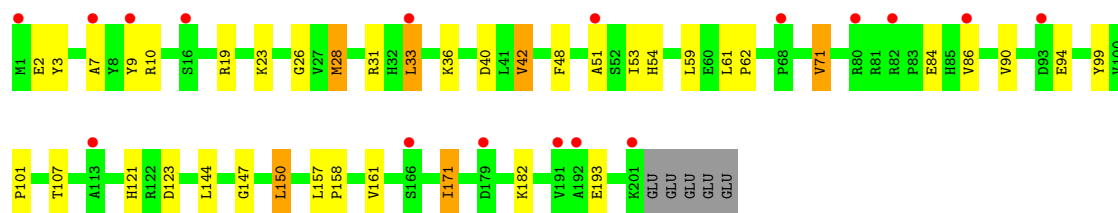


- Molecule 21: 50S ribosomal protein L25

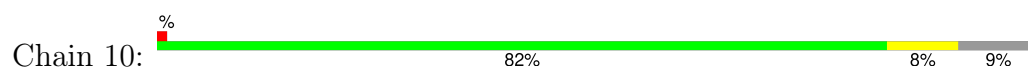


- Molecule 21: 50S ribosomal protein L25

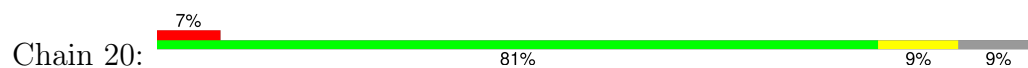




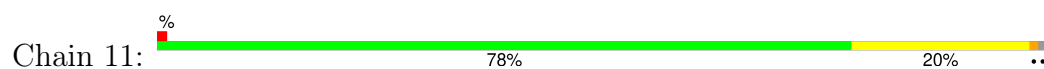
• Molecule 22: 50S ribosomal protein L27



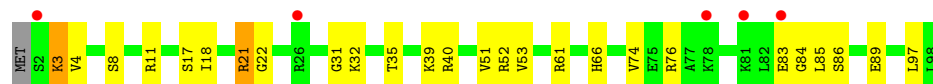
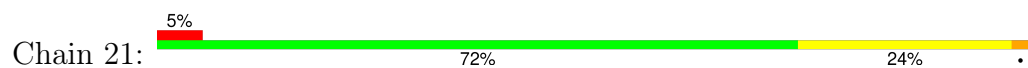
• Molecule 22: 50S ribosomal protein L27



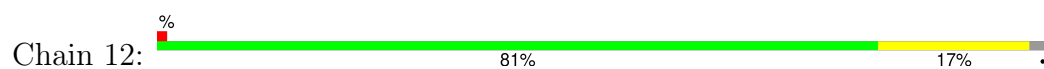
• Molecule 23: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29

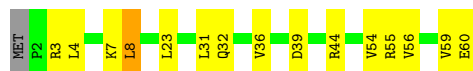


• Molecule 24: 50S ribosomal protein L29

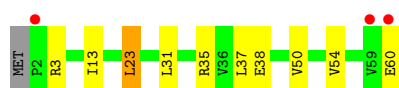
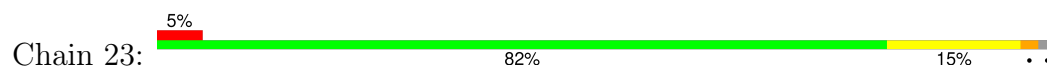




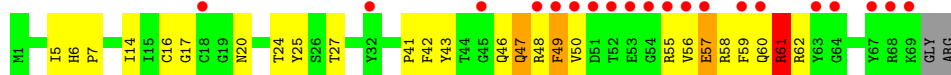
- Molecule 25: 50S ribosomal protein L30



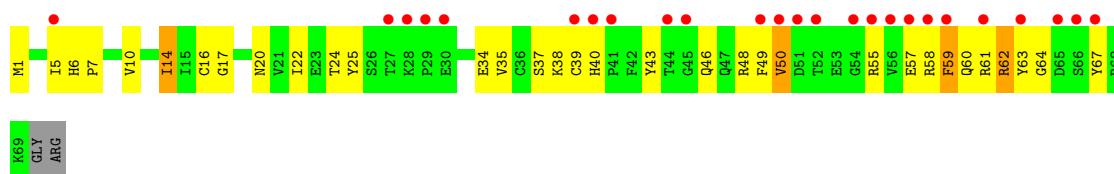
- Molecule 25: 50S ribosomal protein L30



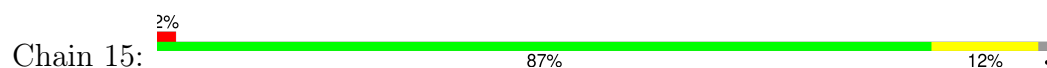
- Molecule 26: 50S ribosomal protein L31



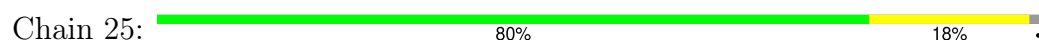
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

Chain 16:  89% 9% .



- Molecule 28: 50S ribosomal protein L33

Chain 26:  76% 19% . .



- Molecule 29: 50S ribosomal protein L34

Chain 17:  8% 82% 14% . .



- Molecule 29: 50S ribosomal protein L34

Chain 27:  10% 82% 12% . .



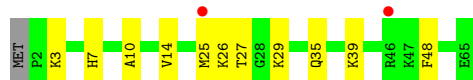
- Molecule 30: 50S ribosomal protein L35

Chain 18:  2% 72% 25% . .



- Molecule 30: 50S ribosomal protein L35

Chain 28:  3% 82% 17% .

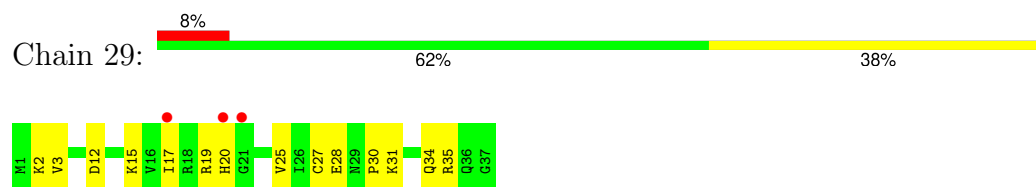


- Molecule 31: 50S ribosomal protein L36

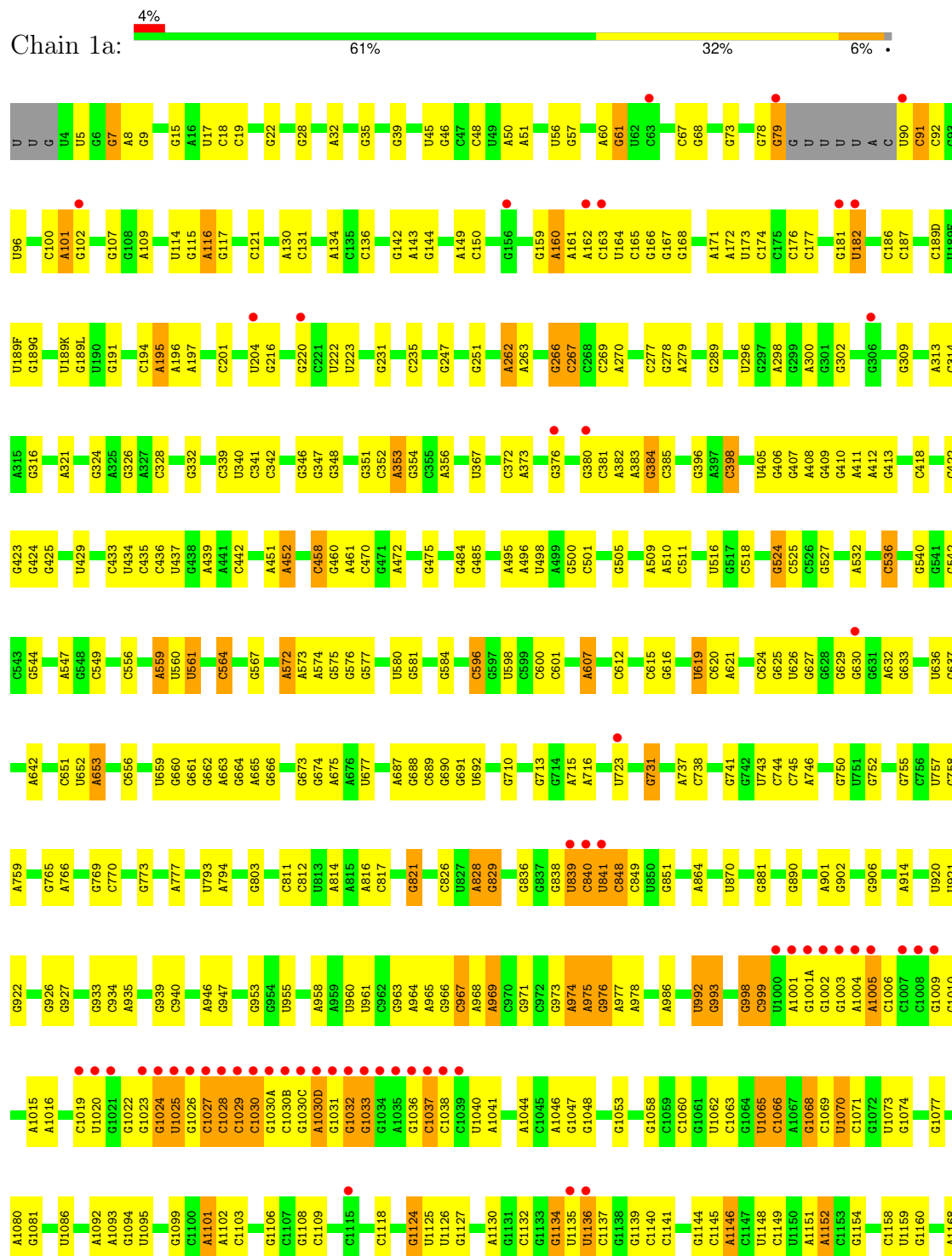
Chain 19:  3% 84% 16%

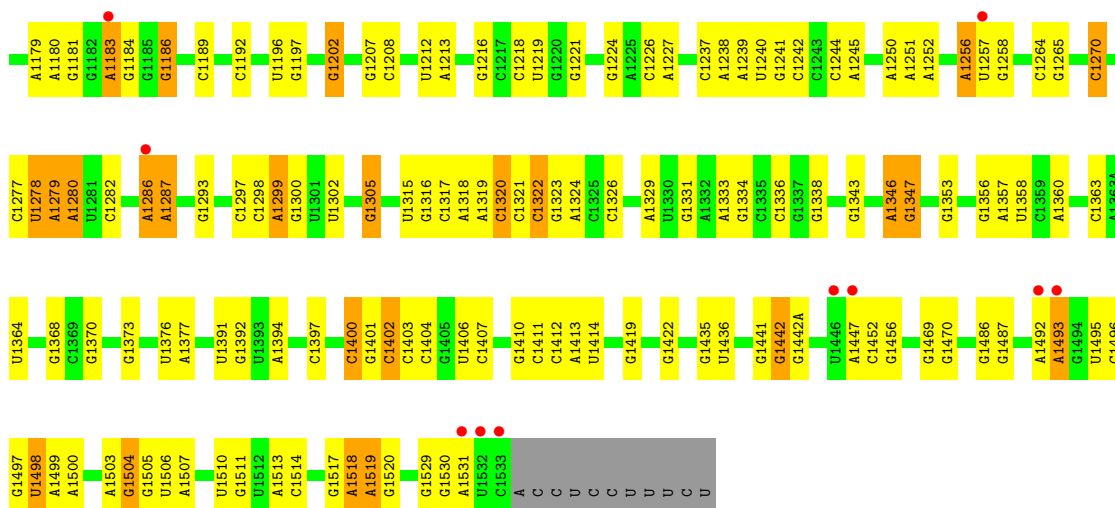


• Molecule 31: 50S ribosomal protein L36

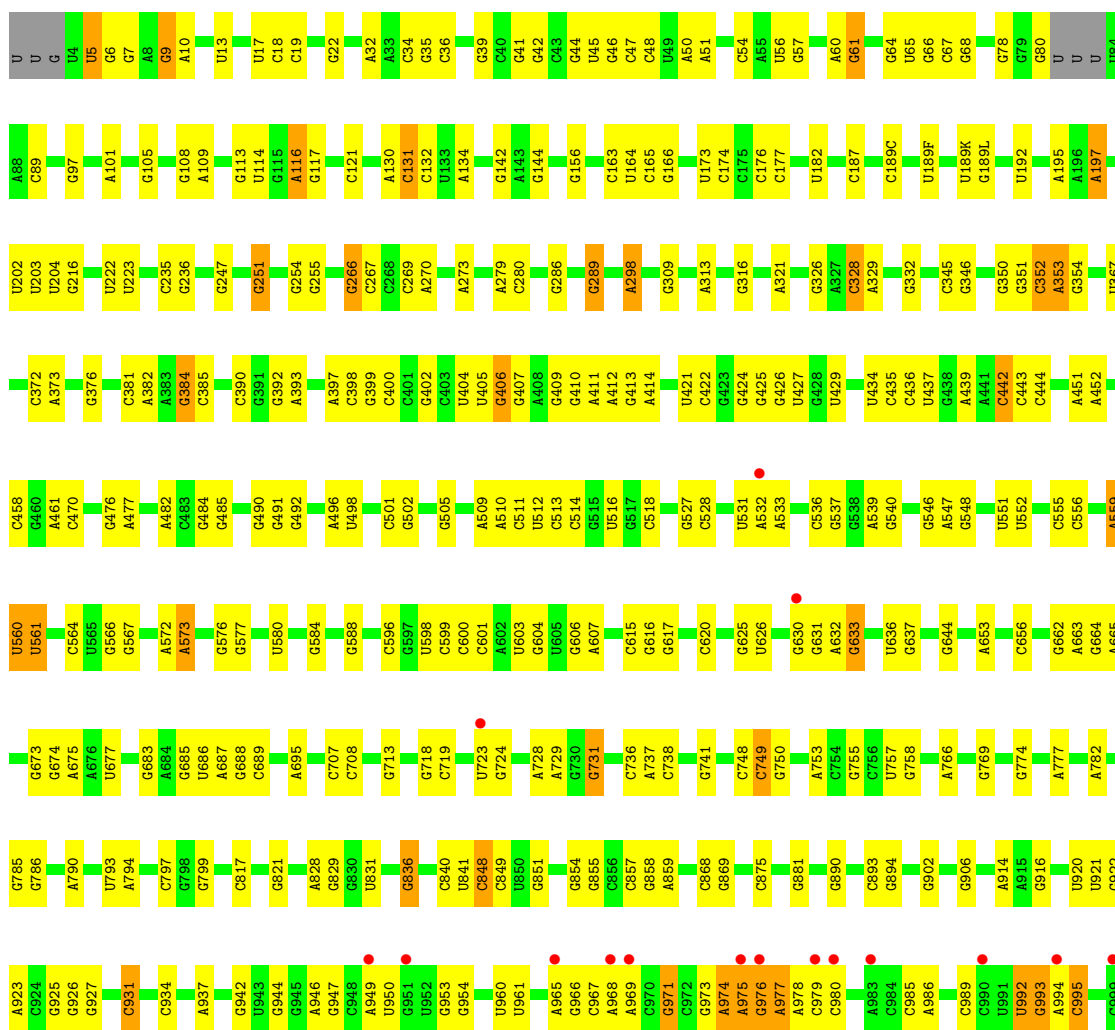


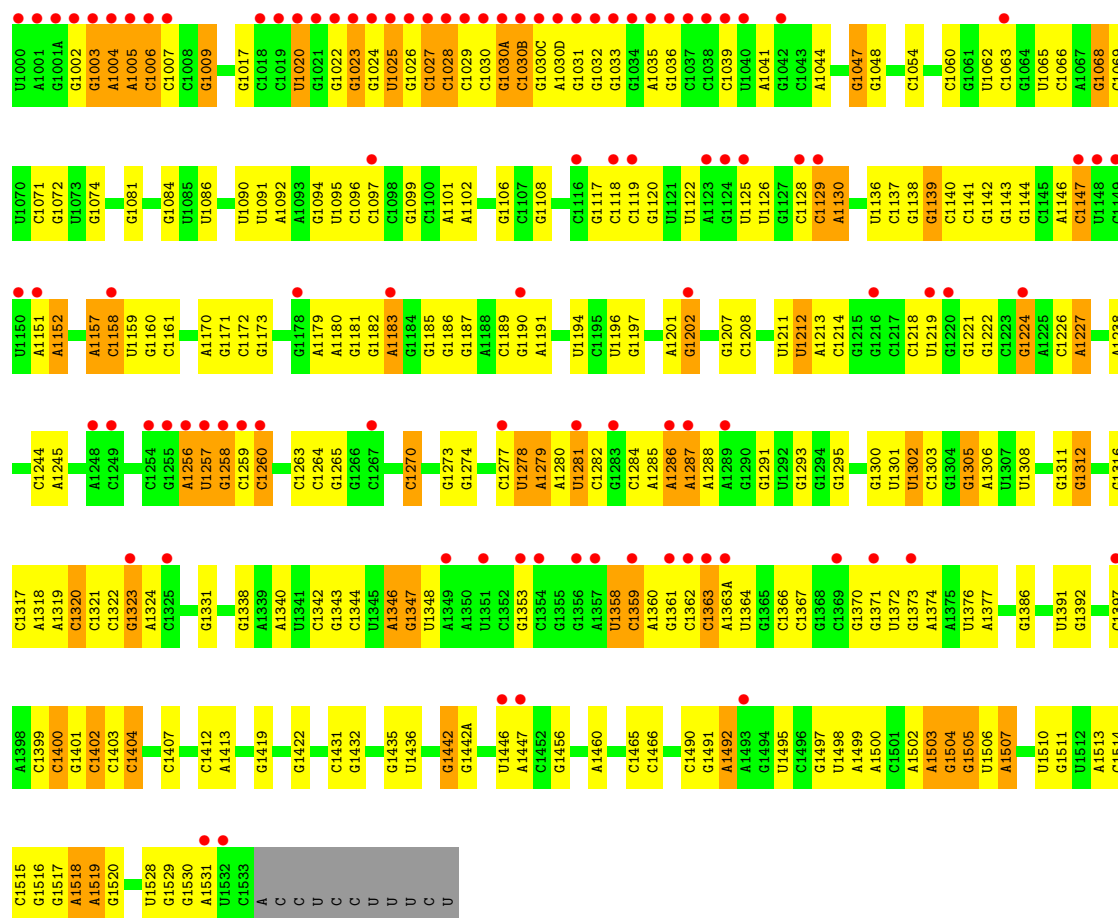
• Molecule 32: 16S Ribosomal RNA



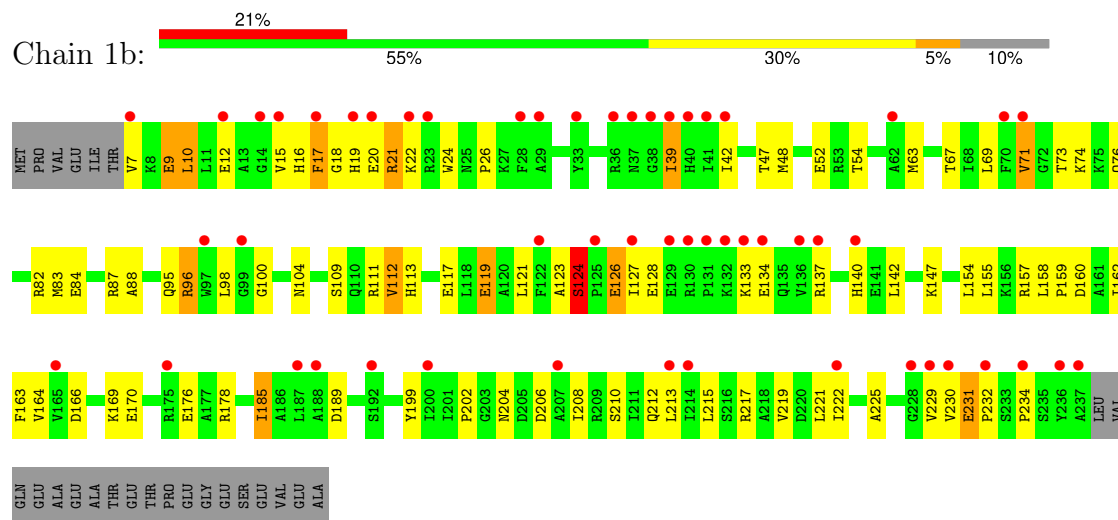


- Molecule 32: 16S Ribosomal RNA

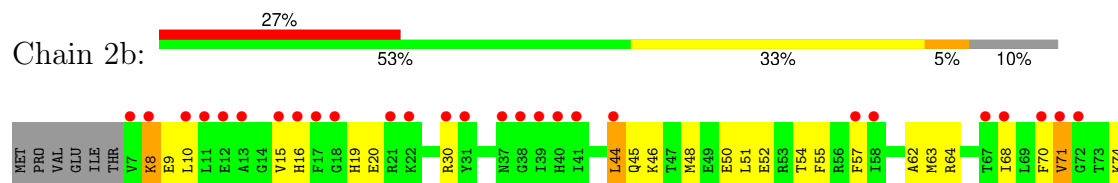


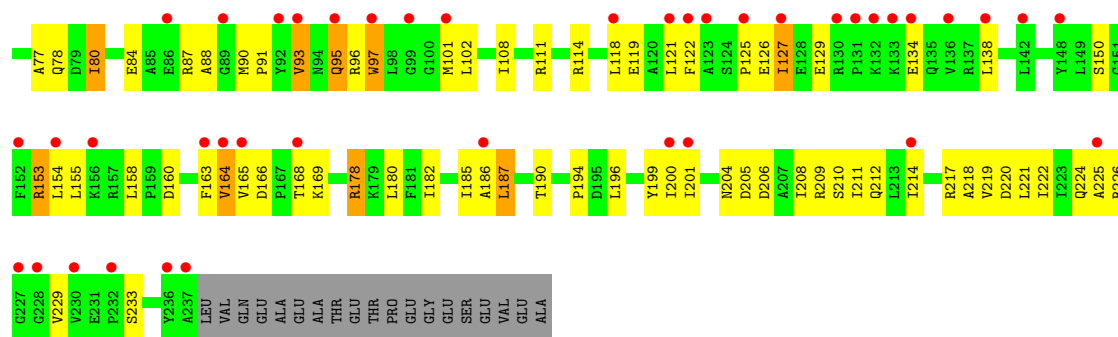


• Molecule 33: 30S ribosomal protein S2

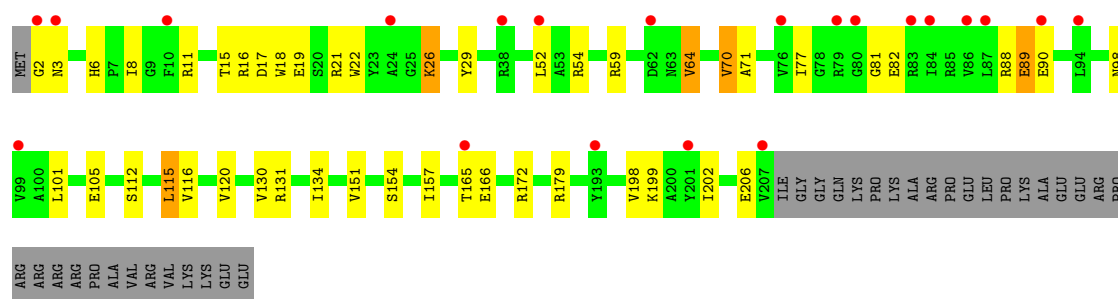


• Molecule 33: 30S ribosomal protein S2

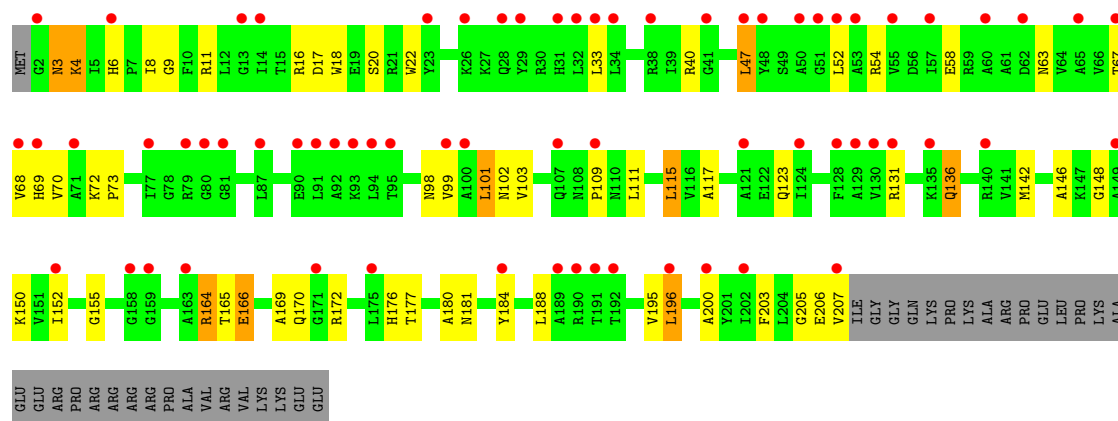




- Molecule 34: 30S ribosomal protein S3

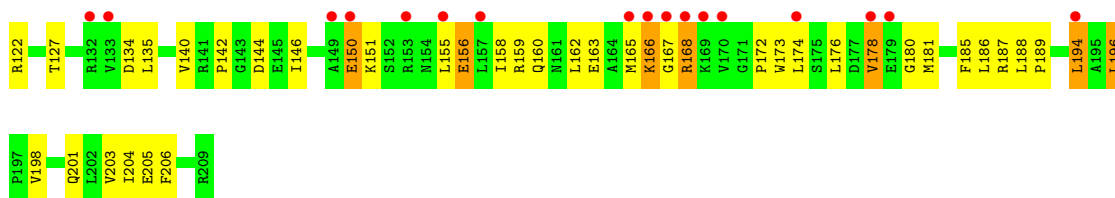


- Molecule 34: 30S ribosomal protein S3

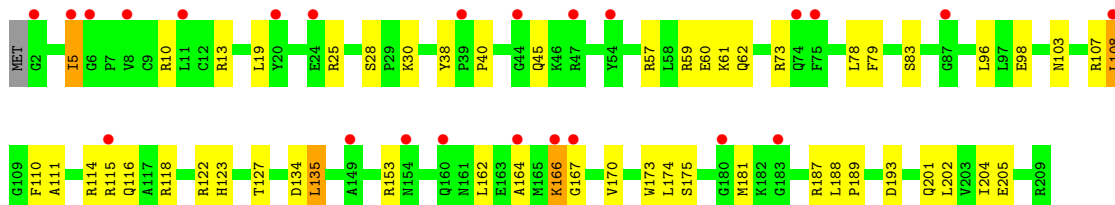
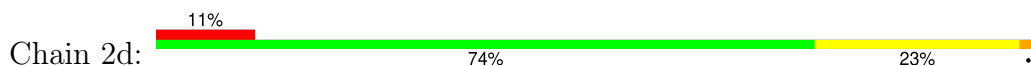


- Molecule 35: 30S ribosomal protein S4

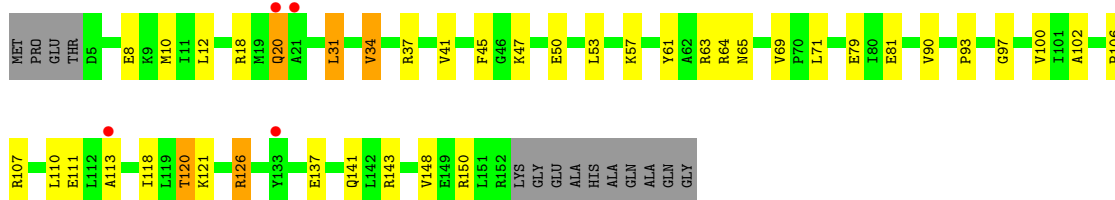




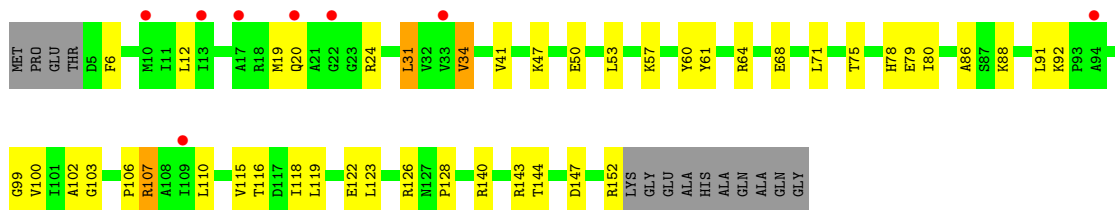
- Molecule 35: 30S ribosomal protein S4



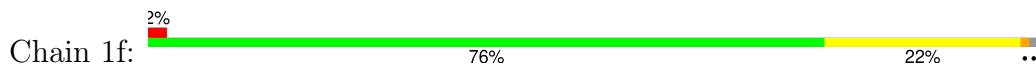
- Molecule 36: 30S ribosomal protein S5



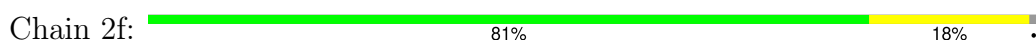
- Molecule 36: 30S ribosomal protein S5

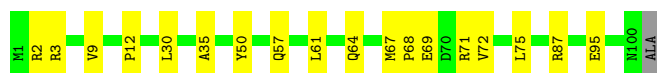


- Molecule 37: 30S ribosomal protein S6

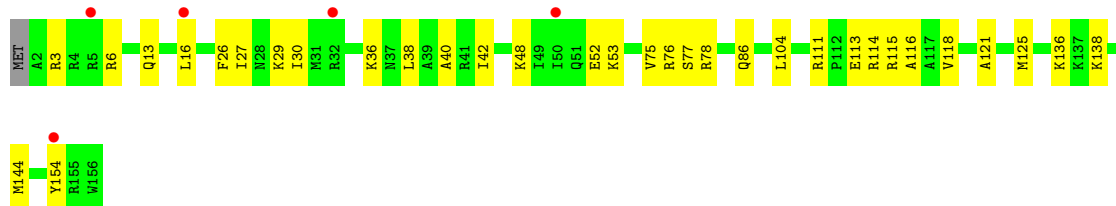
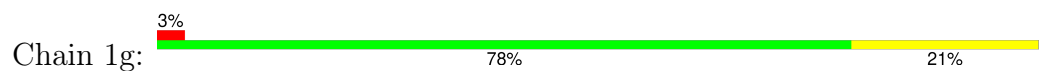


- Molecule 37: 30S ribosomal protein S6

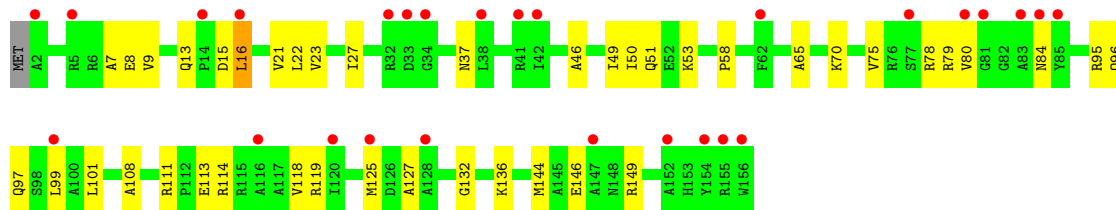
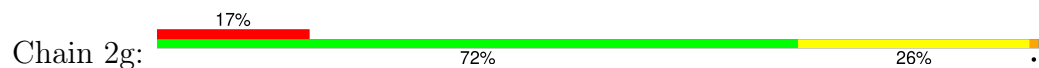




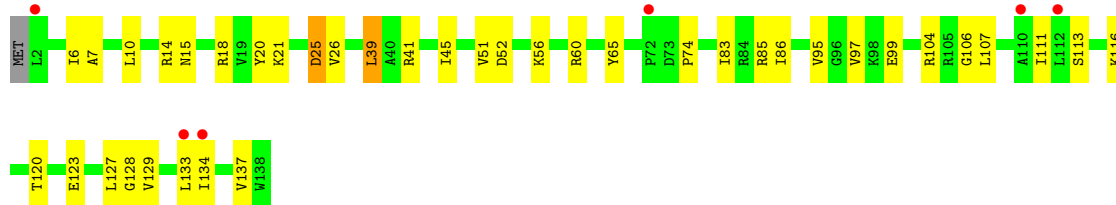
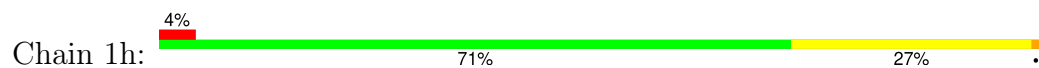
- Molecule 38: 30S ribosomal protein S7



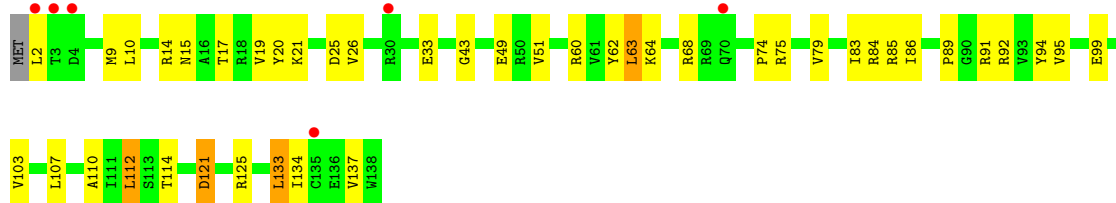
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

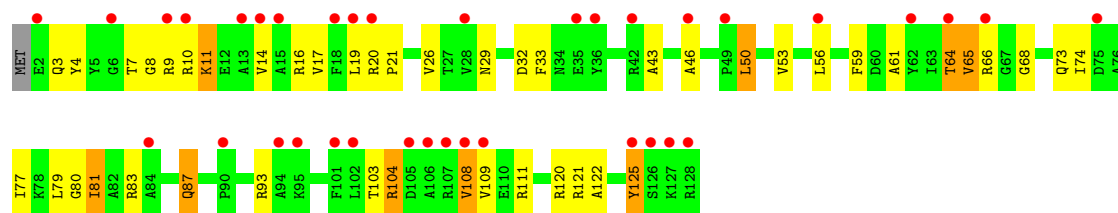


- Molecule 39: 30S ribosomal protein S8

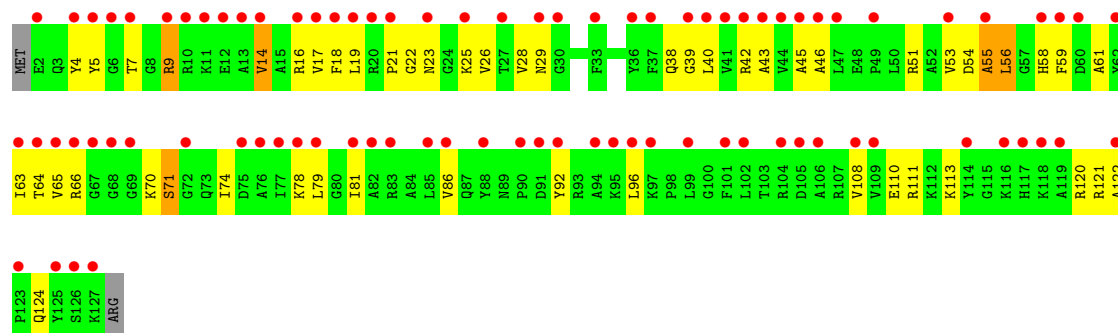


- Molecule 40: 30S ribosomal protein S9

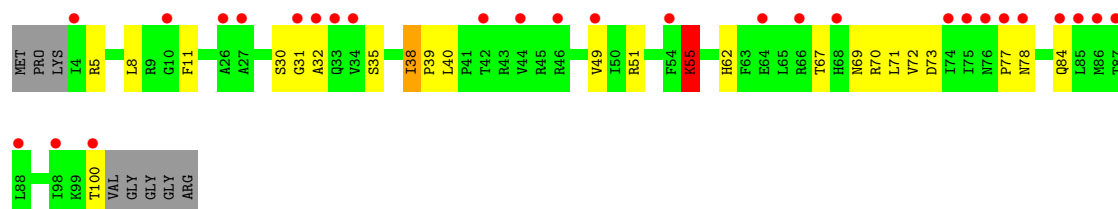




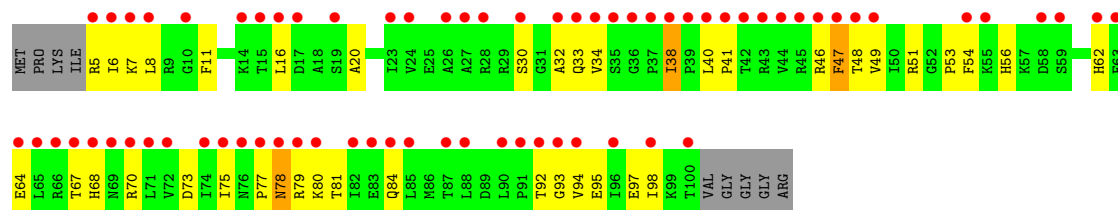
• Molecule 40: 30S ribosomal protein S9



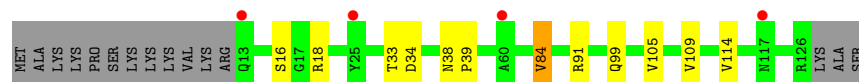
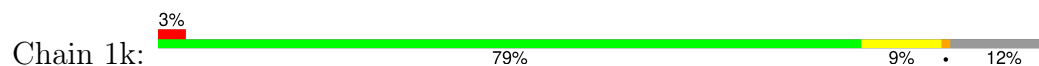
• Molecule 41: 30S ribosomal protein S10



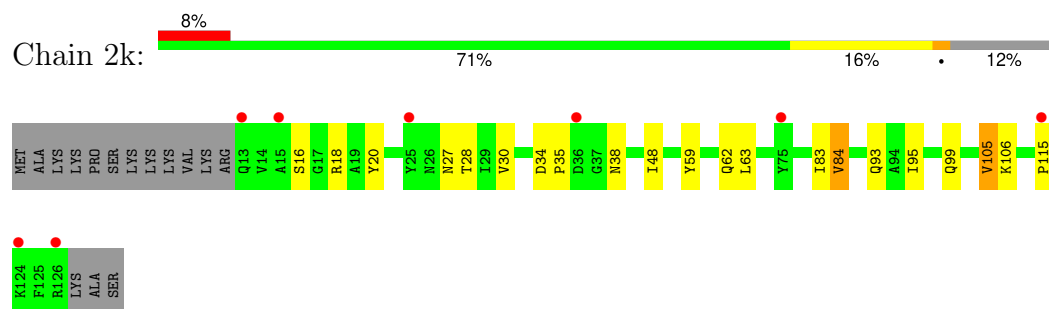
• Molecule 41: 30S ribosomal protein S10



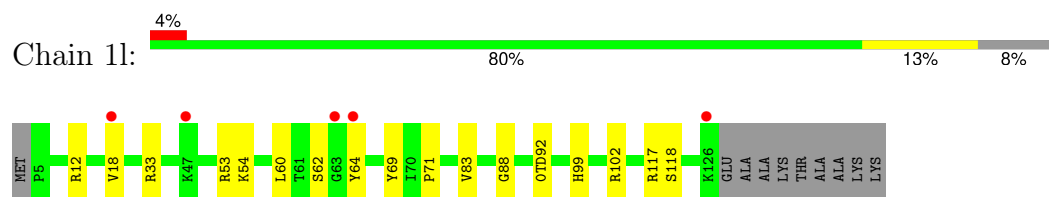
• Molecule 42: 30S ribosomal protein S11



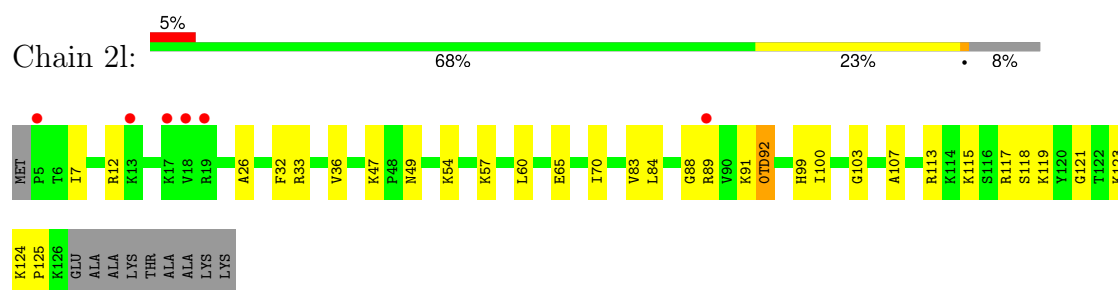
- Molecule 42: 30S ribosomal protein S11



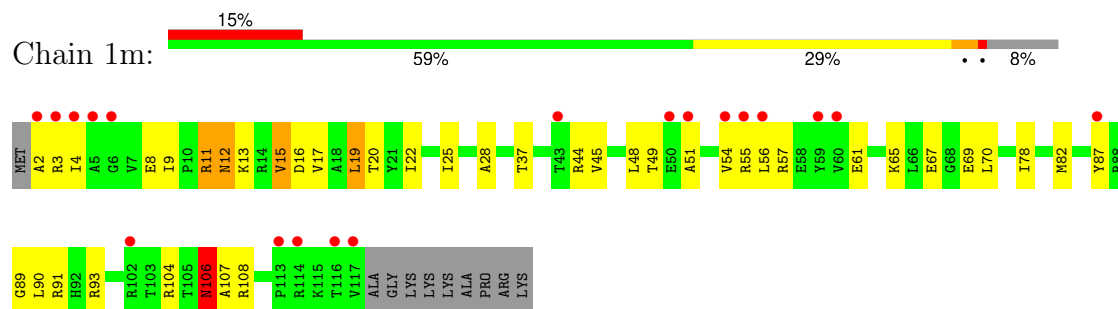
- Molecule 43: 30S ribosomal protein S12



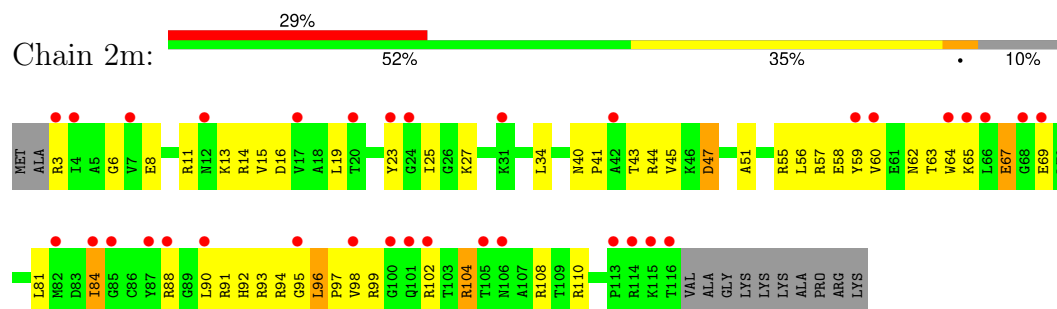
- Molecule 43: 30S ribosomal protein S12



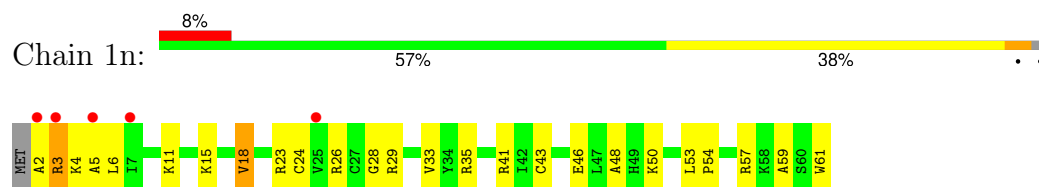
- Molecule 44: 30S ribosomal protein S13



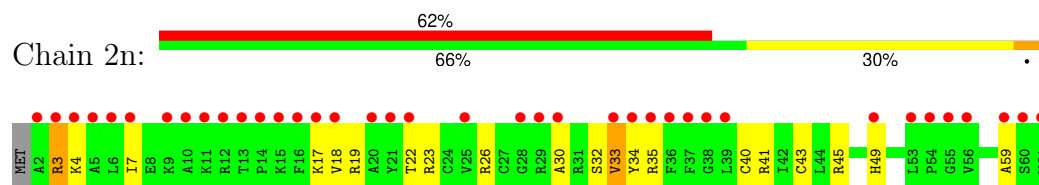
- Molecule 44: 30S ribosomal protein S13



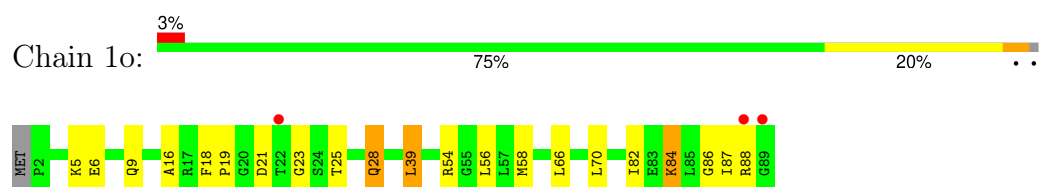
- Molecule 45: 30S ribosomal protein S14 type Z



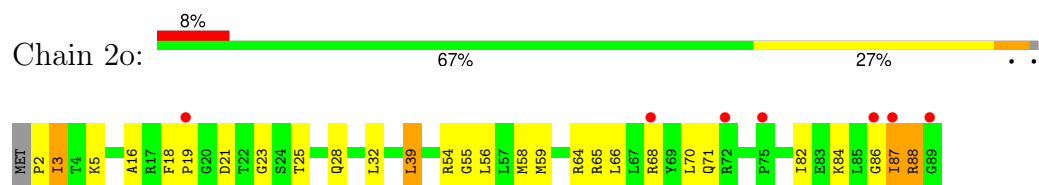
- Molecule 45: 30S ribosomal protein S14 type Z



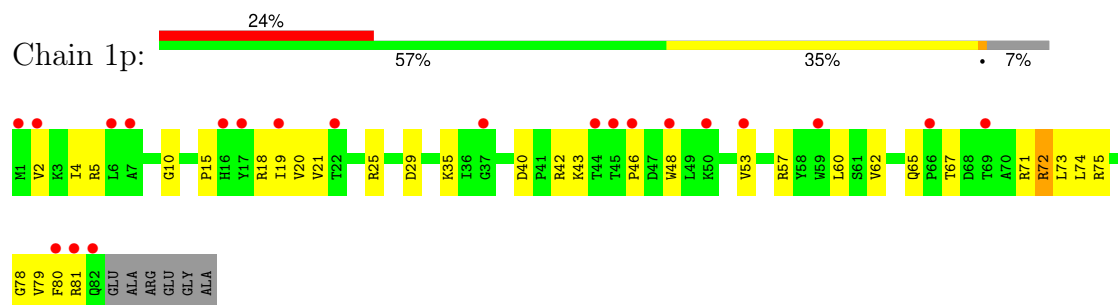
- Molecule 46: 30S ribosomal protein S15



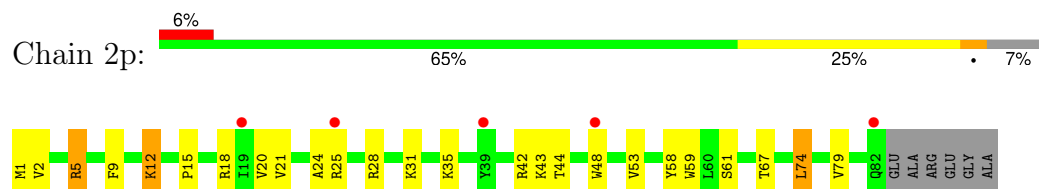
- Molecule 46: 30S ribosomal protein S15



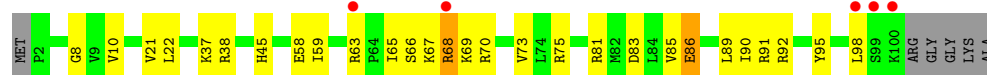
- Molecule 47: 30S ribosomal protein S16



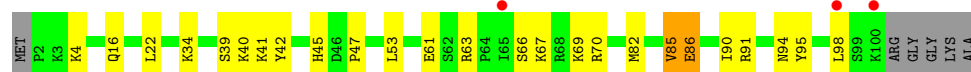
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



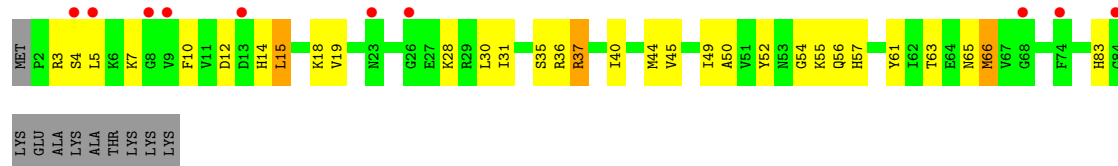
- Molecule 49: 30S ribosomal protein S18



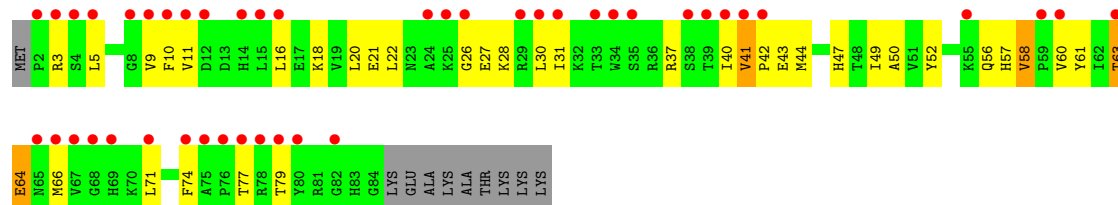
- Molecule 49: 30S ribosomal protein S18



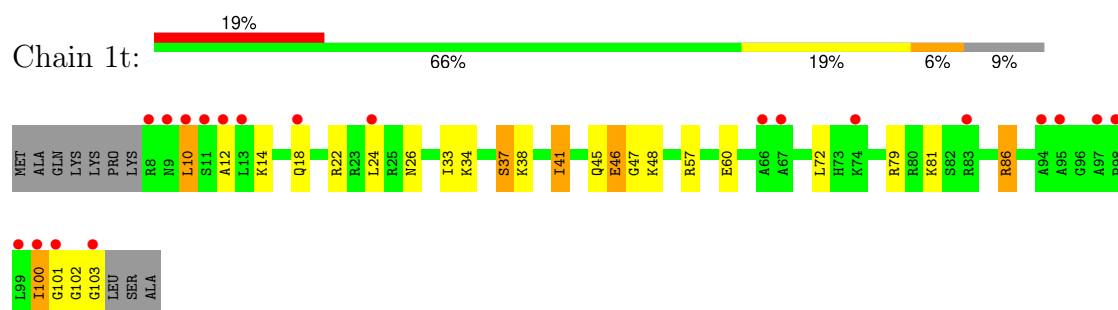
- Molecule 50: 30S ribosomal protein S19



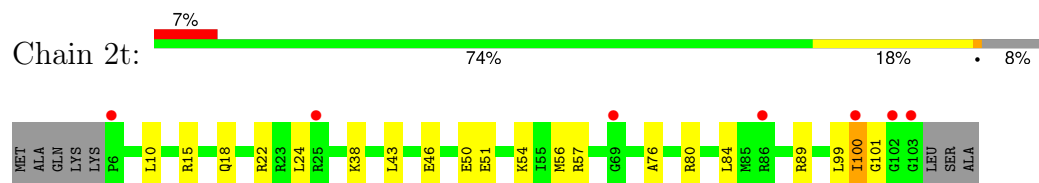
- Molecule 50: 30S ribosomal protein S19



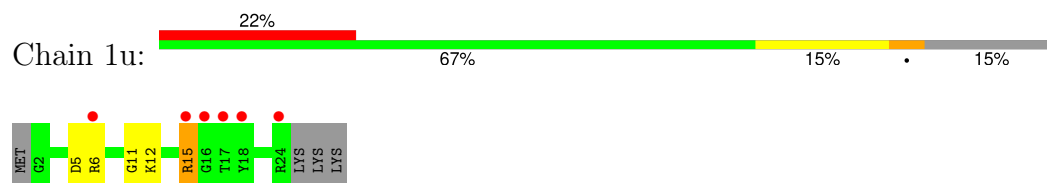
- Molecule 51: 30S ribosomal protein S20



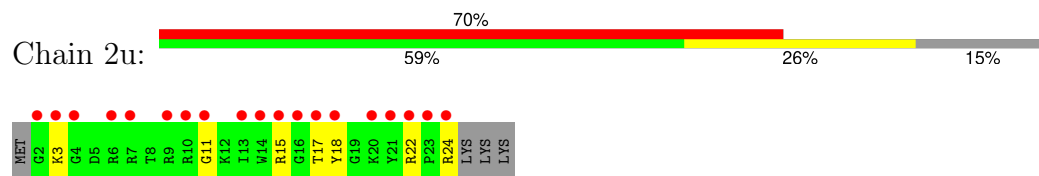
- Molecule 51: 30S ribosomal protein S20



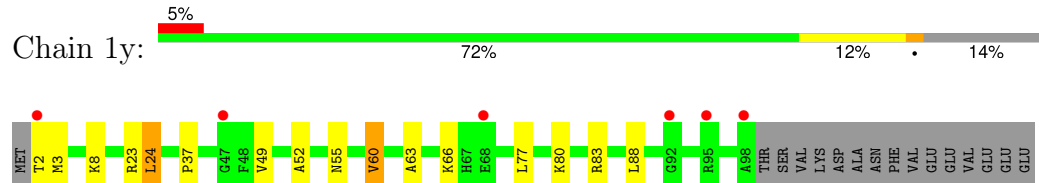
- Molecule 52: 30S ribosomal protein Thx



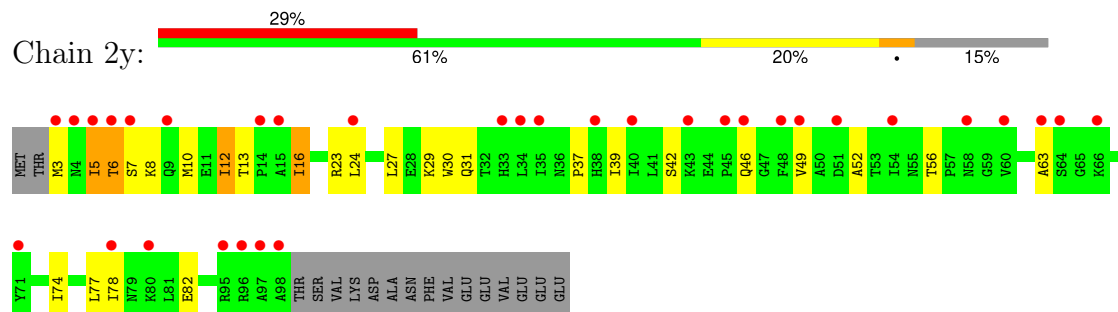
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.90Å 449.76Å 620.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.00 – 2.60 122.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (122.00-2.60) 99.8 (122.00-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.203 , 0.241 0.205 , 0.242	Depositor DCC
R_{free} test set	88927 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	297563	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: MG, OMC, PSU, OMG, G7M, CPF, 5MU, 2MA, 5MC, M2G, 0TD, MPD, SF4, ZN, UR3, MA6, 2MG, OMU, 4OC

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	0.19	0/69031	0.36	0/107754
1	2A	0.16	0/68903	0.34	0/107552
2	1B	0.15	0/2876	0.31	0/4486
2	2B	0.13	0/2878	0.27	0/4490
3	1D	0.19	0/2181	0.43	0/2940
3	2D	0.15	0/2186	0.41	0/2944
4	1E	0.17	0/1592	0.41	0/2149
4	2E	0.16	0/1592	0.39	0/2149
5	1F	0.17	0/1619	0.38	0/2193
5	2F	0.15	0/1615	0.41	0/2188
6	1G	0.14	0/1451	0.37	0/1961
6	2G	0.14	0/1449	0.35	0/1957
7	1H	0.15	0/1356	0.36	0/1834
7	2H	0.14	0/1350	0.37	0/1826
8	1I	0.15	0/1109	0.38	0/1512
8	2I	0.13	0/1091	0.36	0/1490
9	1N	0.16	0/1148	0.37	0/1547
9	2N	0.13	0/1144	0.33	0/1543
10	1O	0.17	0/943	0.40	0/1269
10	2O	0.15	0/943	0.37	0/1269
11	1P	0.18	0/1152	0.41	0/1533
11	2P	0.15	0/1152	0.42	0/1533
12	1Q	0.17	0/1143	0.40	0/1527
12	2Q	0.13	0/1143	0.35	0/1527
13	1R	0.17	0/982	0.40	0/1312
13	2R	0.15	0/982	0.39	0/1312
14	1S	0.15	0/887	0.37	0/1180
14	2S	0.14	0/880	0.38	0/1172
15	1T	0.17	0/1105	0.43	0/1477
15	2T	0.15	0/1097	0.39	0/1468
16	1U	0.18	0/977	0.38	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.13	0/977	0.34	0/1301
17	1V	0.16	0/786	0.38	0/1053
17	2V	0.14	0/782	0.34	0/1049
18	1W	0.18	0/897	0.38	0/1205
18	2W	0.15	0/897	0.35	0/1205
19	1X	0.17	0/764	0.41	0/1025
19	2X	0.14	0/764	0.39	0/1025
20	1Y	0.17	0/823	0.44	0/1099
20	2Y	0.13	0/823	0.37	0/1100
21	1Z	0.14	0/1620	0.34	0/2200
21	2Z	0.13	0/1590	0.36	0/2162
22	10	0.18	0/616	0.45	0/821
22	20	0.15	0/616	0.41	0/821
23	11	0.17	0/761	0.38	0/1013
23	21	0.16	0/766	0.36	0/1018
24	12	0.15	0/590	0.37	0/781
24	22	0.14	0/594	0.38	0/785
25	13	0.17	0/474	0.41	0/635
25	23	0.13	0/469	0.34	0/630
26	14	0.18	0/559	0.54	0/754
26	24	0.22	0/549	0.58	2/741 (0.3%)
27	15	0.17	0/473	0.44	0/639
27	25	0.18	0/469	0.42	0/635
28	16	0.17	0/460	0.40	0/613
28	26	0.15	0/456	0.35	0/608
29	17	0.20	0/426	0.43	0/561
29	27	0.19	0/426	0.45	0/561
30	18	0.17	0/525	0.39	0/691
30	28	0.14	0/525	0.35	0/691
31	19	0.17	0/310	0.41	0/407
31	29	0.15	0/310	0.36	0/407
32	1a	0.14	0/35795	0.31	0/55864
32	2a	0.14	0/35890	0.31	0/56012
33	1b	0.15	0/1876	0.41	0/2533
33	2b	0.17	0/1860	0.41	0/2518
34	1c	0.14	0/1582	0.37	0/2137
34	2c	0.15	0/1566	0.36	0/2119
35	1d	0.14	0/1695	0.38	0/2274
35	2d	0.14	0/1698	0.37	0/2277
36	1e	0.15	0/1149	0.39	0/1548
36	2e	0.14	0/1149	0.37	0/1548
37	1f	0.14	0/827	0.35	0/1120
37	2f	0.13	0/829	0.35	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.13	0/1254	0.33	0/1683
38	2g	0.13	0/1248	0.32	0/1676
39	1h	0.13	0/1118	0.36	0/1506
39	2h	0.13	0/1108	0.36	0/1494
40	1i	0.14	0/1005	0.39	0/1351
40	2i	0.15	0/985	0.39	0/1329
41	1j	0.14	0/732	0.35	0/993
41	2j	0.16	0/723	0.40	0/984
42	1k	0.14	0/849	0.36	0/1150
42	2k	0.14	0/848	0.38	0/1149
43	1l	0.14	0/937	0.37	0/1260
43	2l	0.14	0/937	0.37	0/1260
44	1m	0.15	0/924	0.41	0/1242
44	2m	0.16	0/905	0.47	1/1217 (0.1%)
45	1n	0.13	0/501	0.36	0/664
45	2n	0.14	0/501	0.36	0/664
46	1o	0.14	0/739	0.33	0/985
46	2o	0.14	0/739	0.36	0/985
47	1p	0.15	0/697	0.44	0/939
47	2p	0.13	0/693	0.39	0/935
48	1q	0.14	0/836	0.36	0/1117
48	2q	0.14	0/836	0.37	0/1117
49	1r	0.13	0/560	0.35	0/746
49	2r	0.14	0/560	0.34	0/746
50	1s	0.13	0/663	0.40	0/895
50	2s	0.13	0/660	0.35	0/893
51	1t	0.15	0/734	0.43	0/969
51	2t	0.14	0/736	0.36	0/976
52	1u	0.13	0/203	0.36	0/266
52	2u	0.21	0/203	0.47	0/266
53	1y	0.17	0/776	0.31	0/1048
53	2y	0.12	0/761	0.29	0/1030
All	All	0.16	0/309941	0.35	3/463239 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	24	59	PHE	CA-C-N	5.29	131.22	121.70
26	24	59	PHE	C-N-CA	5.29	131.22	121.70
44	2m	84	ILE	N-CA-C	-5.06	106.66	112.98

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
33	1b	231	GLU	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31207	449	0
1	2A	61758	0	31153	518	0
2	1B	2572	0	1305	12	0
2	2B	2573	0	1306	29	0
3	1D	2131	0	2207	36	0
3	2D	2136	0	2218	34	0
4	1E	1559	0	1618	26	0
4	2E	1559	0	1618	28	0
5	1F	1584	0	1625	26	0
5	2F	1580	0	1619	33	0
6	1G	1426	0	1445	31	0
6	2G	1424	0	1441	54	0
7	1H	1330	0	1407	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	2H	1324	0	1402	39	0
8	1I	1094	0	1127	21	0
8	2I	1076	0	1094	16	0
9	1N	1121	0	1195	15	0
9	2N	1117	0	1184	19	0
10	1O	933	0	996	16	0
10	2O	933	0	996	12	0
11	1P	1135	0	1212	25	0
11	2P	1135	0	1212	17	0
12	1Q	1122	0	1179	10	0
12	2Q	1122	0	1179	17	0
13	1R	968	0	1033	15	0
13	2R	968	0	1033	14	0
14	1S	877	0	938	17	0
14	2S	870	0	923	27	0
15	1T	1091	0	1151	25	0
15	2T	1083	0	1136	17	0
16	1U	959	0	1019	12	0
16	2U	959	0	1019	15	0
17	1V	775	0	841	12	0
17	2V	771	0	830	13	0
18	1W	886	0	940	9	0
18	2W	886	0	940	10	0
19	1X	750	0	814	13	0
19	2X	750	0	814	6	0
20	1Y	810	0	892	13	0
20	2Y	810	0	887	12	0
21	1Z	1587	0	1598	21	0
21	2Z	1557	0	1564	28	0
22	10	608	0	622	6	0
22	20	608	0	622	5	0
23	11	754	0	823	14	0
23	21	759	0	837	17	0
24	12	588	0	643	8	0
24	22	592	0	654	10	0
25	13	469	0	518	8	0
25	23	464	0	514	6	0
26	14	546	0	522	15	0
26	24	536	0	514	25	0
27	15	459	0	476	4	0
27	25	455	0	465	5	0
28	16	453	0	473	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	26	449	0	469	9	0
29	17	418	0	467	9	0
29	27	418	0	467	4	0
30	18	517	0	582	14	0
30	28	517	0	582	8	0
31	19	307	0	335	3	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	335	0
32	2a	32331	0	16338	352	0
33	1b	1842	0	1862	47	0
33	2b	1825	0	1828	61	0
34	1c	1558	0	1557	28	0
34	2c	1542	0	1517	40	0
35	1d	1665	0	1687	56	0
35	2d	1668	0	1703	37	0
36	1e	1133	0	1191	30	0
36	2e	1133	0	1191	27	0
37	1f	814	0	808	14	0
37	2f	816	0	808	13	0
38	1g	1235	0	1249	18	0
38	2g	1229	0	1238	20	0
39	1h	1098	0	1143	24	0
39	2h	1088	0	1126	24	0
40	1i	986	0	990	34	0
40	2i	966	0	953	33	0
41	1j	719	0	672	15	0
41	2j	710	0	661	34	0
42	1k	834	0	838	6	0
42	2k	833	0	836	16	0
43	1l	932	0	981	10	0
43	2l	932	0	981	20	0
44	1m	914	0	954	27	0
44	2m	895	0	920	31	0
45	1n	492	0	529	21	0
45	2n	492	0	529	17	0
46	1o	728	0	760	13	0
46	2o	728	0	760	15	0
47	1p	681	0	697	18	0
47	2p	677	0	686	15	0
48	1q	823	0	891	19	0
48	2q	823	0	891	22	0
49	1r	555	0	618	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	2r	555	0	618	11	0
50	1s	648	0	658	24	0
50	2s	645	0	635	31	0
51	1t	732	0	809	15	0
51	2t	733	0	795	13	0
52	1u	199	0	208	3	0
52	2u	199	0	208	3	0
53	1y	764	0	786	16	0
53	2y	749	0	757	20	0
54	10	7	0	0	0	0
54	11	5	0	0	0	0
54	13	4	0	0	0	0
54	14	1	0	0	0	0
54	15	8	0	0	0	0
54	17	7	0	0	0	0
54	18	3	0	0	0	0
54	19	2	0	0	0	0
54	1A	1056	0	0	0	0
54	1B	29	0	0	0	0
54	1D	18	0	0	0	0
54	1E	9	0	0	0	0
54	1F	19	0	0	0	0
54	1G	4	0	0	0	0
54	1H	3	0	0	0	0
54	1N	5	0	0	0	0
54	1O	1	0	0	0	0
54	1P	6	0	0	0	0
54	1Q	5	0	0	0	0
54	1R	6	0	0	0	0
54	1T	5	0	0	0	0
54	1U	7	0	0	0	0
54	1V	6	0	0	0	0
54	1W	3	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	277	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	2	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1k	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	3	0	0	0	0
54	1o	1	0	0	0	0
54	1t	1	0	0	0	0
54	1y	4	0	0	0	0
54	20	3	0	0	0	0
54	21	1	0	0	0	0
54	23	2	0	0	0	0
54	25	1	0	0	0	0
54	27	1	0	0	0	0
54	28	2	0	0	0	0
54	2A	741	0	0	0	0
54	2B	18	0	0	0	0
54	2D	12	0	0	0	0
54	2E	7	0	0	0	0
54	2F	4	0	0	0	0
54	2G	3	0	0	0	0
54	2N	1	0	0	0	0
54	2O	2	0	0	0	0
54	2Q	3	0	0	0	0
54	2R	3	0	0	0	0
54	2T	3	0	0	0	0
54	2V	3	0	0	0	0
54	2W	3	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	195	0	0	0	0
54	2d	1	0	0	0	0
54	2e	1	0	0	0	0
54	2f	2	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2n	1	0	0	0	0
54	2o	1	0	0	0	0
54	2p	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	24	0	17	1	0
55	2A	24	0	17	3	0
56	18	8	0	14	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1A	8	0	14	1	0
56	1O	8	0	14	1	0
56	1a	8	0	14	4	0
56	2A	16	0	28	1	0
56	2B	8	0	14	0	0
57	1B	12	0	12	1	0
57	1F	12	0	12	2	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	0	0
60	10	25	0	0	0	0
60	11	28	0	0	0	0
60	12	13	0	0	3	0
60	13	25	0	0	2	0
60	14	3	0	0	0	0
60	15	28	0	0	0	0
60	16	20	0	0	0	0
60	17	13	0	0	0	0
60	18	28	0	0	1	0
60	19	8	0	0	0	0
60	1A	3927	0	0	79	0
60	1B	89	0	0	5	0
60	1D	110	0	0	3	0
60	1E	72	0	0	3	0
60	1F	67	0	0	1	0
60	1G	16	0	0	0	0
60	1H	14	0	0	0	0
60	1I	5	0	0	0	0
60	1N	52	0	0	0	0
60	1O	25	0	0	1	0
60	1P	65	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1Q	41	0	0	1	0
60	1R	32	0	0	1	0
60	1S	8	0	0	1	0
60	1T	36	0	0	2	0
60	1U	43	0	0	3	0
60	1V	36	0	0	0	0
60	1W	28	0	0	1	0
60	1X	26	0	0	1	0
60	1Y	17	0	0	2	0
60	1Z	11	0	0	0	0
60	1a	496	0	0	22	0
60	1b	1	0	0	0	0
60	1c	1	0	0	0	0
60	1d	9	0	0	1	0
60	1e	10	0	0	1	0
60	1f	1	0	0	0	0
60	1h	1	0	0	0	0
60	1j	1	0	0	0	0
60	1k	1	0	0	0	0
60	1l	4	0	0	0	0
60	1o	4	0	0	0	0
60	1p	1	0	0	0	0
60	1y	5	0	0	0	0
60	20	10	0	0	0	0
60	21	17	0	0	2	0
60	22	2	0	0	0	0
60	23	2	0	0	1	0
60	25	7	0	0	0	0
60	26	6	0	0	1	0
60	27	9	0	0	0	0
60	28	15	0	0	0	0
60	2A	2249	0	0	87	0
60	2B	42	0	0	3	0
60	2D	47	0	0	1	0
60	2E	28	0	0	1	0
60	2F	23	0	0	0	0
60	2G	4	0	0	0	0
60	2H	1	0	0	1	0
60	2N	6	0	0	1	0
60	2O	15	0	0	0	0
60	2P	21	0	0	1	0
60	2Q	18	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2R	22	0	0	2	0
60	2S	2	0	0	0	0
60	2T	12	0	0	0	0
60	2U	16	0	0	3	0
60	2V	8	0	0	0	0
60	2W	19	0	0	0	0
60	2X	8	0	0	0	0
60	2Y	4	0	0	0	0
60	2Z	8	0	0	0	0
60	2a	404	0	0	22	0
60	2d	3	0	0	1	0
60	2e	3	0	0	0	0
60	2f	3	0	0	0	0
60	2j	2	0	0	1	0
60	2l	5	0	0	1	0
60	2o	2	0	0	1	0
60	2p	1	0	0	0	0
60	2q	1	0	0	0	0
60	2r	3	0	0	0	0
60	2t	3	0	0	0	0
60	2u	1	0	0	0	0
60	2y	1	0	0	0	0
All	All	297563	0	194555	3101	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 7.

All (3101) 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	1.39	1.19
1:1A:1082:U:O4	1:1A:1086:A:N1	1.97	0.97
32:1a:1086:U:H3	32:1a:1099:G:H22	1.16	0.94
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.35	0.90
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.37	0.87
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.37	0.87
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.56	0.86
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.58	0.86
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.58	0.84
1:2A:2427:C:OP1	60:2A:3806:HOH:O	1.95	0.84
32:1a:664:G:H22	32:1a:741:G:H1	1.26	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:231:GLU:HB3	33:1b:232:PRO:HD3	1.61	0.83
32:1a:1441:G:H5''	32:1a:1442:G:H5'	1.59	0.82
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.61	0.82
29:17:24:THR:HG22	29:17:27:GLY:H	1.43	0.81
1:2A:826:U:OP1	60:2A:3806:HOH:O	1.98	0.81
32:1a:975:A:H4'	32:1a:976:G:H5''	1.62	0.81
1:2A:2602:A:H1'	1:2A:2603:G:H5''	1.61	0.80
1:2A:2107:C:H42	1:2A:2182:G:H1	1.27	0.80
32:2a:1500:A:OP1	60:2a:3202:HOH:O	1.99	0.80
1:1A:1064:C:H3'	1:1A:1065:U:H5''	1.62	0.80
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.64	0.80
32:1a:1003:G:H2'	32:1a:1004:A:H4'	1.63	0.80
4:2E:110:GLY:O	60:2R:301:HOH:O	1.99	0.80
32:1a:73:G:H1	32:1a:96:U:H3	1.30	0.79
1:1A:2137:C:H42	1:1A:2154:G:H1	1.28	0.79
29:27:24:THR:HG22	29:27:27:GLY:H	1.46	0.79
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.65	0.78
1:2A:194:G:OP2	60:2A:3807:HOH:O	2.02	0.77
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.65	0.77
36:2e:140:ARG:O	36:2e:143:ARG:NH2	2.17	0.77
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.17	0.77
1:1A:1082:U:H3	1:1A:1086:A:H61	0.80	0.77
33:2b:77:ALA:HB2	33:2b:211:ILE:HD13	1.66	0.77
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.18	0.77
1:2A:2136:C:C2	1:2A:2155:G:N2	2.53	0.77
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.49	0.77
1:1A:1041:C:H42	1:1A:1114:G:H1	1.34	0.76
36:1e:37:ARG:HH12	36:1e:111:GLU:HG2	1.51	0.76
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.19	0.76
32:2a:1129:C:OP1	40:2i:16:ARG:NH1	2.18	0.76
1:2A:2206:G:H5''	1:2A:2207:G:C8	2.20	0.76
22:20:10:THR:HG22	22:20:12:ASN:H	1.48	0.76
51:2t:50:GLU:HG3	51:2t:100:ILE:HD11	1.68	0.76
1:2A:962:G:OP1	60:2A:3809:HOH:O	2.04	0.76
1:1A:2464:C:O2'	60:1A:4106:HOH:O	2.04	0.76
32:2a:953:G:H4'	53:2y:6:THR:HG22	1.66	0.76
4:1E:119:ARG:HD3	4:1E:160:TYR:HB2	1.66	0.75
32:1a:1373:G:H5''	38:1g:36:LYS:HE2	1.68	0.75
1:2A:2156:G:N7	1:2A:2157:G:N2	2.35	0.75
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.68	0.75
8:1I:68:LEU:HD21	8:1I:109:ILE:HD11	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:792:G:O6	60:2A:3810:HOH:O	2.04	0.75
1:2A:881:G:H1	1:2A:895:U:H3	1.34	0.75
1:1A:1085:A:O2'	1:1A:1104:C:O2'	2.05	0.74
1:2A:1602:U:O4	60:2A:3808:HOH:O	2.04	0.74
33:1b:134:GLU:HG3	33:1b:137:ARG:HH21	1.50	0.74
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.67	0.74
32:2a:1500:A:OP2	60:2a:3203:HOH:O	2.05	0.74
32:2a:1285:A:H4'	32:2a:1286:A:H5'	1.68	0.74
1:1A:1271:G:OP2	60:1A:4105:HOH:O	2.04	0.74
1:2A:1315:C:OP2	60:2A:3812:HOH:O	2.06	0.74
35:1d:107:ARG:HH21	35:1d:194:LEU:HD21	1.52	0.74
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.70	0.74
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.51	0.73
32:2a:975:A:H4'	32:2a:976:G:H5''	1.68	0.73
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.69	0.73
26:14:16:CYS:SG	26:14:17:GLY:N	2.62	0.73
26:24:16:CYS:SG	26:24:17:GLY:N	2.60	0.73
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.68	0.73
37:2f:68:PRO:HG2	37:2f:71:ARG:HH11	1.54	0.73
1:1A:271(M):G:H21	8:1I:50:ARG:HD3	1.54	0.73
39:2h:89:PRO:HA	39:2h:92:ARG:HE	1.53	0.73
1:2A:72:U:OP1	60:2A:3811:HOH:O	2.05	0.73
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.22	0.72
1:2A:1314:C:OP1	60:2A:3812:HOH:O	2.07	0.72
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.22	0.72
32:1a:1158:C:H5	32:1a:1181:G:H1	1.36	0.72
1:1A:217:G:OP2	60:1A:4107:HOH:O	2.06	0.72
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.71	0.72
16:1U:33:ARG:NH1	60:1U:301:HOH:O	2.22	0.72
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.23	0.72
32:2a:501:C:OP1	43:2l:117:ARG:NH2	2.22	0.72
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.71	0.72
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.22	0.72
1:1A:1143:A:OP1	9:1N:25:ARG:NH2	2.22	0.72
1:1A:376:C:OP1	60:1A:4108:HOH:O	2.06	0.72
26:24:59:PHE:HA	26:24:60:GLN:C	2.15	0.72
3:1D:108:PRO:HD2	3:1D:111:LEU:HG	1.70	0.72
1:2A:2128:C:H42	1:2A:2160:G:H1	1.38	0.72
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.72	0.72
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.71	0.71
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1647:G:OP1	60:2A:3814:HOH:O	2.08	0.71
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.23	0.71
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.53	0.71
33:1b:15:VAL:HG21	33:1b:213:LEU:HD13	1.72	0.71
1:2A:989:G:O2'	60:2A:3813:HOH:O	2.07	0.71
2:2B:66:A:H61	2:2B:109:C:H5'	1.55	0.71
1:1A:2499:C:OP1	60:1A:4109:HOH:O	2.08	0.71
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.24	0.71
12:2Q:75:THR:HG21	12:2Q:87:LYS:HE3	1.71	0.71
21:2Z:144:LEU:HD21	21:2Z:150:LEU:HD13	1.70	0.71
19:1X:76:ARG:NH1	60:1X:101:HOH:O	2.24	0.71
1:2A:2099:U:H3	1:2A:2190:G:H1	1.38	0.71
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.24	0.71
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.72	0.71
1:2A:963:U:OP2	60:2A:3809:HOH:O	2.09	0.71
36:2e:102:ALA:HB1	36:2e:106:PRO:HG2	1.73	0.71
57:1F:320:ARG:N	60:1F:401:HOH:O	2.24	0.71
32:2a:1360:A:OP2	45:2n:35:ARG:NH2	2.24	0.71
32:1a:964:A:OP1	60:1a:1901:HOH:O	2.09	0.71
33:2b:8:LYS:HG2	33:2b:9:GLU:H	1.56	0.70
1:1A:2133:G:H3'	1:1A:2157:G:H21	1.55	0.70
35:1d:155:LEU:HB3	35:1d:158:ILE:HG12	1.72	0.70
32:1a:656:C:O2'	46:1o:28:GLN:NE2	2.25	0.70
1:2A:2615:U:OP1	60:2A:3815:HOH:O	2.09	0.70
8:2I:72:LEU:HA	8:2I:75:LEU:HD22	1.73	0.70
32:2a:980:C:OP2	60:2a:3205:HOH:O	2.10	0.70
25:13:8:LEU:HD13	25:13:31:LEU:HD23	1.74	0.70
40:2i:40:LEU:HD11	40:2i:70:LYS:HD2	1.73	0.70
47:1p:53:VAL:HG13	47:1p:79:VAL:HG12	1.73	0.70
32:2a:1189:C:O2	60:2a:3204:HOH:O	2.09	0.70
1:1A:521:G:O6	60:1A:4111:HOH:O	2.09	0.69
1:1A:1023:U:OP2	60:1A:4112:HOH:O	2.10	0.69
35:1d:172:PRO:HB2	35:1d:187:ARG:HH21	1.56	0.69
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.74	0.69
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.56	0.69
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.74	0.69
33:2b:8:LYS:HG3	33:2b:48:MET:HG2	1.74	0.69
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.08	0.69
32:2a:573:A:OP2	60:2a:3206:HOH:O	2.10	0.69
1:1A:1173:G:O2'	1:1A:1174:A:O5'	2.10	0.69
32:1a:992:U:H4'	32:1a:993:G:H5'	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.72	0.69
42:1k:99:GLN:HG2	42:1k:105:VAL:HG21	1.74	0.69
1:2A:2499:C:OP1	60:2A:3816:HOH:O	2.09	0.69
32:2a:656:C:O2'	46:2o:28:GLN:NE2	2.24	0.69
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.23	0.69
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.75	0.69
1:2A:827:U:OP1	60:2A:3817:HOH:O	2.10	0.69
1:1A:1315:C:OP2	60:1A:4114:HOH:O	2.11	0.69
32:1a:1047:G:OP1	45:1n:4:LYS:NZ	2.21	0.69
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.25	0.69
1:1A:1071:G:N7	60:1A:4191:HOH:O	2.26	0.69
35:1d:15:GLU:OE2	35:1d:66:ARG:NH1	2.26	0.69
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.75	0.69
1:2A:511:U:OP2	60:2A:3801:HOH:O	2.09	0.69
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.10	0.69
1:2A:2732:G:O6	60:2A:3819:HOH:O	2.11	0.69
33:1b:63:MET:HG3	33:1b:225:ALA:HB1	1.75	0.69
14:2S:21:THR:HG23	14:2S:23:ARG:H	1.58	0.69
32:2a:402:G:N7	60:2a:3229:HOH:O	2.25	0.69
1:1A:2427:C:OP1	60:1A:4115:HOH:O	2.11	0.68
1:1A:2822:G:OP2	60:1A:4110:HOH:O	2.09	0.68
1:2A:1271:G:OP2	60:2A:3814:HOH:O	2.11	0.68
32:1a:1189:C:OP1	41:1j:51:ARG:NH2	2.26	0.68
44:1m:12:ASN:O	44:1m:44:ARG:NH1	2.26	0.68
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.76	0.68
5:1F:197:ASP:N	5:1F:197:ASP:OD1	2.26	0.68
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.26	0.68
32:2a:1086:U:H3	32:2a:1099:G:H22	1.41	0.68
3:2D:237:GLU:OE2	60:2D:401:HOH:O	2.12	0.68
4:2E:119:ARG:HD3	4:2E:160:TYR:HB2	1.76	0.68
32:1a:1025:U:O2	32:1a:1036:G:O6	2.11	0.68
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.76	0.68
32:2a:117:G:OP2	60:2a:3207:HOH:O	2.11	0.68
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.74	0.68
1:1A:1779:U:OP2	60:1A:4118:HOH:O	2.12	0.68
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	1.74	0.68
49:2r:26:LEU:HD21	49:2r:42:ARG:HD3	1.76	0.67
1:2A:2430:A:OP2	60:2A:3817:HOH:O	2.12	0.67
1:2A:2448:A:OP1	60:2A:3816:HOH:O	2.13	0.67
6:1G:139:LEU:HD21	6:1G:149:VAL:HG11	1.77	0.67
1:1A:1648:C:OP1	60:1A:4105:HOH:O	2.11	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2447:G:OP2	60:1A:4113:HOH:O	2.11	0.67
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.77	0.67
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.76	0.67
1:1A:1024:G:OP2	60:1A:4112:HOH:O	2.12	0.67
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.26	0.67
39:1h:95:VAL:HB	39:1h:99:GLU:HG3	1.76	0.67
1:2A:731:C:OP1	60:2A:3822:HOH:O	2.12	0.67
1:2A:745:G:O6	60:2A:3818:HOH:O	2.10	0.67
1:2A:1050:A:H2'	1:2A:1051:G:H8	1.60	0.67
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.26	0.67
11:2P:29:LYS:HD3	11:2P:30:THR:HG23	1.76	0.67
34:2c:155:GLY:HA3	34:2c:196:LEU:HD12	1.75	0.67
41:2j:62:HIS:HB3	45:2n:59:ALA:HB3	1.76	0.67
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.13	0.67
1:2A:2706:G:N7	60:2A:3917:HOH:O	2.28	0.67
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.77	0.67
1:2A:2429:G:OP1	60:2A:3806:HOH:O	2.13	0.67
32:2a:1030:C:N3	32:2a:1031:G:N2	2.43	0.67
1:1A:749:C:OP2	60:1A:4117:HOH:O	2.12	0.67
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	1.75	0.67
40:1i:79:LEU:HD22	40:1i:104:ARG:HB2	1.76	0.67
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.77	0.67
1:2A:1364:G:OP2	23:21:3:LYS:HG3	1.95	0.67
44:2m:91:ARG:NE	44:2m:97:PRO:O	2.28	0.67
48:2q:67:LYS:O	48:2q:69:LYS:N	2.27	0.67
1:1A:1670:C:OP2	60:1A:4123:HOH:O	2.13	0.67
1:1A:1757:U:OP1	60:1A:4120:HOH:O	2.13	0.67
45:1n:24:CYS:HB3	45:1n:28:GLY:H	1.60	0.67
1:2A:740:U:OP2	60:2A:3826:HOH:O	2.13	0.67
1:2A:805:G:OP1	60:2A:3824:HOH:O	2.13	0.66
1:2A:1993:U:OP2	60:2A:3828:HOH:O	2.14	0.66
35:2d:166:LYS:HE2	35:2d:167:GLY:N	2.08	0.66
1:2A:2006:C:OP2	60:2A:3827:HOH:O	2.13	0.66
2:2B:49:C:OP1	60:2B:301:HOH:O	2.13	0.66
32:2a:977:A:N6	32:2a:1224:G:OP1	2.28	0.66
1:1A:1358:G:OP2	60:1A:4121:HOH:O	2.13	0.66
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.27	0.66
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.77	0.66
51:2t:50:GLU:HB2	51:2t:99:LEU:HD12	1.77	0.66
1:2A:62:C:OP1	60:2A:3821:HOH:O	2.12	0.66
1:2A:526:A:OP1	60:2A:3823:HOH:O	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:187:ARG:NH2	35:2d:193:ASP:OD2	2.29	0.66
18:1W:17:VAL:HG12	18:1W:76:VAL:HG21	1.78	0.66
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.78	0.66
1:2A:2610:C:O2'	60:2A:3820:HOH:O	2.12	0.66
6:2G:55:LYS:HA	6:2G:58:GLN:HB3	1.77	0.66
32:1a:166:G:H2'	32:1a:167:G:H8	1.61	0.66
1:2A:2377:A:N6	60:2A:3914:HOH:O	2.28	0.66
2:2B:75:G:N2	60:2B:306:HOH:O	2.28	0.66
42:2k:117:ASN:N	42:2k:117:ASN:OD1	2.29	0.66
1:2A:2139:C:N4	1:2A:2152:G:H1	1.92	0.66
33:2b:164:VAL:HG13	33:2b:186:ALA:HB2	1.76	0.66
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.76	0.66
40:2i:29:ASN:HD21	40:2i:65:VAL:H	1.43	0.66
1:1A:220:G:O6	60:1A:4116:HOH:O	2.11	0.66
32:1a:35:G:O2'	43:1l:118:SER:O	2.11	0.66
1:2A:1840:G:OP2	60:2A:3829:HOH:O	2.14	0.66
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.61	0.66
1:1A:2116:G:OP2	1:1A:2166:G:N2	2.29	0.66
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.28	0.66
1:1A:1865:G:OP1	60:1A:4125:HOH:O	2.14	0.66
26:24:46:GLN:O	26:24:48:ARG:N	2.26	0.66
32:1a:324:G:N7	60:1a:1925:HOH:O	2.28	0.65
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.29	0.65
2:1B:81:G:N7	57:1B:230:ARG:NH2	2.38	0.65
18:1W:18:ARG:NH1	18:1W:76:VAL:O	2.29	0.65
32:1a:803:G:OP1	60:1a:1902:HOH:O	2.13	0.65
44:1m:65:LYS:HE2	44:1m:69:GLU:HG2	1.78	0.65
1:2A:1971:A:OP1	60:2A:3825:HOH:O	2.13	0.65
32:2a:1005:A:OP2	32:2a:1024:G:N2	2.30	0.65
1:1A:1756:G:OP2	60:1A:4119:HOH:O	2.13	0.65
32:1a:117:G:N7	60:1a:1927:HOH:O	2.29	0.65
40:1i:17:VAL:HG21	40:1i:81:ILE:HG22	1.79	0.65
1:2A:2139:C:H42	1:2A:2152:G:H1	1.43	0.65
34:2c:109:PRO:HB3	34:2c:115:LEU:HD23	1.78	0.65
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.61	0.65
1:2A:493:G:OP2	60:2A:3835:HOH:O	2.15	0.65
1:2A:1023:U:OP2	60:2A:3833:HOH:O	2.15	0.65
32:2a:617:G:OP2	60:2a:3208:HOH:O	2.13	0.65
20:1Y:28:LYS:HG3	20:1Y:40:GLU:HG2	1.77	0.65
34:1c:11:ARG:HB3	34:1c:15:THR:HB	1.76	0.65
36:1e:50:GLU:HB2	36:1e:53:LEU:HD13	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:59:PHE:HB2	26:24:62:ARG:HH21	1.62	0.65
11:1P:141:ALA:HA	25:23:38:GLU:HG2	1.77	0.65
40:1i:121:ARG:NH1	40:1i:122:ALA:O	2.28	0.65
47:1p:75:ARG:HG3	47:1p:80:PHE:HD2	1.61	0.65
1:2A:1075:C:H2'	1:2A:1076:C:H5'	1.78	0.65
1:1A:219:G:OP2	60:1A:4124:HOH:O	2.13	0.65
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.11	0.65
1:2A:2107:C:N4	1:2A:2182:G:H1	1.95	0.65
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.77	0.65
36:1e:8:GLU:HG2	36:1e:34:VAL:HG23	1.78	0.65
1:2A:1153:C:OP2	60:2A:3832:HOH:O	2.15	0.65
1:1A:1332:G:OP1	60:1A:4114:HOH:O	2.14	0.65
32:1a:405:U:O4	35:1d:2:GLY:N	2.30	0.65
44:1m:37:THR:O	44:1m:55:ARG:NH1	2.26	0.65
23:11:52:ARG:NH2	23:11:55:GLY:O	2.29	0.64
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.24	0.64
1:2A:1332:G:OP1	60:2A:3812:HOH:O	2.14	0.64
1:1A:135:G:N7	60:1A:4220:HOH:O	2.30	0.64
1:1A:271(Q):G:O6	60:1A:4122:HOH:O	2.13	0.64
1:1A:365:C:OP2	60:1A:4129:HOH:O	2.14	0.64
1:1A:2743:C:OP1	31:19:33:LYS:NZ	2.30	0.64
11:1P:42:SER:O	60:1P:301:HOH:O	2.15	0.64
1:2A:1076:C:H4'	1:2A:1077:A:OP1	1.96	0.64
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.30	0.64
1:1A:249:C:O2'	11:1P:64:LYS:NZ	2.19	0.64
1:1A:1340:U:OP1	19:1X:16:LYS:NZ	2.30	0.64
1:1A:2683:C:OP1	15:1T:53:ARG:NH2	2.31	0.64
1:1A:1026:U:OP1	60:1A:4112:HOH:O	2.14	0.64
1:1A:2639:A:OP2	60:1A:4128:HOH:O	2.14	0.64
32:1a:189(K):U:H2'	32:1a:189(L):G:H8	1.62	0.64
1:2A:2100:G:H1	1:2A:2189:U:H3	1.43	0.64
32:2a:427:U:OP1	35:2d:13:ARG:NH2	2.30	0.64
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.32	0.64
1:2A:1814:G:OP1	60:2A:3834:HOH:O	2.15	0.64
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.79	0.64
1:1A:2049:G:N7	60:1A:4227:HOH:O	2.30	0.64
39:1h:86:ILE:HG13	39:1h:133:LEU:HD22	1.79	0.64
1:2A:1006:C:OP2	60:2A:3830:HOH:O	2.14	0.64
1:2A:2406:U:OP1	60:2A:3831:HOH:O	2.14	0.64
32:2a:35:G:O2'	43:2l:118:SER:O	2.15	0.64
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:812:C:N3	60:1a:1930:HOH:O	2.29	0.64
1:2A:1041:C:H42	1:2A:1114:G:H1	1.44	0.64
11:2P:54:GLY:O	60:2P:201:HOH:O	2.15	0.64
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.78	0.64
1:1A:2137:C:N4	1:1A:2154:G:H1	1.95	0.64
1:2A:2526:G:O6	60:2A:3836:HOH:O	2.15	0.64
23:21:31:GLY:O	60:21:201:HOH:O	2.15	0.64
1:1A:2126:A:H4'	1:1A:2127:G:O5'	1.97	0.64
15:1T:56:GLY:O	15:1T:59:THR:HG23	1.98	0.64
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.78	0.64
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.31	0.64
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.80	0.64
52:2u:17:THR:O	52:2u:22:ARG:NH1	2.29	0.63
32:1a:1025:U:C2	32:1a:1036:G:O6	2.51	0.63
32:2a:954:G:H21	32:2a:1227:A:H62	1.46	0.63
1:1A:2448:A:OP1	60:1A:4109:HOH:O	2.16	0.63
38:1g:27:ILE:HD12	38:1g:40:ALA:HA	1.81	0.63
1:2A:641:C:O2'	1:2A:2350:C:OP1	2.14	0.63
1:2A:2049:G:N7	60:2A:3946:HOH:O	2.30	0.63
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.31	0.63
32:2a:1141:C:H2'	32:2a:1142:G:H8	1.63	0.63
20:1Y:23:ARG:NH1	60:1Y:602:HOH:O	2.31	0.63
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.29	0.63
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.98	0.63
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.29	0.63
32:1a:596:C:OP2	60:1a:1903:HOH:O	2.15	0.63
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.80	0.63
32:1a:953:G:N7	44:1m:104:ARG:NH2	2.45	0.63
1:2A:2128:C:N4	1:2A:2160:G:H1	1.97	0.63
32:2a:36:C:OP1	43:2l:123:LYS:NZ	2.32	0.63
33:2b:93:VAL:HG11	33:2b:101:MET:HE1	1.79	0.63
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.64	0.63
1:2A:2602:A:H4'	1:2A:2603:G:OP1	1.99	0.63
32:2a:1222:G:O6	60:2a:3205:HOH:O	2.14	0.63
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.34	0.63
32:1a:946:A:H2'	32:1a:947:G:C8	2.34	0.63
50:2s:18:LYS:HA	50:2s:21:GLU:HB2	1.80	0.63
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.33	0.63
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.32	0.63
1:2A:1761:C:N3	60:2A:3950:HOH:O	2.31	0.63
50:2s:41:VAL:HG12	50:2s:44:MET:HG3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.80	0.62
44:2m:81:LEU:HD13	44:2m:88:ARG:HD2	1.81	0.62
2:1B:59:A:N6	60:1B:301:HOH:O	2.25	0.62
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.81	0.62
50:1s:18:LYS:HD3	50:1s:31:ILE:HD12	1.79	0.62
1:2A:1062:G:HO2'	1:2A:1063:G:H8	1.46	0.62
1:1A:1356:G:OP1	60:1A:4130:HOH:O	2.15	0.62
32:1a:187:C:H5''	51:1t:86:ARG:HD2	1.81	0.62
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.81	0.62
8:2I:92:VAL:HG23	8:2I:120:ILE:HB	1.81	0.62
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.32	0.62
1:1A:1203:G:O6	60:1A:4127:HOH:O	2.14	0.62
32:1a:612:C:O2	32:1a:629:G:N2	2.32	0.62
36:1e:100:VAL:O	36:1e:107:ARG:NH2	2.32	0.62
1:2A:2126:A:H4'	1:2A:2127:G:O5'	1.98	0.62
34:2c:6:HIS:HD2	34:2c:9:GLY:H	1.45	0.62
40:2i:42:ARG:NH1	40:2i:71:SER:O	2.33	0.62
1:2A:1762:A:N1	60:2A:3953:HOH:O	2.31	0.62
1:1A:942:G:O6	60:1A:4131:HOH:O	2.15	0.62
1:2A:2105:C:N4	1:2A:2106:G:O6	2.32	0.62
32:2a:1126:U:H3	41:2j:40:LEU:HD21	1.64	0.62
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.65	0.62
1:1A:1173:G:OP2	60:1A:4133:HOH:O	2.16	0.62
32:1a:1016:A:OP1	45:1n:15:LYS:NZ	2.30	0.62
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	1.81	0.62
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.82	0.62
39:2h:121:ASP:OD1	39:2h:121:ASP:N	2.33	0.62
1:1A:1542:A:O2'	60:1A:4134:HOH:O	2.16	0.62
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.82	0.62
28:16:13:CYS:SG	28:16:47:THR:HG21	2.39	0.62
1:2A:1064:C:H3'	1:2A:1065:U:H5'	1.81	0.62
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.81	0.62
51:1t:33:ILE:O	51:1t:37:SER:OG	2.18	0.62
32:2a:548:G:OP1	60:2a:3209:HOH:O	2.16	0.62
26:14:57:GLU:HB2	26:14:58:ARG:HA	1.82	0.62
32:1a:160:A:H2'	32:1a:161:A:O4'	2.00	0.62
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.64	0.62
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.82	0.62
34:2c:8:ILE:HD12	34:2c:16:ARG:HD2	1.81	0.62
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.81	0.61
33:1b:10:LEU:HA	33:1b:48:MET:HE1	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.33	0.61
1:1A:2763:G:OP2	60:1A:4132:HOH:O	2.15	0.61
32:1a:1179:A:OP2	40:1i:93:ARG:NH2	2.33	0.61
33:1b:123:ALA:O	33:1b:124:SER:HB2	2.00	0.61
34:1c:154:SER:HB3	34:1c:165:THR:HG22	1.82	0.61
1:2A:2453:A:OP1	60:2A:3839:HOH:O	2.16	0.61
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.83	0.61
7:2H:9:ILE:HB	7:2H:50:VAL:HG23	1.81	0.61
32:2a:662:G:H2'	32:2a:663:A:C8	2.36	0.61
32:2a:673:G:H2'	32:2a:674:G:C8	2.35	0.61
33:2b:63:MET:HG2	33:2b:225:ALA:HB1	1.81	0.61
39:2h:9:MET:HG3	39:2h:26:VAL:HG11	1.82	0.61
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.81	0.61
1:2A:1754:C:P	15:2T:96:ARG:HH12	2.23	0.61
11:1P:94:GLU:HG3	11:1P:124:LYS:HD3	1.81	0.61
6:2G:105:LYS:NZ	6:2G:143:GLU:OE2	2.30	0.61
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.82	0.61
20:2Y:83:THR:HG21	20:2Y:99:CYS:HB2	1.81	0.61
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.82	0.61
19:1X:60:ARG:HH22	29:17:47:ARG:HH12	1.47	0.61
35:1d:167:GLY:H	35:1d:168:ARG:NH1	1.99	0.61
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.32	0.61
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.83	0.61
1:2A:336:C:HO2'	20:2Y:35:TYR:HH	1.48	0.61
38:1g:111:ARG:NH1	38:1g:113:GLU:OE2	2.29	0.61
32:2a:406:G:H4'	35:2d:5:ILE:HD11	1.83	0.61
36:2e:12:LEU:HD12	36:2e:128:PRO:HB2	1.82	0.61
1:1A:1647:G:OP1	60:1A:4105:HOH:O	2.16	0.61
4:1E:28:ALA:HB3	4:1E:93:VAL:HG13	1.83	0.61
32:2a:1071:C:H2'	32:2a:1072:G:H8	1.65	0.61
42:2k:62:GLN:HB2	42:2k:93:GLN:HG3	1.82	0.61
1:1A:870:A:OP1	12:1Q:6:ARG:NH1	2.34	0.61
1:2A:1064:C:H3'	1:2A:1065:U:C5'	2.30	0.61
1:2A:1065:U:H4'	1:2A:1066:U:H5'	1.83	0.61
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.33	0.60
1:2A:1062:G:C5	1:2A:1070:A:H1'	2.36	0.60
34:2c:73:PRO:HB3	34:2c:103:VAL:HG11	1.81	0.60
37:2f:35:ALA:HB2	37:2f:67:MET:HE2	1.81	0.60
1:1A:335:C:H4'	20:1Y:73:ARG:HD2	1.83	0.60
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.84	0.60
1:2A:965:C:OP2	60:2A:3838:HOH:O	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.36	0.60
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.66	0.60
34:2c:181:ASN:N	34:2c:205:GLY:O	2.34	0.60
1:1A:11:G:H2'	1:1A:12:U:H5'	1.83	0.60
10:1O:107:ARG:HG3	10:1O:112:MET:HE1	1.83	0.60
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.33	0.60
1:2A:1568:G:N7	60:2A:3952:HOH:O	2.31	0.60
32:2a:1030:C:N4	32:2a:1031:G:N1	2.48	0.60
36:2e:50:GLU:HB2	36:2e:53:LEU:HD13	1.82	0.60
40:1i:8:GLY:HA2	40:1i:79:LEU:HD23	1.84	0.60
1:2A:2152:G:H2'	1:2A:2153:G:C8	2.36	0.60
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.67	0.60
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.34	0.60
32:2a:1003:G:H3'	32:2a:1003:G:N3	2.17	0.60
24:12:59:ARG:NH2	60:12:102:HOH:O	2.34	0.60
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.35	0.60
6:2G:39:ILE:HG21	6:2G:60:LEU:HD11	1.84	0.60
15:2T:39:ARG:NH2	32:2a:345:C:OP2	2.31	0.60
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.30	0.60
1:1A:489:G:N7	18:1W:49:LYS:NZ	2.49	0.60
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.17	0.60
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.83	0.60
48:1q:67:LYS:O	48:1q:69:LYS:N	2.33	0.60
1:2A:956:G:H5''	12:2Q:77:LYS:HD2	1.84	0.60
9:2N:21:LYS:NZ	9:2N:140:VAL:OXT	2.34	0.60
26:24:14:ILE:HD11	26:24:24:THR:HG21	1.84	0.60
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.82	0.60
32:1a:1202:G:N2	45:1n:46:GLU:OE2	2.35	0.60
1:2A:1057:A:N6	1:2A:1087:G:OP1	2.35	0.60
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.66	0.60
23:21:76:ARG:HH22	23:21:97:LEU:HB3	1.67	0.60
32:2a:67:C:H2'	32:2a:68:G:C8	2.37	0.60
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.17	0.60
1:1A:2130:U:O2'	1:1A:2133:G:O2'	2.19	0.60
4:1E:77:ILE:HD13	4:1E:195:LEU:HD13	1.82	0.60
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.32	0.60
32:1a:1069:C:OP2	60:1a:1904:HOH:O	2.15	0.60
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.32	0.60
1:2A:2582:G:OP2	60:2A:3840:HOH:O	2.17	0.60
16:2U:5:LYS:NZ	60:2U:202:HOH:O	2.33	0.60
1:1A:987:G:O2'	1:1A:1000:A:N3	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1702:G:N7	60:1A:4247:HOH:O	2.32	0.60
1:1A:2719:G:OP2	60:1A:4135:HOH:O	2.17	0.60
3:1D:88:ARG:NH1	60:1D:402:HOH:O	2.24	0.60
43:1l:33:ARG:HE	43:1l:62:SER:HB3	1.67	0.60
1:2A:1014:U:H2'	1:2A:1015:G:H8	1.67	0.60
14:2S:35:ILE:H	14:2S:53:SER:HB3	1.66	0.60
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.83	0.60
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.84	0.59
46:1o:82:ILE:HD12	46:1o:88:ARG:HB2	1.84	0.59
49:1r:51:LEU:HD22	49:1r:55:ARG:HE	1.67	0.59
32:2a:289:G:OP2	60:2a:3207:HOH:O	2.16	0.59
1:1A:784:A:H5'	1:1A:785:G:OP1	2.02	0.59
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.36	0.59
6:1G:59:GLU:OE1	6:1G:153:ARG:NH2	2.32	0.59
15:1T:51:ARG:HG3	15:1T:98:LYS:HE3	1.84	0.59
33:1b:21:ARG:HA	33:1b:39:ILE:HA	1.84	0.59
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.84	0.59
1:1A:1470:G:N2	1:1A:1520:G:OP2	2.27	0.59
32:1a:1145:C:H4'	32:1a:1146:A:H5''	1.84	0.59
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.18	0.59
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.85	0.59
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.35	0.59
40:2i:53:VAL:O	40:2i:55:ALA:N	2.35	0.59
32:1a:560:U:O2'	32:1a:561:U:OP2	2.19	0.59
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.02	0.59
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.36	0.59
32:1a:1360:A:OP2	45:1n:35:ARG:NH2	2.36	0.59
32:1a:1495:U:OP1	53:1y:23:ARG:NH2	2.31	0.59
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.84	0.59
1:2A:387:U:OP1	60:2A:3837:HOH:O	2.16	0.59
1:2A:1830:C:OP2	60:2A:3841:HOH:O	2.17	0.59
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.37	0.59
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.83	0.59
1:1A:1721:G:H8	1:1A:1741:A:H62	1.49	0.59
51:1t:38:LYS:HA	51:1t:41:ILE:HB	1.85	0.59
6:2G:19:LEU:HD13	6:2G:32:PRO:HD2	1.83	0.59
50:2s:22:LEU:HD13	50:2s:28:LYS:H	1.68	0.59
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.36	0.59
1:1A:2852:G:N7	60:1A:4248:HOH:O	2.32	0.59
32:1a:1103:C:OP1	33:1b:96:ARG:NH2	2.36	0.59
1:2A:1094:U:OP1	1:2A:1096:A:N6	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1291:G:H4'	40:2i:39:GLY:HA3	1.85	0.59
34:2c:6:HIS:CD2	34:2c:9:GLY:H	2.20	0.59
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.38	0.59
1:1A:958:U:H5''	12:1Q:14:ARG:HD3	1.84	0.59
1:1A:2167:U:H2'	1:1A:2168:G:C8	2.38	0.59
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.36	0.59
1:2A:979:G:N7	60:2A:3862:HOH:O	2.32	0.59
1:2A:2206:G:H8	1:2A:2207:G:N7	2.01	0.59
32:1a:973:G:H3'	32:1a:974:A:H5''	1.85	0.58
1:2A:1087:G:H22	1:2A:1102:C:H42	1.50	0.58
1:2A:2218:U:O4'	23:21:52:ARG:NH2	2.36	0.58
24:22:9:GLN:HE22	24:22:56:GLN:HB3	1.67	0.58
25:23:13:ILE:O	60:23:201:HOH:O	2.17	0.58
32:2a:992:U:H4'	32:2a:993:G:O5'	2.02	0.58
1:1A:1030:G:OP1	60:1A:4138:HOH:O	2.17	0.58
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.38	0.58
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.36	0.58
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.37	0.58
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.51	0.58
32:2a:1030(A):G:H1'	32:2a:1030(C):G:N7	2.17	0.58
32:2a:1047:G:H5''	45:2n:4:LYS:HD2	1.84	0.58
3:1D:69:ARG:HE	3:1D:130:ALA:HB2	1.67	0.58
35:1d:88:VAL:HA	36:1e:97:GLY:HA3	1.84	0.58
35:1d:140:VAL:HG11	35:1d:146:ILE:HD11	1.84	0.58
35:1d:166:LYS:HE3	35:1d:168:ARG:HH12	1.68	0.58
1:2A:764:A:H2	3:2D:219:PRO:HG3	1.67	0.58
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.36	0.58
32:2a:1221:G:OP1	32:2a:1320:C:N4	2.36	0.58
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.85	0.58
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.84	0.58
32:1a:814:A:OP2	60:1a:1906:HOH:O	2.17	0.58
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.85	0.58
51:1t:46:GLU:HG3	51:1t:48:LYS:HD2	1.83	0.58
1:2A:1009:A:OP2	60:2A:3842:HOH:O	2.17	0.58
32:1a:407:G:H5''	35:1d:115:ARG:HB3	1.85	0.58
32:1a:811:C:O2'	32:1a:901:A:N1	2.37	0.58
1:2A:1017:G:N7	60:2A:3957:HOH:O	2.32	0.58
21:2Z:9:TYR:HE2	21:2Z:61:LEU:HB3	1.67	0.58
32:1a:1003:G:C2	32:1a:1004:A:H1'	2.39	0.58
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.39	0.58
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1372:U:H5''	40:2i:71:SER:HB3	1.84	0.58
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.66	0.58
47:2p:15:PRO:HD2	47:2p:42:ARG:HD3	1.86	0.58
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.19	0.58
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.39	0.58
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.86	0.58
11:2P:59:LEU:HD21	30:28:10:ALA:HA	1.86	0.58
34:2c:63:ASN:HB2	34:2c:98:ASN:HB2	1.86	0.58
40:2i:14:VAL:HG23	40:2i:66:ARG:HB2	1.86	0.58
1:1A:889:C:O2'	1:1A:890:A:O5'	2.21	0.58
1:1A:1011:G:OP1	16:1U:77:SER:OG	2.20	0.58
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.86	0.58
1:2A:2640:G:O3'	9:2N:74:ARG:NH2	2.22	0.58
32:2a:1129:C:H42	32:2a:1143:G:H1	1.51	0.58
32:2a:1278:U:H5''	32:2a:1279:A:H5'	1.83	0.58
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.69	0.58
32:1a:965:A:OP2	53:1y:8:LYS:NZ	2.36	0.58
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.36	0.58
1:2A:668:G:H5'	1:2A:669:G:OP2	2.03	0.58
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.86	0.58
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.69	0.58
31:29:15:LYS:HE2	31:29:17:ILE:HD11	1.86	0.58
32:2a:1244:C:H2'	32:2a:1245:A:H8	1.69	0.58
1:1A:630:G:OP2	30:18:15:LYS:NZ	2.30	0.58
8:1I:77:LEU:HB3	8:1I:142:VAL:HG22	1.86	0.58
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.69	0.58
44:1m:49:THR:HG22	44:1m:51:ALA:H	1.69	0.58
5:2F:20:LEU:HD23	5:2F:21:ALA:H	1.68	0.58
23:21:86:SER:OG	23:21:89:GLU:OE1	2.14	0.58
33:2b:158:LEU:HD21	33:2b:180:LEU:HD13	1.85	0.58
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.85	0.57
35:1d:50:ARG:HH12	36:1e:10:MET:HE3	1.68	0.57
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	1.85	0.57
26:24:34:GLU:HG2	26:24:35:VAL:HG23	1.85	0.57
32:2a:13:U:OP1	60:2a:3210:HOH:O	2.17	0.57
35:2d:201:GLN:NE2	36:2e:116:THR:O	2.37	0.57
24:12:54:LYS:NZ	60:12:101:HOH:O	2.32	0.57
1:2A:2116:G:H3'	1:2A:2117:A:C8	2.39	0.57
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	1.86	0.57
41:2j:77:PRO:O	41:2j:81:THR:OG1	2.21	0.57
1:2A:154(A):C:H42	1:2A:171:G:H1	1.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.86	0.57
41:2j:47:PHE:HB3	45:2n:34:TYR:HE1	1.69	0.57
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.37	0.57
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG11	1.85	0.57
1:2A:1098:A:H3'	1:2A:1099:G:H8	1.69	0.57
6:2G:15:VAL:HA	6:2G:175:LEU:HD23	1.85	0.57
1:1A:762:U:OP1	60:1A:4140:HOH:O	2.17	0.57
38:1g:77:SER:OG	38:1g:86:GLN:NE2	2.37	0.57
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.86	0.57
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.20	0.57
13:2R:12:ARG:O	13:2R:17:ARG:NH1	2.38	0.57
47:2p:42:ARG:HB3	47:2p:44:THR:HG23	1.87	0.57
1:1A:1669:A:OP2	60:1A:4123:HOH:O	2.18	0.57
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.38	0.57
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.40	0.57
33:1b:74:LYS:NZ	33:1b:206:ASP:OD1	2.36	0.57
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.21	0.57
1:2A:1062:G:O2'	1:2A:1063:G:H5'	2.05	0.57
32:2a:1172:C:H2'	32:2a:1173:G:H8	1.69	0.57
39:2h:19:VAL:HG23	39:2h:21:LYS:HD3	1.87	0.57
1:1A:123:G:OP2	60:1A:4136:HOH:O	2.17	0.57
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.85	0.57
32:1a:1106:G:H5''	34:1c:172:ARG:HG3	1.87	0.57
42:1k:109:VAL:HG22	49:1r:86:VAL:HG22	1.87	0.57
50:1s:31:ILE:HB	50:1s:49:ILE:HG13	1.86	0.57
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.86	0.57
41:2j:78:ASN:O	41:2j:80:LYS:N	2.37	0.57
46:2o:55:GLY:HA2	46:2o:58:MET:HE3	1.84	0.57
1:1A:1082:U:N3	1:1A:1086:A:N6	2.19	0.57
1:1A:1395:A:OP1	60:1A:4139:HOH:O	2.17	0.57
32:1a:17:U:H2'	32:1a:18:C:C6	2.40	0.57
35:1d:109:GLY:HA3	35:1d:165:MET:HG3	1.86	0.57
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	1.86	0.57
1:2A:2319:G:N2	14:2S:3:ARG:HD3	2.13	0.57
21:2Z:10:ARG:NH1	21:2Z:26:GLY:O	2.37	0.57
33:2b:78:GLN:NE2	33:2b:95:GLN:OE1	2.37	0.57
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.86	0.57
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.86	0.57
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.38	0.57
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.40	0.57
1:2A:1111:A:C2	1:2A:1112:G:H1'	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2111:C:H42	1:2A:2147:G:H22	1.52	0.57
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.38	0.57
33:2b:80:ILE:HD13	33:2b:211:ILE:HG22	1.87	0.57
34:2c:111:LEU:HD22	34:2c:146:ALA:HB2	1.86	0.57
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.87	0.57
1:2A:2104:G:O6	1:2A:2185:C:N3	2.38	0.57
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.40	0.57
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.70	0.57
1:1A:811:U:OP1	60:1A:4137:HOH:O	2.17	0.56
7:1H:124:GLU:HG2	7:1H:132:ARG:HB3	1.86	0.56
32:1a:1326:C:OP1	52:1u:12:LYS:NZ	2.38	0.56
34:1c:29:TYR:OH	45:1n:54:PRO:O	2.23	0.56
47:1p:4:ILE:HG22	47:1p:19:ILE:HD11	1.86	0.56
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.87	0.56
32:2a:1129:C:N4	32:2a:1143:G:H1	2.03	0.56
1:2A:309:G:N3	1:2A:329:G:O2'	2.38	0.56
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.86	0.56
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.86	0.56
32:1a:67:C:H2'	32:1a:68:G:C8	2.40	0.56
32:1a:1003:G:C2'	32:1a:1004:A:H4'	2.32	0.56
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.39	0.56
40:1i:16:ARG:HB2	40:1i:64:THR:HG22	1.87	0.56
1:2A:446:G:OP1	16:2U:3:ARG:NH1	2.38	0.56
1:2A:476:G:OP1	60:2A:3845:HOH:O	2.18	0.56
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.05	0.56
1:2A:2431:U:OP1	60:2A:3843:HOH:O	2.17	0.56
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.32	0.56
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.86	0.56
26:24:59:PHE:HA	26:24:61:ARG:N	2.20	0.56
32:2a:501:C:H2'	32:2a:502:G:C8	2.40	0.56
32:2a:664:G:H22	32:2a:741:G:H1	1.53	0.56
32:2a:1187:G:H5'	40:2i:113:LYS:HE2	1.85	0.56
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.86	0.56
35:2d:173:TRP:CD1	35:2d:189:PRO:HG3	2.39	0.56
1:1A:330:A:H2	1:1A:1210:A:HO2'	1.52	0.56
50:1s:55:LYS:HG3	50:1s:56:GLN:HG2	1.87	0.56
1:2A:889:C:O2'	1:2A:890:A:O5'	2.24	0.56
52:2u:11:GLY:O	52:2u:15:ARG:HG3	2.06	0.56
1:1A:760:G:OP1	60:1A:4141:HOH:O	2.17	0.56
25:13:39:ASP:OD2	25:13:44:ARG:NH2	2.37	0.56
32:1a:79:G:H1	32:1a:90:U:H3	1.50	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2149:G:C2	1:2A:2150:U:H1'	2.41	0.56
2:2B:75:G:O3'	21:2Z:10:ARG:NH2	2.39	0.56
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.86	0.56
35:2d:61:LYS:NZ	35:2d:62:GLN:OE1	2.35	0.56
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.22	0.56
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.38	0.56
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.88	0.56
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.71	0.56
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.41	0.56
47:2p:21:VAL:HG21	47:2p:59:TRP:CD1	2.41	0.56
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.86	0.56
48:2q:82:MET:HA	48:2q:85:VAL:HG13	1.87	0.56
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.18	0.56
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.86	0.56
25:13:55:ARG:NH1	60:13:202:HOH:O	2.38	0.56
32:1a:574:A:OP2	60:1a:1908:HOH:O	2.18	0.56
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.88	0.56
1:2A:1912:A:OP1	60:2A:3846:HOH:O	2.18	0.56
6:2G:145:THR:HG22	6:2G:148:MET:HG2	1.88	0.56
11:2P:95:VAL:HG23	11:2P:125:VAL:HA	1.87	0.56
31:29:2:LYS:NZ	31:29:31:LYS:O	2.35	0.56
32:2a:978:A:O2'	32:2a:1322:C:N3	2.36	0.56
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.22	0.56
19:1X:54:VAL:HG22	19:1X:81:VAL:HG12	1.88	0.56
4:2E:13:ARG:HG2	15:2T:58:ASN:HD21	1.71	0.56
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.39	0.56
38:2g:111:ARG:HB2	38:2g:119:ARG:HD2	1.88	0.56
41:2j:7:LYS:HB2	41:2j:97:GLU:HB2	1.88	0.56
47:2p:43:LYS:HG2	47:2p:48:TRP:CD2	2.41	0.56
1:1A:1334:G:OP2	60:1A:4142:HOH:O	2.18	0.56
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.86	0.56
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.41	0.56
6:2G:112:PRO:HG3	26:24:43:TYR:HE2	1.70	0.56
51:2t:43:LEU:HD13	51:2t:51:GLU:HB3	1.88	0.56
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.88	0.55
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.87	0.55
41:1j:30:SER:OG	41:1j:84:GLN:NE2	2.39	0.55
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.87	0.55
1:2A:800:A:H8	1:2A:800:A:OP1	1.89	0.55
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.41	0.55
60:2A:3877:HOH:O	11:2P:37:GLY:HA3	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:85:LEU:HD13	11:2P:120:ALA:HB2	1.88	0.55
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.38	0.55
32:1a:1158:C:H5	32:1a:1181:G:N1	2.05	0.55
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.33	0.55
1:2A:1111:A:H2	1:2A:1112:G:H1'	1.72	0.55
32:2a:64:G:H4'	32:2a:65:U:H3'	1.88	0.55
1:1A:493:G:OP2	60:1A:4143:HOH:O	2.18	0.55
4:1E:127:ASP:OD2	60:1E:402:HOH:O	2.18	0.55
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.32	0.55
34:1c:15:THR:HG22	34:1c:16:ARG:HG3	1.89	0.55
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.87	0.55
4:2E:119:ARG:HG2	4:2E:120:TRP:CD1	2.42	0.55
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	1.87	0.55
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.71	0.55
4:1E:185:LYS:NZ	60:1E:405:HOH:O	2.40	0.55
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.39	0.55
36:2e:71:LEU:HD21	36:2e:115:VAL:HG22	1.88	0.55
32:1a:222:U:H2'	32:1a:223:U:C6	2.41	0.55
1:2A:1084:A:H3'	1:2A:1085:A:H4'	1.88	0.55
32:2a:222:U:H2'	32:2a:223:U:C6	2.41	0.55
32:2a:1092:A:H1'	32:2a:1183:A:H62	1.72	0.55
32:2a:1518:MA6:H93	32:2a:1519:MA6:H102	1.86	0.55
34:2c:6:HIS:NE2	34:2c:8:ILE:HB	2.22	0.55
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.41	0.55
32:1a:314:C:OP2	60:1a:1907:HOH:O	2.18	0.55
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.54	0.55
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.39	0.55
1:2A:2112:G:H2'	1:2A:2113:U:C6	2.41	0.55
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.40	0.55
33:2b:16:HIS:CG	33:2b:210:SER:HB3	2.42	0.55
1:1A:1364:G:N7	23:11:3:LYS:HE2	2.21	0.55
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.39	0.55
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.37	0.55
32:1a:1108:G:O6	60:1a:1905:HOH:O	2.17	0.55
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.40	0.55
9:2N:71:ILE:HG21	9:2N:84:LYS:HD3	1.89	0.55
34:2c:117:ALA:HB2	34:2c:200:ALA:HB2	1.89	0.55
37:2f:68:PRO:HB2	37:2f:71:ARG:HD2	1.88	0.55
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.89	0.55
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.72	0.55
32:1a:425:G:O3'	35:1d:45:GLN:NE2	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.22	0.55
37:1f:45:LEU:HD12	37:1f:59:TYR:HD1	1.72	0.55
44:1m:15:VAL:HG11	44:1m:48:LEU:HD21	1.87	0.55
1:2A:2180:U:H2'	1:2A:2181:G:C8	2.41	0.55
4:2E:127:ASP:OD2	60:2E:401:HOH:O	2.18	0.55
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.42	0.55
32:1a:437:U:H5'	35:1d:155:LEU:HD21	1.89	0.55
39:1h:39:LEU:HB3	39:1h:45:ILE:HG12	1.89	0.55
1:2A:1721:G:H8	1:2A:1741:A:H62	1.55	0.55
32:2a:986:A:N3	50:2s:52:TYR:OH	2.29	0.55
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	1.89	0.55
34:2c:6:HIS:HB3	45:2n:49:HIS:ND1	2.21	0.55
34:2c:67:THR:HG23	34:2c:102:ASN:HB2	1.88	0.55
44:2m:60:VAL:HG13	44:2m:64:TRP:HE3	1.71	0.55
1:1A:2526:G:N2	60:1A:4361:HOH:O	2.40	0.54
6:1G:66:GLN:NE2	6:1G:93:THR:O	2.33	0.54
32:1a:376:G:H4'	47:1p:5:ARG:HH11	1.72	0.54
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.36	0.54
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.42	0.54
32:2a:1027:C:H5''	32:2a:1028:C:C5	2.42	0.54
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.72	0.54
38:2g:46:ALA:HA	38:2g:49:ILE:HD12	1.88	0.54
32:1a:864:A:OP1	60:1a:1909:HOH:O	2.18	0.54
48:1q:58:GLU:OE2	48:1q:75:ARG:NH2	2.40	0.54
1:2A:1530:C:H42	1:2A:1539:G:H1	1.53	0.54
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.43	0.54
32:2a:937:A:OP2	60:2a:3212:HOH:O	2.18	0.54
38:2g:149:ARG:HD2	42:2k:59:TYR:CZ	2.42	0.54
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.40	0.54
32:1a:79:G:N2	32:1a:90:U:O2	2.40	0.54
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.91	0.54
41:1j:8:LEU:HB2	41:1j:70:ARG:HB2	1.89	0.54
7:2H:24:VAL:HG22	7:2H:35:VAL:HB	1.90	0.54
32:2a:411:A:OP2	35:2d:25:ARG:NH2	2.40	0.54
32:2a:1035:A:HO2'	32:2a:1036:G:H8	1.53	0.54
32:2a:1505:G:OP1	60:2a:3202:HOH:O	2.19	0.54
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.43	0.54
17:1V:21:ARG:NH1	17:1V:93:GLU:OE1	2.40	0.54
32:1a:1030(C):G:N7	32:1a:1031:G:N2	2.55	0.54
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.90	0.54
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.26	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:36:ARG:NH2	4:2E:88:GLY:O	2.40	0.54
6:2G:32:PRO:HB2	6:2G:172:LEU:HD22	1.89	0.54
13:2R:87:TYR:OH	13:2R:117:VAL:O	2.20	0.54
25:23:3:ARG:HG3	25:23:38:GLU:HA	1.89	0.54
32:2a:425:G:O3'	35:2d:45:GLN:NE2	2.32	0.54
32:2a:1005:A:H1'	32:2a:1025:U:N3	2.22	0.54
33:2b:111:ARG:HH11	33:2b:111:ARG:HA	1.73	0.54
44:2m:16:ASP:HB2	44:2m:27:LYS:HE3	1.90	0.54
1:1A:226:G:H21	1:1A:228:A:H62	1.55	0.54
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.07	0.54
22:10:10:THR:HG22	22:10:12:ASN:H	1.73	0.54
32:1a:396:G:O2'	32:1a:398:C:OP1	2.17	0.54
1:2A:7:G:H1	1:2A:2896:C:H42	1.56	0.54
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.41	0.54
3:2D:25:THR:HG21	3:2D:113:VAL:HG11	1.89	0.54
32:2a:677:U:H3	32:2a:713:G:H22	1.53	0.54
34:2c:188:LEU:HD11	34:2c:195:VAL:HB	1.90	0.54
32:1a:677:U:H3	32:1a:713:G:H22	1.55	0.54
1:2A:991:C:OP2	60:2A:3844:HOH:O	2.18	0.54
17:2V:1:MET:HE1	17:2V:44:LYS:H	1.72	0.54
38:2g:97:GLN:HE21	38:2g:101:LEU:HD11	1.72	0.54
1:1A:548:A:H61	17:1V:19:LYS:H	1.54	0.54
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.43	0.54
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.42	0.54
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.88	0.54
35:1d:156:GLU:O	35:1d:160:GLN:HG2	2.07	0.54
39:1h:116:LYS:HD2	39:1h:129:VAL:HG11	1.89	0.54
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	1.89	0.54
26:24:20:ASN:HD21	26:24:38:LYS:HD3	1.72	0.54
32:2a:134:A:N6	47:2p:25:ARG:HH22	2.05	0.54
35:2d:25:ARG:NH1	35:2d:30:LYS:O	2.41	0.54
50:2s:22:LEU:HD12	50:2s:31:ILE:HD11	1.89	0.54
1:1A:1252:G:N3	16:1U:33:ARG:HG2	2.23	0.54
32:1a:1005:A:O2'	32:1a:1037:C:O2'	2.26	0.54
32:1a:1030:C:N4	32:1a:1032:G:O6	2.40	0.54
53:1y:2:THR:OG1	53:1y:3:MET:N	2.40	0.54
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.39	0.54
35:2d:122:ARG:NH1	35:2d:134:ASP:O	2.41	0.54
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.42	0.54
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.43	0.54
1:2A:247:G:H4'	1:2A:386:G:C5	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2171:A:H4'	1:2A:2172:U:OP1	2.07	0.54
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.08	0.54
32:2a:644:G:H5'	39:2h:92:ARG:HH12	1.73	0.54
32:2a:931:C:H42	32:2a:1386:G:H1	1.55	0.54
40:2i:78:LYS:HA	40:2i:81:ILE:HG22	1.89	0.54
18:1W:4:LYS:NZ	60:1W:302:HOH:O	2.37	0.54
21:1Z:103:ARG:HD3	21:1Z:136:PHE:CG	2.43	0.54
24:12:16:LEU:O	24:12:67:LYS:NZ	2.41	0.54
32:1a:79:G:N1	32:1a:90:U:N3	2.52	0.54
32:1a:176:C:H2'	32:1a:177:C:H6	1.72	0.54
32:1a:1297:C:O2'	38:1g:114:ARG:NH1	2.38	0.54
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.88	0.54
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.73	0.54
1:2A:2155:G:C2	1:2A:2156:G:H1'	2.43	0.54
1:2A:2313:C:H4'	6:2G:91:ARG:HD3	1.90	0.54
26:24:62:ARG:O	26:24:64:GLY:N	2.41	0.54
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.43	0.54
48:2q:4:LYS:H	48:2q:61:GLU:HG2	1.72	0.54
1:1A:2508:G:OP1	60:1A:4144:HOH:O	2.18	0.53
26:14:16:CYS:HB3	26:14:20:ASN:HB3	1.89	0.53
32:1a:1135:U:H4'	32:1a:1136:U:H5	1.73	0.53
1:2A:2104:G:N7	1:2A:2186:G:N2	2.56	0.53
7:2H:95:ARG:HB2	7:2H:128:PRO:HB3	1.90	0.53
32:2a:273:A:H1'	48:2q:16:GLN:NE2	2.23	0.53
32:2a:975:A:N1	41:2j:48:THR:HB	2.23	0.53
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.43	0.53
1:1A:671:C:N4	60:1A:4375:HOH:O	2.41	0.53
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE2	1.90	0.53
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.89	0.53
51:1t:60:GLU:HG3	51:1t:81:LYS:HE3	1.89	0.53
1:2A:588:U:H2'	1:2A:589:C:C6	2.42	0.53
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.89	0.53
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.07	0.53
33:2b:8:LYS:H	33:2b:8:LYS:HD3	1.73	0.53
35:2d:78:LEU:HD22	35:2d:96:LEU:HB3	1.89	0.53
5:1F:12:LEU:HD22	5:1F:124:LEU:HD21	1.90	0.53
19:1X:60:ARG:NH2	29:17:47:ARG:HH12	2.06	0.53
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.90	0.53
32:2a:286:G:O6	60:2a:3211:HOH:O	2.17	0.53
32:2a:1291:G:OP1	38:2g:37:ASN:ND2	2.40	0.53
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:123:LEU:HD23	8:1I:144:VAL:HG12	1.91	0.53
26:14:7:PRO:HB2	26:14:27:THR:HG21	1.90	0.53
32:1a:411:A:OP1	35:1d:30:LYS:NZ	2.41	0.53
1:2A:370:G:OP2	1:2A:370:G:H8	1.92	0.53
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.42	0.53
21:2Z:54:HIS:HE2	21:2Z:123:ASP:HB3	1.74	0.53
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.41	0.53
32:2a:978:A:H61	32:2a:1316:G:H1'	1.72	0.53
32:2a:993:G:H2'	32:2a:995:C:H41	1.72	0.53
1:1A:1634:A:OP2	60:1A:4147:HOH:O	2.19	0.53
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.41	0.53
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.73	0.53
32:1a:262:A:H2'	32:1a:263:A:C8	2.44	0.53
32:1a:1414:U:H3	32:1a:1486:G:H1	1.56	0.53
8:2I:62:LYS:HG2	8:2I:133:HIS:NE2	2.23	0.53
32:2a:1244:C:H2'	32:2a:1245:A:C8	2.44	0.53
36:2e:80:ILE:HG22	36:2e:91:LEU:HB2	1.89	0.53
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.42	0.53
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.08	0.53
7:1H:27:LYS:HG2	7:1H:32:GLU:HG2	1.91	0.53
32:1a:142:G:O2'	32:1a:196:A:N1	2.40	0.53
32:1a:673:G:H2'	32:1a:674:G:C8	2.42	0.53
32:1a:1030(C):G:H2'	32:1a:1030(D):A:H8	1.72	0.53
39:1h:113:SER:HB2	39:1h:134:ILE:HD11	1.90	0.53
47:1p:57:ARG:HE	47:1p:79:VAL:HA	1.74	0.53
1:2A:1762:A:N6	60:2A:3950:HOH:O	2.41	0.53
5:2F:165:ARG:HA	5:2F:168:ARG:HD2	1.91	0.53
13:2R:45:ARG:NH2	60:2R:304:HOH:O	2.38	0.53
32:2a:17:U:H2'	32:2a:18:C:C6	2.43	0.53
32:2a:536:C:OP2	60:2a:3213:HOH:O	2.18	0.53
32:2a:748:C:H4'	32:2a:749:C:O5'	2.08	0.53
1:2A:1247:A:OP1	5:2F:95:ARG:NH2	2.39	0.53
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.73	0.53
3:2D:147:LEU:HD13	3:2D:155:LEU:HD21	1.91	0.53
10:2O:64:ARG:HB2	10:2O:79:PHE:CD2	2.43	0.53
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.44	0.53
33:2b:80:ILE:HD11	33:2b:212:GLN:HA	1.91	0.53
34:2c:70:VAL:HG22	34:2c:72:LYS:H	1.73	0.53
17:1V:21:ARG:HD3	17:1V:91:TYR:CD1	2.44	0.53
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.43	0.53
41:2j:53:PRO:O	45:2n:41:ARG:NH2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:65:LYS:HG2	44:2m:69:GLU:HB3	1.90	0.53
50:2s:31:ILE:HD12	50:2s:49:ILE:HD11	1.91	0.53
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.90	0.53
1:1A:1754:C:OP1	15:1T:96:ARG:NH1	2.41	0.53
3:1D:71:ASP:HB3	3:1D:103:ARG:HH22	1.74	0.53
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.42	0.53
1:2A:2319:G:N1	14:2S:3:ARG:HA	2.24	0.53
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.57	0.53
5:2F:164:ARG:O	5:2F:168:ARG:HG3	2.08	0.53
1:1A:2117:A:N6	1:1A:2171:A:N1	2.57	0.53
1:2A:2237:G:OP1	60:2A:3849:HOH:O	2.19	0.53
29:27:35:ARG:HG3	29:27:42:LEU:HD11	1.90	0.53
32:2a:539:A:OP2	43:2l:115:LYS:NZ	2.42	0.53
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.91	0.53
51:2t:57:ARG:HH22	51:2t:100:ILE:HD12	1.73	0.53
53:2y:52:ALA:HB2	53:2y:77:LEU:HD21	1.90	0.53
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.44	0.52
32:1a:1347:G:N2	32:1a:1373:G:H2'	2.24	0.52
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.42	0.52
46:2o:18:PHE:HB2	46:2o:19:PRO:HD2	1.91	0.52
1:1A:1300:U:H4'	1:1A:1301:A:H5'	1.91	0.52
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.25	0.52
32:1a:165:C:H2'	32:1a:166:G:C8	2.44	0.52
38:1g:115:ARG:HB2	38:1g:118:VAL:HG12	1.89	0.52
49:1r:37:VAL:HG22	49:1r:78:LEU:HB3	1.91	0.52
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.92	0.52
1:1A:813:U:H2'	1:1A:814:C:C6	2.44	0.52
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.44	0.52
1:2A:1067:A:H4'	1:2A:1068:G:OP2	2.09	0.52
32:2a:279:A:OP2	48:2q:95:TYR:OH	2.21	0.52
35:2d:57:ARG:NH2	35:2d:205:GLU:OE1	2.39	0.52
37:2f:30:LEU:HB3	37:2f:35:ALA:HB3	1.91	0.52
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.91	0.52
32:1a:890:G:O2'	32:1a:906:G:O6	2.20	0.52
35:1d:87:GLY:N	60:1d:402:HOH:O	2.38	0.52
1:2A:1087:G:H22	1:2A:1102:C:N4	2.07	0.52
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.91	0.52
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.44	0.52
32:2a:1054:C:H41	53:2y:46:GLN:HE21	1.56	0.52
1:1A:1068:G:O2'	1:1A:1096:A:O2'	2.12	0.52
1:1A:1086:A:H3'	1:1A:1086:A:N3	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2681:C:OP2	4:1E:109:LYS:NZ	2.37	0.52
2:1B:82:G:OP2	60:1B:302:HOH:O	2.19	0.52
36:1e:79:GLU:HG3	36:1e:93:PRO:HD2	1.92	0.52
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.42	0.52
32:2a:309:G:O2'	32:2a:607:A:N1	2.42	0.52
32:2a:407:G:OP1	35:2d:115:ARG:NH2	2.42	0.52
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.44	0.52
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.24	0.52
40:2i:92:TYR:HB3	40:2i:96:LEU:HD12	1.92	0.52
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.41	0.52
44:2m:13:LYS:O	44:2m:45:VAL:HG23	2.09	0.52
1:1A:41:C:OP2	60:1A:4148:HOH:O	2.19	0.52
1:1A:300:A:H2'	1:1A:334:C:H1'	1.90	0.52
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.45	0.52
15:1T:112:ARG:HG2	15:1T:115:ARG:HH21	1.75	0.52
32:1a:737:A:H2'	32:1a:738:C:C6	2.45	0.52
39:1h:14:ARG:O	39:1h:18:ARG:HG2	2.09	0.52
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.22	0.52
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.92	0.52
1:2A:2140:C:H2'	1:2A:2141:G:H8	1.74	0.52
1:2A:2184:G:N1	1:2A:2185:C:O2	2.42	0.52
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.09	0.52
6:2G:113:ARG:HD2	6:2G:140:ILE:HA	1.91	0.52
14:2S:93:LYS:HZ2	14:2S:95:HIS:HB2	1.74	0.52
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.44	0.52
33:2b:57:PHE:HE2	33:2b:185:ILE:HD11	1.75	0.52
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.44	0.52
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.45	0.52
20:1Y:92:ASN:N	20:1Y:92:ASN:HD22	2.07	0.52
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.25	0.52
33:1b:47:THR:HA	33:1b:202:PRO:HG2	1.92	0.52
35:1d:79:PHE:HE1	35:1d:204:ILE:HD13	1.74	0.52
32:2a:954:G:O6	44:2m:104:ARG:NH1	2.43	0.52
33:2b:50:GLU:O	33:2b:54:THR:N	2.28	0.52
33:2b:122:PHE:HA	33:2b:127:ILE:HG12	1.92	0.52
34:2c:22:TRP:HA	41:2j:93:GLY:HA2	1.91	0.52
41:2j:32:ALA:HB1	41:2j:33:GLN:HG2	1.91	0.52
14:1S:3:ARG:NH2	60:1S:204:HOH:O	2.42	0.52
14:1S:11:LYS:HG3	14:1S:91:PRO:HD3	1.90	0.52
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.42	0.52
32:1a:600:C:H2'	32:1a:601:C:H6	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.91	0.52
32:1a:1124:G:N7	32:1a:1145:C:O2'	2.41	0.52
37:1f:38:GLU:OE1	37:1f:64:GLN:NE2	2.41	0.52
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.74	0.52
7:2H:87:LEU:HD23	7:2H:164:TYR:HA	1.90	0.52
50:2s:10:PHE:HE2	50:2s:37:ARG:HD2	1.75	0.52
1:1A:307:G:H21	1:1A:330:A:H62	1.57	0.52
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.10	0.52
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.45	0.52
1:1A:2308:G:O2'	1:1A:2310:A:N7	2.38	0.52
3:1D:242:ARG:HD2	3:1D:246:PRO:HG3	1.91	0.52
4:1E:7:VAL:HG13	4:1E:27:LEU:HB3	1.92	0.52
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.34	0.52
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.16	0.52
32:2a:9:G:H2'	32:2a:10:A:H8	1.75	0.52
32:2a:546:G:OP1	35:2d:73:ARG:HG2	2.09	0.52
32:2a:1030(A):G:H21	32:2a:1030(C):G:H3'	1.74	0.52
32:2a:1492:A:H5''	43:2l:47:LYS:HD3	1.91	0.52
35:2d:166:LYS:HE2	35:2d:167:GLY:H	1.74	0.52
1:1A:1843:C:H5'	3:1D:253:GLN:NE2	2.25	0.52
32:1a:56:U:H2'	32:1a:57:G:C8	2.45	0.52
33:1b:88:ALA:HB2	33:1b:219:VAL:HG13	1.92	0.52
47:1p:71:ARG:HG3	47:1p:80:PHE:CE2	2.45	0.52
1:2A:2104:G:N7	1:2A:2186:G:C2	2.78	0.52
32:2a:1286:A:H2'	32:2a:1287:A:H4'	1.90	0.52
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.24	0.52
38:2g:132:GLY:O	38:2g:136:LYS:HG2	2.10	0.52
32:1a:1005:A:HO2'	32:1a:1037:C:HO2'	1.56	0.51
34:1c:17:ASP:O	34:1c:54:ARG:NH2	2.36	0.51
48:1q:67:LYS:C	48:1q:69:LYS:H	2.18	0.51
32:2a:1005:A:H1'	32:2a:1025:U:C2	2.45	0.51
1:1A:2314:C:H2'	1:1A:2315:G:C8	2.45	0.51
1:1A:2759:G:N7	60:1A:4276:HOH:O	2.34	0.51
3:1D:134:ARG:HG3	3:1D:135:PHE:CE1	2.45	0.51
25:13:59:VAL:HG23	25:13:60:GLU:HG2	1.92	0.51
40:1i:9:ARG:HG2	40:1i:14:VAL:HG13	1.92	0.51
1:2A:2104:G:N2	1:2A:2105:C:C4	2.77	0.51
6:2G:64:THR:HB	6:2G:94:LEU:HD11	1.92	0.51
32:2a:41:G:H2'	32:2a:42:G:C8	2.45	0.51
32:2a:1191:A:OP2	34:2c:3:ASN:ND2	2.44	0.51
39:2h:49:GLU:OE2	39:2h:62:TYR:OH	2.23	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:75:VAL:HG11	38:1g:144:MET:HG2	1.92	0.51
42:1k:34:ASP:OD1	42:1k:38:ASN:N	2.43	0.51
21:2Z:157:LEU:HB3	21:2Z:161:VAL:HG23	1.92	0.51
32:2a:328:C:H4'	32:2a:329:A:H5'	1.92	0.51
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.74	0.51
32:2a:1291:G:O2'	40:2i:38:GLN:OE1	2.28	0.51
1:1A:184:C:H2'	1:1A:185:U:C6	2.45	0.51
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.10	0.51
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.45	0.51
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.46	0.51
15:1T:85:LYS:NZ	15:1T:87:ASP:OD2	2.42	0.51
32:1a:100:C:H2'	32:1a:101:A:C8	2.45	0.51
33:1b:231:GLU:HB3	33:1b:232:PRO:CD	2.38	0.51
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.29	0.51
1:2A:1062:G:O2'	1:2A:1063:G:H8	1.93	0.51
7:2H:173:PRO:O	60:2H:201:HOH:O	2.19	0.51
24:22:1:MET:SD	24:22:56:GLN:NE2	2.83	0.51
26:24:14:ILE:HB	26:24:22:ILE:HD13	1.93	0.51
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.26	0.51
31:19:24:TYR:CE1	31:19:35:ARG:HG3	2.45	0.51
32:1a:838:G:H5'	32:1a:839:U:OP2	2.11	0.51
33:1b:19:HIS:NE2	33:1b:189:ASP:OD2	2.44	0.51
47:1p:43:LYS:HG2	47:1p:48:TRP:CE2	2.46	0.51
1:2A:1428:C:O2'	1:2A:1569:A:OP2	2.20	0.51
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.91	0.51
4:2E:178:GLU:CD	4:2E:178:GLU:H	2.18	0.51
7:2H:5:GLY:O	7:2H:65:HIS:NE2	2.43	0.51
7:2H:59:ARG:O	7:2H:63:SER:OG	2.28	0.51
12:2Q:58:PHE:O	12:2Q:60:ARG:N	2.40	0.51
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.10	0.51
3:1D:204:ILE:O	60:1D:401:HOH:O	2.19	0.51
4:1E:170:LEU:HB3	4:1E:184:VAL:HG22	1.93	0.51
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	1.91	0.51
26:14:61:ARG:HG3	26:14:62:ARG:H	1.76	0.51
32:1a:757:U:H2'	32:1a:758:G:O4'	2.11	0.51
32:1a:1492:A:H4'	32:1a:1493:A:C6	2.45	0.51
1:2A:1110:G:H1'	1:2A:1111:A:C8	2.45	0.51
1:2A:2550:G:OP1	60:2A:3847:HOH:O	2.19	0.51
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.92	0.51
33:2b:178:ARG:HH22	39:2h:74:PRO:HB3	1.76	0.51
1:1A:1378:A:OP1	29:17:10:ARG:NH2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2133:G:H1'	1:1A:2158:A:H2	1.75	0.51
1:1A:2791:C:H5'	1:1A:2893:G:N2	2.26	0.51
32:1a:715:A:H2'	32:1a:716:A:C8	2.46	0.51
32:1a:998:G:H2'	32:1a:999:C:C6	2.45	0.51
32:1a:1368:G:OP1	40:1i:111:ARG:NH2	2.42	0.51
1:2A:1648:C:OP1	60:2A:3814:HOH:O	2.19	0.51
32:2a:1108:G:H5'	34:2c:176:HIS:CD2	2.46	0.51
34:2c:131:ARG:HH11	34:2c:166:GLU:HG2	1.75	0.51
43:2l:49:ASN:ND2	43:2l:92:OTD:SB	2.82	0.51
1:1A:2790:A:H2'	1:1A:2790:A:N3	2.25	0.51
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.92	0.51
32:1a:309:G:O2'	32:1a:607:A:N1	2.41	0.51
32:2a:737:A:H2'	32:2a:738:C:C6	2.46	0.51
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.45	0.51
44:2m:95:GLY:O	44:2m:110:ARG:HG3	2.10	0.51
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.39	0.51
1:1A:1078:U:H4'	1:1A:1079:C:H5'	1.93	0.51
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.46	0.51
32:1a:161:A:N1	32:1a:347:G:O2'	2.38	0.51
32:1a:191:G:H1'	51:1t:103:GLY:HA3	1.92	0.51
56:1a:1878:MPD:H12	56:1a:1878:MPD:H52	1.93	0.51
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.76	0.51
47:1p:18:ARG:HD3	47:1p:35:LYS:HE2	1.92	0.51
48:1q:45:HIS:CD2	48:1q:65:ILE:HG12	2.46	0.51
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.25	0.51
1:2A:1066:U:O2'	1:2A:1068:G:OP2	2.28	0.51
1:2A:1566:A:OP1	3:2D:211:ARG:NH1	2.42	0.51
18:2W:18:ARG:HG3	18:2W:76:VAL:HB	1.93	0.51
33:2b:178:ARG:HH12	39:2h:68:ARG:HH22	1.58	0.51
1:1A:588:U:H2'	1:1A:589:C:C6	2.46	0.51
4:1E:66:HIS:O	60:1E:403:HOH:O	2.20	0.51
32:1a:1160:G:OP1	33:1b:133:LYS:NZ	2.44	0.51
32:1a:1221:G:OP1	32:1a:1320:C:N4	2.42	0.51
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.32	0.51
33:1b:87:ARG:HB2	33:1b:219:VAL:HG11	1.91	0.51
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.46	0.51
1:2A:510:C:OP1	60:2A:3801:HOH:O	2.18	0.51
1:2A:1102:C:H2'	1:2A:1103:A:H8	1.76	0.51
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.76	0.51
1:2A:2680:C:H5'	4:2E:189:PRO:HA	1.93	0.51
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:106:LEU:HD12	6:2G:110:ALA:HB3	1.92	0.51
8:2I:2:LYS:HD3	8:2I:18:VAL:HG12	1.92	0.51
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.29	0.51
32:2a:1030(C):G:H2'	32:2a:1030(D):A:C8	2.46	0.51
32:2a:1172:C:H2'	32:2a:1173:G:C8	2.46	0.51
1:1A:2336:A:H61	22:10:43:THR:CG2	2.24	0.50
1:1A:2453:A:OP1	60:1A:4149:HOH:O	2.19	0.50
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.29	0.50
6:1G:67:LYS:HD3	26:14:5:ILE:HB	1.92	0.50
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.93	0.50
32:1a:1244:C:H2'	32:1a:1245:A:C8	2.46	0.50
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.36	0.50
37:1f:14:LEU:HB3	37:1f:18:GLN:HB2	1.92	0.50
40:1i:7:THR:O	40:1i:83:ARG:NH1	2.44	0.50
1:2A:265:A:N1	1:2A:427:U:O2'	2.42	0.50
1:2A:2122:U:H3	1:2A:2176:A:H61	1.58	0.50
1:2A:2405:G:H5'	11:2P:75:ILE:HD13	1.93	0.50
1:2A:2689:U:H4'	1:2A:2690:C:H5'	1.93	0.50
4:2E:5:LEU:HD11	4:2E:79:ARG:HB2	1.94	0.50
21:2Z:48:PHE:HE1	21:2Z:71:VAL:HG11	1.76	0.50
21:2Z:150:LEU:HB3	21:2Z:171:ILE:HD11	1.91	0.50
33:2b:121:LEU:HG	33:2b:127:ILE:HG23	1.93	0.50
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.46	0.50
32:1a:624:C:H2'	32:1a:625:G:H8	1.74	0.50
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.46	0.50
40:1i:50:LEU:HA	40:1i:53:VAL:HG22	1.93	0.50
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.10	0.50
12:2Q:11:LYS:HD3	12:2Q:87:LYS:HG2	1.93	0.50
32:2a:9:G:H2'	32:2a:10:A:C8	2.47	0.50
32:2a:881:G:P	43:2l:12:ARG:HH22	2.35	0.50
41:2j:46:ARG:HG2	41:2j:64:GLU:HB3	1.94	0.50
1:1A:2292:C:OP1	14:1S:17:ARG:NH2	2.44	0.50
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.46	0.50
2:1B:23:G:O6	60:1B:301:HOH:O	2.18	0.50
13:1R:24:GLN:NE2	60:1R:303:HOH:O	2.44	0.50
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	1.93	0.50
33:1b:96:ARG:HG2	33:1b:98:LEU:HD23	1.92	0.50
37:1f:69:GLU:O	37:1f:72:VAL:HG12	2.12	0.50
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.76	0.50
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.76	0.50
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.34	0.50
33:2b:102:LEU:HD23	33:2b:182:ILE:HD12	1.93	0.50
35:2d:111:ALA:HA	35:2d:116:GLN:HE21	1.76	0.50
53:2y:74:ILE:O	53:2y:78:ILE:HG12	2.11	0.50
35:1d:168:ARG:N	35:1d:168:ARG:HH11	2.10	0.50
48:1q:45:HIS:HD2	48:1q:65:ILE:HG12	1.77	0.50
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.11	0.50
1:2A:2168:G:O2'	1:2A:2170:A:N7	2.36	0.50
1:2A:2823:A:O2'	60:2A:3852:HOH:O	2.20	0.50
32:2a:1004:A:H5''	32:2a:1025:U:C5	2.46	0.50
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.38	0.50
1:1A:286:C:H2'	1:1A:287:C:C6	2.47	0.50
1:1A:897:C:H2'	1:1A:898:C:C6	2.46	0.50
1:1A:1082:U:C4	1:1A:1086:A:N1	2.78	0.50
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.12	0.50
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	1.93	0.50
1:2A:212:G:H2'	1:2A:213:A:O4'	2.11	0.50
1:2A:1798:U:OP2	3:2D:274:ARG:NH2	2.45	0.50
2:2B:8:U:H5'	14:2S:15:ARG:NH1	2.27	0.50
32:2a:584:G:H5'	48:2q:91:ARG:HH22	1.77	0.50
32:2a:1108:G:H5'	34:2c:176:HIS:HD2	1.76	0.50
34:2c:47:LEU:HD13	34:2c:68:VAL:HG11	1.93	0.50
1:1A:312:G:OP2	60:1A:4150:HOH:O	2.19	0.50
1:1A:796:C:H2'	1:1A:797:C:C6	2.47	0.50
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.47	0.50
32:1a:710:G:H5''	37:1f:54:LYS:HE3	1.94	0.50
38:1g:48:LYS:O	38:1g:52:GLU:HG2	2.12	0.50
50:1s:15:LEU:O	50:1s:19:VAL:HG23	2.12	0.50
1:2A:2602:A:H1'	1:2A:2603:G:C5'	2.39	0.50
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.94	0.50
6:2G:19:LEU:HG	6:2G:175:LEU:HD22	1.93	0.50
6:2G:108:ASN:HA	26:24:37:SER:HB3	1.93	0.50
21:2Z:54:HIS:HB3	21:2Z:101:PRO:HD3	1.93	0.50
32:2a:56:U:H2'	32:2a:57:G:C8	2.46	0.50
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.76	0.50
53:2y:3:MET:HB2	53:2y:37:PRO:HD2	1.93	0.50
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.47	0.50
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.47	0.50
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.11	0.50
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.94	0.50
32:1a:171:A:H2'	32:1a:172:A:C8	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.44	0.50
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.47	0.50
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.45	0.50
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.94	0.50
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.46	0.50
1:2A:2390:U:P	30:28:35:GLN:HE22	2.35	0.50
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.76	0.50
6:2G:39:ILE:HD11	6:2G:102:PHE:CZ	2.47	0.50
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.94	0.50
1:1A:826:U:OP1	60:1A:4115:HOH:O	2.20	0.50
1:1A:2206:G:H5'	1:1A:2207:G:C5	2.47	0.50
2:1B:58:A:OP2	60:1B:303:HOH:O	2.20	0.50
8:1I:57:ARG:O	8:1I:61:ARG:HG2	2.12	0.50
15:1T:54:ARG:HA	15:1T:59:THR:HB	1.94	0.50
32:1a:300:A:O2'	32:1a:564:C:N3	2.36	0.50
32:1a:472:A:O3'	47:1p:81:ARG:HA	2.12	0.50
32:1a:1239:A:H62	32:1a:1299:A:N6	2.10	0.50
32:1a:1401:G:OP1	53:1y:80:LYS:NZ	2.45	0.50
34:1c:77:ILE:HG22	34:1c:81:GLY:HA2	1.94	0.50
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.12	0.50
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.94	0.50
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.12	0.50
32:2a:501:C:H2'	32:2a:502:G:H8	1.75	0.50
32:2a:632:A:H3'	32:2a:633:G:H8	1.76	0.50
40:2i:42:ARG:NH2	40:2i:71:SER:OG	2.45	0.50
41:2j:5:ARG:N	60:2j:302:HOH:O	2.45	0.50
41:2j:16:LEU:O	41:2j:20:ALA:N	2.31	0.50
1:1A:1382:G:N7	60:1A:4278:HOH:O	2.35	0.50
32:1a:266:G:H2'	32:1a:266:G:N3	2.26	0.50
32:1a:662:G:H2'	32:1a:663:A:C8	2.47	0.50
32:1a:1239:A:O2'	38:1g:114:ARG:O	2.29	0.50
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.47	0.50
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.46	0.50
32:2a:1068:G:N2	32:2a:1191:A:N3	2.48	0.50
33:2b:15:VAL:HB	33:2b:209:ARG:HB3	1.93	0.50
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.37	0.50
50:2s:27:GLU:OE1	50:2s:47:HIS:NE2	2.45	0.50
1:1A:578:A:H3'	60:1A:4296:HOH:O	2.12	0.49
1:1A:2789:C:O2	1:1A:2894:G:N1	2.45	0.49
32:1a:803:G:OP1	60:1a:1910:HOH:O	2.20	0.49
32:1a:1298:C:P	38:1g:114:ARG:HH22	2.34	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:37:ARG:NH1	36:1e:111:GLU:HG2	2.21	0.49
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.12	0.49
23:21:17:SER:O	60:21:202:HOH:O	2.20	0.49
32:2a:1028:C:H2'	32:2a:1033:G:N2	2.27	0.49
43:2l:103:GLY:N	43:2l:107:ALA:O	2.43	0.49
1:1A:330:A:H2	1:1A:1210:A:O2'	1.95	0.49
1:1A:639:U:H2'	1:1A:640:C:C6	2.47	0.49
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.11	0.49
32:1a:920:U:H2'	32:1a:921:U:C6	2.47	0.49
33:1b:9:GLU:OE2	33:1b:217:ARG:NH1	2.45	0.49
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.29	0.49
1:2A:1084:A:N6	1:2A:1086:A:N7	2.60	0.49
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.94	0.49
5:2F:140:LEU:HD13	5:2F:170:LEU:HD21	1.94	0.49
32:2a:620:C:C2	35:2d:135:LEU:HG	2.47	0.49
32:2a:1004:A:H5''	32:2a:1025:U:H5	1.77	0.49
1:1A:247:G:H4'	1:1A:386:G:C5	2.46	0.49
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.47	0.49
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.47	0.49
21:1Z:103:ARG:HD3	21:1Z:136:PHE:CD1	2.47	0.49
37:1f:27:GLN:HA	37:1f:30:LEU:HD12	1.94	0.49
1:2A:1065:U:H3	1:2A:1073:A:H61	1.59	0.49
32:2a:1028:C:H2'	32:2a:1033:G:H22	1.77	0.49
1:1A:1920:OMC:HM22	1:1A:1921:G:H5'	1.94	0.49
1:1A:2336:A:H61	22:10:43:THR:HG22	1.77	0.49
13:1R:59:ASP:OD1	13:1R:59:ASP:N	2.45	0.49
25:13:3:ARG:NE	25:13:60:GLU:OE2	2.45	0.49
35:1d:150:GLU:OE1	35:1d:151:LYS:N	2.43	0.49
40:1i:10:ARG:HG3	40:1i:11:LYS:H	1.77	0.49
48:1q:81:ARG:NH1	48:1q:83:ASP:OD2	2.46	0.49
1:2A:586:A:N1	1:2A:809:G:O2'	2.42	0.49
21:2Z:3:TYR:CG	21:2Z:51:ALA:HB2	2.48	0.49
32:2a:434:U:H2'	32:2a:435:C:C6	2.47	0.49
38:2g:70:LYS:HB3	38:2g:96:GLN:HB3	1.94	0.49
50:2s:40:ILE:HD11	50:2s:74:PHE:HE2	1.77	0.49
16:1U:49:HIS:HA	16:1U:52:ARG:HG2	1.93	0.49
32:1a:316:G:OP2	32:1a:351:G:O2'	2.29	0.49
32:1a:1003:G:N2	32:1a:1004:A:H1'	2.27	0.49
1:2A:1062:G:H5'	1:2A:1070:A:H5'	1.95	0.49
1:2A:2102:U:O2	1:2A:2187:G:O6	2.30	0.49
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.41	0.49
3:1D:37:LEU:HD13	3:1D:62:TYR:HB2	1.94	0.49
3:1D:106:ILE:HG12	60:1D:469:HOH:O	2.11	0.49
32:1a:8:A:N6	35:1d:205:GLU:O	2.44	0.49
32:1a:380:G:N2	32:1a:383:A:OP2	2.44	0.49
32:1a:1216:G:OP1	45:1n:2:ALA:HA	2.12	0.49
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.12	0.49
36:1e:148:VAL:HG21	39:1h:107:LEU:HB3	1.93	0.49
1:2A:1756:G:H4'	1:2A:1758:G:O4'	2.11	0.49
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.94	0.49
44:2m:19:LEU:HD11	44:2m:56:LEU:HD21	1.95	0.49
48:2q:67:LYS:C	48:2q:69:LYS:H	2.18	0.49
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.13	0.49
6:1G:66:GLN:OE1	6:1G:98:ARG:NE	2.46	0.49
32:1a:1216:G:H5''	45:1n:5:ALA:HB2	1.95	0.49
35:1d:172:PRO:HB2	35:1d:187:ARG:NH2	2.26	0.49
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	1.95	0.49
32:2a:192:U:H5'	51:2t:101:GLY:HA3	1.95	0.49
34:2c:123:GLN:HE22	34:2c:136:GLN:HE22	1.60	0.49
1:1A:548:A:O2'	1:1A:549:G:OP1	2.30	0.49
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.47	0.49
32:1a:130:A:H5'	48:1q:63:ARG:HE	1.77	0.49
39:1h:104:ARG:C	39:1h:106:GLY:H	2.20	0.49
1:2A:876:C:H2'	1:2A:877:U:O4'	2.12	0.49
2:2B:22:U:H2'	2:2B:23:G:C8	2.47	0.49
2:2B:115:G:O2'	14:2S:50:SER:OG	2.30	0.49
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.34	0.49
38:2g:79:ARG:HA	38:2g:84:ASN:HA	1.95	0.49
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.20	0.49
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.95	0.49
32:1a:652:U:O4	32:1a:752:G:O2'	2.30	0.49
32:1a:1401:G:N7	53:1y:83:ARG:NH1	2.38	0.49
45:1n:46:GLU:O	45:1n:50:LYS:HG3	2.13	0.49
1:2A:885:C:H2'	1:2A:886:C:O4'	2.13	0.49
1:2A:1014:U:H2'	1:2A:1015:G:C8	2.46	0.49
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.47	0.49
3:2D:102:LYS:C	3:2D:103:ARG:HG2	2.37	0.49
28:26:8:LYS:NZ	60:26:602:HOH:O	2.42	0.49
28:26:14:THR:OG1	28:26:48:VAL:O	2.27	0.49
32:2a:164:U:H2'	32:2a:165:C:C6	2.48	0.49
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:2y:12:ILE:HG23	53:2y:16:ILE:HG23	1.94	0.49
1:1A:774:A:N3	1:1A:774:A:H2'	2.28	0.49
8:1I:133:HIS:ND1	8:1I:134:PRO:O	2.44	0.49
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.86	0.49
33:1b:21:ARG:HG3	33:1b:22:LYS:H	1.77	0.49
33:1b:54:THR:HG23	33:1b:199:TYR:HB3	1.94	0.49
48:1q:8:GLY:HA3	48:1q:22:LEU:O	2.13	0.49
1:2A:796:C:H2'	1:2A:797:C:C6	2.47	0.49
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.95	0.49
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.48	0.49
4:2E:48:GLN:NE2	4:2E:78:LEU:HD13	2.28	0.49
6:2G:57:ALA:HB2	6:2G:90:LEU:HD13	1.94	0.49
32:2a:881:G:OP2	43:2l:12:ARG:NH2	2.46	0.49
1:1A:1020:A:N1	1:1A:1141:U:O2'	2.38	0.48
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.46	0.48
32:1a:524:G:H2'	32:1a:525:C:C6	2.47	0.48
1:2A:2847:U:OP1	15:2T:98:LYS:NZ	2.46	0.48
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.78	0.48
16:2U:27:LEU:HA	16:2U:30:LYS:HB2	1.94	0.48
32:2a:757:U:H2'	32:2a:758:G:O4'	2.13	0.48
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.14	0.48
18:1W:86:LEU:HB2	18:1W:96:ILE:HG13	1.95	0.48
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.95	0.48
1:2A:747:U:O2	1:2A:2014:A:H1'	2.13	0.48
1:2A:1110:G:H1'	1:2A:1111:A:H8	1.76	0.48
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.45	0.48
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.48	0.48
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.13	0.48
6:2G:77:ILE:HG21	6:2G:80:PHE:CD2	2.48	0.48
6:2G:122:PRO:HG3	6:2G:182:LYS:C	2.38	0.48
7:2H:13:LYS:HE2	7:2H:14:GLY:HA2	1.95	0.48
32:2a:1069:C:OP1	60:2a:3215:HOH:O	2.20	0.48
32:2a:1403:C:H2'	32:2a:1404:5MC:HM53	1.95	0.48
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.75	0.48
1:1A:2296:U:OP2	14:1S:9:ARG:NH2	2.46	0.48
1:1A:2319:G:N2	14:1S:3:ARG:HA	2.28	0.48
24:12:1:MET:N	60:12:103:HOH:O	2.44	0.48
32:1a:269:C:H2'	32:1a:270:A:C8	2.48	0.48
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.48	0.48
37:1f:19:LEU:HD11	37:1f:59:TYR:CE1	2.47	0.48
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.48	0.48
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.46	0.48
26:24:1:MET:HB3	26:24:6:HIS:CD2	2.48	0.48
32:2a:890:G:O2'	32:2a:906:G:O6	2.26	0.48
32:2a:1054:C:H41	53:2y:46:GLN:HG3	1.78	0.48
42:2k:16:SER:OG	42:2k:106:LYS:NZ	2.41	0.48
47:2p:74:LEU:HD23	47:2p:79:VAL:HG11	1.94	0.48
1:1A:620:G:N3	1:1A:620:G:H5'	2.28	0.48
32:1a:939:G:N7	60:1a:1955:HOH:O	2.35	0.48
35:1d:3:ARG:NH1	35:1d:5:ILE:HG22	2.29	0.48
53:1y:55:ASN:OD1	53:1y:60:VAL:HG12	2.13	0.48
1:2A:686:G:N2	1:2A:788:A:H61	2.11	0.48
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.49	0.48
7:2H:25:LYS:HE3	7:2H:27:LYS:NZ	2.29	0.48
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.49	0.48
32:2a:266:G:H3'	48:2q:67:LYS:HB2	1.94	0.48
32:2a:965:A:C8	53:2y:8:LYS:HD2	2.48	0.48
33:2b:178:ARG:HE	33:2b:178:ARG:HB3	1.41	0.48
1:1A:228:A:H8	1:1A:229:A:H5'	1.78	0.48
1:1A:1919:A:N1	32:1a:1495:U:O2'	2.33	0.48
1:1A:2550:G:OP1	60:1A:4123:HOH:O	2.20	0.48
32:1a:1400:5MC:C2	53:1y:63:ALA:HA	2.48	0.48
44:1m:2:ALA:N	44:1m:8:GLU:OE1	2.46	0.48
47:1p:57:ARG:NH2	47:1p:78:GLY:O	2.47	0.48
53:1y:49:VAL:HG22	53:1y:66:LYS:HG2	1.94	0.48
2:2B:13:A:N1	2:2B:69:G:O2'	2.45	0.48
7:2H:88:LEU:HD21	7:2H:165:ALA:HA	1.95	0.48
7:2H:89:ILE:O	7:2H:129:THR:HG23	2.14	0.48
32:2a:443:C:H2'	32:2a:444:C:C6	2.49	0.48
32:2a:979:C:O2	45:2n:19:ARG:NE	2.42	0.48
33:2b:87:ARG:CZ	33:2b:233:SER:HB3	2.42	0.48
50:2s:50:ALA:HA	50:2s:58:VAL:O	2.13	0.48
1:1A:1762:A:H2'	60:1A:7559:HOH:O	2.12	0.48
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.95	0.48
21:1Z:52:SER:HB3	21:1Z:54:HIS:ND1	2.29	0.48
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.62	0.48
1:2A:774:A:H2'	1:2A:774:A:N3	2.28	0.48
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.48	0.48
1:2A:2133:G:C2	1:2A:2157:G:H2'	2.47	0.48
1:2A:2186:G:C2	1:2A:2187:G:C5	3.02	0.48
1:2A:2378:A:O2'	14:2S:21:THR:HG21	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:14:U:OP2	2:2B:70:C:O2'	2.28	0.48
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.96	0.48
6:2G:61:ALA:O	6:2G:65:GLY:N	2.45	0.48
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.47	0.48
33:2b:15:VAL:HG23	33:2b:16:HIS:HD2	1.78	0.48
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.49	0.48
8:1I:4:ILE:HD11	8:1I:44:LEU:HD13	1.94	0.48
8:1I:31:LEU:HD21	8:1I:38:LEU:HD13	1.94	0.48
15:1T:1:MET:HE2	15:1T:3:ARG:HG3	1.95	0.48
32:1a:1005:A:C2	32:1a:1025:U:H1'	2.48	0.48
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.49	0.48
1:2A:451:C:H5'	60:2A:3871:HOH:O	2.12	0.48
1:2A:752:A:H3'	29:27:1:MET:HE1	1.95	0.48
1:2A:1827:C:O2'	1:2A:1970:A:N3	2.34	0.48
27:25:51:TYR:CE2	27:25:56:LYS:HD3	2.49	0.48
1:1A:1096:A:H3'	1:1A:1097:U:H5''	1.95	0.48
1:1A:1359:A:H61	1:1A:1372:U:H3	1.61	0.48
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.96	0.48
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.96	0.48
32:1a:15:G:H21	36:1e:18:ARG:HA	1.77	0.48
32:1a:1024:G:H2'	32:1a:1024:G:N3	2.28	0.48
32:1a:1226:C:N4	44:1m:104:ARG:HD2	2.28	0.48
32:1a:1250:A:H4'	40:1i:68:GLY:N	2.29	0.48
38:1g:26:PHE:O	38:1g:30:ILE:HG13	2.14	0.48
50:1s:63:THR:HG23	50:1s:66:MET:HE3	1.95	0.48
51:1t:47:GLY:HA2	51:1t:48:LYS:HB2	1.96	0.48
1:2A:27:G:O2'	1:2A:28:A:OP2	2.30	0.48
1:2A:361:G:O2'	1:2A:362:U:H5'	2.14	0.48
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.13	0.48
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.48	0.48
1:2A:2321:G:O2'	1:2A:2322:A:OP1	2.30	0.48
6:2G:80:PHE:O	6:2G:82:LEU:N	2.47	0.48
6:2G:109:VAL:HG11	6:2G:142:PRO:HB3	1.95	0.48
32:2a:1212:U:H4'	32:2a:1213:A:C8	2.48	0.48
1:1A:1075:C:OP2	12:1Q:59:ARG:HD3	2.13	0.48
32:1a:745:C:H2'	32:1a:746:A:C8	2.48	0.48
40:1i:3:GLN:NE2	40:1i:20:ARG:HH21	2.12	0.48
41:1j:31:GLY:HA2	41:1j:32:ALA:HA	1.49	0.48
1:2A:11:G:H2'	1:2A:12:U:H5'	1.96	0.48
1:2A:999:U:OP2	60:2A:3832:HOH:O	2.20	0.48
1:2A:1047:G:H2'	1:2A:1110:G:H22	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.14	0.48
16:2U:10:ARG:NH2	60:2U:203:HOH:O	2.38	0.48
26:24:1:MET:HE2	26:24:6:HIS:CG	2.49	0.48
32:2a:7:G:H5'	32:2a:298:A:O4'	2.14	0.48
32:2a:254:G:H21	48:2q:16:GLN:NE2	2.11	0.48
44:2m:59:TYR:O	44:2m:63:THR:OG1	2.30	0.48
53:2y:5:ILE:HG23	53:2y:39:ILE:HB	1.95	0.48
1:1A:1500:G:O2'	3:1D:100:GLY:O	2.30	0.48
1:1A:2365:G:O6	30:18:39:LYS:HE3	2.14	0.48
4:1E:181:LEU:HD11	15:1T:6:LEU:HD23	1.96	0.48
28:16:9:LEU:HD13	28:16:51:GLU:HG3	1.95	0.48
32:1a:142:G:H2'	32:1a:143:A:C8	2.48	0.48
32:1a:166:G:H2'	32:1a:167:G:C8	2.45	0.48
32:1a:881:G:P	43:1l:12:ARG:HH22	2.36	0.48
34:1c:134:ILE:HG23	34:1c:151:VAL:HB	1.96	0.48
1:2A:1068:G:H3'	1:2A:1096:A:OP2	2.13	0.48
1:2A:2165:G:H2'	1:2A:2166:G:O4'	2.14	0.48
7:2H:117:PRO:HG3	7:2H:123:PHE:CE2	2.49	0.48
11:2P:138:LEU:HD23	11:2P:145:PRO:HB3	1.95	0.48
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.96	0.48
1:1A:1041:C:H5'	1:1A:1042:G:OP2	2.14	0.47
1:1A:1045:A:H5'	1:1A:1046:A:H5'	1.95	0.47
1:1A:1877:A:H5'	1:1A:1878:G:OP2	2.14	0.47
3:1D:71:ASP:HB3	3:1D:103:ARG:NH2	2.29	0.47
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.97	0.47
35:1d:167:GLY:H	35:1d:168:ARG:HH12	1.60	0.47
36:1e:45:PHE:CD2	36:1e:47:LYS:HE2	2.49	0.47
44:1m:3:ARG:NH2	44:1m:11:ARG:HG2	2.29	0.47
50:1s:12:ASP:HB3	50:1s:14:HIS:CD2	2.49	0.47
53:1y:3:MET:HG2	53:1y:37:PRO:HG2	1.96	0.47
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.48	0.47
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.49	0.47
14:2S:25:ARG:HD3	14:2S:42:ASP:OD2	2.14	0.47
28:26:34:LEU:HB2	28:26:51:GLU:HB2	1.95	0.47
32:2a:56:U:H2'	32:2a:57:G:H8	1.79	0.47
32:2a:537:G:H5''	43:2l:113:ARG:NH1	2.29	0.47
32:2a:1141:C:H2'	32:2a:1142:G:C8	2.47	0.47
4:1E:59:VAL:HG21	4:1E:74:PRO:HB3	1.96	0.47
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.95	0.47
27:15:49:CYS:HA	27:15:60:VAL:HG11	1.96	0.47
32:1a:186:C:H2'	32:1a:187:C:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:964:A:N3	32:1a:969:A:O2'	2.46	0.47
35:1d:163:GLU:O	35:1d:166:LYS:HG2	2.13	0.47
39:1h:97:VAL:HG21	39:1h:128:GLY:HA2	1.96	0.47
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.14	0.47
1:2A:2128:C:O2'	1:2A:2174:C:H4'	2.13	0.47
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.47	0.47
7:2H:127:GLU:C	7:2H:129:THR:H	2.22	0.47
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.29	0.47
32:2a:1030:C:N4	32:2a:1031:G:H1	2.12	0.47
39:2h:95:VAL:HB	39:2h:99:GLU:HG3	1.97	0.47
50:2s:9:VAL:O	50:2s:11:VAL:N	2.45	0.47
1:1A:185:U:H2'	1:1A:186:G:C8	2.49	0.47
1:1A:2135:A:H62	1:1A:2156:G:H21	1.60	0.47
1:1A:2144:U:H2'	1:1A:2147:G:H1	1.79	0.47
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.44	0.47
10:1O:115:VAL:O	56:1a:1878:MPD:H13	2.14	0.47
18:1W:1:MET:HE2	18:1W:62:HIS:HB3	1.95	0.47
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.79	0.47
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.96	0.47
43:1l:54:LYS:HD2	43:1l:54:LYS:N	2.28	0.47
50:1s:3:ARG:NH2	50:1s:7:LYS:HE2	2.30	0.47
1:2A:272:G:N7	1:2A:421:U:H2'	2.28	0.47
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.49	0.47
5:2F:122:LYS:HD2	5:2F:191:ARG:HD2	1.97	0.47
32:2a:799:G:OP2	60:2a:3216:HOH:O	2.20	0.47
32:2a:920:U:H2'	32:2a:921:U:C6	2.49	0.47
44:2m:15:VAL:O	44:2m:19:LEU:HG	2.14	0.47
1:1A:2165:G:H2'	1:1A:2166:G:C8	2.50	0.47
32:1a:536:C:OP2	60:1a:1912:HOH:O	2.20	0.47
33:1b:73:THR:OG1	33:1b:170:GLU:OE2	2.23	0.47
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.39	0.47
1:2A:854:G:H2'	1:2A:855:G:C8	2.49	0.47
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.44	0.47
7:2H:103:LEU:O	7:2H:114:VAL:HA	2.14	0.47
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.97	0.47
16:2U:90:VAL:HG12	16:2U:95:LEU:HG	1.96	0.47
17:2V:5:VAL:HG11	17:2V:57:VAL:HG21	1.95	0.47
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.97	0.47
32:2a:973:G:H1'	41:2j:54:PHE:CD1	2.49	0.47
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.95	0.47
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:116:HIS:N	42:2k:117:ASN:HA	2.28	0.47
1:1A:636:G:OP1	11:1P:132:LYS:HE2	2.15	0.47
1:1A:956:G:O6	60:1A:4146:HOH:O	2.19	0.47
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.50	0.47
1:1A:2893:G:H4'	1:1A:2894:G:O5'	2.14	0.47
32:1a:407:G:OP1	35:1d:115:ARG:HD3	2.14	0.47
32:1a:1277:C:H1'	32:1a:1282:C:O2	2.14	0.47
36:1e:90:VAL:O	36:1e:120:THR:HA	2.15	0.47
1:2A:2810:A:N6	1:2A:2891:G:O2'	2.45	0.47
9:2N:19:GLU:HG3	9:2N:59:LYS:HB3	1.96	0.47
44:2m:90:LEU:HD21	44:2m:93:ARG:HH21	1.79	0.47
48:2q:94:ASN:O	48:2q:98:LEU:HD23	2.15	0.47
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.49	0.47
32:1a:45:U:H2'	32:1a:46:G:C8	2.50	0.47
32:1a:828:A:H2'	32:1a:829:G:O4'	2.14	0.47
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.33	0.47
45:1n:26:ARG:HD3	45:1n:43:CYS:HB3	1.95	0.47
1:2A:1919:A:N1	32:2a:1495:U:O2'	2.40	0.47
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.80	0.47
32:2a:921:U:O2	36:2e:19:MET:HB2	2.13	0.47
41:2j:8:LEU:HB2	41:2j:70:ARG:HB2	1.96	0.47
1:1A:207:A:H2'	1:1A:208:C:O4'	2.13	0.47
1:1A:969:U:H2'	1:1A:970:C:C6	2.50	0.47
1:1A:1179:C:H2'	1:1A:1180:C:H6	1.80	0.47
1:1A:1289:C:H2'	1:1A:1290:C:C6	2.50	0.47
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.32	0.47
1:1A:2140:C:H2'	1:1A:2141:G:H8	1.79	0.47
1:1A:2162:G:H4'	1:1A:2172:U:O2'	2.15	0.47
1:1A:2393:A:O2'	11:1P:60:MET:O	2.30	0.47
6:1G:50:ALA:C	6:1G:52:ILE:H	2.22	0.47
8:1I:72:LEU:HD12	8:1I:138:ILE:HG21	1.96	0.47
32:1a:626:U:H2'	32:1a:627:G:C8	2.50	0.47
32:1a:940:C:OP1	38:1g:29:LYS:NZ	2.48	0.47
32:1a:974:A:OP2	45:1n:29:ARG:NH1	2.47	0.47
32:1a:1264:C:H2'	32:1a:1265:G:C8	2.50	0.47
32:1a:1496:C:OP2	60:1a:1913:HOH:O	2.21	0.47
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.96	0.47
34:1c:88:ARG:NH2	34:1c:101:LEU:O	2.47	0.47
35:1d:108:LEU:HD12	35:1d:174:LEU:HD13	1.96	0.47
37:1f:78:GLU:O	37:1f:81:ILE:HG22	2.15	0.47
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.29	0.47
1:2A:2104:G:H21	1:2A:2105:C:N4	2.12	0.47
1:2A:2527:C:H5''	31:29:30:PRO:HB2	1.97	0.47
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.97	0.47
6:2G:66:GLN:OE1	6:2G:98:ARG:NE	2.48	0.47
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.30	0.47
17:2V:62:LEU:HD23	17:2V:93:GLU:HG2	1.96	0.47
32:2a:1264:C:H2'	32:2a:1265:G:C8	2.49	0.47
34:2c:3:ASN:N	34:2c:3:ASN:OD1	2.46	0.47
34:2c:17:ASP:OD1	34:2c:18:TRP:N	2.48	0.47
41:2j:16:LEU:HD23	41:2j:94:VAL:HG22	1.96	0.47
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.79	0.47
50:2s:22:LEU:O	50:2s:26:GLY:N	2.48	0.47
14:1S:59:LYS:HE2	14:1S:60:GLY:H	1.79	0.47
32:1a:176:C:H2'	32:1a:177:C:C6	2.49	0.47
32:1a:434:U:H2'	32:1a:435:C:C6	2.50	0.47
32:1a:501:C:H1'	32:1a:549:C:H1'	1.97	0.47
32:1a:653:A:OP1	39:1h:56:LYS:NZ	2.44	0.47
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.50	0.47
32:1a:1498:UR3:H4'	32:1a:1519:MA6:H2	1.96	0.47
44:1m:78:ILE:HG22	44:1m:82:MET:HE2	1.96	0.47
50:1s:3:ARG:HH21	50:1s:7:LYS:HB3	1.79	0.47
1:2A:639:U:H2'	1:2A:640:C:C6	2.50	0.47
1:2A:2117:A:H5'	1:2A:2147:G:O2'	2.14	0.47
4:2E:105:THR:OG1	4:2E:199:ARG:NH2	2.47	0.47
15:2T:54:ARG:HA	15:2T:59:THR:HG23	1.97	0.47
32:2a:1030(A):G:H2'	32:2a:1030(B):C:H5''	1.96	0.47
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.15	0.47
11:1P:86:LYS:HB3	11:1P:118:GLY:HA3	1.95	0.47
26:14:55:ARG:H	26:14:56:VAL:HA	1.80	0.47
32:1a:624:C:H2'	32:1a:625:G:C8	2.50	0.47
44:1m:89:GLY:O	44:1m:93:ARG:HG3	2.15	0.47
1:2A:2152:G:H2'	1:2A:2153:G:H8	1.78	0.47
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.15	0.47
4:2E:119:ARG:HG2	4:2E:120:TRP:NE1	2.30	0.47
6:2G:22:ARG:HH21	6:2G:171:ALA:HB2	1.79	0.47
9:2N:18:ALA:HA	9:2N:21:LYS:HD2	1.96	0.47
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.50	0.47
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.66	0.47
32:2a:269:C:H2'	32:2a:270:A:C8	2.49	0.47
32:2a:689:C:OP1	42:2k:27:ASN:ND2	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:19:HIS:CE1	33:2b:206:ASP:HB2	2.50	0.47
40:2i:110:GLU:OE2	40:2i:113:LYS:NZ	2.41	0.47
44:2m:84:ILE:HB	50:2s:66:MET:HE2	1.96	0.47
1:1A:305:U:H2'	1:1A:306:U:C6	2.50	0.47
1:1A:1073:A:H2	1:1A:1074:G:H8	1.63	0.47
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.33	0.47
1:1A:2689:U:H4'	1:1A:2690:C:H5'	1.96	0.47
1:1A:2882:A:OP1	13:1R:96:ARG:HD3	2.15	0.47
32:1a:7:G:H21	36:1e:121:LYS:HG2	1.80	0.47
41:1j:5:ARG:NE	41:1j:73:ASP:OD1	2.30	0.47
1:2A:495:G:N3	18:2W:61:ASN:ND2	2.61	0.47
1:2A:1104:C:H2'	1:2A:1105:U:C6	2.50	0.47
1:2A:1230:C:H2'	1:2A:1231:G:C8	2.50	0.47
1:2A:1287:A:O4'	13:2R:104:ARG:HD3	2.14	0.47
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.15	0.47
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.50	0.47
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.48	0.47
8:2I:1:MET:HE2	8:2I:38:LEU:HD21	1.97	0.47
24:22:38:GLN:HB3	24:22:44:LEU:HB2	1.97	0.47
32:2a:636:U:H2'	32:2a:637:G:C8	2.50	0.47
32:2a:854:G:O6	60:2a:3214:HOH:O	2.20	0.47
34:2c:164:ARG:HG2	34:2c:165:THR:H	1.80	0.47
50:2s:61:TYR:HE2	50:2s:63:THR:HG23	1.79	0.47
1:1A:752:A:H3'	29:17:1:MET:HE1	1.96	0.46
1:1A:1062:G:H1'	1:1A:1088:A:H62	1.80	0.46
1:1A:2145:C:H2'	1:1A:2147:G:N2	2.30	0.46
2:1B:66:A:H61	2:1B:108:U:H2'	1.81	0.46
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.13	0.46
9:1N:12:ARG:HD3	9:1N:14:VAL:HG23	1.97	0.46
15:1T:16:ARG:NH2	15:1T:83:ILE:O	2.48	0.46
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.30	0.46
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.30	0.46
3:2D:106:ILE:HD11	3:2D:143:HIS:HD2	1.79	0.46
6:2G:173:LEU:HB3	6:2G:178:PHE:CD2	2.50	0.46
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.96	0.46
32:2a:512:U:H2'	32:2a:513:C:C6	2.50	0.46
32:2a:588:G:H4'	39:2h:2:LEU:HD23	1.97	0.46
32:2a:944:G:N1	32:2a:1338:G:OP2	2.44	0.46
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.50	0.46
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.50	0.46
60:1A:4421:HOH:O	29:17:32:LYS:HE2	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:12:LEU:HD13	5:1F:124:LEU:HD11	1.95	0.46
11:1P:121:LYS:O	11:1P:123:LEU:N	2.48	0.46
32:1a:7:G:H5'	32:1a:298:A:O4'	2.14	0.46
32:1a:580:U:H2'	32:1a:581:G:O4'	2.14	0.46
32:1a:1278:U:H5'	32:1a:1279:A:O4'	2.15	0.46
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.50	0.46
36:1e:102:ALA:HB1	36:1e:106:PRO:HG2	1.97	0.46
47:1p:40:ASP:HB3	47:1p:48:TRP:HB2	1.97	0.46
1:2A:1053:C:H2'	1:2A:1054:A:H8	1.80	0.46
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.50	0.46
1:2A:2353:G:N7	60:2A:3981:HOH:O	2.35	0.46
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.31	0.46
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.95	0.46
39:2h:103:VAL:HG21	39:2h:110:ALA:HB2	1.97	0.46
44:2m:3:ARG:HB2	44:2m:8:GLU:HA	1.96	0.46
47:2p:18:ARG:HD3	47:2p:35:LYS:HD3	1.96	0.46
1:1A:2096:U:H3	1:1A:2193:G:H1	1.63	0.46
2:1B:92:C:OP2	60:1B:304:HOH:O	2.20	0.46
6:1G:179:PRO:HB2	26:14:42:PHE:HE2	1.81	0.46
7:1H:105:LEU:HD11	7:1H:148:ILE:HG23	1.97	0.46
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.58	0.46
32:1a:773:G:OP1	60:1a:1911:HOH:O	2.20	0.46
1:2A:299:A:N1	1:2A:322:A:O2'	2.39	0.46
1:2A:1050:A:H2'	1:2A:1051:G:C8	2.45	0.46
32:2a:381:C:H2'	32:2a:382:A:O4'	2.16	0.46
32:2a:973:G:H3'	32:2a:974:A:H5''	1.98	0.46
35:2d:173:TRP:CD1	35:2d:174:LEU:HG	2.51	0.46
36:2e:6:PHE:HB3	36:2e:34:VAL:HG22	1.96	0.46
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.96	0.46
1:1A:363(A):A:H2'	1:1A:363(B):G:H8	1.81	0.46
1:1A:652(C):G:N2	1:1A:653:A:H1'	2.30	0.46
1:1A:802:A:OP1	60:1A:4151:HOH:O	2.21	0.46
1:1A:1952:A:OP1	10:1O:44:LYS:NZ	2.40	0.46
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.51	0.46
1:1A:2602:A:H4'	1:1A:2603:G:OP1	2.16	0.46
6:1G:5:VAL:HG13	6:1G:8:LYS:HE2	1.96	0.46
32:1a:1058:G:OP1	34:1c:199:LYS:HE3	2.16	0.46
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.30	0.46
48:1q:10:VAL:HG22	48:1q:21:VAL:HG22	1.97	0.46
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.80	0.46
1:2A:1055:G:H3'	1:2A:1056:G:H8	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.30	0.46
13:2R:8:ARG:HE	13:2R:43:GLU:HG2	1.80	0.46
16:2U:49:HIS:HA	16:2U:52:ARG:HG2	1.98	0.46
24:22:3:LEU:O	24:22:7:ARG:HG3	2.15	0.46
25:23:23:LEU:HD13	25:23:50:VAL:HG11	1.97	0.46
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.51	0.46
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.98	0.46
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.80	0.46
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.15	0.46
32:2a:1503:A:H5'	32:2a:1531:A:H1'	1.97	0.46
36:2e:12:LEU:HB3	36:2e:31:LEU:HB2	1.98	0.46
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.97	0.46
38:2g:50:ILE:HD11	38:2g:58:PRO:HA	1.96	0.46
51:2t:56:MET:HE2	51:2t:56:MET:HB3	1.87	0.46
1:1A:1056:G:H5''	1:1A:1057:A:O4'	2.15	0.46
1:1A:2319:G:H1	14:1S:3:ARG:NH1	2.14	0.46
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.50	0.46
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.51	0.46
7:1H:159:GLU:HG2	7:1H:169:VAL:HG11	1.97	0.46
29:17:47:ARG:HE	29:17:47:ARG:HB3	1.59	0.46
32:1a:955:U:O2'	50:1s:83:HIS:HD2	1.99	0.46
36:1e:137:GLU:OE2	36:1e:141:GLN:NE2	2.40	0.46
1:2A:84:A:N1	1:2A:98:G:O2'	2.37	0.46
1:2A:1815:A:OP2	3:2D:54:ARG:NH2	2.48	0.46
7:2H:46:GLU:HB2	7:2H:49:VAL:HG12	1.98	0.46
28:26:26:ASN:HB3	28:26:29:ASN:HB2	1.97	0.46
32:2a:255:G:OP1	48:2q:69:LYS:NZ	2.42	0.46
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.14	0.46
32:2a:1129:C:H1'	32:2a:1130:A:N7	2.31	0.46
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.98	0.46
50:2s:41:VAL:HG13	50:2s:43:GLU:H	1.81	0.46
7:1H:40:GLU:OE1	7:1H:60:ARG:NH1	2.47	0.46
18:1W:68:ARG:NH1	18:1W:112:GLY:H	2.14	0.46
32:1a:161:A:H2'	32:1a:162:A:C8	2.51	0.46
32:1a:381:C:OP1	60:1a:1914:HOH:O	2.21	0.46
32:1a:1124:G:N2	32:1a:1125:U:O4	2.45	0.46
33:1b:76:GLN:HB3	33:1b:208:ILE:HG22	1.97	0.46
34:1c:19:GLU:HG2	34:1c:54:ARG:NE	2.31	0.46
35:1d:85:LYS:HG3	35:1d:86:LYS:H	1.81	0.46
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.98	0.46
1:2A:1041:C:N4	1:2A:1114:G:H1	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2469:A:H4'	12:2Q:56:ARG:HG2	1.98	0.46
1:2A:2657:A:O3'	7:2H:160:LYS:NZ	2.49	0.46
7:2H:3:ARG:NH2	7:2H:62:LYS:O	2.48	0.46
32:2a:1060:C:HO2'	41:2j:56:HIS:HD1	1.64	0.46
1:1A:221:A:N1	1:1A:265:A:O2'	2.43	0.46
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.51	0.46
1:1A:800:A:H8	1:1A:800:A:OP1	1.97	0.46
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.50	0.46
1:1A:2319:G:H22	14:1S:3:ARG:HA	1.81	0.46
60:1A:4223:HOH:O	11:1P:37:GLY:HA3	2.16	0.46
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.50	0.46
35:1d:61:LYS:HG3	35:1d:203:VAL:HG13	1.98	0.46
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.51	0.46
60:2B:314:HOH:O	21:2Z:31:ARG:HG3	2.16	0.46
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.15	0.46
32:2a:731:G:H5'	32:2a:766:A:H4'	1.96	0.46
33:2b:30:ARG:NH2	33:2b:194:PRO:HB2	2.30	0.46
36:2e:92:LYS:HB3	36:2e:119:LEU:HB2	1.98	0.46
42:2k:59:TYR:CE2	42:2k:63:LEU:HD11	2.51	0.46
1:1A:566:U:H5''	11:1P:29:LYS:HE3	1.98	0.46
1:1A:1721:G:H5'	1:1A:1722:A:OP2	2.14	0.46
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.64	0.46
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.59	0.46
32:1a:575:G:O2'	32:1a:821:G:H5'	2.16	0.46
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.51	0.46
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.97	0.46
39:1h:111:ILE:HG22	39:1h:134:ILE:HD12	1.98	0.46
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.29	0.46
1:2A:2585:U:O2'	55:2A:3741:CPF:H161	2.16	0.46
1:2A:2641:G:OP1	9:2N:74:ARG:NH1	2.49	0.46
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.15	0.46
14:2S:19:LYS:HG2	14:2S:42:ASP:OD2	2.15	0.46
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.51	0.46
32:2a:1504:G:OP1	32:2a:1507:A:H4'	2.16	0.46
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.30	0.46
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.51	0.46
1:1A:2138:C:H2'	1:1A:2139:C:C5	2.51	0.46
1:1A:2168:G:C2	1:1A:2171:A:C8	3.04	0.46
8:1I:77:LEU:HD21	8:1I:100:ALA:HB3	1.98	0.46
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.97	0.46
35:1d:61:LYS:HD3	35:1d:206:PHE:CE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.16	0.46
1:2A:218:A:C2	1:2A:235:U:H4'	2.51	0.46
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.39	0.46
32:2a:1279:A:H2'	32:2a:1279:A:N3	2.30	0.46
32:2a:1342:C:H2'	32:2a:1343:G:H8	1.81	0.46
33:2b:44:LEU:H	33:2b:44:LEU:HD12	1.80	0.46
39:2h:112:LEU:HA	39:2h:134:ILE:HG12	1.98	0.46
44:2m:40:ASN:HB3	44:2m:43:THR:HG23	1.98	0.46
53:2y:24:LEU:HG	53:2y:27:LEU:HD12	1.98	0.46
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.30	0.46
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.51	0.46
25:13:4:LEU:O	25:13:36:VAL:HA	2.16	0.46
32:1a:978:A:O2'	32:1a:1322:C:N3	2.41	0.46
32:1a:1093:A:N3	32:1a:1109:C:O2'	2.47	0.46
36:1e:107:ARG:NH1	60:1e:301:HOH:O	2.49	0.46
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.51	0.46
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.98	0.46
9:2N:104:LYS:HE2	9:2N:117:PHE:CZ	2.51	0.46
32:2a:1002:G:H2'	32:2a:1003:G:C8	2.51	0.46
33:2b:201:ILE:HG21	33:2b:214:ILE:HG12	1.97	0.46
35:2d:59:ARG:HD3	35:2d:59:ARG:HA	1.62	0.46
1:1A:528:A:OP1	60:1A:4152:HOH:O	2.21	0.45
1:1A:910:A:N1	1:1A:2277:G:H1'	2.31	0.45
1:1A:922:U:H2'	1:1A:923:C:C6	2.51	0.45
1:1A:2618:G:H21	4:1E:150:VAL:HG21	1.81	0.45
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.15	0.45
8:1I:14:ASP:O	8:1I:17:GLN:HB3	2.16	0.45
19:1X:94:GLY:HA3	19:1X:95:LEU:C	2.42	0.45
21:1Z:152:ALA:O	21:1Z:155:LEU:HB2	2.17	0.45
32:1a:164:U:H2'	32:1a:165:C:C6	2.50	0.45
35:1d:196:LEU:O	35:1d:198:VAL:N	2.48	0.45
40:1i:65:VAL:HG21	40:1i:73:GLN:HB3	1.98	0.45
53:1y:23:ARG:HA	53:1y:23:ARG:HD2	1.81	0.45
1:2A:890:A:H2'	1:2A:892:G:O4'	2.15	0.45
1:2A:1065:U:H4'	1:2A:1066:U:C5'	2.46	0.45
1:2A:2227:A:O2'	60:2A:3854:HOH:O	2.21	0.45
6:2G:54:GLU:O	6:2G:58:GLN:N	2.46	0.45
8:2I:26:ALA:O	8:2I:31:LEU:HB2	2.16	0.45
9:2N:28:THR:HG22	9:2N:29:LYS:HG3	1.98	0.45
32:2a:490:G:H2'	32:2a:491:G:C8	2.51	0.45
32:2a:560:U:H4'	32:2a:561:U:O5'	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1003:G:C5	32:2a:1004:A:H1'	2.51	0.45
32:2a:1030:C:N4	32:2a:1032:G:H1	2.13	0.45
32:2a:1265:G:H1	32:2a:1270:C:H42	1.65	0.45
32:2a:1277:C:H4'	32:2a:1281:U:H5	1.81	0.45
44:2m:19:LEU:HB3	44:2m:25:ILE:HG21	1.99	0.45
47:2p:5:ARG:HH21	47:2p:24:ALA:HA	1.82	0.45
1:1A:2115:G:H2'	1:1A:2117:A:H62	1.82	0.45
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.16	0.45
1:1A:2849:U:P	15:1T:95:ARG:HH12	2.39	0.45
14:1S:59:LYS:NZ	14:1S:68:GLN:HE22	2.14	0.45
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.65	0.45
32:1a:664:G:N2	32:1a:741:G:H1	2.06	0.45
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.48	0.45
32:1a:1237:C:H3'	32:1a:1336:C:H41	1.82	0.45
32:1a:1401:G:O6	53:1y:83:ARG:NH2	2.39	0.45
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.51	0.45
35:1d:162:LEU:HD13	35:1d:181:MET:HG2	1.99	0.45
39:1h:6:ILE:HB	39:1h:85:ARG:NH1	2.31	0.45
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.49	0.45
1:2A:1057:A:O2'	1:2A:1058:G:OP1	2.33	0.45
7:2H:25:LYS:HE3	7:2H:27:LYS:HZ1	1.80	0.45
20:2Y:19:LYS:HZ3	20:2Y:20:TYR:HE2	1.65	0.45
24:22:51:ARG:O	24:22:55:ARG:HG3	2.16	0.45
26:24:59:PHE:HB3	26:24:61:ARG:HB2	1.97	0.45
32:2a:109:A:C6	32:2a:326:G:C6	3.04	0.45
32:2a:1342:C:H2'	32:2a:1343:G:C8	2.51	0.45
38:2g:16:LEU:HD13	40:2i:45:ALA:HB2	1.97	0.45
1:1A:1063:G:N1	1:1A:1074:G:O6	2.49	0.45
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.17	0.45
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.32	0.45
17:1V:95:LEU:HD23	17:1V:97:LYS:HE3	1.98	0.45
33:1b:95:GLN:HG3	33:1b:147:LYS:O	2.16	0.45
44:1m:87:TYR:HA	44:1m:90:LEU:HD12	1.98	0.45
1:2A:684:G:OP1	29:27:16:HIS:ND1	2.48	0.45
1:2A:2531:A:C8	7:2H:175:LYS:HG3	2.51	0.45
21:2Z:28:MET:HE3	21:2Z:59:LEU:HD12	1.97	0.45
23:21:76:ARG:NH2	23:21:97:LEU:HB3	2.30	0.45
32:2a:1002:G:N2	32:2a:1039:C:C2	2.84	0.45
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.24	0.45
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.17	0.45
49:2r:40:LEU:HB3	49:2r:79:LEU:HD11	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:41:VAL:HG22	50:2s:42:PRO:HD2	1.98	0.45
1:1A:185:U:H4'	1:1A:218:A:H4'	1.98	0.45
1:1A:579:G:H2'	1:1A:580:C:C6	2.51	0.45
1:1A:744:G:OP1	4:1E:132:HIS:ND1	2.42	0.45
1:1A:888:C:O5'	44:1m:93:ARG:HD2	2.16	0.45
1:1A:1364:G:C8	23:11:3:LYS:HE2	2.51	0.45
1:1A:2099:U:H3	1:1A:2190:G:H1	1.63	0.45
6:1G:114:ILE:HG12	6:1G:140:ILE:HD13	1.98	0.45
7:1H:121:ILE:HG13	7:1H:144:VAL:HG21	1.97	0.45
9:1N:33:LEU:HD12	9:1N:38:HIS:CE1	2.51	0.45
11:1P:70:GLN:NE2	60:1P:307:HOH:O	2.50	0.45
32:1a:1148:U:O3'	40:1i:14:VAL:HG11	2.17	0.45
44:1m:22:ILE:HB	44:1m:25:ILE:HD12	1.99	0.45
1:2A:2641:G:P	9:2N:74:ARG:HH22	2.37	0.45
4:2E:170:LEU:HB3	4:2E:184:VAL:HG22	1.99	0.45
32:2a:130:A:H5'	48:2q:63:ARG:HE	1.80	0.45
32:2a:923:A:O2'	32:2a:1399:C:OP2	2.30	0.45
32:2a:1130:A:H5'	40:2i:18:PHE:CE1	2.51	0.45
36:2e:152:ARG:HB3	39:2h:43:GLY:HA3	1.98	0.45
4:1E:73:GLU:H	4:1E:73:GLU:CD	2.24	0.45
32:1a:1069:C:O2'	32:1a:1192:C:H1'	2.16	0.45
32:1a:1343:G:O2'	40:1i:121:ARG:HD2	2.17	0.45
33:1b:9:GLU:H	33:1b:9:GLU:HG3	1.41	0.45
44:1m:11:ARG:C	44:1m:13:LYS:H	2.25	0.45
1:2A:1007:C:H5''	9:2N:35:ARG:NH1	2.32	0.45
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.51	0.45
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.33	0.45
2:2B:28:C:H2'	2:2B:29:A:O4'	2.17	0.45
4:2E:50:GLY:HA2	4:2E:77:ILE:O	2.17	0.45
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.97	0.45
8:2I:130:TYR:HD2	8:2I:138:ILE:HD12	1.81	0.45
21:2Z:23:LYS:NZ	21:2Z:40:ASP:OD1	2.34	0.45
32:2a:925:G:H1'	32:2a:1502:A:C4	2.52	0.45
39:2h:51:VAL:HG11	39:2h:60:ARG:HH11	1.82	0.45
1:1A:251:A:C5	1:1A:252:G:H1'	2.52	0.45
1:1A:1171:G:H3'	1:1A:1173:G:H5'	1.97	0.45
1:1A:1512:U:H2'	1:1A:1513:C:C6	2.51	0.45
1:1A:2100:G:H1	1:1A:2189:U:H3	1.64	0.45
6:1G:52:ILE:H	6:1G:52:ILE:HG13	1.43	0.45
20:1Y:30:VAL:HG22	20:1Y:37:VAL:HG12	1.99	0.45
32:1a:710:G:OP1	37:1f:54:LYS:HE2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:986:A:H1'	50:1s:54:GLY:O	2.16	0.45
32:1a:1002:G:C6	32:1a:1003:G:C2	3.05	0.45
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.16	0.45
33:1b:71:VAL:HB	33:1b:164:VAL:HG22	1.98	0.45
1:2A:286:C:H2'	1:2A:287:C:C6	2.51	0.45
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.17	0.45
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.52	0.45
17:2V:24:LYS:HE2	17:2V:24:LYS:HB3	1.83	0.45
32:2a:1074:G:OP1	36:2e:64:ARG:NH1	2.48	0.45
32:2a:1096:C:H2'	32:2a:1097:C:H6	1.82	0.45
1:1A:604:G:OP2	11:1P:90:ARG:NH1	2.50	0.45
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.32	0.45
1:1A:1064:C:H3'	1:1A:1065:U:C5'	2.40	0.45
1:1A:1935:G:H1'	1:1A:1964:G:N2	2.31	0.45
1:1A:2206:G:H2'	1:1A:2207:G:C2	2.52	0.45
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.52	0.45
6:1G:43:LEU:C	6:1G:45:GLU:H	2.24	0.45
6:1G:45:GLU:H	6:1G:45:GLU:HG2	1.52	0.45
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.51	0.45
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.16	0.45
42:1k:33:THR:HG22	42:1k:39:PRO:HA	1.98	0.45
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.99	0.45
1:2A:362:U:O2'	1:2A:363:G:H5'	2.16	0.45
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.51	0.45
16:2U:32:PHE:N	60:2U:204:HOH:O	2.46	0.45
25:23:3:ARG:NH1	25:23:60:GLU:O	2.48	0.45
32:2a:176:C:H2'	32:2a:177:C:C6	2.52	0.45
32:2a:384:G:H2'	32:2a:385:C:C6	2.52	0.45
32:2a:437:U:O2'	35:2d:123:HIS:HD2	2.00	0.45
32:2a:1170:A:C4	32:2a:1171:G:H1'	2.52	0.45
32:2a:1312:G:H5'	50:2s:5:LEU:HD21	1.98	0.45
33:2b:114:ARG:HH12	33:2b:118:LEU:HD13	1.82	0.45
1:1A:882:G:H1	1:1A:894:C:H42	1.64	0.45
1:1A:1287:A:H8	13:1R:104:ARG:HD3	1.81	0.45
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.17	0.45
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.48	0.45
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.98	0.45
21:1Z:144:LEU:HD11	21:1Z:150:LEU:HD22	1.98	0.45
32:1a:278:G:OP2	48:1q:92:ARG:NH2	2.50	0.45
32:1a:636:U:H2'	32:1a:637:G:C8	2.52	0.45
32:1a:811:C:N4	60:1a:1930:HOH:O	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:121:ALA:O	38:1g:125:MET:HG3	2.16	0.45
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.16	0.45
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.51	0.45
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.52	0.45
1:2A:2820:A:OP1	13:2R:2:ARG:NH2	2.49	0.45
4:2E:89:ASP:OD2	4:2E:89:ASP:N	2.50	0.45
6:2G:33:ARG:NH2	6:2G:162:THR:HG21	2.32	0.45
6:2G:39:ILE:HD11	6:2G:102:PHE:CE1	2.51	0.45
6:2G:103:LEU:O	6:2G:107:LEU:HG	2.17	0.45
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.16	0.45
21:2Z:61:LEU:H	21:2Z:61:LEU:HD12	1.81	0.45
32:2a:559:A:H4'	32:2a:560:U:H3'	1.99	0.45
36:2e:78:HIS:HD2	39:2h:107:LEU:HD12	1.82	0.45
42:2k:20:TYR:CE1	42:2k:83:ILE:HD12	2.52	0.45
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.99	0.45
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.48	0.45
20:1Y:56:PRO:C	20:1Y:58:GLY:H	2.25	0.45
32:1a:750:G:N3	46:1o:23:GLY:HA3	2.31	0.45
32:1a:1019:C:H2'	32:1a:1020:U:O4'	2.17	0.45
32:1a:1027:C:H2'	32:1a:1028:C:C6	2.52	0.45
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.31	0.45
34:1c:59:ARG:HG2	34:1c:64:VAL:HB	1.99	0.45
1:2A:297:C:OP1	20:2Y:87:LYS:HG3	2.16	0.45
1:2A:2595:G:N2	1:2A:2598:A:OP2	2.47	0.45
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.52	0.45
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.51	0.45
17:2V:6:LYS:HB2	17:2V:38:LEU:HD11	1.99	0.45
17:2V:52:VAL:HG23	17:2V:55:ALA:HB3	1.98	0.45
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.52	0.45
48:2q:45:HIS:CD2	48:2q:47:PRO:HG3	2.52	0.45
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.17	0.45
1:1A:2304:G:H22	1:1A:2312:U:H3	1.66	0.45
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.67	0.45
32:1a:615:C:H2'	32:1a:616:G:O4'	2.17	0.45
1:2A:9:U:O2'	1:2A:10:G:OP1	2.33	0.45
1:2A:30:G:H2'	1:2A:31:C:C6	2.51	0.45
1:2A:813:U:H2'	1:2A:814:C:C6	2.52	0.45
1:2A:1500:G:O2'	3:2D:100:GLY:O	2.29	0.45
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.32	0.45
1:2A:2306:C:N4	6:2G:42:GLY:O	2.47	0.45
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2850:A:N7	1:2A:2868:A:O2'	2.45	0.45
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.99	0.45
1:1A:614:U:H2'	1:1A:614(A):U:O4'	2.16	0.44
21:1Z:98:MET:HE3	21:1Z:98:MET:HB2	1.81	0.44
22:10:43:THR:O	22:10:43:THR:HG23	2.18	0.44
53:1y:24:LEU:HD23	53:1y:24:LEU:HA	1.88	0.44
1:2A:205:G:O6	23:21:39:LYS:NZ	2.34	0.44
1:2A:922:U:H2'	1:2A:923:C:C6	2.51	0.44
1:2A:1084:A:H3'	1:2A:1085:A:C4'	2.47	0.44
1:2A:2564:A:OP1	1:2A:2648:C:H4'	2.17	0.44
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.82	0.44
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.99	0.44
32:2a:1023:G:H3'	32:2a:1024:G:C8	2.51	0.44
32:2a:1071:C:H2'	32:2a:1072:G:C8	2.50	0.44
32:2a:1318:A:O2'	50:2s:37:ARG:HB2	2.18	0.44
33:2b:16:HIS:CB	33:2b:210:SER:HB3	2.47	0.44
35:2d:108:LEU:HD13	35:2d:174:LEU:HD13	1.99	0.44
1:1A:784:A:C5	3:1D:229:VAL:HG21	2.52	0.44
1:1A:1857:G:C6	1:1A:1858:G:C6	3.05	0.44
1:1A:2142:C:H2'	1:1A:2143:C:C6	2.53	0.44
39:1h:51:VAL:HG21	39:1h:60:ARG:HD2	1.99	0.44
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.99	0.44
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.50	0.44
1:2A:234:C:H2'	1:2A:235:U:C6	2.53	0.44
1:2A:234:C:H2'	1:2A:235:U:H6	1.82	0.44
1:2A:380:U:H5'	23:21:18:ILE:HD12	1.99	0.44
1:2A:911:A:N6	12:2Q:11:LYS:O	2.44	0.44
6:2G:62:LEU:HB3	6:2G:143:GLU:HB3	1.98	0.44
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.17	0.44
32:2a:736:C:H2'	32:2a:737:A:C8	2.52	0.44
32:2a:977:A:O3'	32:2a:980:C:N4	2.50	0.44
32:2a:1308:U:OP2	44:2m:99:ARG:HG3	2.17	0.44
33:2b:119:GLU:OE1	33:2b:153:ARG:NH1	2.48	0.44
44:2m:27:LYS:HA	44:2m:27:LYS:HD2	1.75	0.44
46:2o:82:ILE:HD12	46:2o:88:ARG:HB2	1.99	0.44
50:2s:18:LYS:HD3	50:2s:31:ILE:HG23	1.99	0.44
1:1A:1187:G:OP1	17:1V:81:TYR:OH	2.26	0.44
1:1A:1957:C:OP1	60:1A:4154:HOH:O	2.21	0.44
1:1A:2140:C:H2'	1:1A:2141:G:C8	2.53	0.44
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.53	0.44
32:1a:277:C:H5''	48:1q:68:ARG:NH2	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:120:THR:H	39:1h:123:GLU:HB2	1.81	0.44
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	2.00	0.44
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.53	0.44
3:2D:26:LYS:HE2	3:2D:28:GLU:O	2.17	0.44
6:2G:9:ARG:O	6:2G:13:GLU:HB2	2.18	0.44
7:2H:102:ALA:HA	7:2H:117:PRO:HD3	1.99	0.44
14:2S:93:LYS:NZ	14:2S:95:HIS:HB2	2.33	0.44
18:2W:60:ASN:HD22	18:2W:60:ASN:N	2.15	0.44
28:26:23:THR:OG1	28:26:24:GLU:N	2.49	0.44
32:2a:607:A:C2	47:2p:31:LYS:HG3	2.51	0.44
32:2a:1278:U:H5'	32:2a:1279:A:C4	2.53	0.44
32:2a:1465:C:H2'	32:2a:1466:C:O4'	2.16	0.44
40:2i:51:ARG:HG2	40:2i:56:LEU:HD21	1.99	0.44
48:2q:22:LEU:HD11	48:2q:39:SER:HB2	1.98	0.44
51:2t:57:ARG:HH12	51:2t:100:ILE:HB	1.83	0.44
53:2y:7:SER:HB3	53:2y:10:MET:O	2.18	0.44
1:1A:2134:A:O2'	1:1A:2159:G:N3	2.50	0.44
12:1Q:58:PHE:O	12:1Q:60:ARG:N	2.49	0.44
14:1S:58:LEU:HD23	14:1S:58:LEU:HA	1.82	0.44
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.15	0.44
32:1a:1251:A:H2'	32:1a:1252:A:C8	2.53	0.44
32:1a:1320:C:H2'	32:1a:1321:C:O4'	2.16	0.44
37:1f:45:LEU:HD12	37:1f:59:TYR:CD1	2.51	0.44
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.82	0.44
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	1.99	0.44
7:2H:16:SER:O	7:2H:26:VAL:HA	2.18	0.44
11:2P:88:LEU:HD11	11:2P:114:ILE:HD12	1.99	0.44
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.52	0.44
1:1A:2563:U:H4'	10:1O:28:SER:HA	1.99	0.44
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.52	0.44
21:1Z:125:LEU:HB3	21:1Z:165:VAL:HG13	1.99	0.44
32:1a:1092:A:H1'	32:1a:1183:A:N6	2.31	0.44
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.52	0.44
35:1d:142:PRO:HA	35:1d:185:PHE:HD2	1.82	0.44
39:1h:7:ALA:HB2	39:1h:85:ARG:HG3	1.99	0.44
1:2A:154(A):C:N4	1:2A:171:G:H1	2.16	0.44
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.18	0.44
2:2B:114:C:HO2'	14:2S:47:THR:H	1.66	0.44
7:2H:124:GLU:HB2	7:2H:132:ARG:HB3	1.99	0.44
17:2V:62:LEU:HD21	17:2V:95:LEU:HB2	1.99	0.44
32:2a:44:G:OP2	47:2p:12:LYS:NZ	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:560:U:H5'	32:2a:566:G:N2	2.32	0.44
32:2a:662:G:O2'	32:2a:836:G:OP1	2.35	0.44
32:2a:707:C:H2'	32:2a:708:C:C6	2.53	0.44
34:2c:54:ARG:HB2	34:2c:69:HIS:HB2	1.99	0.44
35:2d:79:PHE:CE1	35:2d:204:ILE:HD13	2.51	0.44
38:2g:23:VAL:O	38:2g:27:ILE:HG13	2.17	0.44
52:2u:18:TYR:CE1	52:2u:24:ARG:HB2	2.52	0.44
1:1A:271(L):U:H5'	8:1I:50:ARG:HH12	1.81	0.44
1:1A:2820:A:P	13:1R:2:ARG:HH22	2.39	0.44
2:1B:48:A:H2'	2:1B:49:C:C6	2.52	0.44
9:1N:73:THR:HA	9:1N:83:LYS:O	2.17	0.44
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.99	0.44
13:1R:83:ILE:O	13:1R:86:ARG:HG2	2.16	0.44
32:1a:1027:C:H2'	32:1a:1028:C:C5	2.52	0.44
1:2A:322:A:OP1	5:2F:168:ARG:HD3	2.17	0.44
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.18	0.44
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.32	0.44
5:2F:120:GLU:HB2	5:2F:122:LYS:HG2	1.99	0.44
32:2a:857:C:H2'	32:2a:858:G:O4'	2.18	0.44
34:2c:6:HIS:CD2	45:2n:49:HIS:HB3	2.53	0.44
1:1A:613:G:N2	1:1A:614(C):A:O2'	2.50	0.44
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.33	0.44
1:1A:1364:G:OP2	23:11:3:LYS:HD3	2.18	0.44
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.17	0.44
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.51	0.44
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	2.00	0.44
21:1Z:3:TYR:CD2	21:1Z:51:ALA:HB2	2.52	0.44
1:2A:93:G:H2'	1:2A:94:C:C6	2.53	0.44
1:2A:253:C:O2'	60:2A:3855:HOH:O	2.21	0.44
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.81	0.44
7:2H:148:ILE:HA	7:2H:151:ILE:HD12	2.00	0.44
20:2Y:56:PRO:C	20:2Y:58:GLY:H	2.26	0.44
32:2a:19:C:H5''	36:2e:86:ALA:HB3	2.00	0.44
32:2a:598:U:H4'	39:2h:94:TYR:CD2	2.53	0.44
32:2a:1090:U:H2'	32:2a:1091:U:C6	2.52	0.44
32:2a:1263:C:H2'	32:2a:1264:C:C6	2.53	0.44
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.53	0.44
35:2d:153:ARG:NH1	60:2d:401:HOH:O	2.50	0.44
36:2e:103:GLY:O	36:2e:107:ARG:HB3	2.17	0.44
44:2m:94:ARG:HB3	44:2m:96:LEU:HD12	2.00	0.44
1:1A:1250:G:H5''	60:1U:330:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1289:C:H2'	1:1A:1290:C:H6	1.83	0.44
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.18	0.44
10:1O:3:GLN:NE2	60:1O:308:HOH:O	2.51	0.44
13:1R:104:ARG:HD2	13:1R:107:ASP:OD1	2.17	0.44
15:1T:108:ARG:HA	15:1T:111:ARG:HH11	1.83	0.44
18:1W:86:LEU:HD22	18:1W:96:ILE:HD11	2.00	0.44
26:14:59:PHE:CZ	50:1s:45:VAL:HG21	2.53	0.44
32:1a:1048:G:OP1	45:1n:3:ARG:HB3	2.17	0.44
32:1a:1074:G:OP1	36:1e:64:ARG:NH1	2.51	0.44
33:1b:215:LEU:O	33:1b:219:VAL:HG23	2.18	0.44
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.33	0.44
40:1i:9:ARG:O	40:1i:104:ARG:HG3	2.18	0.44
44:1m:106:ASN:HB2	44:1m:107:ALA:H	1.46	0.44
1:2A:494:G:H3'	60:2A:4010:HOH:O	2.18	0.44
1:2A:898:C:H2'	1:2A:899:A:O4'	2.17	0.44
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.18	0.44
1:2A:2184:G:H2'	1:2A:2185:C:O4'	2.18	0.44
1:2A:2189:U:H2'	1:2A:2190:G:C8	2.53	0.44
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.51	0.44
19:2X:21:PHE:CZ	19:2X:92:LEU:HB3	2.52	0.44
32:2a:404:U:H2'	32:2a:405:U:C6	2.53	0.44
32:2a:875:C:H1'	39:2h:15:ASN:HD21	1.83	0.44
32:2a:946:A:H2'	32:2a:947:G:C8	2.53	0.44
32:2a:1151:A:O2'	32:2a:1152:A:H8	2.01	0.44
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.83	0.44
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.18	0.44
37:2f:3:ARG:HD3	37:2f:64:GLN:NE2	2.33	0.44
40:2i:28:VAL:HG13	40:2i:63:ILE:HG22	1.99	0.44
51:2t:76:ALA:O	51:2t:80:ARG:HG3	2.18	0.44
1:1A:1071:G:H1'	1:1A:1089:G:C8	2.53	0.44
1:1A:2038:G:O6	60:1A:4153:HOH:O	2.21	0.44
1:1A:2258:C:OP2	60:1A:4155:HOH:O	2.21	0.44
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.33	0.44
32:1a:235:C:H5'	48:1q:70:ARG:HG3	1.99	0.44
32:1a:384:G:H2'	32:1a:385:C:C6	2.53	0.44
32:1a:418:C:H1'	32:1a:540:G:O2'	2.17	0.44
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.18	0.44
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.53	0.44
32:1a:1400:5MC:N3	53:1y:63:ALA:HA	2.33	0.44
35:1d:53:ASP:HB3	35:1d:57:ARG:NH1	2.33	0.44
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:4:ILE:O	44:1m:4:ILE:HG13	2.18	0.44
44:1m:16:ASP:N	44:1m:16:ASP:OD1	2.51	0.44
1:2A:27:G:N2	1:2A:512:G:H1'	2.31	0.44
1:2A:583:G:OP2	16:2U:10:ARG:HD2	2.17	0.44
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.18	0.44
2:2B:4:C:H2'	2:2B:5:C:C6	2.53	0.44
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.50	0.44
6:2G:145:THR:HG23	6:2G:147:ASP:H	1.82	0.44
15:2T:8:LYS:HB3	15:2T:8:LYS:HE2	1.81	0.44
32:2a:114:U:H1'	32:2a:353:A:H1'	1.99	0.44
32:2a:625:G:H2'	32:2a:626:U:H6	1.83	0.44
32:2a:1212:U:H4'	32:2a:1213:A:N7	2.33	0.44
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.53	0.44
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.52	0.44
32:2a:1516:G:H2'	32:2a:1518:MA6:OP2	2.18	0.44
33:2b:55:PHE:CD1	33:2b:221:LEU:HD22	2.53	0.44
33:2b:97:TRP:CE2	33:2b:101:MET:HE2	2.53	0.44
38:2g:95:ARG:HE	38:2g:99:LEU:HD11	1.82	0.44
39:2h:121:ASP:HB2	39:2h:125:ARG:NH2	2.32	0.44
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	1.99	0.44
1:1A:299:A:N1	1:1A:322:A:O2'	2.44	0.43
1:1A:2648:C:H2'	1:1A:2649:U:C6	2.53	0.43
6:1G:120:LEU:HB3	6:1G:131:TYR:OH	2.18	0.43
13:1R:38:VAL:HB	13:1R:39:PRO:HD3	2.00	0.43
32:1a:1040:U:H2'	32:1a:1041:A:H8	1.82	0.43
33:1b:100:GLY:N	33:1b:176:GLU:OE2	2.41	0.43
34:1c:71:ALA:HB2	34:1c:115:LEU:HD21	1.99	0.43
36:1e:69:VAL:O	36:1e:71:LEU:N	2.51	0.43
39:1h:20:TYR:HA	39:1h:65:TYR:CZ	2.52	0.43
40:1i:4:TYR:HA	40:1i:87:GLN:HE21	1.82	0.43
46:1o:84:LYS:O	46:1o:84:LYS:HD3	2.17	0.43
48:1q:86:GLU:O	48:1q:90:ILE:HG12	2.17	0.43
1:2A:455:C:N3	1:2A:472:A:H2'	2.33	0.43
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.50	0.43
1:2A:1166:C:H2'	1:2A:1167:U:C6	2.53	0.43
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.53	0.43
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.53	0.43
5:2F:148:LEU:HD22	5:2F:154:VAL:HG21	1.99	0.43
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.53	0.43
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	1.99	0.43
15:2T:16:ARG:NH2	15:2T:83:ILE:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:102:ILE:HA	15:2T:105:LEU:HD12	2.00	0.43
28:26:34:LEU:HD23	28:26:34:LEU:HA	1.86	0.43
32:2a:949:A:H1'	32:2a:1364:U:H3	1.81	0.43
32:2a:1273:G:H3'	32:2a:1274:G:C8	2.48	0.43
33:2b:70:PHE:CD1	33:2b:163:PHE:HB3	2.53	0.43
33:2b:153:ARG:HE	33:2b:153:ARG:HB2	1.54	0.43
34:2c:8:ILE:HG23	34:2c:16:ARG:HD3	2.00	0.43
35:2d:166:LYS:H	35:2d:166:LYS:HD3	1.82	0.43
41:2j:47:PHE:HB3	45:2n:34:TYR:CE1	2.52	0.43
43:2l:26:ALA:HB1	43:2l:60:LEU:HD12	2.00	0.43
46:2o:65:ARG:HG2	46:2o:68:ARG:HH21	1.83	0.43
48:2q:40:LYS:HD3	48:2q:42:TYR:CZ	2.53	0.43
1:1A:210:C:OP2	29:17:29:LYS:NZ	2.51	0.43
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.43	0.43
4:1E:55:ASN:HB3	4:1E:58:ARG:HG3	2.01	0.43
7:1H:157:TYR:CE1	7:1H:172:LYS:HG3	2.53	0.43
32:1a:116:A:H61	32:1a:313:A:H1'	1.83	0.43
35:1d:3:ARG:HD3	35:1d:118:ARG:NE	2.34	0.43
51:1t:57:ARG:HH22	51:1t:100:ILE:HD12	1.82	0.43
1:2A:171:G:H2'	1:2A:172:C:C6	2.53	0.43
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.18	0.43
1:2A:1101:U:H2'	1:2A:1102:C:H6	1.84	0.43
1:2A:1470:G:N7	60:2A:3992:HOH:O	2.36	0.43
1:2A:2137:C:H2'	1:2A:2138:C:C6	2.53	0.43
2:2B:80:U:H2'	2:2B:81:G:C8	2.52	0.43
6:2G:40:ASN:HB3	6:2G:156:ASP:HB2	1.99	0.43
21:2Z:36:LYS:HB2	21:2Z:36:LYS:HE3	1.80	0.43
32:2a:567:G:H1'	60:2a:3283:HOH:O	2.18	0.43
32:2a:1316:G:H5''	45:2n:17:LYS:NZ	2.32	0.43
33:2b:222:ILE:O	33:2b:226:ARG:HB2	2.18	0.43
43:2l:54:LYS:NZ	60:2l:201:HOH:O	2.38	0.43
51:2t:18:GLN:O	51:2t:22:ARG:HG3	2.18	0.43
1:1A:1176:G:H1'	1:1A:1177:A:H5''	1.99	0.43
1:1A:1826:G:H4'	3:1D:242:ARG:NH1	2.33	0.43
2:1B:4:C:H42	2:1B:117:G:H1	1.65	0.43
6:1G:77:ILE:HB	6:1G:82:LEU:HB2	2.01	0.43
32:1a:17:U:H1'	32:1a:1080:A:N3	2.33	0.43
32:1a:1127:G:H5'	32:1a:1280:A:O2'	2.18	0.43
32:1a:1239:A:H62	32:1a:1299:A:H61	1.66	0.43
32:1a:1265:G:H1	32:1a:1270:C:H42	1.65	0.43
34:1c:179:ARG:HG3	34:1c:206:GLU:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1055:G:H3'	1:2A:1056:G:C8	2.54	0.43
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.01	0.43
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.35	0.43
1:2A:2130:U:O2'	1:2A:2133:G:H4'	2.17	0.43
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.52	0.43
3:2D:101:GLU:OE2	3:2D:103:ARG:NH1	2.48	0.43
6:2G:97:ASP:HA	6:2G:100:TRP:CD1	2.50	0.43
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.40	0.43
14:2S:67:ARG:HE	14:2S:67:ARG:HB2	1.65	0.43
32:2a:131:C:H2'	32:2a:132:C:C6	2.53	0.43
32:2a:953:G:H4'	53:2y:6:THR:CG2	2.42	0.43
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.53	0.43
34:2c:3:ASN:HB2	34:2c:4:LYS:H	1.70	0.43
44:2m:92:HIS:CE1	44:2m:98:VAL:HG21	2.53	0.43
53:2y:24:LEU:HD12	53:2y:78:ILE:HD12	2.00	0.43
1:1A:747:U:O2	1:1A:2014:A:H1'	2.18	0.43
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.17	0.43
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.19	0.43
32:1a:114:U:H1'	32:1a:353:A:H1'	2.00	0.43
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.86	0.43
1:2A:77:C:OP2	60:2A:3857:HOH:O	2.21	0.43
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.53	0.43
1:2A:390:A:N6	60:2A:4170:HOH:O	2.50	0.43
1:2A:521:G:O6	60:2A:3851:HOH:O	2.19	0.43
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.30	0.43
1:2A:2254:C:N4	60:2A:3882:HOH:O	2.51	0.43
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.60	0.43
60:2A:4752:HOH:O	5:2F:74:ARG:HD2	2.18	0.43
6:2G:86:MET:HE3	6:2G:86:MET:HB2	1.93	0.43
27:25:20:ARG:HG2	27:25:23:HIS:CE1	2.53	0.43
27:25:41:PRO:O	27:25:44:THR:OG1	2.36	0.43
32:2a:551:U:H2'	32:2a:552:U:C6	2.52	0.43
38:2g:53:LYS:HD2	38:2g:125:MET:HE1	2.01	0.43
41:2j:38:ILE:O	41:2j:38:ILE:HG12	2.18	0.43
1:1A:1800:C:OP1	3:1D:264:LYS:NZ	2.50	0.43
1:1A:2096:U:H2'	1:1A:2097:C:C6	2.54	0.43
1:1A:2896:C:H2'	1:1A:2897:U:C6	2.53	0.43
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.84	0.43
32:1a:279:A:OP2	48:1q:95:TYR:OH	2.34	0.43
35:1d:168:ARG:HA	35:1d:168:ARG:HD3	1.47	0.43
46:1o:6:GLU:N	46:1o:6:GLU:OE2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:616:G:H5'	5:2F:205:ARG:HD3	2.00	0.43
1:2A:810:U:C4	11:2P:29:LYS:O	2.71	0.43
1:2A:1048:A:N1	1:2A:1112:G:O2'	2.45	0.43
1:2A:1288:U:OP1	1:2A:1289:C:N4	2.45	0.43
1:2A:2660:A:H2'	1:2A:2661:G:O4'	2.18	0.43
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	2.01	0.43
9:2N:4:TYR:HB2	16:2U:101:ARG:NH1	2.34	0.43
32:2a:442:C:H42	32:2a:492:G:H1	1.66	0.43
32:2a:600:C:H2'	32:2a:601:C:C6	2.53	0.43
32:2a:1323:G:H4'	32:2a:1363:C:C2	2.53	0.43
33:2b:15:VAL:HG23	33:2b:16:HIS:CD2	2.53	0.43
1:1A:286:C:H2'	1:1A:287:C:H6	1.83	0.43
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.33	0.43
1:1A:1509(B):A:H2'	1:1A:1510:G:O4'	2.19	0.43
1:1A:1766:U:H2'	1:1A:1767:C:H6	1.83	0.43
1:1A:2590:A:H2'	1:1A:2591:C:C6	2.54	0.43
4:1E:4:ILE:HD13	4:1E:28:ALA:HB1	2.01	0.43
32:1a:181:G:H4'	32:1a:182:U:H5'	2.01	0.43
32:1a:1036:G:H5''	32:1a:1037:C:C5	2.54	0.43
50:1s:36:ARG:NH1	50:1s:52:TYR:O	2.47	0.43
1:2A:35:G:H2'	1:2A:36:G:O4'	2.19	0.43
1:2A:1598:C:H2'	1:2A:1599:C:C6	2.53	0.43
1:2A:2105:C:H42	1:2A:2184:G:H1	1.66	0.43
4:2E:72:VAL:HG12	4:2E:73:GLU:O	2.18	0.43
21:2Z:7:ALA:O	21:2Z:62:PRO:HD3	2.19	0.43
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.19	0.43
32:2a:45:U:H2'	32:2a:46:G:C8	2.53	0.43
38:2g:146:GLU:OE1	38:2g:149:ARG:NE	2.52	0.43
43:2l:88:GLY:O	43:2l:99:HIS:HD2	2.01	0.43
46:2o:32:LEU:HD22	46:2o:59:MET:HG2	2.00	0.43
1:1A:1007:C:H5''	9:1N:35:ARG:NH1	2.33	0.43
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.19	0.43
1:1A:1614:A:C2	18:1W:93:ALA:HB2	2.53	0.43
1:1A:1773:A:C5	1:1A:1829:A:H1'	2.53	0.43
1:1A:2114:A:H2'	1:1A:2115:G:O4'	2.18	0.43
10:1O:16:ALA:HB2	10:1O:52:VAL:HG21	2.01	0.43
15:1T:108:ARG:HA	15:1T:111:ARG:NH1	2.34	0.43
19:1X:60:ARG:NH1	29:17:47:ARG:HH22	2.17	0.43
27:15:34:PRO:HG2	27:15:35:GLU:OE1	2.19	0.43
32:1a:90:U:O2'	32:1a:91:C:H5'	2.19	0.43
32:1a:826:C:O2	39:1h:15:ASN:ND2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	2.01	0.43
36:1e:150:ARG:HE	36:1e:150:ARG:HB2	1.62	0.43
47:1p:60:LEU:HD21	47:1p:80:PHE:HE1	1.83	0.43
48:1q:59:ILE:HG22	48:1q:73:VAL:HA	2.01	0.43
50:1s:40:ILE:HA	50:1s:44:MET:SD	2.59	0.43
1:2A:1277:G:O2'	13:2R:24:GLN:HG2	2.19	0.43
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.48	0.43
26:24:67:TYR:HB3	50:2s:16:LEU:HD11	2.01	0.43
32:2a:187:C:O2'	51:2t:89:ARG:HD3	2.18	0.43
32:2a:718:G:H5'	42:2k:117:ASN:OD1	2.19	0.43
40:2i:5:TYR:OH	40:2i:16:ARG:HG2	2.19	0.43
41:2j:68:HIS:N	41:2j:68:HIS:CD2	2.86	0.43
46:2o:82:ILE:O	46:2o:86:GLY:N	2.51	0.43
1:1A:583:G:OP2	16:1U:10:ARG:HD2	2.19	0.43
1:1A:2137:C:N3	1:1A:2154:G:N2	2.63	0.43
8:1I:132:PRO:HD2	8:1I:136:VAL:O	2.19	0.43
12:1Q:21:THR:HG21	12:1Q:101:ARG:HG3	2.00	0.43
32:1a:382:A:H2'	32:1a:383:A:C8	2.54	0.43
32:1a:946:A:O2'	32:1a:1333:A:N3	2.49	0.43
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.53	0.43
33:1b:121:LEU:HD12	33:1b:126:GLU:HB3	2.00	0.43
47:1p:15:PRO:HD2	47:1p:42:ARG:HD3	2.01	0.43
1:2A:392:C:H5''	1:2A:409:C:H5''	2.01	0.43
1:2A:1580:A:H8	1:2A:1580:A:OP2	2.01	0.43
2:2B:24:G:N7	2:2B:56:G:H2'	2.34	0.43
2:2B:58:A:H2'	2:2B:59:A:O4'	2.19	0.43
6:2G:15:VAL:HG21	6:2G:176:LEU:HD23	2.00	0.43
8:2I:91:SER:HB3	8:2I:121:LYS:HD3	2.01	0.43
9:2N:73:THR:HB	9:2N:82:LEU:HD11	2.01	0.43
26:24:34:GLU:HB2	44:2m:57:ARG:NE	2.34	0.43
32:2a:116:A:H61	32:2a:313:A:H1'	1.84	0.43
32:2a:606:G:H5''	32:2a:607:A:H5'	2.01	0.43
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.54	0.43
39:2h:17:THR:HG22	39:2h:63:LEU:HG	2.01	0.43
44:2m:51:ALA:O	44:2m:55:ARG:HB2	2.19	0.43
46:2o:68:ARG:NH1	60:2o:201:HOH:O	2.52	0.43
1:1A:1140:C:O3'	9:1N:25:ARG:NH1	2.52	0.43
1:1A:1274:A:N3	1:1A:1297:C:H1'	2.34	0.43
1:1A:2650:U:H2'	1:1A:2651:C:C6	2.53	0.43
56:1A:4058:MPD:HM2	56:1A:4058:MPD:H4	1.71	0.43
12:1Q:101:ARG:HD2	60:1Q:308:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:3:TYR:CE2	21:1Z:51:ALA:HB2	2.54	0.43
26:14:24:THR:OG1	26:14:25:TYR:N	2.52	0.43
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.44	0.43
32:1a:636:U:H2'	32:1a:637:G:H8	1.83	0.43
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.19	0.43
44:1m:3:ARG:HH22	44:1m:11:ARG:HG2	1.83	0.43
46:1o:82:ILE:O	46:1o:86:GLY:N	2.51	0.43
1:2A:2330:G:H2'	1:2A:2331:G:O4'	2.19	0.43
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.54	0.43
2:2B:66:A:N6	2:2B:109:C:H5'	2.29	0.43
10:2O:64:ARG:HB2	10:2O:79:PHE:CG	2.54	0.43
32:2a:1201:A:H4'	32:2a:1202:G:H5''	2.00	0.43
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.32	0.43
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.34	0.43
33:2b:187:LEU:HB2	33:2b:201:ILE:HB	2.01	0.43
36:2e:60:TYR:CE2	36:2e:64:ARG:HD3	2.53	0.43
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.34	0.43
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.19	0.43
1:1A:2548:G:O6	60:1A:4157:HOH:O	2.22	0.43
4:1E:178:GLU:H	4:1E:178:GLU:CD	2.27	0.43
8:1I:27:ARG:HD2	23:11:71:TYR:CE2	2.54	0.43
12:1Q:108:GLY:HA3	21:1Z:116:VAL:HG13	2.01	0.43
26:14:41:PRO:HB3	26:14:47:GLN:O	2.19	0.43
32:1a:598:U:O4	60:1a:1903:HOH:O	2.21	0.43
32:1a:967:5MC:H4'	40:1i:125:TYR:HE1	1.83	0.43
32:1a:1151:A:O2'	32:1a:1152:A:H8	2.02	0.43
35:1d:122:ARG:HA	35:1d:122:ARG:HD2	1.68	0.43
1:2A:609:A:H2'	1:2A:610:G:O4'	2.19	0.43
1:2A:760:G:H2'	1:2A:761:A:O4'	2.19	0.43
1:2A:859:G:O2'	1:2A:916:G:O6	2.33	0.43
1:2A:1590:U:H2'	1:2A:1591:G:C8	2.54	0.43
10:2O:36:GLY:HA3	10:2O:109:LYS:HD2	2.00	0.43
16:2U:52:ARG:HA	16:2U:55:ARG:HG3	2.01	0.43
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB2	2.00	0.43
32:2a:251:G:N7	60:2a:3253:HOH:O	2.36	0.43
32:2a:407:G:H5''	35:2d:115:ARG:HB3	2.01	0.43
32:2a:435:C:H2'	32:2a:436:C:H6	1.83	0.43
32:2a:973:G:H1'	41:2j:54:PHE:HD1	1.82	0.43
32:2a:1106:G:H5''	34:2c:172:ARG:HG2	2.01	0.43
36:2e:88:LYS:HE2	36:2e:123:LEU:HD12	1.99	0.43
47:2p:58:TYR:O	47:2p:61:SER:OG	2.23	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:191:A:H2'	1:1A:192:C:C6	2.54	0.42
1:1A:493:G:H2'	1:1A:494:G:O4'	2.19	0.42
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.54	0.42
1:1A:2182:G:H2'	1:1A:2183:C:C6	2.54	0.42
32:1a:194:C:H2'	32:1a:195:A:H5''	2.00	0.42
32:1a:409:G:H1	32:1a:433:C:H42	1.67	0.42
35:1d:166:LYS:HE3	35:1d:168:ARG:NH1	2.34	0.42
40:1i:21:PRO:HA	40:1i:59:PHE:HA	2.01	0.42
1:2A:196:A:N3	1:2A:196:A:H2'	2.34	0.42
1:2A:896:A:H5''	21:2Z:147:GLY:HA3	2.01	0.42
2:2B:16:G:H1	2:2B:68:C:H42	1.67	0.42
13:2R:59:ASP:OD1	13:2R:59:ASP:N	2.51	0.42
14:2S:105:ALA:O	14:2S:110:LEU:HB2	2.19	0.42
32:2a:273:A:H1'	48:2q:16:GLN:HE21	1.83	0.42
32:2a:555:C:H2'	32:2a:556:C:C6	2.54	0.42
34:2c:180:ALA:HB1	34:2c:203:PHE:CE1	2.53	0.42
42:2k:115:PRO:C	42:2k:117:ASN:HA	2.44	0.42
48:2q:45:HIS:NE2	48:2q:47:PRO:HG3	2.34	0.42
1:1A:2019:A:O4'	16:1U:34:LYS:HE3	2.18	0.42
1:1A:2030:A:H4'	1:1A:2031:A:C8	2.54	0.42
1:1A:2119:A:O2'	1:1A:2120:G:H5'	2.18	0.42
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.18	0.42
1:1A:2314:C:H2'	1:1A:2315:G:H8	1.82	0.42
15:1T:51:ARG:NH1	60:1T:301:HOH:O	2.32	0.42
16:1U:34:LYS:HD3	16:1U:34:LYS:HA	1.69	0.42
17:1V:52:VAL:CG2	17:1V:55:ALA:HB3	2.50	0.42
32:1a:60:A:H4'	32:1a:61:G:H5'	2.00	0.42
32:1a:60:A:N1	32:1a:107:G:O2'	2.50	0.42
32:1a:584:G:H5'	48:1q:91:ARG:NH2	2.33	0.42
36:1e:57:LYS:HG2	36:1e:61:TYR:CE2	2.54	0.42
40:1i:29:ASN:OD1	40:1i:65:VAL:N	2.50	0.42
53:1y:52:ALA:HB2	53:1y:77:LEU:HD21	2.01	0.42
1:2A:588:U:H1'	5:2F:90:PHE:CG	2.54	0.42
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.19	0.42
1:2A:2104:G:O6	1:2A:2185:C:C4	2.72	0.42
4:2E:54:GLN:OE1	4:2E:55:ASN:N	2.52	0.42
7:2H:12:PRO:O	7:2H:15:VAL:HG22	2.19	0.42
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	2.00	0.42
18:2W:80:PRO:O	18:2W:100:THR:HB	2.19	0.42
32:2a:60:A:H4'	32:2a:61:G:O5'	2.20	0.42
32:2a:513:C:H2'	32:2a:514:C:C6	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.54	0.42
53:2y:23:ARG:HG3	53:2y:78:ILE:HG13	2.00	0.42
1:1A:569:U:C4	1:1A:570:G:C6	3.07	0.42
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.54	0.42
5:1F:11:VAL:O	5:1F:17:ARG:HA	2.19	0.42
7:1H:41:MET:HE2	7:1H:65:HIS:HA	2.01	0.42
24:12:2:LYS:O	24:12:6:VAL:HG23	2.18	0.42
32:1a:500:G:H2'	32:1a:501:C:C6	2.54	0.42
32:1a:848:C:H2'	32:1a:849:C:C6	2.54	0.42
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.54	0.42
40:1i:77:ILE:O	40:1i:81:ILE:HG23	2.19	0.42
52:1u:6:ARG:HE	52:1u:15:ARG:NH1	2.16	0.42
1:2A:8:A:H2'	1:2A:9:U:C6	2.54	0.42
1:2A:78:A:H2'	1:2A:79:G:C8	2.54	0.42
1:2A:1092:C:O2	1:2A:1092:C:H2'	2.20	0.42
1:2A:1101:U:H2'	1:2A:1102:C:C6	2.54	0.42
1:2A:2047:U:O2'	1:2A:2823:A:N1	2.50	0.42
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.54	0.42
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	2.01	0.42
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.29	0.42
20:2Y:68:HIS:ND1	20:2Y:70:SER:HB3	2.34	0.42
24:22:17:SER:N	24:22:20:GLU:OE1	2.47	0.42
26:24:50:VAL:HG11	44:2m:64:TRP:C	2.44	0.42
38:2g:13:GLN:HE21	38:2g:13:GLN:HB2	1.63	0.42
44:2m:47:ASP:N	44:2m:47:ASP:OD1	2.53	0.42
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.19	0.42
1:1A:1843:C:H5'	3:1D:253:GLN:HE22	1.84	0.42
1:1A:2059:A:H2'	1:1A:2503:2MA:HM23	2.02	0.42
4:1E:9:VAL:HB	15:1T:3:ARG:HG2	2.02	0.42
9:1N:21:LYS:NZ	9:1N:140:VAL:OXT	2.52	0.42
30:18:47:LYS:NZ	56:18:104:MPD:H51	2.34	0.42
32:1a:167:G:H2'	32:1a:168:G:C8	2.54	0.42
32:1a:691:G:H2'	32:1a:692:U:C6	2.54	0.42
32:1a:838:G:H2'	32:1a:839:U:H2'	2.01	0.42
1:2A:706:A:H2'	1:2A:707:G:O4'	2.19	0.42
1:2A:994:C:O2'	1:2A:996:A:OP1	2.34	0.42
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.19	0.42
1:2A:2066:C:H5''	60:2A:5757:HOH:O	2.18	0.42
1:2A:2185:C:N4	1:2A:2186:G:O6	2.53	0.42
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.54	0.42
1:2A:2801(A):A:N3	1:2A:2895:U:H1'	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	2.02	0.42
6:2G:18:GLU:OE2	6:2G:21:ARG:NH2	2.49	0.42
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.52	0.42
32:2a:673:G:O3'	37:2f:87:ARG:NH2	2.52	0.42
32:2a:1400:5MC:C2	53:2y:63:ALA:HA	2.54	0.42
33:2b:74:LYS:O	33:2b:78:GLN:N	2.53	0.42
33:2b:134:GLU:O	33:2b:138:LEU:HG	2.18	0.42
35:2d:162:LEU:HD13	35:2d:181:MET:HG2	2.01	0.42
41:2j:30:SER:HB3	41:2j:81:THR:HG22	2.02	0.42
1:1A:621:A:OP2	11:1P:108:LYS:NZ	2.51	0.42
1:1A:686:G:N2	1:1A:788:A:H61	2.16	0.42
1:1A:839:U:H2'	1:1A:840:C:C6	2.54	0.42
1:1A:1013:C:OP2	60:1A:4156:HOH:O	2.21	0.42
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.35	0.42
1:1A:1359:A:N6	1:1A:1372:U:H3	2.16	0.42
1:1A:1486:A:H2'	1:1A:1487:G:H8	1.85	0.42
1:1A:2115:G:H2'	1:1A:2117:A:N6	2.33	0.42
1:1A:2805:G:H2'	1:1A:2807:G:C8	2.54	0.42
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.49	0.42
8:1I:9:LEU:HD13	8:1I:9:LEU:HA	1.86	0.42
11:1P:59:LEU:HG	30:18:58:ILE:HG12	2.01	0.42
23:11:23:LYS:HB2	23:11:23:LYS:HE3	1.84	0.42
34:1c:89:GLU:HG3	34:1c:90:GLU:N	2.35	0.42
1:2A:26:G:C6	1:2A:27:G:N1	2.88	0.42
1:2A:855:G:H2'	1:2A:856:C:C6	2.54	0.42
1:2A:1642:G:N7	60:2A:4002:HOH:O	2.37	0.42
1:2A:2189:U:H2'	1:2A:2190:G:H8	1.82	0.42
1:2A:2515:C:H2'	1:2A:2516:G:H8	1.85	0.42
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.18	0.42
6:2G:107:LEU:HD21	6:2G:178:PHE:CE1	2.54	0.42
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.36	0.42
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HG13	2.02	0.42
32:2a:683:G:O6	60:2a:3218:HOH:O	2.22	0.42
32:2a:1258:G:H2'	32:2a:1259:C:C6	2.54	0.42
35:2d:10:ARG:HB2	35:2d:40:PRO:HG3	2.01	0.42
39:2h:20:TYR:HE2	39:2h:75:ARG:HD2	1.85	0.42
1:1A:196:A:H2'	1:1A:196:A:N3	2.34	0.42
1:1A:264:C:O2'	1:1A:265:A:H2'	2.19	0.42
1:1A:817:C:H4'	1:1A:932:G:C5	2.55	0.42
1:1A:1270:C:H5''	1:1A:1271:G:O5'	2.19	0.42
27:15:35:GLU:OE1	27:15:35:GLU:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:567:G:N3	60:1a:1959:HOH:O	2.37	0.42
32:1a:1315:U:H2'	32:1a:1316:G:O4'	2.20	0.42
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.19	0.42
35:1d:158:ILE:HG13	35:1d:159:ARG:N	2.34	0.42
50:1s:61:TYR:CE2	50:1s:63:THR:HG22	2.55	0.42
1:2A:263:C:H2'	1:2A:264:C:O4'	2.19	0.42
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.52	0.42
1:2A:1063:G:O2'	1:2A:1064:C:H5''	2.19	0.42
1:2A:1501:C:O4'	3:2D:100:GLY:HA2	2.20	0.42
1:2A:2224:G:H4'	1:2A:2226:C:C2	2.54	0.42
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.53	0.42
3:2D:106:ILE:HD11	3:2D:143:HIS:CD2	2.54	0.42
3:2D:175:LEU:HD12	3:2D:185:VAL:HG21	2.01	0.42
6:2G:41:GLN:O	6:2G:43:LEU:N	2.53	0.42
20:2Y:47:LYS:NZ	20:2Y:48:ALA:O	2.51	0.42
32:2a:580:U:H5''	46:2o:58:MET:HG2	2.02	0.42
32:2a:1009:G:H1	32:2a:1020:U:H3	1.67	0.42
33:2b:165:VAL:HA	33:2b:187:LEU:HD23	2.01	0.42
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	2.01	0.42
34:2c:20:SER:HB2	34:2c:40:ARG:HH21	1.84	0.42
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	2.02	0.42
46:2o:2:PRO:HB2	46:2o:3:ILE:H	1.60	0.42
50:2s:20:LEU:HD21	50:2s:43:GLU:HG2	2.00	0.42
1:1A:263:C:H2'	1:1A:264:C:O4'	2.20	0.42
1:1A:2128:C:H42	1:1A:2160:G:H1	1.66	0.42
6:1G:82:LEU:HD21	6:1G:88:ILE:HG21	2.02	0.42
7:1H:124:GLU:CG	7:1H:132:ARG:HB3	2.50	0.42
9:1N:62:VAL:CG1	9:1N:66:LYS:HB2	2.50	0.42
11:1P:49:ARG:NH1	30:18:61:LEU:HD23	2.35	0.42
32:1a:5:U:H1'	60:1a:1986:HOH:O	2.19	0.42
32:1a:266:G:H5''	32:1a:267:C:C5	2.55	0.42
32:1a:620:C:H2'	32:1a:621:A:O4'	2.20	0.42
32:1a:840:C:H5''	32:1a:841:U:C4	2.55	0.42
32:1a:1030(C):G:H2'	32:1a:1030(D):A:C8	2.54	0.42
32:1a:1256:A:OP2	34:1c:26:LYS:NZ	2.34	0.42
34:1c:18:TRP:CZ2	45:1n:57:ARG:HD2	2.55	0.42
37:1f:99:ALA:HB1	49:1r:23:LYS:HE3	2.00	0.42
1:2A:321:G:O2'	1:2A:340:A:N3	2.51	0.42
1:2A:1063:G:H2'	1:2A:1065:U:H6	1.84	0.42
1:2A:1262:A:OP2	18:2W:97:LYS:NZ	2.53	0.42
1:2A:2659:G:H4'	7:2H:175:LYS:HD3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2A:3741:CPF:H142	55:2A:3741:CPF:H9	1.52	0.42
2:2B:90:A:N7	2:2B:91:C:H1'	2.35	0.42
7:2H:98:LEU:HD22	7:2H:125:VAL:HG23	2.00	0.42
26:24:57:GLU:HA	26:24:58:ARG:HA	1.59	0.42
32:2a:399:G:H2'	32:2a:400:C:C6	2.54	0.42
33:2b:127:ILE:C	33:2b:129:GLU:H	2.28	0.42
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.35	0.42
45:2n:32:SER:O	45:2n:40:CYS:HA	2.19	0.42
50:2s:52:TYR:HD1	50:2s:57:HIS:CD2	2.38	0.42
1:1A:11:G:N7	60:1A:4309:HOH:O	2.37	0.42
1:1A:1007:C:OP1	9:1N:35:ARG:NH1	2.53	0.42
1:1A:1073:A:H2	1:1A:1074:G:C8	2.38	0.42
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.84	0.42
1:1A:1509(A):A:H2'	1:1A:1509(B):A:O4'	2.19	0.42
5:1F:95:ARG:HD3	5:1F:97:TYR:CZ	2.55	0.42
15:1T:91:ARG:HB2	15:1T:121:ILE:HG13	2.02	0.42
15:1T:93:ARG:NH2	60:1T:304:HOH:O	2.51	0.42
26:14:46:GLN:O	26:14:48:ARG:N	2.53	0.42
32:1a:435:C:H2'	32:1a:436:C:H6	1.85	0.42
32:1a:674:G:H2'	32:1a:675:A:C8	2.54	0.42
33:1b:157:ARG:HG2	33:1b:158:LEU:H	1.85	0.42
36:1e:61:TYR:HA	36:1e:64:ARG:HB3	2.01	0.42
37:1f:9:VAL:HB	37:1f:87:ARG:HB2	2.01	0.42
41:1j:55:LYS:H	41:1j:55:LYS:HG3	1.51	0.42
46:1o:18:PHE:HB2	46:1o:19:PRO:HD2	2.01	0.42
48:1q:85:VAL:O	48:1q:89:LEU:HG	2.20	0.42
1:2A:723:G:H2'	1:2A:724:U:O4'	2.20	0.42
1:2A:954:G:H5''	12:2Q:13:GLN:HB3	2.01	0.42
1:2A:1772:G:O6	56:2A:3743:MPD:H32	2.20	0.42
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.52	0.42
21:2Z:144:LEU:HD11	21:2Z:150:LEU:HD22	2.02	0.42
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.22	0.42
32:2a:674:G:H2'	32:2a:675:A:C8	2.55	0.42
32:2a:1404:5MC:O2	32:2a:1519:MA6:O2'	2.32	0.42
33:2b:74:LYS:H	33:2b:74:LYS:HG3	1.53	0.42
42:2k:115:PRO:HB2	42:2k:117:ASN:C	2.44	0.42
1:1A:763:G:OP1	60:1A:4160:HOH:O	2.22	0.42
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.55	0.42
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.55	0.42
32:1a:339:C:H2'	32:1a:340:U:C6	2.55	0.42
32:1a:743:U:H2'	32:1a:744:C:C6	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:18:ARG:HB2	42:1k:33:THR:OG1	2.20	0.42
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	2.01	0.42
1:2A:244:A:H4'	11:2P:74:GLU:HB2	2.01	0.42
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.55	0.42
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.54	0.42
1:2A:2570:G:O6	60:2A:3859:HOH:O	2.22	0.42
1:2A:2826:A:N7	60:2A:3995:HOH:O	2.37	0.42
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	2.01	0.42
12:2Q:112:GLU:HG3	12:2Q:113:GLN:N	2.35	0.42
28:26:12:GLU:OE1	28:26:19:ARG:NH1	2.53	0.42
32:2a:235:C:H2'	32:2a:236:G:H8	1.85	0.42
32:2a:790:A:H4'	53:2y:31:GLN:OE1	2.20	0.42
32:2a:985:C:H2'	32:2a:986:A:C8	2.54	0.42
32:2a:1143:G:H2'	32:2a:1144:G:C8	2.55	0.42
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.51	0.42
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.34	0.42
32:2a:1359:C:O2'	32:2a:1361:G:N7	2.53	0.42
33:2b:71:VAL:HG23	33:2b:164:VAL:HB	2.01	0.42
41:2j:81:THR:O	41:2j:84:GLN:HG2	2.20	0.42
53:2y:10:MET:HE2	53:2y:12:ILE:HD11	2.02	0.42
7:1H:84:SER:OG	7:1H:132:ARG:NH1	2.53	0.42
8:1I:69:LYS:HG3	8:1I:138:ILE:HG12	2.01	0.42
17:1V:52:VAL:HG21	17:1V:55:ALA:HB3	2.01	0.42
32:1a:109:A:C6	32:1a:326:G:C6	3.07	0.42
32:1a:458:C:H2'	32:1a:460:G:O4'	2.19	0.42
32:1a:1028:C:H2'	32:1a:1029:C:H4'	2.02	0.42
38:1g:38:LEU:O	38:1g:42:ILE:HG13	2.20	0.42
43:1l:60:LEU:HD12	43:1l:64:TYR:HB2	2.01	0.42
47:1p:71:ARG:HG3	47:1p:80:PHE:HE2	1.84	0.42
1:2A:579:G:O2'	1:2A:2019:A:OP1	2.33	0.42
1:2A:656:G:H2'	1:2A:657:U:O4'	2.19	0.42
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.54	0.42
2:2B:48:A:H2'	2:2B:49:C:C6	2.55	0.42
7:2H:26:VAL:HG12	7:2H:79:VAL:HG21	2.02	0.42
14:2S:87:PHE:CZ	14:2S:102:ALA:HB2	2.54	0.42
18:2W:32:ALA:O	18:2W:36:LEU:HG	2.20	0.42
32:2a:173:U:H5''	32:2a:197:A:O4'	2.20	0.42
32:2a:280:C:N3	48:2q:39:SER:OG	2.48	0.42
32:2a:598:U:H2'	32:2a:599:C:C6	2.55	0.42
32:2a:603:U:H2'	32:2a:604:G:H8	1.85	0.42
32:2a:664:G:P	49:2r:64:ARG:HH21	2.43	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:91:PRO:HG3	33:2b:155:LEU:HD13	2.02	0.42
45:2n:22:THR:O	45:2n:33:VAL:HG11	2.19	0.42
1:1A:443:A:N7	5:1F:45:ARG:HG2	2.35	0.41
1:1A:1668:A:H4'	1:1A:1669:A:O5'	2.20	0.41
1:1A:1802:A:H2'	1:1A:1803:A:C8	2.55	0.41
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.55	0.41
1:1A:2389:G:H5''	1:1A:2390:U:O4'	2.19	0.41
6:1G:163:ALA:HB1	6:1G:168:GLU:HB2	2.02	0.41
10:1O:116:SER:HA	56:1a:1878:MPD:H11	2.01	0.41
56:1O:202:MPD:H51	15:1T:68:TYR:HE2	1.85	0.41
15:1T:26:ASP:OD1	15:1T:120:ARG:NH2	2.38	0.41
20:1Y:4:LYS:NZ	60:1Y:604:HOH:O	2.53	0.41
20:1Y:86:ARG:HB2	20:1Y:98:VAL:HG23	2.02	0.41
21:1Z:198:LYS:HB3	21:1Z:202:GLU:HB3	2.02	0.41
23:11:71:TYR:O	23:11:74:VAL:HG22	2.20	0.41
32:1a:405:U:H5''	32:1a:495:A:H2	1.84	0.41
32:1a:689:C:H2'	32:1a:690:G:O4'	2.20	0.41
33:1b:18:GLY:HA2	33:1b:204:ASN:HB2	2.03	0.41
35:1d:173:TRP:C	35:1d:186:LEU:HB2	2.45	0.41
40:1i:43:ALA:HA	40:1i:74:ILE:HD13	2.02	0.41
42:1k:84:VAL:HG11	42:1k:91:ARG:HD2	2.01	0.41
49:1r:26:LEU:HG	49:1r:39:VAL:HG13	2.01	0.41
50:1s:10:PHE:HE2	50:1s:37:ARG:HD3	1.84	0.41
1:2A:746:A:H2'	1:2A:2612:C:H5''	2.02	0.41
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.19	0.41
1:2A:1668:A:H4'	1:2A:1669:A:O5'	2.20	0.41
1:2A:2114:A:N6	1:2A:2119:A:OP2	2.53	0.41
1:2A:2295:C:OP1	14:2S:10:ARG:NH1	2.53	0.41
2:2B:24:G:H4'	2:2B:25:A:C8	2.55	0.41
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.20	0.41
7:2H:140:LYS:HE3	7:2H:140:LYS:HB2	1.79	0.41
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	2.02	0.41
21:2Z:158:PRO:O	21:2Z:161:VAL:HG22	2.20	0.41
32:2a:615:C:H2'	32:2a:616:G:O4'	2.20	0.41
33:2b:46:LYS:O	33:2b:50:GLU:HG2	2.20	0.41
35:2d:13:ARG:HD2	35:2d:38:TYR:O	2.19	0.41
38:2g:113:GLU:O	38:2g:119:ARG:NH1	2.46	0.41
40:2i:22:GLY:N	40:2i:58:HIS:O	2.31	0.41
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.20	0.41
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.19	0.41
1:1A:2404:C:O3'	11:1P:77:ARG:NH2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2441:C:OP2	1:1A:2586:C:O2'	2.34	0.41
6:1G:109:VAL:HG21	26:14:14:ILE:HG21	2.01	0.41
10:1O:107:ARG:NH2	15:1T:36:GLU:HG2	2.35	0.41
12:1Q:109:VAL:HG22	12:1Q:113:GLN:CD	2.45	0.41
25:13:55:ARG:HD3	60:13:222:HOH:O	2.20	0.41
32:1a:408:A:OP1	35:1d:113:SER:OG	2.32	0.41
32:1a:1149:C:P	40:1i:9:ARG:HH21	2.42	0.41
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	2.01	0.41
36:1e:71:LEU:HD11	36:1e:113:ALA:O	2.20	0.41
40:1i:4:TYR:HB2	40:1i:19:LEU:HB2	2.02	0.41
1:2A:251:A:C5	1:2A:252:G:H1'	2.55	0.41
1:2A:2343:C:H4'	1:2A:2373:G:O3'	2.20	0.41
3:2D:124:PRO:HB2	3:2D:126:GLN:HG2	2.01	0.41
5:2F:153:SER:HB2	5:2F:189:THR:HG22	2.02	0.41
6:2G:19:LEU:HD11	6:2G:172:LEU:HB2	2.02	0.41
6:2G:126:ASP:HB2	6:2G:130:ASN:H	1.86	0.41
10:2O:16:ALA:HB2	10:2O:52:VAL:HG21	2.02	0.41
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	2.02	0.41
32:2a:5:U:H5''	32:2a:6:G:C5	2.55	0.41
32:2a:41:G:H2'	32:2a:42:G:H8	1.84	0.41
32:2a:1362:C:H2'	32:2a:1363:C:H5''	2.03	0.41
33:2b:48:MET:HA	33:2b:51:LEU:HD12	2.02	0.41
41:2j:6:ILE:HD12	41:2j:98:ILE:HG12	2.01	0.41
43:2l:89:ARG:HH21	43:2l:91:LYS:HA	1.84	0.41
1:1A:185:U:H2'	1:1A:186:G:H8	1.84	0.41
1:1A:489:G:H2'	1:1A:491:G:O4'	2.20	0.41
1:1A:1301:A:C8	1:1A:1303:G:C8	3.07	0.41
1:1A:2038:G:H2'	1:1A:2039:C:O4'	2.20	0.41
1:1A:2572:A:N7	4:1E:145:LYS:HB2	2.35	0.41
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	2.01	0.41
5:1F:140:LEU:HD12	5:1F:140:LEU:HA	1.83	0.41
5:1F:195:ASP:HB2	5:1F:198:ALA:H	1.85	0.41
11:1P:95:VAL:HG23	11:1P:125:VAL:HA	2.02	0.41
32:1a:302:G:O2'	32:1a:556:C:H5''	2.20	0.41
32:1a:1070:U:H2'	32:1a:1071:C:H6	1.85	0.41
35:1d:176:LEU:HG	35:1d:178:VAL:HG22	2.01	0.41
36:1e:31:LEU:HD23	36:1e:31:LEU:HA	1.92	0.41
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	2.02	0.41
41:1j:35:SER:CB	41:1j:73:ASP:HB2	2.48	0.41
44:1m:57:ARG:O	44:1m:61:GLU:HG3	2.20	0.41
1:2A:470:A:OP1	5:2F:59:TYR:HE1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:735:A:N7	1:2A:761:A:H2	2.18	0.41
1:2A:1069:A:H2'	1:2A:1073:A:N7	2.35	0.41
1:2A:1479:G:H5''	1:2A:1560:G:H4'	2.02	0.41
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.20	0.41
1:2A:1803:A:H4'	3:2D:259:THR:HG23	2.02	0.41
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.19	0.41
2:2B:42:C:C4	2:2B:43:C:C4	3.08	0.41
5:2F:176:LEU:HD23	5:2F:176:LEU:HA	1.88	0.41
9:2N:96:GLU:HB2	9:2N:122:VAL:HG12	2.02	0.41
31:29:19:ARG:HG2	31:29:20:HIS:ND1	2.36	0.41
32:2a:373:A:O2'	32:2a:451:A:N7	2.53	0.41
32:2a:625:G:H2'	32:2a:626:U:C6	2.56	0.41
32:2a:662:G:H2'	32:2a:663:A:H8	1.81	0.41
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.56	0.41
51:2t:38:LYS:HB3	51:2t:38:LYS:HE2	1.85	0.41
53:2y:29:LYS:HG2	53:2y:30:TRP:CE3	2.55	0.41
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.48	0.41
1:1A:2135:A:H62	1:1A:2156:G:N2	2.17	0.41
1:1A:2816:C:O2	1:1A:2883:A:O2'	2.37	0.41
60:1A:4665:HOH:O	16:1U:55:ARG:HB3	2.20	0.41
4:1E:2:LYS:NZ	4:1E:95:ILE:O	2.41	0.41
8:1I:38:LEU:HB3	8:1I:40:THR:HG23	2.03	0.41
17:1V:58:VAL:HG12	17:1V:97:LYS:HB2	2.01	0.41
32:1a:624:C:H4'	47:1p:10:GLY:C	2.45	0.41
32:1a:1073:U:O2'	33:1b:104:ASN:OD1	2.21	0.41
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.54	0.41
32:1a:1373:G:N7	40:1i:11:LYS:NZ	2.68	0.41
37:1f:18:GLN:O	37:1f:22:GLU:HG2	2.20	0.41
45:1n:6:LEU:HB3	45:1n:23:ARG:NH2	2.34	0.41
1:2A:39:C:H2'	1:2A:40:C:C6	2.56	0.41
1:2A:208:C:H2'	1:2A:209:C:C6	2.55	0.41
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.21	0.41
1:2A:2028:U:H2'	1:2A:2029:G:O4'	2.20	0.41
1:2A:2118:U:O2'	1:2A:2119:A:H5''	2.21	0.41
55:2A:3741:CPF:H1	55:2A:3741:CPF:H131	1.73	0.41
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.84	0.41
7:2H:98:LEU:HD12	7:2H:98:LEU:HA	1.91	0.41
32:2a:376:G:H5''	47:2p:5:ARG:HD3	2.03	0.41
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.20	0.41
32:2a:1318:A:H4'	50:2s:10:PHE:CE2	2.55	0.41
32:2a:1318:A:H5''	50:2s:3:ARG:NH2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:114:ARG:O	35:2d:118:ARG:N	2.49	0.41
36:2e:19:MET:SD	36:2e:24:ARG:HB3	2.60	0.41
48:2q:22:LEU:HD13	48:2q:41:LYS:HG2	2.02	0.41
1:1A:1781:C:N4	60:1A:4680:HOH:O	2.53	0.41
1:1A:2557:G:H2'	1:1A:2558:C:C6	2.55	0.41
21:1Z:136:PHE:HE1	21:1Z:138:GLU:HG3	1.84	0.41
32:1a:196:A:N3	32:1a:222:U:H1'	2.36	0.41
32:1a:848:C:H2'	32:1a:849:C:H6	1.85	0.41
32:1a:1010:G:N2	32:1a:1020:U:H1'	2.36	0.41
32:1a:1029:C:N4	32:1a:1030:C:H41	2.18	0.41
32:1a:1317:C:H5	45:1n:18:VAL:HG21	1.85	0.41
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.85	0.41
34:1c:17:ASP:OD1	34:1c:21:ARG:HD3	2.20	0.41
35:1d:178:VAL:C	35:1d:180:GLY:H	2.27	0.41
51:1t:72:LEU:HD23	51:1t:72:LEU:HA	1.85	0.41
53:1y:3:MET:HE3	53:1y:3:MET:HB3	1.81	0.41
1:2A:854:G:H2'	1:2A:855:G:H8	1.85	0.41
1:2A:2109:U:H2'	1:2A:2110:G:C8	2.55	0.41
1:2A:2185:C:N4	1:2A:2186:G:C6	2.88	0.41
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.20	0.41
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.55	0.41
1:2A:2711:A:OP1	1:2A:2712:U:H3'	2.20	0.41
5:2F:140:LEU:HD12	5:2F:140:LEU:HA	1.84	0.41
21:2Z:53:ILE:HG22	21:2Z:71:VAL:O	2.21	0.41
30:28:26:LYS:HD2	30:28:48:PHE:CD2	2.56	0.41
32:2a:539:A:H2'	32:2a:540:G:C8	2.56	0.41
32:2a:685:G:O2'	32:2a:686:U:H5'	2.20	0.41
32:2a:1151:A:H5''	41:2j:41:PRO:HA	2.03	0.41
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.54	0.41
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.86	0.41
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.53	0.41
1:1A:2232:U:P	23:11:40:ARG:HH12	2.43	0.41
6:1G:82:LEU:HD23	6:1G:82:LEU:HA	1.85	0.41
32:1a:690:G:C6	32:1a:691:G:C6	3.08	0.41
44:1m:108:ARG:HA	44:1m:108:ARG:HD3	1.90	0.41
51:1t:14:LYS:O	51:1t:18:GLN:HG3	2.20	0.41
1:2A:29:U:H2'	1:2A:30:G:C8	2.56	0.41
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.56	0.41
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.20	0.41
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.55	0.41
22:20:27:GLU:HB2	22:20:69:PHE:HD1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.55	0.41
32:2a:1490:C:H2'	32:2a:1491:G:C8	2.56	0.41
35:2d:164:ALA:C	35:2d:166:LYS:HD3	2.45	0.41
36:2e:144:THR:H	36:2e:147:ASP:HB2	1.85	0.41
1:1A:567:A:OP2	11:1P:29:LYS:NZ	2.49	0.41
1:1A:1094:U:H1'	1:1A:1097:U:H5	1.86	0.41
1:1A:1111:A:N3	1:1A:1112:G:H1'	2.35	0.41
1:1A:1448:G:O2'	1:1A:1528(A):A:N1	2.51	0.41
1:1A:2139:C:H2'	1:1A:2140:C:H6	1.85	0.41
1:1A:2774:C:H2'	1:1A:2775:A:O4'	2.20	0.41
3:1D:43:ARG:HA	3:1D:48:ARG:O	2.20	0.41
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.55	0.41
8:1I:140:LEU:HD23	8:1I:140:LEU:HA	1.87	0.41
23:11:23:LYS:HB3	23:11:29:GLY:HA3	2.02	0.41
23:11:56:GLN:HE21	23:11:87:PRO:HG3	1.85	0.41
30:18:42:ARG:HD2	60:18:202:HOH:O	2.20	0.41
32:1a:149:A:H2'	32:1a:150:C:C6	2.56	0.41
32:1a:263:A:OP1	51:1t:79:ARG:NH1	2.54	0.41
32:1a:659:U:H2'	32:1a:660:G:C8	2.56	0.41
32:1a:731:G:H5'	32:1a:766:A:H4'	2.03	0.41
32:1a:765:G:C6	32:1a:812:C:C2	3.08	0.41
32:1a:1140:C:H2'	32:1a:1141:C:H6	1.86	0.41
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.20	0.41
32:1a:1179:A:H2'	32:1a:1180:A:O4'	2.20	0.41
32:1a:1394:A:N1	32:1a:1500:A:O2'	2.49	0.41
33:1b:109:SER:HA	33:1b:112:VAL:HG13	2.01	0.41
48:1q:37:LYS:O	48:1q:38:ARG:NH2	2.51	0.41
1:2A:1383:C:O2	60:2A:3853:HOH:O	2.21	0.41
5:2F:130:ALA:H	5:2F:142:TRP:CD1	2.38	0.41
6:2G:67:LYS:HE3	26:24:5:ILE:HD12	2.03	0.41
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	2.01	0.41
19:2X:28:PHE:CE1	19:2X:92:LEU:HD11	2.55	0.41
31:29:3:VAL:HA	31:29:35:ARG:O	2.21	0.41
32:2a:786:G:C2	32:2a:797:C:C2	3.09	0.41
32:2a:831:U:H3	32:2a:855:G:H1	1.68	0.41
32:2a:848:C:H2'	32:2a:849:C:C6	2.56	0.41
33:2b:74:LYS:HD2	33:2b:166:ASP:HB2	2.03	0.41
34:2c:99:VAL:O	34:2c:101:LEU:N	2.54	0.41
42:2k:34:ASP:OD1	42:2k:38:ASN:N	2.53	0.41
43:2l:57:LYS:NZ	43:2l:65:GLU:HG2	2.35	0.41
1:1A:668:G:H5'	1:1A:669:G:OP2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1179:C:H2'	1:1A:1180:C:C6	2.55	0.41
6:1G:12:TYR:HA	6:1G:16:ARG:HG3	2.03	0.41
32:1a:1299:A:N3	32:1a:1299:A:H5''	2.35	0.41
36:1e:143:ARG:HA	36:1e:143:ARG:HD3	1.91	0.41
1:2A:241:A:H5''	60:2A:5634:HOH:O	2.20	0.41
1:2A:839:U:H2'	1:2A:840:C:C6	2.55	0.41
1:2A:1048:A:OP2	1:2A:1109:C:N4	2.54	0.41
1:2A:1528(A):A:H2'	1:2A:1529:G:O4'	2.21	0.41
1:2A:2336:A:H61	22:20:43:THR:CG2	2.34	0.41
2:2B:43:C:H5''	26:24:1:MET:HG2	2.02	0.41
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	2.03	0.41
17:2V:25:LEU:HD12	17:2V:94:LEU:HD21	2.03	0.41
21:2Z:48:PHE:CE1	21:2Z:71:VAL:HG11	2.55	0.41
32:2a:34:C:H2'	32:2a:35:G:C8	2.55	0.41
32:2a:435:C:H2'	32:2a:436:C:C6	2.56	0.41
32:2a:1048:G:OP1	45:2n:3:ARG:HB3	2.21	0.41
41:2j:8:LEU:HB3	41:2j:16:LEU:HD22	2.02	0.41
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.74	0.41
42:2k:84:VAL:HG21	42:2k:95:ILE:HD11	2.02	0.41
1:1A:78:A:H2'	1:1A:79:G:H8	1.86	0.41
1:1A:197:A:N6	1:1A:2430:A:O2'	2.54	0.41
1:1A:530:G:N1	1:1A:2023:G:OP1	2.40	0.41
1:1A:531:C:H4'	1:1A:532:A:H5''	2.03	0.41
1:1A:904:C:O2'	21:1Z:169:GLU:OE2	2.38	0.41
1:1A:1050:A:H2'	1:1A:1051:G:O4'	2.20	0.41
1:1A:1064:C:N3	1:1A:1074:G:C6	2.89	0.41
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.85	0.41
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.56	0.41
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.56	0.41
1:1A:1999:C:H5''	1:1A:2723:C:O2'	2.21	0.41
1:1A:2187:G:H5'	1:1A:2188:C:OP2	2.21	0.41
1:1A:2447:G:N2	1:1A:2450:A:OP2	2.54	0.41
55:1A:4056:CPF:H11	55:1A:4056:CPF:H9	1.56	0.41
6:1G:43:LEU:O	6:1G:45:GLU:N	2.52	0.41
10:1O:8:LEU:HB2	10:1O:19:ILE:HG13	2.02	0.41
16:1U:101:ARG:NH2	60:1U:308:HOH:O	2.50	0.41
21:1Z:52:SER:HB3	21:1Z:54:HIS:HD1	1.86	0.41
32:1a:19:C:O2'	32:1a:572:A:N1	2.53	0.41
32:1a:136:C:O2'	47:1p:65:GLN:NE2	2.30	0.41
32:1a:341:C:H2'	32:1a:342:C:C6	2.56	0.41
32:1a:382:A:H2'	32:1a:383:A:H8	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:814:A:H2'	32:1a:816:A:H5''	2.02	0.41
32:1a:958:A:C5	50:1s:55:LYS:HD2	2.56	0.41
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.56	0.41
32:1a:1319:A:OP2	50:1s:3:ARG:HD2	2.21	0.41
33:1b:83:MET:SD	33:1b:234:PRO:HB2	2.61	0.41
34:1c:130:VAL:HG21	34:1c:157:ILE:HG23	2.03	0.41
35:1d:18:LYS:HD3	35:1d:20:TYR:CZ	2.55	0.41
35:1d:59:ARG:NH1	35:1d:59:ARG:HA	2.35	0.41
51:1t:101:GLY:HA3	51:1t:102:GLY:HA2	1.91	0.41
1:2A:530:G:H4'	1:2A:531:C:OP1	2.20	0.41
1:2A:570:G:H2'	1:2A:2030:A:C5	2.56	0.41
1:2A:740:U:H2'	1:2A:741:G:C8	2.56	0.41
1:2A:973:A:OP1	1:2A:973:A:H8	2.04	0.41
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.56	0.41
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.56	0.41
1:2A:2036:C:OP2	60:2A:3860:HOH:O	2.22	0.41
1:2A:2111:C:N4	1:2A:2147:G:H22	2.16	0.41
1:2A:2391:G:O6	1:2A:2425:A:H8	2.04	0.41
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.21	0.41
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.21	0.41
8:2I:77:LEU:HD22	8:2I:101:LEU:HG	2.02	0.41
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	2.02	0.41
24:22:23:LYS:HD2	24:22:23:LYS:H	1.85	0.41
32:2a:113:G:N3	32:2a:353:A:O2'	2.49	0.41
32:2a:392:G:H2'	32:2a:393:A:H8	1.86	0.41
32:2a:728:A:H2'	32:2a:729:A:C8	2.55	0.41
32:2a:782:A:O3'	32:2a:1515:C:H4'	2.21	0.41
33:2b:62:ALA:C	33:2b:64:ARG:H	2.29	0.41
37:2f:12:PRO:HG3	37:2f:57:GLN:O	2.21	0.41
37:2f:35:ALA:HA	37:2f:67:MET:HB3	2.03	0.41
39:2h:14:ARG:NH1	39:2h:83:ILE:O	2.54	0.41
41:2j:70:ARG:HD3	41:2j:70:ARG:HA	1.94	0.41
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.44	0.41
43:2l:119:LYS:C	43:2l:121:GLY:H	2.28	0.41
44:2m:108:ARG:HD3	44:2m:108:ARG:HA	1.58	0.41
49:2r:37:VAL:HG22	49:2r:78:LEU:HB3	2.03	0.41
53:2y:78:ILE:O	53:2y:82:GLU:HG3	2.21	0.41
1:1A:548:A:N6	17:1V:19:LYS:H	2.17	0.41
1:1A:1094:U:O2'	1:1A:1096:A:N7	2.51	0.41
3:1D:132:PRO:HG3	3:1D:190:TYR:CE2	2.56	0.41
19:1X:12:VAL:HG21	19:1X:27:THR:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:11:80:LEU:HB3	23:11:82:LEU:HG	2.02	0.41
32:1a:28:G:O2'	32:1a:296:U:OP1	2.28	0.41
32:1a:1004:A:N7	32:1a:1036:G:N1	2.69	0.41
32:1a:1040:U:H2'	32:1a:1041:A:C8	2.55	0.41
32:1a:1186:G:H21	45:1n:61:TRP:C	2.30	0.41
40:1i:3:GLN:HE22	40:1i:20:ARG:HH21	1.68	0.41
45:1n:3:ARG:HD3	45:1n:3:ARG:C	2.46	0.41
1:2A:581:C:H2'	1:2A:582:G:C8	2.55	0.41
1:2A:856:C:H2'	1:2A:857:C:C6	2.56	0.41
1:2A:897:C:H2'	1:2A:898:C:C6	2.56	0.41
1:2A:1117:G:H2'	1:2A:1118:C:C6	2.56	0.41
1:2A:2168:G:N2	1:2A:2171:A:OP2	2.54	0.41
3:2D:16:MET:HE3	3:2D:16:MET:HB2	1.93	0.41
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.51	0.41
5:2F:29:ASN:H	5:2F:112:MET:CE	2.34	0.41
12:2Q:109:VAL:HG22	12:2Q:113:GLN:OE1	2.21	0.41
20:2Y:94:LYS:HD3	20:2Y:94:LYS:HA	1.91	0.41
32:2a:54:C:H2'	32:2a:352:C:H41	1.85	0.41
32:2a:868:C:H2'	32:2a:869:G:O4'	2.20	0.41
41:2j:11:PHE:HE1	41:2j:67:THR:HG22	1.86	0.41
43:2l:124:LYS:HA	43:2l:125:PRO:HD3	1.97	0.41
49:2r:39:VAL:O	49:2r:42:ARG:HG3	2.20	0.41
1:1A:400:G:N7	60:1A:4315:HOH:O	2.37	0.40
1:1A:586:A:N1	1:1A:809:G:O2'	2.51	0.40
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.56	0.40
1:1A:884:C:H2'	1:1A:885:C:O4'	2.21	0.40
1:1A:1394:U:H2'	1:1A:1395:A:O4'	2.21	0.40
1:1A:1668:A:O2'	1:1A:1674:G:N7	2.47	0.40
1:1A:1803:A:H4'	3:1D:259:THR:HG23	2.03	0.40
1:1A:1833:U:O2'	1:1A:1969:A:N1	2.52	0.40
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.56	0.40
3:1D:142:VAL:HG23	3:1D:193:VAL:HA	2.03	0.40
7:1H:98:LEU:HD12	7:1H:98:LEU:HA	1.88	0.40
13:1R:26:LYS:HE2	13:1R:70:LEU:O	2.21	0.40
19:1X:5:TYR:CZ	24:12:30:ARG:HB2	2.57	0.40
19:1X:84:ALA:HB3	19:1X:87:GLN:CD	2.46	0.40
32:1a:186:C:H2'	32:1a:187:C:H6	1.86	0.40
32:1a:1101:A:OP2	33:1b:96:ARG:NH1	2.54	0.40
33:1b:178:ARG:NH2	39:1h:74:PRO:HB3	2.36	0.40
38:1g:111:ARG:HD3	38:1g:113:GLU:OE2	2.21	0.40
46:1o:5:LYS:O	46:1o:9:GLN:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:530:G:O6	60:2A:3858:HOH:O	2.21	0.40
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.56	0.40
1:2A:1918:A:O2'	1:2A:1920:OMC:N4	2.53	0.40
1:2A:2106:G:C4	1:2A:2107:C:H1'	2.56	0.40
1:2A:2370:G:C6	1:2A:2371:G:C6	3.09	0.40
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.65	0.40
14:2S:18:ILE:O	14:2S:21:THR:HG22	2.21	0.40
21:2Z:10:ARG:HH11	21:2Z:26:GLY:H	1.69	0.40
26:24:59:PHE:CZ	50:2s:64:GLU:HB3	2.56	0.40
32:2a:1372:U:H2'	32:2a:1373:G:O4'	2.21	0.40
33:2b:55:PHE:CE1	33:2b:218:ALA:HA	2.54	0.40
40:2i:29:ASN:ND2	40:2i:65:VAL:H	2.16	0.40
50:2s:52:TYR:HA	50:2s:56:GLN:O	2.21	0.40
1:1A:30:G:H2'	1:1A:31:C:C6	2.56	0.40
1:1A:660:G:O3'	5:1F:38:ARG:NH2	2.52	0.40
1:1A:709:U:H2'	1:1A:710:G:C8	2.56	0.40
1:1A:1296:G:OP1	1:1A:2709:G:O2'	2.31	0.40
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.56	0.40
1:1A:1509(A):A:H2'	1:1A:1509(B):A:C8	2.56	0.40
1:1A:1768:U:OP1	60:1A:4161:HOH:O	2.22	0.40
1:1A:1795:C:O2	3:1D:255:LYS:NZ	2.53	0.40
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.21	0.40
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.79	0.40
10:1O:64:ARG:HB2	10:1O:79:PHE:CD2	2.57	0.40
32:1a:1134:G:C2	32:1a:1141:C:C2	3.09	0.40
32:1a:1144:G:N2	32:1a:1146:A:H62	2.19	0.40
34:1c:52:LEU:HA	34:1c:70:VAL:HG23	2.03	0.40
34:1c:120:VAL:HB	34:1c:198:VAL:HG11	2.03	0.40
39:1h:25:ASP:OD1	39:1h:60:ARG:HG3	2.20	0.40
40:1i:108:VAL:HG12	40:1i:109:VAL:H	1.85	0.40
41:1j:62:HIS:HB3	45:1n:59:ALA:HB3	2.03	0.40
1:2A:606:U:H4'	1:2A:658:C:H4'	2.02	0.40
1:2A:981:A:OP1	60:2A:3862:HOH:O	2.22	0.40
1:2A:2291:U:O2'	1:2A:2374:C:O2	2.36	0.40
8:2I:81:VAL:O	8:2I:146:ALA:HA	2.21	0.40
9:2N:50:ASP:OD1	60:2N:301:HOH:O	2.22	0.40
24:22:64:LEU:O	24:22:68:ARG:HG2	2.21	0.40
32:2a:67:C:H2'	32:2a:68:G:H8	1.86	0.40
32:2a:353:A:H5'	32:2a:353:A:H8	1.87	0.40
32:2a:1002:G:C2	32:2a:1003:G:N7	2.90	0.40
32:2a:1054:C:N4	53:2y:46:GLN:HE21	2.19	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:101:MET:HG2	33:2b:108:ILE:HG21	2.04	0.40
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	2.02	0.40
49:2r:25:THR:OG1	49:2r:26:LEU:HD22	2.21	0.40
1:1A:476:G:H4'	1:1A:502:A:N1	2.37	0.40
1:1A:1766:U:H2'	1:1A:1767:C:C6	2.55	0.40
1:1A:2122:U:H2'	1:1A:2123:G:O4'	2.21	0.40
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.54	0.40
1:1A:2443:C:OP1	5:1F:68:LYS:HD3	2.21	0.40
3:1D:132:PRO:HD3	3:1D:190:TYR:CZ	2.57	0.40
3:1D:275:LYS:HB2	3:1D:276:LYS:H	1.74	0.40
4:1E:111:ARG:HA	13:1R:1:MET:SD	2.60	0.40
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.56	0.40
23:11:3:LYS:O	23:11:12:PRO:HD3	2.20	0.40
32:1a:115:G:H4'	32:1a:116:A:O5'	2.21	0.40
32:1a:642:A:N3	39:1h:113:SER:OG	2.41	0.40
33:1b:219:VAL:HA	33:1b:222:ILE:HD12	2.03	0.40
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.86	0.40
50:1s:55:LYS:HE3	50:1s:55:LYS:HB2	1.90	0.40
1:2A:441:U:H2'	1:2A:442:G:C8	2.56	0.40
1:2A:1075:C:OP1	12:2Q:59:ARG:HD3	2.21	0.40
1:2A:1530:C:N4	1:2A:1539:G:H1	2.17	0.40
1:2A:1752:C:H2'	1:2A:1753:G:C8	2.56	0.40
1:2A:1882:C:H2'	1:2A:1883:G:O4'	2.21	0.40
2:2B:95:C:H2'	2:2B:96:U:C6	2.57	0.40
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.84	0.40
6:2G:61:ALA:HB1	26:24:7:PRO:CG	2.51	0.40
15:2T:41:ARG:NH2	32:2a:346:G:OP1	2.51	0.40
25:23:35:ARG:HE	25:23:37:LEU:HD21	1.86	0.40
26:24:1:MET:HB3	26:24:6:HIS:NE2	2.36	0.40
32:2a:165:C:H2'	32:2a:166:G:H8	1.87	0.40
32:2a:603:U:H2'	32:2a:604:G:C8	2.55	0.40
32:2a:1244:C:H42	32:2a:1293:G:H1	1.69	0.40
35:2d:110:PHE:N	35:2d:110:PHE:CD1	2.89	0.40
35:2d:201:GLN:NE2	36:2e:99:GLY:HA2	2.36	0.40
38:2g:108:ALA:HA	38:2g:111:ARG:HD2	2.02	0.40
40:2i:53:VAL:C	40:2i:55:ALA:H	2.29	0.40
43:2l:7:ILE:HG21	48:2q:34:LYS:HB2	2.02	0.40
49:2r:52:PRO:HB2	49:2r:54:ARG:HG2	2.03	0.40
51:2t:54:LYS:HB3	51:2t:54:LYS:HE2	1.82	0.40
1:1A:795:C:H2'	1:1A:796:C:C6	2.56	0.40
1:1A:1260:G:H2'	1:1A:1261:C:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2179:C:H2'	1:1A:2180:U:H6	1.85	0.40
1:1A:2682:U:O2'	15:1T:58:ASN:ND2	2.54	0.40
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.57	0.40
23:11:67:ILE:N	23:11:68:PRO:HD2	2.36	0.40
24:12:65:ASN:O	24:12:69:ARG:HG3	2.21	0.40
32:1a:1065:U:H1'	32:1a:1066:C:OP2	2.21	0.40
32:1a:1318:A:H5''	50:1s:3:ARG:NH1	2.36	0.40
32:1a:1329:A:P	44:1m:28:ALA:HB3	2.61	0.40
35:1d:65:ARG:HG3	35:1d:70:ILE:HG23	2.02	0.40
35:1d:107:ARG:NH2	35:1d:194:LEU:HD21	2.29	0.40
39:1h:104:ARG:HA	39:1h:104:ARG:HD3	1.91	0.40
50:1s:3:ARG:NH1	50:1s:10:PHE:HB2	2.37	0.40
53:1y:88:LEU:HD23	53:1y:88:LEU:HA	1.93	0.40
1:2A:576:U:H2'	1:2A:577:G:C8	2.56	0.40
1:2A:784:A:C5	3:2D:229:VAL:HG21	2.56	0.40
1:2A:1072:C:N4	1:2A:1093:G:H1	2.19	0.40
1:2A:1449:A:N3	1:2A:1529:G:H1'	2.36	0.40
1:2A:2717:G:O2'	15:2T:96:ARG:HD3	2.21	0.40
60:2A:4684:HOH:O	5:2F:74:ARG:HG3	2.21	0.40
2:2B:91:C:H5'	12:2Q:18:LYS:HA	2.04	0.40
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	2.04	0.40
23:21:22:GLY:O	23:21:32:LYS:NZ	2.46	0.40
31:29:27:CYS:SG	31:29:28:GLU:N	2.94	0.40
32:2a:950:U:OP2	44:2m:102:ARG:HD3	2.21	0.40
32:2a:971:G:H1	32:2a:1363(A):A:H5'	1.86	0.40
32:2a:1256:A:H5'	32:2a:1257:U:OP1	2.22	0.40
34:2c:8:ILE:HG12	34:2c:184:TYR:HB3	2.04	0.40
48:2q:86:GLU:O	48:2q:90:ILE:HG12	2.21	0.40
1:1A:614(A):U:H5''	57:1F:320:ARG:N	2.37	0.40
1:1A:651:G:OP1	30:18:17:THR:OG1	2.35	0.40
1:1A:721:C:H2'	1:1A:722:A:H8	1.87	0.40
1:1A:729:G:C5	3:1D:208:LYS:HB2	2.57	0.40
1:1A:818:G:H4'	1:1A:838:C:O3'	2.22	0.40
1:1A:1040:C:H2'	1:1A:1041:C:O4'	2.21	0.40
1:1A:1152:C:H4'	16:1U:77:SER:HA	2.04	0.40
1:1A:1508:A:H4'	1:1A:1509(A):A:C5	2.57	0.40
32:1a:167:G:H2'	32:1a:168:G:H8	1.86	0.40
32:1a:346:G:H3'	56:1a:1878:MPD:O4	2.21	0.40
32:1a:881:G:OP2	43:1l:12:ARG:NH2	2.52	0.40
33:1b:119:GLU:O	33:1b:123:ALA:N	2.54	0.40
1:2A:116:C:H2'	1:2A:117:G:O4'	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:422:A:H2'	1:2A:423:A:C8	2.56	0.40
1:2A:784:A:O4'	3:2D:227:ASN:ND2	2.55	0.40
1:2A:2153:G:H2'	1:2A:2154:G:H8	1.86	0.40
2:2B:33:G:C6	2:2B:34:U:C4	3.10	0.40
32:2a:409:G:H2'	32:2a:410:G:O4'	2.21	0.40
32:2a:674:G:H2'	32:2a:675:A:H8	1.85	0.40
32:2a:893:C:H2'	32:2a:894:G:C8	2.57	0.40
32:2a:1002:G:N3	32:2a:1003:G:N7	2.70	0.40
38:2g:78:ARG:HE	38:2g:80:VAL:HG21	1.87	0.40
38:2g:113:GLU:HG3	38:2g:118:VAL:HG12	2.04	0.40
41:2j:6:ILE:HA	41:2j:97:GLU:O	2.22	0.40
47:2p:9:PHE:CE1	47:2p:18:ARG:HD2	2.57	0.40
49:2r:59:SER:OG	49:2r:62:GLU:HG2	2.22	0.40
50:2s:58:VAL:O	50:2s:60:VAL:HG23	2.22	0.40
50:2s:61:TYR:CE2	50:2s:63:THR:HG23	2.57	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%)	261 (96%)	12 (4%)	0	100	100
3	2D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	30	51
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	46
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	12	28
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24	46
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	46
6	1G	179/182 (98%)	171 (96%)	4 (2%)	4 (2%)	5	10
6	2G	179/182 (98%)	164 (92%)	12 (7%)	3 (2%)	7	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	1H	172/180 (96%)	161 (94%)	11 (6%)	0	100	100
7	2H	171/180 (95%)	155 (91%)	16 (9%)	0	100	100
8	1I	145/148 (98%)	132 (91%)	13 (9%)	0	100	100
8	2I	144/148 (97%)	134 (93%)	10 (7%)	0	100	100
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	38
11	2P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18	38
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	28
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	28
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	25
19	2X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	25
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	1Z	201/206 (98%)	191 (95%)	9 (4%)	1 (0%)	24	46
21	2Z	199/206 (97%)	186 (94%)	13 (6%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	20	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	25
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
26	24	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
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%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	198 (86%)	26 (11%)	5 (2%)	5	10
33	2b	229/256 (90%)	201 (88%)	22 (10%)	6 (3%)	4	7
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100	100
34	2c	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	24	46
35	1d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
35	2d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
36	1e	146/162 (90%)	139 (95%)	7 (5%)	0	100	100
36	2e	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	2g	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	18	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	114 (91%)	10 (8%)	1 (1%)	16	34
40	2i	124/128 (97%)	109 (88%)	12 (10%)	3 (2%)	4	9
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	5
41	2j	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	3	5
42	1k	112/129 (87%)	105 (94%)	7 (6%)	0	100	100
42	2k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	14	30
43	1l	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
43	2l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
44	1m	114/126 (90%)	104 (91%)	8 (7%)	2 (2%)	6	14
44	2m	112/126 (89%)	97 (87%)	12 (11%)	3 (3%)	4	7
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	23
46	2o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	5	9
47	1p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	9	21
47	2p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12	28
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
51	1t	94/106 (89%)	88 (94%)	6 (6%)	0	100	100
51	2t	96/106 (91%)	91 (95%)	5 (5%)	0	100	100
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	2
53	1y	95/113 (84%)	95 (100%)	0	0	100	100
53	2y	94/113 (83%)	92 (98%)	2 (2%)	0	100	100
All	All	11629/12354 (94%)	10978 (94%)	588 (5%)	63 (0%)	24	46

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	1b	21	ARG
33	1b	124	SER
44	1m	67	GLU
44	1m	106	ASN
5	2F	130	ALA
26	24	62	ARG
5	1F	130	ALA
6	1G	50	ALA
19	1X	94	GLY
21	1Z	52	SER
26	14	57	GLU
33	1b	17	PHE
41	1j	55	LYS
4	2E	71	GLY
6	2G	78	SER
17	2V	79	VAL
19	2X	94	GLY
26	24	63	TYR
40	2i	43	ALA
40	2i	54	ASP
41	2j	79	ARG
46	2o	88	ARG
40	1i	11	LYS
41	1j	77	PRO
41	1j	78	ASN
6	2G	81	LYS
23	21	3	LYS
33	2b	95	GLN
34	2c	4	LYS
38	2g	7	ALA
40	2i	55	ALA
44	2m	23	TYR
4	1E	52	LEU
11	1P	29	LYS
26	14	61	ARG
33	1b	20	GLU
48	1q	68	ARG
33	2b	10	LEU
33	2b	20	GLU
33	2b	125	PRO
41	2j	78	ASN
6	1G	51	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	1Q	59	ARG
26	14	47	GLN
26	14	49	PHE
46	1o	87	ILE
47	1p	46	PRO
6	2G	42	GLY
26	24	55	ARG
33	2b	190	THR
41	2j	75	ILE
46	2o	87	ILE
6	1G	48	GLU
33	1b	127	ILE
4	2E	52	LEU
33	2b	150	SER
44	2m	67	GLU
52	2u	3	LYS
44	2m	6	GLY
6	1G	44	GLY
42	2k	105	VAL
17	1V	79	VAL
3	2D	125	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	199 (93%)	15 (7%)	14	31
3	2D	215/218 (99%)	199 (93%)	16 (7%)	13	29
4	1E	164/166 (99%)	150 (92%)	14 (8%)	10	22
4	2E	164/166 (99%)	152 (93%)	12 (7%)	13	29
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8	18
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	18
6	1G	144/156 (92%)	134 (93%)	10 (7%)	14	32
6	2G	142/156 (91%)	128 (90%)	14 (10%)	7	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	1H	144/148 (97%)	134 (93%)	10 (7%)	14	32
7	2H	143/148 (97%)	129 (90%)	14 (10%)	7	17
8	1I	111/124 (90%)	104 (94%)	7 (6%)	16	36
8	2I	108/124 (87%)	100 (93%)	8 (7%)	13	29
9	1N	119/119 (100%)	109 (92%)	10 (8%)	10	23
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	27
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68	86
10	2O	100/100 (100%)	98 (98%)	2 (2%)	48	74
11	1P	115/116 (99%)	110 (96%)	5 (4%)	26	51
11	2P	115/116 (99%)	104 (90%)	11 (10%)	8	17
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13	30
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	36
13	1R	101/101 (100%)	94 (93%)	7 (7%)	14	32
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	20
14	1S	87/88 (99%)	79 (91%)	8 (9%)	8	19
14	2S	85/88 (97%)	79 (93%)	6 (7%)	13	31
15	1T	115/127 (91%)	110 (96%)	5 (4%)	26	51
15	2T	113/127 (89%)	109 (96%)	4 (4%)	32	59
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34	62
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34	62
17	1V	81/82 (99%)	78 (96%)	3 (4%)	30	57
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	16
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19	40
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	33
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	55
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	68
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	14	31
20	2Y	86/91 (94%)	81 (94%)	5 (6%)	18	39
21	1Z	169/179 (94%)	155 (92%)	14 (8%)	10	23
21	2Z	165/179 (92%)	152 (92%)	13 (8%)	11	26
22	10	61/67 (91%)	59 (97%)	2 (3%)	33	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	20	61/67 (91%)	60 (98%)	1 (2%)	55	79
23	11	79/83 (95%)	74 (94%)	5 (6%)	16	36
23	21	81/83 (98%)	76 (94%)	5 (6%)	16	36
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	63
24	22	66/67 (98%)	60 (91%)	6 (9%)	9	19
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	26
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	37
26	14	58/63 (92%)	54 (93%)	4 (7%)	14	32
26	24	54/63 (86%)	48 (89%)	6 (11%)	6	12
27	15	51/52 (98%)	49 (96%)	2 (4%)	28	55
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	55
28	16	51/52 (98%)	50 (98%)	1 (2%)	48	74
28	26	50/52 (96%)	48 (96%)	2 (4%)	28	55
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	47
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	17
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	40
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	40
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	65
33	1b	191/220 (87%)	164 (86%)	27 (14%)	3	6
33	2b	187/220 (85%)	163 (87%)	24 (13%)	4	8
34	1c	144/188 (77%)	135 (94%)	9 (6%)	16	36
34	2c	140/188 (74%)	127 (91%)	13 (9%)	8	18
35	1d	171/181 (94%)	155 (91%)	16 (9%)	8	18
35	2d	172/181 (95%)	160 (93%)	12 (7%)	14	31
36	1e	114/123 (93%)	107 (94%)	7 (6%)	17	37
36	2e	114/123 (93%)	106 (93%)	8 (7%)	14	31
37	1f	85/90 (94%)	79 (93%)	6 (7%)	13	31
37	2f	85/90 (94%)	82 (96%)	3 (4%)	32	59
38	1g	120/127 (94%)	112 (93%)	8 (7%)	15	33
38	2g	119/127 (94%)	109 (92%)	10 (8%)	10	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	1h	116/119 (98%)	110 (95%)	6 (5%)	21	44
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8	17
40	1i	91/99 (92%)	81 (89%)	10 (11%)	6	13
40	2i	88/99 (89%)	77 (88%)	11 (12%)	4	9
41	1j	68/92 (74%)	64 (94%)	4 (6%)	18	38
41	2j	68/92 (74%)	63 (93%)	5 (7%)	13	29
42	1k	83/99 (84%)	80 (96%)	3 (4%)	31	58
42	2k	83/99 (84%)	79 (95%)	4 (5%)	23	47
43	1l	96/108 (89%)	94 (98%)	2 (2%)	47	73
43	2l	96/108 (89%)	93 (97%)	3 (3%)	35	63
44	1m	90/101 (89%)	82 (91%)	8 (9%)	9	20
44	2m	87/101 (86%)	82 (94%)	5 (6%)	18	40
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	24
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	24
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21	45
46	2o	78/80 (98%)	70 (90%)	8 (10%)	7	15
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	8
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	15
48	1q	94/97 (97%)	92 (98%)	2 (2%)	47	73
48	2q	94/97 (97%)	91 (97%)	3 (3%)	34	62
49	1r	59/77 (77%)	58 (98%)	1 (2%)	53	78
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	60
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7	15
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7	14
51	1t	71/82 (87%)	62 (87%)	9 (13%)	4	9
51	2t	70/82 (85%)	65 (93%)	5 (7%)	13	31
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	40
52	2u	18/22 (82%)	18 (100%)	0	100	100
53	1y	82/98 (84%)	80 (98%)	2 (2%)	43	70
53	2y	79/98 (81%)	71 (90%)	8 (10%)	7	15
All	All	9524/10260 (93%)	8854 (93%)	670 (7%)	14	31

All (670) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	7	LYS
3	1D	35	LYS
3	1D	71	ASP
3	1D	99	ASP
3	1D	111	LEU
3	1D	113	VAL
3	1D	116	GLN
3	1D	141	VAL
3	1D	142	VAL
3	1D	173	VAL
3	1D	193	VAL
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	275	LYS
4	1E	7	VAL
4	1E	9	VAL
4	1E	41	LYS
4	1E	52	LEU
4	1E	72	VAL
4	1E	75	VAL
4	1E	93	VAL
4	1E	116	VAL
4	1E	119	ARG
4	1E	163	GLU
4	1E	178	GLU
4	1E	181	LEU
4	1E	184	VAL
4	1E	188	VAL
5	1F	12	LEU
5	1F	18	ARG
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	132	VAL
5	1F	140	LEU
5	1F	157	VAL
5	1F	158	THR
5	1F	162	LEU
5	1F	183	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	192	LEU
5	1F	197	ASP
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	45	GLU
6	1G	47	LYS
6	1G	52	ILE
6	1G	53	LEU
6	1G	82	LEU
6	1G	159	VAL
6	1G	181	ARG
7	1H	15	VAL
7	1H	18	GLU
7	1H	71	LEU
7	1H	81	GLU
7	1H	98	LEU
7	1H	107	VAL
7	1H	119	GLU
7	1H	122	THR
7	1H	127	GLU
7	1H	149	ARG
8	1I	9	LEU
8	1I	38	LEU
8	1I	44	LEU
8	1I	78	THR
8	1I	92	VAL
8	1I	109	ILE
8	1I	140	LEU
9	1N	5	VAL
9	1N	12	ARG
9	1N	14	VAL
9	1N	33	LEU
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	67	LEU
9	1N	121	LYS
9	1N	133	GLN
10	1O	69	ILE
11	1P	3	LEU
11	1P	59	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	1P	95	VAL
11	1P	99	LEU
11	1P	119	GLU
12	1Q	7	MET
12	1Q	16	ARG
12	1Q	21	THR
12	1Q	55	VAL
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	112	GLU
12	1Q	133	ARG
13	1R	6	SER
13	1R	29	LEU
13	1R	33	ARG
13	1R	44	LEU
13	1R	75	LEU
13	1R	100	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	14	VAL
14	1S	48	LEU
14	1S	50	SER
14	1S	59	LYS
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	39	ARG
15	1T	49	VAL
15	1T	53	ARG
15	1T	59	THR
15	1T	89	VAL
16	1U	59	ARG
16	1U	77	SER
16	1U	104	GLN
17	1V	44	LYS
17	1V	51	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	100	THR
18	1W	107	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	1X	35	THR
19	1X	38	GLU
19	1X	66	LEU
20	1Y	7	VAL
20	1Y	43	ASN
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	92	ASN
20	1Y	107	ASP
21	1Z	61	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	93	ASP
21	1Z	94	GLU
21	1Z	107	THR
21	1Z	126	VAL
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	162	GLU
21	1Z	170	THR
21	1Z	171	ILE
21	1Z	191	VAL
22	10	49	LYS
22	10	74	ARG
23	11	30	VAL
23	11	46	LEU
23	11	74	VAL
23	11	95	LEU
23	11	98	LEU
24	12	9	GLN
24	12	53	LEU
25	13	8	LEU
25	13	23	LEU
25	13	54	VAL
25	13	56	VAL
26	14	49	PHE
26	14	50	VAL
26	14	60	GLN
26	14	61	ARG
27	15	6	VAL
27	15	58	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	16	52	VAL
29	17	24	THR
29	17	43	THR
30	18	14	VAL
30	18	46	ARG
30	18	58	ILE
31	19	17	ILE
33	1b	7	VAL
33	1b	9	GLU
33	1b	10	LEU
33	1b	12	GLU
33	1b	39	ILE
33	1b	52	GLU
33	1b	67	THR
33	1b	71	VAL
33	1b	82	ARG
33	1b	96	ARG
33	1b	111	ARG
33	1b	112	VAL
33	1b	113	HIS
33	1b	117	GLU
33	1b	119	GLU
33	1b	124	SER
33	1b	126	GLU
33	1b	128	GLU
33	1b	140	HIS
33	1b	142	LEU
33	1b	154	LEU
33	1b	160	ASP
33	1b	185	ILE
33	1b	212	GLN
33	1b	221	LEU
33	1b	229	VAL
33	1b	230	VAL
34	1c	26	LYS
34	1c	64	VAL
34	1c	70	VAL
34	1c	82	GLU
34	1c	89	GLU
34	1c	98	ASN
34	1c	105	GLU
34	1c	112	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	115	LEU
35	1d	59	ARG
35	1d	83	SER
35	1d	85	LYS
35	1d	112	VAL
35	1d	127	THR
35	1d	135	LEU
35	1d	144	ASP
35	1d	150	GLU
35	1d	156	GLU
35	1d	166	LYS
35	1d	168	ARG
35	1d	178	VAL
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
35	1d	201	GLN
36	1e	20	GLN
36	1e	31	LEU
36	1e	34	VAL
36	1e	41	VAL
36	1e	65	ASN
36	1e	120	THR
36	1e	126	ARG
37	1f	1	MET
37	1f	10	LEU
37	1f	61	LEU
37	1f	69	GLU
37	1f	73	ASN
37	1f	86	ARG
38	1g	6	ARG
38	1g	13	GLN
38	1g	16	LEU
38	1g	53	LYS
38	1g	76	ARG
38	1g	104	LEU
38	1g	136	LYS
38	1g	138	LYS
39	1h	25	ASP
39	1h	26	VAL
39	1h	39	LEU
39	1h	52	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	1h	127	LEU
39	1h	137	VAL
40	1i	50	LEU
40	1i	64	THR
40	1i	65	VAL
40	1i	66	ARG
40	1i	81	ILE
40	1i	87	GLN
40	1i	103	THR
40	1i	104	ARG
40	1i	108	VAL
40	1i	125	TYR
41	1j	38	ILE
41	1j	55	LYS
41	1j	72	VAL
41	1j	100	THR
42	1k	16	SER
42	1k	84	VAL
42	1k	114	VAL
43	1l	18	VAL
43	1l	83	VAL
44	1m	9	ILE
44	1m	11	ARG
44	1m	12	ASN
44	1m	15	VAL
44	1m	19	LEU
44	1m	54	VAL
44	1m	70	LEU
44	1m	106	ASN
45	1n	3	ARG
45	1n	11	LYS
45	1n	18	VAL
45	1n	33	VAL
46	1o	28	GLN
46	1o	39	LEU
46	1o	66	LEU
46	1o	84	LYS
47	1p	2	VAL
47	1p	20	VAL
47	1p	21	VAL
47	1p	29	ASP
47	1p	62	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	1p	67	THR
47	1p	72	ARG
47	1p	73	LEU
47	1p	74	LEU
48	1q	86	GLU
48	1q	98	LEU
49	1r	82	THR
50	1s	4	SER
50	1s	5	LEU
50	1s	15	LEU
50	1s	28	LYS
50	1s	30	LEU
50	1s	37	ARG
50	1s	66	MET
51	1t	10	LEU
51	1t	24	LEU
51	1t	34	LYS
51	1t	37	SER
51	1t	41	ILE
51	1t	45	GLN
51	1t	46	GLU
51	1t	86	ARG
51	1t	100	ILE
52	1u	15	ARG
53	1y	24	LEU
53	1y	60	VAL
3	2D	3	VAL
3	2D	61	LEU
3	2D	69	ARG
3	2D	99	ASP
3	2D	103	ARG
3	2D	113	VAL
3	2D	138	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	173	VAL
3	2D	193	VAL
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	7	VAL
4	2E	9	VAL
4	2E	52	LEU
4	2E	75	VAL
4	2E	77	ILE
4	2E	116	VAL
4	2E	119	ARG
4	2E	163	GLU
4	2E	170	LEU
4	2E	178	GLU
4	2E	181	LEU
4	2E	184	VAL
5	2F	20	LEU
5	2F	24	LEU
5	2F	27	GLU
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	107	LYS
5	2F	126	VAL
5	2F	140	LEU
5	2F	165	ARG
5	2F	168	ARG
5	2F	170	LEU
5	2F	183	VAL
5	2F	197	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	31	VAL
6	2G	43	LEU
6	2G	53	LEU
6	2G	60	LEU
6	2G	88	ILE
6	2G	116	ASP
6	2G	126	ASP
6	2G	133	LEU
6	2G	138	GLN
6	2G	149	VAL
6	2G	159	VAL
6	2G	162	THR
7	2H	4	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	2H	18	GLU
7	2H	33	LEU
7	2H	43	VAL
7	2H	44	VAL
7	2H	45	VAL
7	2H	50	VAL
7	2H	63	SER
7	2H	70	THR
7	2H	88	LEU
7	2H	92	ILE
7	2H	105	LEU
7	2H	136	ILE
7	2H	137	ASP
8	2I	38	LEU
8	2I	64	GLU
8	2I	68	LEU
8	2I	75	LEU
8	2I	76	THR
8	2I	121	LYS
8	2I	123	LEU
8	2I	127	VAL
9	2N	9	VAL
9	2N	28	THR
9	2N	33	LEU
9	2N	46	VAL
9	2N	62	VAL
9	2N	67	LEU
9	2N	85	ILE
9	2N	99	LEU
9	2N	115	ARG
10	2O	61	VAL
10	2O	70	LYS
11	2P	3	LEU
11	2P	29	LYS
11	2P	30	THR
11	2P	59	LEU
11	2P	71	VAL
11	2P	95	VAL
11	2P	96	THR
11	2P	123	LEU
11	2P	125	VAL
11	2P	126	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	2P	133	SER
12	2Q	7	MET
12	2Q	35	VAL
12	2Q	55	VAL
12	2Q	98	LYS
12	2Q	109	VAL
12	2Q	112	GLU
12	2Q	130	LYS
13	2R	29	LEU
13	2R	33	ARG
13	2R	44	LEU
13	2R	75	LEU
13	2R	86	ARG
13	2R	96	ARG
13	2R	100	LEU
13	2R	114	VAL
13	2R	117	VAL
14	2S	28	VAL
14	2S	44	LYS
14	2S	48	LEU
14	2S	52	SER
14	2S	53	SER
14	2S	85	VAL
15	2T	28	VAL
15	2T	34	VAL
15	2T	89	VAL
15	2T	107	ASP
16	2U	31	SER
16	2U	104	GLN
16	2U	111	GLU
17	2V	32	THR
17	2V	35	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	62	LEU
17	2V	71	LEU
17	2V	72	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	60	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	2W	100	THR
18	2W	107	LEU
19	2X	88	LYS
19	2X	90	GLU
20	2Y	19	LYS
20	2Y	42	VAL
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	99	CYS
21	2Z	2	GLU
21	2Z	28	MET
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	71	VAL
21	2Z	86	VAL
21	2Z	94	GLU
21	2Z	107	THR
21	2Z	121	HIS
21	2Z	150	LEU
21	2Z	171	ILE
21	2Z	182	LYS
21	2Z	193	GLU
22	20	36	ILE
23	21	4	VAL
23	21	21	ARG
23	21	40	ARG
23	21	51	VAL
23	21	85	LEU
24	22	1	MET
24	22	17	SER
24	22	32	LEU
24	22	52	ASP
24	22	53	LEU
24	22	64	LEU
25	23	23	LEU
25	23	31	LEU
25	23	54	VAL
26	24	10	VAL
26	24	14	ILE
26	24	39	CYS
26	24	40	HIS
26	24	49	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	24	50	VAL
27	25	6	VAL
27	25	58	LEU
28	26	14	THR
28	26	48	VAL
29	27	1	MET
29	27	24	THR
29	27	43	THR
29	27	46	VAL
30	28	3	LYS
30	28	14	VAL
30	28	29	LYS
31	29	12	ASP
33	2b	8	LYS
33	2b	44	LEU
33	2b	45	GLN
33	2b	52	GLU
33	2b	68	ILE
33	2b	71	VAL
33	2b	80	ILE
33	2b	90	MET
33	2b	93	VAL
33	2b	96	ARG
33	2b	97	TRP
33	2b	127	ILE
33	2b	153	ARG
33	2b	154	LEU
33	2b	160	ASP
33	2b	164	VAL
33	2b	168	THR
33	2b	178	ARG
33	2b	187	LEU
33	2b	196	LEU
33	2b	200	ILE
33	2b	208	ILE
33	2b	224	GLN
33	2b	229	VAL
34	2c	3	ASN
34	2c	33	LEU
34	2c	47	LEU
34	2c	52	LEU
34	2c	101	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	115	LEU
34	2c	136	GLN
34	2c	152	ILE
34	2c	164	ARG
34	2c	166	GLU
34	2c	196	LEU
34	2c	206	GLU
34	2c	207	VAL
35	2d	5	ILE
35	2d	19	LEU
35	2d	28	SER
35	2d	83	SER
35	2d	107	ARG
35	2d	108	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	166	LYS
35	2d	170	VAL
35	2d	175	SER
35	2d	188	LEU
36	2e	31	LEU
36	2e	34	VAL
36	2e	41	VAL
36	2e	47	LYS
36	2e	68	GLU
36	2e	75	THR
36	2e	79	GLU
36	2e	107	ARG
37	2f	61	LEU
37	2f	72	VAL
37	2f	95	GLU
38	2g	8	GLU
38	2g	9	VAL
38	2g	15	ASP
38	2g	16	LEU
38	2g	21	VAL
38	2g	22	LEU
38	2g	51	GLN
38	2g	75	VAL
38	2g	114	ARG
38	2g	144	MET
39	2h	25	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	2h	33	GLU
39	2h	63	LEU
39	2h	84	ARG
39	2h	85	ARG
39	2h	91	ARG
39	2h	112	LEU
39	2h	114	THR
39	2h	121	ASP
39	2h	133	LEU
39	2h	137	VAL
40	2i	7	THR
40	2i	9	ARG
40	2i	14	VAL
40	2i	17	VAL
40	2i	23	ASN
40	2i	25	LYS
40	2i	56	LEU
40	2i	71	SER
40	2i	86	VAL
40	2i	108	VAL
40	2i	111	ARG
41	2j	34	VAL
41	2j	38	ILE
41	2j	47	PHE
41	2j	73	ASP
41	2j	95	GLU
42	2k	30	VAL
42	2k	48	ILE
42	2k	84	VAL
42	2k	117	ASN
43	2l	33	ARG
43	2l	36	VAL
43	2l	83	VAL
44	2m	11	ARG
44	2m	47	ASP
44	2m	67	GLU
44	2m	96	LEU
44	2m	104	ARG
45	2n	3	ARG
45	2n	7	ILE
45	2n	18	VAL
45	2n	33	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	2o	3	ILE
46	2o	5	LYS
46	2o	39	LEU
46	2o	64	ARG
46	2o	66	LEU
46	2o	71	GLN
46	2o	84	LYS
46	2o	87	ILE
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG
47	2p	12	LYS
47	2p	20	VAL
47	2p	67	THR
47	2p	74	LEU
48	2q	53	LEU
48	2q	85	VAL
48	2q	86	GLU
49	2r	26	LEU
49	2r	45	SER
50	2s	41	VAL
50	2s	58	VAL
50	2s	63	THR
50	2s	64	GLU
50	2s	71	LEU
50	2s	77	THR
50	2s	79	THR
51	2t	10	LEU
51	2t	24	LEU
51	2t	46	GLU
51	2t	84	LEU
51	2t	100	ILE
53	2y	5	ILE
53	2y	6	THR
53	2y	12	ILE
53	2y	13	THR
53	2y	16	ILE
53	2y	42	SER
53	2y	49	VAL
53	2y	56	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	253	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	133	ASN
5	1F	203	GLN
6	1G	26	GLN
6	1G	40	ASN
6	1G	108	ASN
6	1G	132	ASN
9	1N	94	HIS
9	1N	133	GLN
10	1O	3	GLN
13	1R	13	HIS
13	1R	24	GLN
13	1R	71	GLN
14	1S	68	GLN
15	1T	58	ASN
15	1T	84	GLN
15	1T	123	GLN
16	1U	72	HIS
16	1U	94	ASN
16	1U	117	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	73	GLN
21	1Z	151	HIS
23	11	19	GLN
23	11	56	GLN
25	13	32	GLN
30	18	35	GLN
33	1b	95	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	102	ASN
34	1c	104	GLN
34	1c	162	GLN
35	1d	77	ASN
35	1d	123	HIS
35	1d	129	ASN
35	1d	160	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1e	20	GLN
36	1e	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	64	GLN
38	1g	86	GLN
38	1g	110	GLN
40	1i	3	GLN
40	1i	87	GLN
41	1j	69	ASN
41	1j	84	GLN
42	1k	93	GLN
43	1l	80	HIS
43	1l	99	HIS
46	1o	28	GLN
47	1p	16	HIS
48	1q	45	HIS
48	1q	93	GLN
50	1s	14	HIS
50	1s	83	HIS
51	1t	18	GLN
51	1t	90	GLN
53	1y	9	GLN
53	1y	38	HIS
3	2D	126	GLN
3	2D	253	GLN
5	2F	69	HIS
5	2F	133	ASN
6	2G	26	GLN
6	2G	41	GLN
6	2G	132	ASN
8	2I	43	ASN
8	2I	104	GLN
9	2N	94	HIS
9	2N	133	GLN
10	2O	3	GLN
11	2P	35	HIS
12	2Q	13	GLN
12	2Q	89	ASN
12	2Q	141	GLN
13	2R	24	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	2R	71	GLN
15	2T	58	ASN
16	2U	94	ASN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
20	2Y	57	GLN
21	2Z	65	GLN
21	2Z	118	GLN
21	2Z	151	HIS
24	22	38	GLN
25	23	32	GLN
26	24	40	HIS
26	24	46	GLN
28	26	20	ASN
30	28	35	GLN
33	2b	19	HIS
33	2b	146	GLN
33	2b	224	GLN
34	2c	6	HIS
34	2c	28	GLN
34	2c	31	HIS
34	2c	136	GLN
34	2c	139	GLN
34	2c	176	HIS
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	160	GLN
36	2e	38	GLN
36	2e	73	ASN
36	2e	141	GLN
38	2g	13	GLN
38	2g	28	ASN
38	2g	86	GLN
38	2g	97	GLN
39	2h	15	ASN
39	2h	82	HIS
40	2i	29	ASN
40	2i	31	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	84	GLN
42	2k	93	GLN
43	2l	99	HIS
44	2m	62	ASN
46	2o	28	GLN
47	2p	13	HIS
47	2p	16	HIS
48	2q	16	GLN
48	2q	93	GLN
50	2s	83	HIS
53	2y	9	GLN
53	2y	46	GLN
53	2y	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	396 (13%)	27 (0%)
1	2A	2858/2915 (98%)	460 (16%)	32 (1%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	15 (12%)	0
32	1a	1497/1521 (98%)	241 (16%)	0
32	2a	1501/1521 (98%)	254 (16%)	0
All	All	8959/9114 (98%)	1375 (15%)	59 (0%)

All (1375) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	94	C
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	181	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	229	A
1	1A	248	G
1	1A	265	A
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
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	280	C
1	1A	283	A
1	1A	311	A
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	505	A
1	1A	509	C
1	1A	528	A
1	1A	530	G
1	1A	531	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	748	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	882	G
1	1A	886	C
1	1A	887	A
1	1A	888	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	910	A
1	1A	931	G
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1039	G
1	1A	1041	C
1	1A	1042	G
1	1A	1043	C
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1065	U
1	1A	1066	U
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1109	C
1	1A	1110	G
1	1A	1112	G
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1139	G
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1210	A
1	1A	1211	U
1	1A	1220	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1320	C
1	1A	1321	A
1	1A	1345	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	1452	A
1	1A	1455	G
1	1A	1459	G
1	1A	1465	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C
1	1A	1506	C
1	1A	1508	A
1	1A	1509(A)	A
1	1A	1542	A
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1648	C
1	1A	1654	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1936	A
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2103	C
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2112	G
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2119	A
1	1A	2121	G
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2135	A
1	1A	2139	C
1	1A	2142	C
1	1A	2145	C
1	1A	2146	C
1	1A	2147	G
1	1A	2153	G
1	1A	2158	A
1	1A	2159	G
1	1A	2164	C
1	1A	2170	A
1	1A	2173	A
1	1A	2178	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2186	G
1	1A	2187	G
1	1A	2189	U
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2279	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2422	A
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2469	A
1	1A	2470	G
1	1A	2476	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2498	C
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	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	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2893	G
1	1A	2894	G
2	1B	2	C
2	1B	13	A
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	92	C
32	1a	101	A
32	1a	102	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	159	G
32	1a	160	A
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(F)	U
32	1a	189(G)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	231	G
32	1a	247	G
32	1a	251	G
32	1a	262	A
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	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	439	A
32	1a	442	C
32	1a	451	A
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	475	G
32	1a	484	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	532	A
32	1a	536	C
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	564	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	633	G
32	1a	651	C
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	666	G
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	755	G
32	1a	759	A
32	1a	770	C
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	828	A
32	1a	829	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	870	U
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	963	G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	999	C
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(D)	A
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1038	C
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1124	G
32	1a	1126	U
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1159	U
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1186	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1293	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1406	U
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1493	A
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1520	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	12	U
1	2A	14	A
1	2A	34	C
1	2A	45	C
1	2A	55	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
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	141	A
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	277	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	278	A
1	2A	283	A
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	370	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	545	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	740	U
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	815	C
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	880	G
1	2A	881	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	980	A
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	1012	U
1	2A	1013	C
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1041	C
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1055	G
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1072	C
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1095	A
1	2A	1096	A
1	2A	1097	U
1	2A	1105	U
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1170	G
1	2A	1171	G
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1236	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1329	U
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1750	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1918	A
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1938	A
1	2A	1955	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1975	G
1	2A	1984	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2096	U
1	2A	2100	G
1	2A	2101	G
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2111	C
1	2A	2112	G
1	2A	2114	A
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2121	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2130	U
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2144	U
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2163	C
1	2A	2164	C
1	2A	2172	U
1	2A	2173	A
1	2A	2178	C
1	2A	2180	U
1	2A	2181	G
1	2A	2184	G
1	2A	2186	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2269	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2311	A
1	2A	2312	U
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2335	A
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2406	U
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G
1	2A	2474	C
1	2A	2476	A
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
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	2744	G
1	2A	2748	A
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2872	G
1	2A	2880	C
1	2A	2891	G
1	2A	2894	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2896	C
2	2B	2	C
2	2B	7	G
2	2B	9	G
2	2B	13	A
2	2B	30	C
2	2B	33	G
2	2B	35	U
2	2B	45	A
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	106	G
2	2B	109	C
2	2B	110	G
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	61	G
32	2a	66	G
32	2a	78	G
32	2a	80	G
32	2a	89	C
32	2a	97	G
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	156	G
32	2a	163	C
32	2a	174	C
32	2a	182	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	189(C)	C
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	298	A
32	2a	316	G
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	367	U
32	2a	372	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	414	A
32	2a	421	U
32	2a	422	C
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	476	G
32	2a	477	A
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	528	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	631	G
32	2a	633	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	774	G
32	2a	777	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	785	G
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	859	A
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1017	G
32	2a	1020	U
32	2a	1022	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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(A)	G
32	2a	1030(B)	C
32	2a	1041	A
32	2a	1044	A
32	2a	1047	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C
32	2a	1183	A
32	2a	1185	G
32	2a	1186	G
32	2a	1194	U
32	2a	1196	U
32	2a	1197	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1202	G
32	2a	1208	C
32	2a	1211	U
32	2a	1212	U
32	2a	1214	C
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1311	G
32	2a	1312	G
32	2a	1317	C
32	2a	1319	A
32	2a	1320	C
32	2a	1323	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1359	C
32	2a	1363	C
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1460	A
32	2a	1492	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1528	U
32	2a	1529	G
32	2a	1530	G

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	746	A
1	1A	827	U
1	1A	839	U
1	1A	895	U
1	1A	974	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	2126	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2172	U
1	1A	2406	U
1	1A	2430	A
1	1A	2602	A
1	1A	2689	U
1	1A	2756	U
1	1A	2893	G
1	2A	9	U
1	2A	195	A
1	2A	196	A
1	2A	271(M)	G
1	2A	277	C
1	2A	645	C
1	2A	752	A
1	2A	764	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2406	U
1	2A	2601	C
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	2A	2552	54,1	19,22,23	1.18	3 (15%)	25,31,34	1.87	5 (20%)
32	2MG	1a	1207	32,54	23,26,27	1.24	2 (8%)	33,38,41	2.36	9 (27%)
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.12	3 (11%)
1	5MC	1A	1942	54,1	19,22,23	1.59	3 (15%)	26,32,35	1.10	2 (7%)
32	5MC	2a	967	32	19,22,23	1.79	3 (15%)	26,32,35	1.10	2 (7%)
32	PSU	2a	516	32,54	18,21,22	1.36	2 (11%)	21,30,33	2.09	5 (23%)
43	0TD	2l	92	43	8,9,10	4.37	1 (12%)	6,11,13	1.27	1 (16%)
43	0TD	1l	92	43	8,9,10	4.52	1 (12%)	6,11,13	6.96	2 (33%)
32	UR3	2a	1498	32	19,22,23	1.00	2 (10%)	26,32,35	1.73	3 (11%)
1	OMU	1A	2552	54,1	19,22,23	1.24	2 (10%)	25,31,34	1.77	5 (20%)
32	G7M	1a	527	32,54	23,26,27	1.52	3 (13%)	34,39,42	1.71	5 (14%)
1	5MU	2A	1915	1	19,22,23	1.45	4 (21%)	27,32,35	2.20	8 (29%)
1	PSU	1A	1917	54,1	18,21,22	1.36	2 (11%)	21,30,33	1.98	3 (14%)
32	5MC	1a	1407	32	19,22,23	1.71	3 (15%)	26,32,35	1.14	3 (11%)
1	5MC	2A	1962	54,1	19,22,23	1.61	3 (15%)	26,32,35	1.14	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.99	1 (4%)
1	5MU	1A	1939	54,1	19,22,23	1.43	6 (31%)	27,32,35	2.10	6 (22%)
32	M2G	1a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.85	6 (18%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.74	3 (11%)
32	5MC	2a	1400	32	19,22,23	1.66	3 (15%)	26,32,35	1.17	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.63	3 (15%)	26,32,35	1.09	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.34	2 (11%)	21,30,33	2.05	5 (23%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	1.98	9 (27%)
32	PSU	1a	516	32,54	18,21,22	1.38	2 (11%)	21,30,33	1.97	4 (19%)
32	MA6	1a	1519	32	23,26,27	0.42	0	33,38,41	2.03	9 (27%)
32	G7M	2a	527	32,54	23,26,27	1.52	3 (13%)	34,39,42	1.73	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	2a	966	32	24,27,28	1.29	3 (12%)	33,40,43	1.85	6 (18%)
1	5MU	2A	1939	1	19,22,23	1.41	5 (26%)	27,32,35	2.16	6 (22%)
32	4OC	2a	1402	32	20,23,24	0.77	0	25,32,35	1.01	1 (4%)
1	5MC	2A	1942	1	19,22,23	1.72	3 (15%)	26,32,35	1.13	2 (7%)
1	2MA	1A	2503	54,1	22,25,26	1.50	4 (18%)	32,37,40	2.34	7 (21%)
1	OMG	2A	2251	54,1	23,26,27	1.18	3 (13%)	32,38,41	2.02	6 (18%)
32	5MC	1a	1400	32	19,22,23	1.76	3 (15%)	26,32,35	1.14	2 (7%)
1	PSU	1A	2605	1	18,21,22	1.37	3 (16%)	21,30,33	2.03	4 (19%)
1	2MA	2A	2503	54,1	22,25,26	1.50	4 (18%)	32,37,40	2.34	8 (25%)
1	PSU	2A	2605	1	18,21,22	1.32	2 (11%)	21,30,33	2.09	4 (19%)
1	OMC	1A	1920	1	19,22,23	0.78	0	25,31,34	0.85	1 (4%)
32	MA6	2a	1518	32	23,26,27	0.40	0	33,38,41	2.03	9 (27%)
32	MA6	2a	1519	32	23,26,27	0.41	0	33,38,41	2.09	9 (27%)
1	OMG	1A	2251	54,1	23,26,27	1.20	3 (13%)	32,38,41	2.00	6 (18%)
1	5MC	1A	1962	54,1	19,22,23	1.78	3 (15%)	26,32,35	1.20	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.98	1 (4%)
32	2MG	2a	1207	32	23,26,27	1.21	2 (8%)	33,38,41	2.21	7 (21%)
1	5MU	1A	1915	54,1	19,22,23	1.47	6 (31%)	27,32,35	2.18	8 (29%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
32	5MC	2a	1407	32	19,22,23	1.64	2 (10%)	26,32,35	1.16	3 (11%)
32	5MC	1a	967	32	19,22,23	1.67	3 (15%)	26,32,35	1.12	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	32,54	-	0/9/27/28	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	54,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
43	0TD	1l	92	43	-	2/7/12/14	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	54,1	-	0/9/27/28	0/2/2/2
32	G7M	1a	527	32,54	-	1/7/25/26	0/3/3/3
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	54,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	54,1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	5MU	1A	1939	54,1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	G7M	2a	527	32,54	-	3/7/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	1/7/25/26	0/3/3/3
1	OMG	2A	2251	54,1	-	0/9/27/28	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	54,1	-	2/7/25/26	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	MA6	2a	1519	32	-	2/11/29/30	0/3/3/3
1	OMG	1A	2251	54,1	-	0/9/27/28	0/3/3/3
1	5MC	1A	1962	54,1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	1A	1915	54,1	-	2/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.42	1.69	1.82
43	2l	92	0TD	CB-SB	-12.02	1.70	1.82
32	2a	967	5MC	C5-C4	6.61	1.49	1.44
1	1A	1962	5MC	C5-C4	6.61	1.49	1.44
32	1a	1400	5MC	C5-C4	6.47	1.49	1.44
1	2A	1942	5MC	C5-C4	6.32	1.48	1.44
32	1a	1407	5MC	C5-C4	6.23	1.48	1.44
32	2a	1404	5MC	C5-C4	6.16	1.48	1.44
32	2a	1400	5MC	C5-C4	6.02	1.48	1.44
32	1a	967	5MC	C5-C4	6.00	1.48	1.44
32	1a	1404	5MC	C5-C4	5.88	1.48	1.44
32	2a	1407	5MC	C5-C4	5.82	1.48	1.44
1	2A	1962	5MC	C5-C4	5.77	1.48	1.44
1	1A	1942	5MC	C5-C4	5.56	1.48	1.44
32	1a	527	G7M	C5-N7	-4.79	1.33	1.39
32	2a	527	G7M	C5-N7	-4.55	1.33	1.39
1	2A	2503	2MA	C5-C4	4.54	1.47	1.39
1	1A	2503	2MA	C5-C4	4.54	1.47	1.39
32	1a	516	PSU	C6-C5	3.53	1.39	1.35
1	1A	1917	PSU	C6-C5	3.52	1.39	1.35
1	2A	1911	PSU	C6-C5	3.49	1.39	1.35
1	2A	1917	PSU	C6-C5	3.43	1.39	1.35
32	2a	516	PSU	C6-C5	3.36	1.39	1.35
1	1A	1911	PSU	C6-C5	3.32	1.39	1.35
32	2a	527	G7M	C5-C4	3.27	1.46	1.38
32	2a	966	M2G	C5-C4	3.24	1.47	1.38
32	1a	527	G7M	C5-C4	3.21	1.46	1.38
1	2A	2605	PSU	C6-C5	3.19	1.38	1.35
32	1a	966	M2G	C5-C4	3.14	1.47	1.38
1	2A	2251	OMG	C5-C4	3.14	1.47	1.38
32	2a	1207	2MG	C5-C4	3.13	1.47	1.38
32	1a	1207	2MG	C5-C4	3.05	1.47	1.38
1	1A	2251	OMG	C5-C4	3.03	1.47	1.38
32	2a	1407	5MC	C6-C5	3.02	1.39	1.34
1	1A	2605	PSU	C6-C5	3.00	1.38	1.35
1	1A	1939	5MU	C6-C5	2.96	1.39	1.34
32	2a	966	M2G	C2-N2	2.95	1.40	1.35
1	1A	1915	5MU	C2-N1	2.92	1.43	1.38
32	1a	1400	5MC	C6-C5	2.91	1.39	1.34
1	2A	1915	5MU	C2-N1	2.87	1.43	1.38
32	2a	1404	5MC	C6-C5	2.86	1.39	1.34
32	1a	1407	5MC	C6-C5	2.86	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	967	5MC	C6-C5	2.85	1.39	1.34
1	2A	1939	5MU	C6-C5	2.84	1.39	1.34
1	2A	1915	5MU	C6-C5	2.83	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.82	1.33	1.38
32	1a	1404	5MC	C6-C5	2.82	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.80	1.33	1.38
32	1a	967	5MC	C6-C5	2.79	1.39	1.34
1	2A	1962	5MC	C6-C5	2.79	1.39	1.34
1	1A	1942	5MC	C6-C5	2.78	1.39	1.34
1	1A	1915	5MU	C6-C5	2.76	1.39	1.34
32	1a	966	M2G	C2-N2	2.76	1.40	1.35
1	1A	1915	5MU	C4-N3	-2.73	1.33	1.38
1	2A	1942	5MC	C6-C5	2.71	1.39	1.34
32	2a	1400	5MC	C6-C5	2.70	1.39	1.34
1	1A	2503	2MA	C5-N7	-2.67	1.34	1.39
1	1A	2552	OMU	C4-N3	-2.67	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.65	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.63	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.61	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.60	1.33	1.38
1	2A	2552	OMU	C4-N3	-2.59	1.34	1.38
32	2a	516	PSU	C4-N3	-2.59	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.58	1.34	1.38
1	2A	2503	2MA	C5-C6	2.58	1.48	1.41
1	2A	1939	5MU	C4-C5	2.57	1.49	1.44
1	2A	1917	PSU	C4-N3	-2.55	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.55	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.53	1.34	1.38
32	1a	516	PSU	C4-N3	-2.53	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.52	1.34	1.38
32	1a	966	M2G	C6-N1	-2.51	1.34	1.38
1	1A	1962	5MC	C6-C5	2.49	1.38	1.34
32	2a	527	G7M	C6-N1	-2.47	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.42	1.33	1.38
1	1A	2503	2MA	C8-N7	2.41	1.36	1.31
1	1A	2503	2MA	C5-C6	2.40	1.47	1.41
1	2A	2251	OMG	C6-N1	-2.38	1.34	1.38
32	1a	527	G7M	C6-N1	-2.37	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.37	1.34	1.38
1	2A	1915	5MU	C4-C5	2.35	1.48	1.44
1	2A	2503	2MA	C5-N7	-2.33	1.34	1.39
1	1A	1939	5MU	C2-N3	-2.31	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1915	5MU	C4-C5	2.31	1.48	1.44
32	1a	1400	5MC	C6-N1	-2.27	1.34	1.38
32	2a	966	M2G	C6-N1	-2.27	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.27	1.34	1.38
1	2A	2503	2MA	C8-N7	2.27	1.36	1.31
32	2a	1400	5MC	C6-N1	-2.25	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.24	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.24	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.24	1.34	1.38
1	1A	2552	OMU	C2-N3	-2.21	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.21	1.34	1.38
32	1a	967	5MC	C6-N1	-2.18	1.34	1.38
1	1A	1939	5MU	C4-C5	2.18	1.48	1.44
1	2A	2251	OMG	C5-N7	-2.14	1.34	1.39
32	2a	1404	5MC	C6-N1	-2.14	1.34	1.38
32	2a	967	5MC	C6-N1	-2.13	1.34	1.38
1	2A	2552	OMU	C2-N3	-2.13	1.34	1.38
1	1A	2251	OMG	C5-N7	-2.12	1.34	1.39
32	1a	1498	UR3	C6-C5	2.11	1.40	1.35
32	1a	1404	5MC	C6-N1	-2.11	1.34	1.38
32	2a	1498	UR3	C6-C5	2.07	1.39	1.35
1	2A	2552	OMU	C5-C4	-2.06	1.39	1.43
1	2A	1939	5MU	C2-N1	2.05	1.41	1.38
1	1A	1915	5MU	C2-N3	-2.04	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.03	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.02	1.34	1.38
32	2a	1498	UR3	C2-N1	2.02	1.41	1.38
1	1A	2605	PSU	C2-N3	-2.02	1.34	1.37
1	1A	1939	5MU	C2-N1	2.01	1.41	1.38
32	1a	966	M2G	C5-N7	-2.00	1.35	1.39

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-16.76	72.24	102.36
1	1A	2503	2MA	C5-C4-N3	-8.42	118.31	127.18
1	2A	2503	2MA	C5-C4-N3	-8.20	118.55	127.18
32	1a	1207	2MG	C2-N3-C4	7.28	121.11	112.00
32	1a	1498	UR3	C4-N3-C2	-7.03	118.92	124.58
32	2a	1498	UR3	C4-N3-C2	-6.99	118.96	124.58
32	2a	1207	2MG	C2-N3-C4	6.82	120.53	112.00
1	2A	2503	2MA	N3-C4-N9	6.71	135.50	126.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	N3-C4-N9	6.43	135.15	126.99
32	2a	516	PSU	N1-C2-N3	6.41	121.93	115.17
1	2A	1911	PSU	N1-C2-N3	6.37	121.89	115.17
1	2A	2605	PSU	N1-C2-N3	6.32	121.84	115.17
1	2A	2251	OMG	C5-C4-N3	-6.31	118.34	128.39
1	1A	2605	PSU	N1-C2-N3	6.27	121.78	115.17
1	1A	1911	PSU	N1-C2-N3	6.25	121.76	115.17
1	1A	2251	OMG	C5-C4-N3	-6.18	118.55	128.39
1	2A	1917	PSU	N1-C2-N3	6.16	121.67	115.17
32	1a	516	PSU	N1-C2-N3	6.15	121.66	115.17
1	1A	1917	PSU	N1-C2-N3	6.14	121.65	115.17
32	2a	966	M2G	C5-C4-N3	-6.02	118.81	128.39
32	1a	966	M2G	C5-C4-N3	-6.02	118.81	128.39
32	1a	1207	2MG	C5-C4-N3	-5.81	119.14	128.39
32	2a	1207	2MG	C5-C4-N3	-5.55	119.56	128.39
32	2a	527	G7M	N9-C4-N3	5.47	136.90	125.95
32	2a	527	G7M	C5-C4-N3	-5.44	117.88	128.15
32	1a	527	G7M	N9-C4-N3	5.42	136.79	125.95
1	2A	1939	5MU	C4-N3-C2	-5.36	120.32	127.34
32	1a	527	G7M	C5-C4-N3	-5.32	118.09	128.15
1	2A	1939	5MU	N3-C2-N1	5.20	121.67	114.89
1	2A	2251	OMG	C2-N3-C4	5.19	121.24	112.30
1	1A	1939	5MU	N3-C2-N1	5.16	121.61	114.89
1	1A	1939	5MU	C4-N3-C2	-5.16	120.58	127.34
1	1A	1915	5MU	N3-C2-N1	5.13	121.57	114.89
1	2A	1915	5MU	N3-C2-N1	5.12	121.56	114.89
1	1A	2251	OMG	C2-N3-C4	5.12	121.11	112.30
1	2A	2552	OMU	C4-N3-C2	-5.05	120.34	126.61
32	2a	1519	MA6	N1-C2-N3	-4.88	121.20	128.58
32	2a	1518	MA6	N1-C2-N3	-4.85	121.24	128.58
32	2a	527	G7M	C2-N3-C4	4.74	120.46	112.30
1	2A	1915	5MU	C4-N3-C2	-4.72	121.15	127.34
32	1a	527	G7M	C2-N3-C4	4.71	120.42	112.30
1	1A	2552	OMU	C4-N3-C2	-4.70	120.78	126.61
32	1a	1519	MA6	N1-C2-N3	-4.68	121.49	128.58
32	1a	1518	MA6	N1-C2-N3	-4.68	121.50	128.58
1	1A	1915	5MU	C4-N3-C2	-4.68	121.21	127.34
1	2A	2251	OMG	N9-C4-N3	4.61	135.16	125.95
1	1A	2251	OMG	N9-C4-N3	4.57	135.09	125.95
32	2a	966	M2G	C2-N3-C4	4.57	120.96	112.51
32	1a	966	M2G	C2-N3-C4	4.49	120.81	112.51
1	1A	1939	5MU	C5-C4-N3	4.48	119.22	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1519	MA6	C5-C4-N3	-4.45	120.59	126.72
32	1a	966	M2G	N9-C4-N3	4.43	134.82	125.95
32	2a	1519	MA6	C5-C4-N3	-4.41	120.65	126.72
32	2a	1518	MA6	C5-C4-N3	-4.40	120.66	126.72
1	2A	1939	5MU	C5-C4-N3	4.39	119.14	115.32
32	2a	966	M2G	N9-C4-N3	4.38	134.72	125.95
1	2A	2605	PSU	C4-N3-C2	-4.36	120.36	126.37
32	2a	516	PSU	C4-N3-C2	-4.29	120.47	126.37
1	1A	2552	OMU	N3-C2-N1	4.25	120.43	114.89
1	1A	2605	PSU	C4-N3-C2	-4.25	120.52	126.37
1	1A	1911	PSU	C4-N3-C2	-4.23	120.55	126.37
32	1a	1518	MA6	C5-C4-N3	-4.23	120.90	126.72
1	2A	2552	OMU	N3-C2-N1	4.15	120.30	114.89
1	2A	1915	5MU	C5-C4-N3	4.09	118.88	115.32
32	2a	1518	MA6	C2-N1-C6	4.07	121.77	111.83
1	2A	1911	PSU	C4-N3-C2	-4.07	120.77	126.37
32	2a	1519	MA6	C5-N7-C8	4.05	109.81	103.45
1	2A	2552	OMU	C5-C4-N3	4.04	120.46	114.80
32	1a	1518	MA6	C2-N1-C6	4.02	121.65	111.83
1	1A	1915	5MU	C5-C4-N3	4.02	118.82	115.32
1	1A	1917	PSU	C4-N3-C2	-4.02	120.84	126.37
32	2a	1519	MA6	C4-C5-N7	-4.00	106.01	110.58
32	1a	1207	2MG	C6-C5-N7	3.98	137.53	130.29
32	2a	1519	MA6	C2-N1-C6	3.97	121.54	111.83
32	1a	1519	MA6	C2-N1-C6	3.97	121.52	111.83
32	1a	516	PSU	C4-N3-C2	-3.96	120.91	126.37
1	2A	1939	5MU	C5-C6-N1	-3.94	119.03	123.31
32	1a	1519	MA6	C4-C5-N7	-3.92	106.10	110.58
1	1A	1939	5MU	C5-C6-N1	-3.88	119.10	123.31
1	1A	1915	5MU	C1'-N1-C2	3.88	124.55	117.59
1	2A	1917	PSU	C4-N3-C2	-3.86	121.06	126.37
1	2A	1939	5MU	O4-C4-C5	-3.85	120.51	124.92
1	1A	1939	5MU	O4-C4-C5	-3.84	120.52	124.92
1	2A	1915	5MU	C1'-N1-C2	3.84	124.49	117.59
1	1A	2503	2MA	N6-C6-N1	3.83	122.20	117.03
32	2a	1207	2MG	C6-C5-N7	3.83	137.26	130.29
32	2a	1518	MA6	C5-N7-C8	3.82	109.45	103.45
32	1a	1519	MA6	C5-N7-C8	3.80	109.42	103.45
32	1a	1207	2MG	N9-C4-N3	3.77	133.50	125.95
32	1a	1518	MA6	C5-N7-C8	3.74	109.33	103.45
1	2A	1915	5MU	O4-C4-C5	-3.71	120.67	124.92
1	1A	2552	OMU	C5-C4-N3	3.67	119.95	114.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1911	PSU	O2-C2-N1	-3.65	119.02	122.79
1	2A	2605	PSU	O2-C2-N1	-3.65	119.03	122.79
32	2a	1207	2MG	N9-C4-N3	3.64	133.24	125.95
32	2a	1518	MA6	C4-C5-N7	-3.64	106.42	110.58
32	2a	516	PSU	O2-C2-N1	-3.59	119.09	122.79
1	1A	1915	5MU	O4-C4-C5	-3.59	120.81	124.92
32	2a	1519	MA6	N9-C8-N7	-3.58	108.85	113.94
32	1a	1518	MA6	C4-C5-N7	-3.58	106.49	110.58
1	2A	1917	PSU	O2-C2-N1	-3.57	119.11	122.79
32	2a	1400	5MC	C5-C6-N1	-3.54	119.47	123.31
32	1a	1400	5MC	C5-C6-N1	-3.51	119.50	123.31
1	2A	1942	5MC	C5-C6-N1	-3.49	119.52	123.31
1	1A	1917	PSU	O2-C2-N1	-3.45	119.23	122.79
32	2a	1519	MA6	C2-N3-C4	3.43	120.21	111.83
32	2a	1518	MA6	N9-C8-N7	-3.42	109.09	113.94
1	1A	1962	5MC	C5-C6-N1	-3.41	119.61	123.31
1	1A	1942	5MC	C5-C6-N1	-3.39	119.63	123.31
32	2a	1207	2MG	N1-C2-N2	3.39	120.02	116.56
1	1A	2605	PSU	O2-C2-N1	-3.37	119.32	122.79
1	1A	2503	2MA	C4-C5-N7	-3.36	106.74	110.58
32	1a	1518	MA6	N9-C8-N7	-3.36	109.17	113.94
32	2a	1518	MA6	C2-N3-C4	3.36	120.04	111.83
1	2A	2503	2MA	C4-C5-N7	-3.33	106.77	110.58
32	1a	1519	MA6	C2-N3-C4	3.32	119.95	111.83
1	1A	2251	OMG	C6-C5-N7	3.30	136.30	130.29
32	1a	516	PSU	O2-C2-N1	-3.30	119.39	122.79
1	2A	1911	PSU	O2-C2-N1	-3.27	119.42	122.79
32	1a	966	M2G	C6-C5-N7	3.25	136.21	130.29
1	2A	1962	5MC	C5-C6-N1	-3.24	119.79	123.31
1	2A	2552	OMU	O4-C4-C5	-3.24	119.58	125.16
32	2a	966	M2G	C6-C5-N7	3.23	136.18	130.29
32	2a	967	5MC	C5-C6-N1	-3.23	119.80	123.31
32	1a	1518	MA6	C2-N3-C4	3.23	119.72	111.83
32	1a	1519	MA6	N9-C8-N7	-3.21	109.38	113.94
32	1a	1407	5MC	C5-C6-N1	-3.21	119.83	123.31
32	2a	1498	UR3	C5-C4-N3	3.19	119.24	115.04
1	2A	1939	5MU	O2-C2-N1	-3.19	118.65	122.80
32	1a	967	5MC	C5-C6-N1	-3.17	119.87	123.31
32	1a	1207	2MG	N1-C2-N2	3.17	119.79	116.56
32	1a	1404	5MC	C5-C6-N1	-3.17	119.87	123.31
1	2A	2251	OMG	C6-C5-N7	3.12	135.97	130.29
32	2a	1404	5MC	C5-C6-N1	-3.12	119.93	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1915	5MU	C1'-N1-C6	-3.11	116.02	121.15
1	2A	1915	5MU	C1'-N1-C6	-3.10	116.05	121.15
32	1a	1207	2MG	C4-C5-N7	-3.08	105.78	110.67
32	2a	1407	5MC	C5-C6-N1	-3.08	119.97	123.31
32	1a	1498	UR3	C5-C4-N3	3.07	119.08	115.04
1	2A	2503	2MA	N6-C6-N1	3.04	121.13	117.03
1	2A	2503	2MA	C4-N9-C8	2.98	108.87	105.74
32	2a	1207	2MG	C4-C5-N7	-2.97	105.96	110.67
32	2a	1407	5MC	C5-C4-N3	-2.93	118.75	121.75
1	1A	2552	OMU	O4-C4-C5	-2.89	120.17	125.16
32	2a	1207	2MG	N2-C2-N3	-2.89	116.83	120.51
1	2A	2552	OMU	O2-C2-N1	-2.85	119.08	122.80
32	2a	1404	5MC	C5-C4-N3	-2.79	118.89	121.75
32	1a	1400	5MC	C5-C4-N3	-2.78	118.90	121.75
32	2a	1518	MA6	N3-C4-N9	2.77	131.88	127.17
1	1A	1915	5MU	O2-C2-N3	-2.76	116.40	121.49
32	1a	1404	5MC	C5-C4-N3	-2.74	118.95	121.75
32	1a	1402	4OC	C6-C5-C4	2.72	120.28	117.00
32	2a	967	5MC	C5-C4-N3	-2.72	118.97	121.75
1	1A	2251	OMG	C4-C5-N7	-2.71	106.38	110.67
1	2A	1942	5MC	C5-C4-N3	-2.70	118.99	121.75
32	1a	967	5MC	C5-C4-N3	-2.68	119.01	121.75
1	1A	1939	5MU	O2-C2-N1	-2.66	119.33	122.80
32	1a	1518	MA6	N3-C4-N9	2.66	131.69	127.17
1	1A	2503	2MA	C2-N1-C6	2.65	122.18	118.10
1	2A	2503	2MA	C2-N1-C6	2.65	122.17	118.10
32	2a	1519	MA6	N3-C4-N9	2.63	131.63	127.17
32	2a	1400	5MC	C5-C4-N3	-2.61	119.08	121.75
1	1A	1915	5MU	C5-C6-N1	-2.61	120.48	123.31
1	2A	2503	2MA	C5-N7-C8	2.61	107.55	103.45
1	2A	1915	5MU	C5-C6-N1	-2.56	120.54	123.31
1	2A	2251	OMG	C4-C5-N7	-2.56	106.62	110.67
1	2A	1920	OMC	O2-C2-N3	-2.56	118.30	122.33
32	2a	966	M2G	C4-C5-N7	-2.55	106.62	110.67
32	1a	1519	MA6	N3-C4-N9	2.54	131.49	127.17
32	1a	1407	5MC	C5-C4-N3	-2.54	119.15	121.75
32	1a	1519	MA6	C4-C5-C6	2.53	118.52	115.91
32	1a	966	M2G	C4-C5-N7	-2.52	106.67	110.67
1	2A	1962	5MC	C5-C4-N3	-2.52	119.17	121.75
32	2a	1518	MA6	C4-C5-C6	2.51	118.50	115.91
1	1A	1942	5MC	C5-C4-N3	-2.48	119.21	121.75
1	2A	1915	5MU	O2-C2-N3	-2.47	116.94	121.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	C4-C5-C6	2.44	118.43	115.91
1	1A	2503	2MA	C5-N7-C8	2.43	107.27	103.45
1	1A	1962	5MC	C5-C4-N3	-2.41	119.28	121.75
1	1A	2605	PSU	C5-C6-N1	-2.41	118.79	122.14
32	2a	1407	5MC	O2-C2-N3	-2.40	118.55	122.33
32	1a	527	G7M	O6-C6-C5	-2.38	122.70	128.01
32	1a	1207	2MG	N2-C2-N3	-2.36	117.51	120.51
32	1a	1407	5MC	O2-C2-N3	-2.34	118.64	122.33
32	2a	527	G7M	O6-C6-C5	-2.33	122.81	128.01
1	1A	2552	OMU	O2-C2-N1	-2.32	119.77	122.80
1	1A	1962	5MC	CM5-C5-C6	-2.31	119.73	122.85
32	2a	516	PSU	O4'-C1'-C2'	2.28	108.31	105.15
43	1l	92	0TD	OD2-CG-CB	2.28	118.08	113.15
32	2a	516	PSU	C5-C6-N1	-2.28	118.98	122.14
32	2a	1402	4OC	C6-C5-C4	2.27	119.74	117.00
32	2a	1498	UR3	C3U-N3-C4	2.27	121.01	117.87
1	2A	2251	OMG	O6-C6-C5	-2.25	120.58	126.53
1	1A	1911	PSU	C5-C6-N1	-2.25	119.02	122.14
32	2a	1519	MA6	C4-C5-C6	2.24	118.22	115.91
1	1A	2503	2MA	C4-N9-C8	2.21	108.06	105.74
43	2l	92	0TD	OD2-CG-CB	2.21	117.93	113.15
32	1a	1498	UR3	C6-N1-C2	-2.19	120.00	121.80
32	2a	527	G7M	C5-C6-N1	2.17	116.33	111.84
1	2A	2503	2MA	N9-C8-N7	-2.17	110.86	113.94
1	2A	2605	PSU	C5-C6-N1	-2.15	119.16	122.14
32	2a	966	M2G	O6-C6-C5	-2.13	120.90	126.53
32	1a	1207	2MG	O3'-C3'-C2'	2.10	118.54	111.82
32	1a	527	G7M	C5-C6-N1	2.09	116.15	111.84
1	1A	2251	OMG	O6-C6-C5	-2.08	121.03	126.53
32	1a	966	M2G	O6-C6-C5	-2.07	121.07	126.53
32	2a	1404	5MC	O2-C2-N3	-2.07	119.07	122.33
1	1A	1920	OMC	O2-C2-N3	-2.05	119.09	122.33
32	1a	1207	2MG	C8-N7-C5	2.05	107.91	104.26
32	2a	1400	5MC	O2-C2-N3	-2.04	119.11	122.33
32	1a	516	PSU	C5-C6-N1	-2.04	119.31	122.14
1	2A	1911	PSU	C5-C6-N1	-2.02	119.34	122.14
1	1A	1911	PSU	O4'-C1'-C2'	2.01	107.93	105.15

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
43	2l	92	0TD	O-C-CA-CB
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	SB-CB-CG-OD1
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C2'-O2'-CM2
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD2
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	2503	2MA	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	527	G7M	C4'-C5'-O5'-P

There are no ring outliers.

19 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1404	5MC	2	0
43	2l	92	0TD	1	0
1	2A	1915	5MU	1	0
1	1A	1917	PSU	1	0
32	1a	1402	4OC	1	0
1	1A	1939	5MU	1	0
32	1a	1498	UR3	1	0
32	2a	1400	5MC	1	0
32	1a	1518	MA6	1	0
32	1a	1519	MA6	2	0
32	2a	1402	4OC	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	2503	2MA	1	0
32	1a	1400	5MC	2	0
1	1A	1920	OMC	1	0
32	2a	1518	MA6	2	0
32	2a	1519	MA6	2	0
1	2A	1920	OMC	1	0
32	1a	967	5MC	1	0
1	2A	1917	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2572 ligands modelled in this entry, 2559 are monoatomic - leaving 13 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	$\# Z > 2$
55	CPF	1A	4056	54	27,27,27	2.11	6 (22%)	40,40,40	1.79	11 (27%)
56	MPD	1a	1878	-	7,7,7	0.40	0	9,10,10	0.40	0
56	MPD	18	104	-	7,7,7	0.30	0	9,10,10	0.25	0
59	SF4	1d	306	35	0,12,12	-	-	-	-	-
56	MPD	2A	3744	-	7,7,7	0.31	0	9,10,10	0.17	0
56	MPD	1O	202	-	7,7,7	0.31	0	9,10,10	0.19	0
56	MPD	2A	3743	-	7,7,7	0.33	0	9,10,10	0.30	0
55	CPF	2A	3741	54	27,27,27	2.09	6 (22%)	40,40,40	2.22	13 (32%)
56	MPD	2B	219	-	7,7,7	0.31	0	9,10,10	0.23	0
57	ARG	1F	320	-	10,11,11	0.75	1 (10%)	9,13,13	0.87	1 (11%)
57	ARG	1B	230	54	10,11,11	0.76	1 (10%)	9,13,13	0.99	1 (11%)
59	SF4	2d	302	35	0,12,12	-	-	-	-	-
56	MPD	1A	4058	-	7,7,7	0.35	0	9,10,10	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	CPF	1A	4056	54	-	9/12/22/22	0/4/4/4
56	MPD	1a	1878	-	-	5/5/5/5	-
56	MPD	18	104	-	-	4/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
56	MPD	2A	3744	-	-	4/5/5/5	-
56	MPD	1O	202	-	-	2/5/5/5	-
56	MPD	2A	3743	-	-	0/5/5/5	-
55	CPF	2A	3741	54	-	6/12/22/22	0/4/4/4
56	MPD	2B	219	-	-	3/5/5/5	-
57	ARG	1F	320	-	-	3/11/11/11	-
57	ARG	1B	230	54	-	2/11/11/11	-
59	SF4	2d	302	35	-	-	0/6/5/5
56	MPD	1A	4058	-	-	2/5/5/5	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4056	CPF	C2-C3	-5.59	1.39	1.48
55	2A	3741	CPF	C2-C3	-5.56	1.40	1.48
55	2A	3741	CPF	C5-C4	-4.88	1.38	1.48
55	1A	4056	CPF	C10-N1	-4.71	1.34	1.40
55	1A	4056	CPF	C5-C4	-4.62	1.39	1.48
55	2A	3741	CPF	C10-N1	-4.51	1.34	1.40
55	1A	4056	CPF	C1-N1	3.67	1.40	1.34
55	2A	3741	CPF	C1-N1	3.48	1.40	1.34
55	1A	4056	CPF	C8-N2	-3.23	1.34	1.41
55	2A	3741	CPF	C8-N2	-2.80	1.35	1.41
57	1B	230	ARG	OXT-C	-2.24	1.23	1.30
57	1F	320	ARG	OXT-C	-2.17	1.23	1.30
55	2A	3741	CPF	O2-C3	-2.11	1.24	1.30
55	1A	4056	CPF	O2-C3	-2.04	1.25	1.30

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3741	CPF	F1-C7-C8	6.06	124.15	118.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2A	3741	CPF	C9-C8-N2	-4.45	116.11	122.59
55	2A	3741	CPF	C6-C7-C8	-4.44	119.43	123.35
55	2A	3741	CPF	C7-C8-N2	4.16	125.28	120.42
55	1A	4056	CPF	C2-C1-N1	-4.07	119.54	124.42
55	2A	3741	CPF	C14-N2-C17	3.78	120.07	111.57
55	1A	4056	CPF	C14-N2-C17	3.76	120.03	111.57
55	1A	4056	CPF	C6-C7-C8	-3.72	120.06	123.35
55	2A	3741	CPF	C2-C1-N1	-3.45	120.28	124.42
55	2A	3741	CPF	C5-C4-C2	3.32	119.83	115.64
55	1A	4056	CPF	C5-C4-C2	3.24	119.73	115.64
55	2A	3741	CPF	C13-C11-N1	-3.11	113.95	118.87
55	1A	4056	CPF	C9-C8-C7	3.09	119.75	116.53
55	2A	3741	CPF	C17-N2-C8	3.00	123.31	116.19
57	1B	230	ARG	OXT-C-O	-2.84	117.63	124.08
55	1A	4056	CPF	C5-C10-N1	2.68	120.94	118.83
55	1A	4056	CPF	C13-C11-N1	-2.63	114.70	118.87
55	1A	4056	CPF	C9-C8-N2	-2.55	118.88	122.59
57	1F	320	ARG	OXT-C-O	-2.52	118.35	124.08
55	2A	3741	CPF	C12-C11-N1	-2.48	114.94	118.87
55	2A	3741	CPF	O2-C3-C2	2.43	121.38	115.69
55	1A	4056	CPF	O2-C3-C2	2.41	121.33	115.69
55	1A	4056	CPF	C12-C11-N1	-2.22	115.35	118.87
55	2A	3741	CPF	O3-C4-C5	-2.21	118.04	121.57
55	2A	3741	CPF	O2-C3-O1	-2.11	118.87	123.90
55	1A	4056	CPF	O2-C3-O1	-2.07	118.98	123.90

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	4056	CPF	C1-C2-C3-O2
55	1A	4056	CPF	C4-C2-C3-O2
55	1A	4056	CPF	C1-C2-C3-O1
55	1A	4056	CPF	C4-C2-C3-O1
55	1A	4056	CPF	C7-C8-N2-C17
55	2A	3741	CPF	C12-C11-N1-C1
56	1O	202	MPD	C2-C3-C4-C5
56	18	104	MPD	C2-C3-C4-O4
56	1a	1878	MPD	C2-C3-C4-O4
56	1a	1878	MPD	C2-C3-C4-C5
56	2A	3744	MPD	C2-C3-C4-C5
56	2B	219	MPD	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

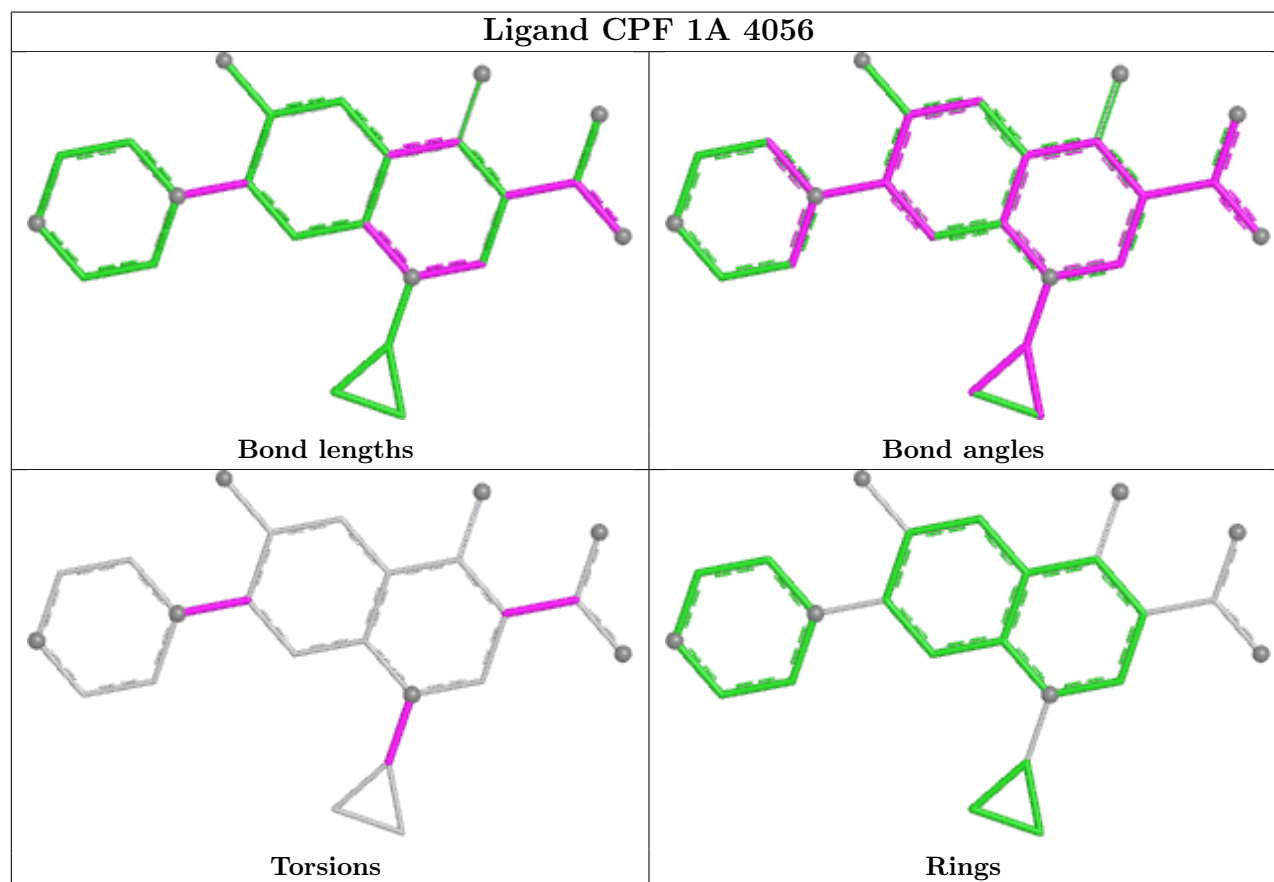
Mol	Chain	Res	Type	Atoms
55	2A	3741	CPF	C13-C11-N1-C1
55	2A	3741	CPF	C9-C8-N2-C17
55	2A	3741	CPF	C12-C11-N1-C10
55	2A	3741	CPF	C7-C8-N2-C17
55	1A	4056	CPF	C13-C11-N1-C1
57	1B	230	ARG	CA-CB-CG-CD
55	2A	3741	CPF	C13-C11-N1-C10
57	1B	230	ARG	NE-CD-CG-CB
55	1A	4056	CPF	C13-C11-N1-C10
55	1A	4056	CPF	C9-C8-N2-C17
56	18	104	MPD	CM-C2-C3-C4
56	1a	1878	MPD	CM-C2-C3-C4
56	2A	3744	MPD	C1-C2-C3-C4
57	1F	320	ARG	CA-CB-CG-CD
56	18	104	MPD	C2-C3-C4-C5
57	1F	320	ARG	NE-CD-CG-CB
55	1A	4056	CPF	C7-C8-N2-C14
56	1A	4058	MPD	O2-C2-C3-C4
56	1O	202	MPD	O2-C2-C3-C4
56	1a	1878	MPD	O2-C2-C3-C4
56	1A	4058	MPD	C2-C3-C4-O4
56	2A	3744	MPD	C2-C3-C4-O4
56	2B	219	MPD	C2-C3-C4-O4
56	18	104	MPD	C1-C2-C3-C4
56	1a	1878	MPD	C1-C2-C3-C4
56	2A	3744	MPD	CM-C2-C3-C4
56	2B	219	MPD	C1-C2-C3-C4
57	1F	320	ARG	OXT-C-CA-CB

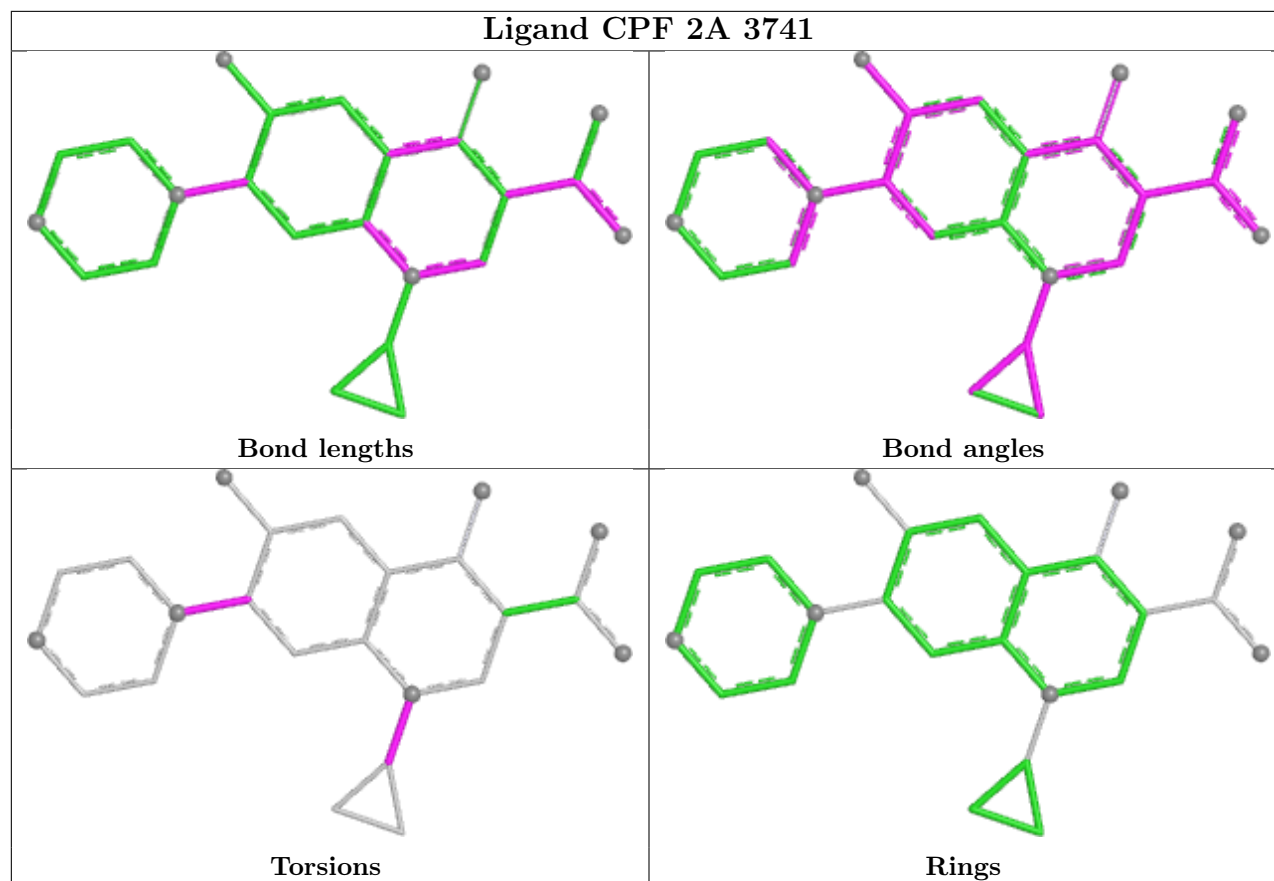
There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1A	4056	CPF	1	0
56	1a	1878	MPD	4	0
56	18	104	MPD	1	0
56	1O	202	MPD	1	0
56	2A	3743	MPD	1	0
55	2A	3741	CPF	3	0
57	1F	320	ARG	2	0
57	1B	230	ARG	1	0
56	1A	4058	MPD	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2861/2915 (98%)	-0.39	154 (5%) 31 26	24, 40, 97, 109	0
1	2A	2856/2915 (97%)	0.06	181 (6%) 26 20	31, 57, 100, 110	0
2	1B	120/121 (99%)	-0.17	2 (1%) 69 64	38, 56, 70, 88	0
2	2B	120/121 (99%)	0.81	6 (5%) 34 28	62, 82, 89, 98	0
3	1D	275/276 (99%)	-0.11	4 (1%) 72 68	25, 39, 55, 76	0
3	2D	275/276 (99%)	0.16	2 (0%) 84 82	32, 50, 63, 78	0
4	1E	204/206 (99%)	-0.07	3 (1%) 72 68	23, 42, 64, 78	0
4	2E	204/206 (99%)	0.18	3 (1%) 72 68	36, 57, 73, 81	0
5	1F	203/210 (96%)	-0.01	2 (0%) 79 76	22, 45, 71, 89	0
5	2F	203/210 (96%)	0.38	1 (0%) 87 85	35, 64, 79, 89	0
6	1G	181/182 (99%)	0.69	13 (7%) 21 17	53, 70, 82, 91	0
6	2G	181/182 (99%)	1.55	45 (24%) 2 1	77, 87, 94, 98	0
7	1H	174/180 (96%)	0.33	7 (4%) 42 37	41, 56, 69, 74	0
7	2H	173/180 (96%)	1.42	32 (18%) 3 3	72, 84, 90, 95	0
8	1I	147/148 (99%)	0.85	10 (6%) 23 19	45, 71, 83, 86	0
8	2I	146/148 (98%)	0.86	5 (3%) 48 42	53, 75, 86, 91	0
9	1N	140/140 (100%)	-0.13	1 (0%) 84 82	30, 43, 64, 79	0
9	2N	140/140 (100%)	0.48	3 (2%) 63 58	48, 64, 78, 86	0
10	1O	122/122 (100%)	-0.11	0 100 100	31, 43, 62, 68	0
10	2O	122/122 (100%)	0.12	0 100 100	46, 55, 68, 75	0
11	1P	149/150 (99%)	-0.00	1 (0%) 84 82	24, 48, 68, 81	0
11	2P	149/150 (99%)	0.52	2 (1%) 75 71	39, 66, 83, 88	0
12	1Q	141/141 (100%)	-0.16	0 100 100	31, 43, 57, 71	0
12	2Q	141/141 (100%)	0.69	6 (4%) 40 34	47, 65, 76, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.15	0 100 100	29, 41, 55, 63	0
13	2R	118/118 (100%)	0.19	0 100 100	40, 54, 64, 70	0
14	1S	110/112 (98%)	0.27	1 (0%) 81 78	43, 55, 67, 72	0
14	2S	110/112 (98%)	1.29	21 (19%) 3 2	67, 76, 82, 89	0
15	1T	131/146 (89%)	0.09	5 (3%) 44 38	38, 47, 70, 81	0
15	2T	131/146 (89%)	0.37	2 (1%) 72 68	47, 59, 76, 86	0
16	1U	116/118 (98%)	-0.29	0 100 100	28, 35, 49, 65	0
16	2U	116/118 (98%)	0.36	0 100 100	42, 59, 72, 80	0
17	1V	101/101 (100%)	-0.17	0 100 100	27, 46, 63, 71	0
17	2V	101/101 (100%)	0.71	3 (2%) 52 47	41, 69, 77, 84	0
18	1W	112/113 (99%)	-0.18	2 (1%) 67 63	28, 36, 54, 84	0
18	2W	112/113 (99%)	0.13	2 (1%) 67 63	41, 50, 66, 91	0
19	1X	95/96 (98%)	-0.00	2 (2%) 63 58	31, 42, 66, 77	0
19	2X	95/96 (98%)	0.53	6 (6%) 26 20	45, 60, 77, 86	0
20	1Y	107/110 (97%)	0.18	1 (0%) 81 78	37, 51, 68, 78	0
20	2Y	107/110 (97%)	0.93	6 (5%) 30 24	59, 70, 79, 90	0
21	1Z	203/206 (98%)	0.42	4 (1%) 65 60	44, 62, 75, 86	0
21	2Z	201/206 (97%)	1.14	17 (8%) 16 13	68, 79, 85, 92	0
22	10	77/85 (90%)	0.08	1 (1%) 75 71	32, 41, 60, 65	0
22	20	77/85 (90%)	0.80	6 (7%) 19 15	50, 65, 74, 77	0
23	11	97/98 (98%)	0.14	1 (1%) 79 76	32, 45, 69, 75	0
23	21	97/98 (98%)	0.55	5 (5%) 33 27	41, 55, 76, 80	0
24	12	70/72 (97%)	0.18	1 (1%) 73 69	40, 51, 62, 83	0
24	22	70/72 (97%)	0.65	1 (1%) 73 69	61, 70, 77, 79	0
25	13	59/60 (98%)	-0.09	0 100 100	31, 42, 66, 72	0
25	23	59/60 (98%)	0.47	3 (5%) 33 28	51, 62, 80, 84	0
26	14	69/71 (97%)	1.32	20 (28%) 1 1	64, 83, 95, 98	0
26	24	69/71 (97%)	1.93	25 (36%) 1 0	85, 92, 99, 103	0
27	15	59/60 (98%)	-0.15	1 (1%) 69 64	26, 40, 63, 74	0
27	25	59/60 (98%)	0.10	0 100 100	35, 52, 69, 79	0
28	16	53/54 (98%)	-0.21	0 100 100	38, 46, 60, 64	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.52	0	100 100	53, 62, 71, 74	0
29	17	48/49 (97%)	-0.11	4 (8%)	17 13	25, 32, 61, 66	0
29	27	48/49 (97%)	0.14	5 (10%)	11 9	34, 41, 69, 77	0
30	18	64/65 (98%)	-0.23	1 (1%)	70 66	29, 37, 46, 54	0
30	28	64/65 (98%)	0.43	2 (3%)	51 45	48, 56, 63, 72	0
31	19	37/37 (100%)	0.05	1 (2%)	56 50	35, 45, 60, 63	0
31	29	37/37 (100%)	1.18	3 (8%)	18 14	61, 70, 79, 81	0
32	1a	1488/1521 (97%)	0.45	66 (4%)	39 33	39, 73, 96, 110	0
32	2a	1492/1521 (98%)	0.71	115 (7%)	19 15	47, 77, 98, 109	0
33	1b	231/256 (90%)	1.39	53 (22%)	2 2	69, 81, 90, 96	0
33	2b	231/256 (90%)	1.62	68 (29%)	1 1	74, 85, 93, 98	0
34	1c	206/239 (86%)	1.06	21 (10%)	12 9	65, 76, 87, 89	0
34	2c	206/239 (86%)	1.79	68 (33%)	1 1	78, 86, 91, 96	0
35	1d	208/209 (99%)	1.04	21 (10%)	12 9	59, 74, 82, 89	0
35	2d	208/209 (99%)	1.13	24 (11%)	9 7	62, 72, 81, 84	0
36	1e	148/162 (91%)	0.63	4 (2%)	56 50	49, 68, 77, 90	0
36	2e	148/162 (91%)	0.96	8 (5%)	31 26	57, 73, 82, 93	0
37	1f	100/101 (99%)	0.47	2 (2%)	65 60	51, 68, 78, 82	0
37	2f	100/101 (99%)	0.59	0	100 100	56, 69, 78, 84	0
38	1g	155/156 (99%)	0.67	5 (3%)	50 44	68, 75, 83, 90	0
38	2g	155/156 (99%)	1.31	27 (17%)	4 3	76, 84, 89, 92	0
39	1h	137/138 (99%)	0.75	6 (4%)	39 33	58, 70, 78, 80	0
39	2h	137/138 (99%)	0.89	6 (4%)	39 33	62, 74, 81, 83	0
40	1i	127/128 (99%)	1.65	36 (28%)	1 1	66, 81, 87, 89	0
40	2i	126/128 (98%)	2.53	85 (67%)	0 0	77, 88, 93, 94	0
41	1j	97/105 (92%)	1.60	28 (28%)	1 1	65, 81, 90, 94	0
41	2j	96/105 (91%)	2.63	70 (72%)	0 0	79, 89, 93, 97	0
42	1k	114/129 (88%)	0.48	4 (3%)	47 41	46, 66, 76, 81	0
42	2k	114/129 (88%)	0.97	10 (8%)	15 12	60, 73, 82, 86	0
43	1l	121/132 (91%)	0.61	5 (4%)	41 36	51, 62, 73, 79	0
43	2l	121/132 (91%)	0.70	6 (4%)	34 28	56, 67, 76, 80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	1.36	19 (16%) 4 3	68, 79, 84, 90	0
44	2m	114/126 (90%)	1.73	36 (31%) 1 1	80, 88, 93, 95	0
45	1n	60/61 (98%)	1.23	5 (8%) 17 13	67, 76, 83, 86	0
45	2n	60/61 (98%)	2.59	38 (63%) 0 0	80, 87, 93, 97	0
46	1o	88/89 (98%)	0.61	3 (3%) 48 42	47, 69, 80, 82	0
46	2o	88/89 (98%)	0.88	7 (7%) 18 14	58, 73, 81, 86	0
47	1p	82/88 (93%)	1.69	21 (25%) 1 1	62, 74, 83, 88	0
47	2p	82/88 (93%)	1.10	5 (6%) 27 22	62, 70, 80, 83	0
48	1q	99/105 (94%)	1.00	5 (5%) 33 28	57, 71, 80, 84	0
48	2q	99/105 (94%)	0.81	3 (3%) 52 47	55, 72, 79, 82	0
49	1r	68/88 (77%)	0.51	2 (2%) 53 48	58, 67, 80, 86	0
49	2r	68/88 (77%)	0.70	2 (2%) 53 48	62, 71, 82, 84	0
50	1s	83/93 (89%)	1.11	10 (12%) 9 7	71, 81, 87, 90	0
50	2s	83/93 (89%)	2.12	44 (53%) 0 0	79, 91, 95, 96	0
51	1t	96/106 (90%)	1.31	20 (20%) 2 2	64, 75, 86, 90	0
51	2t	98/106 (92%)	0.96	7 (7%) 22 17	60, 73, 84, 87	0
52	1u	23/27 (85%)	1.50	6 (26%) 1 1	72, 77, 81, 81	0
52	2u	23/27 (85%)	2.95	19 (82%) 0 0	80, 86, 89, 90	0
53	1y	97/113 (85%)	0.79	6 (6%) 26 21	59, 69, 78, 84	0
53	2y	96/113 (84%)	1.82	33 (34%) 1 1	73, 83, 88, 91	0
All	All	20766/21468 (96%)	0.45	1664 (8%) 18 14	22, 65, 92, 110	0

All (1664) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1076	C	8.4
45	2n	2	ALA	7.8
41	2j	37	PRO	7.2
7	1H	2	SER	7.1
1	1A	1087	G	6.9
26	14	56	VAL	6.8
26	24	56	VAL	6.8
1	2A	2174	C	6.7
1	1A	2602	A	6.7
1	1A	1064	C	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	1n	2	ALA	6.3
40	2i	7	THR	6.2
53	2y	98	ALA	6.1
1	2A	2152	G	5.7
1	1A	1077	A	5.7
1	2A	2153	G	5.6
51	2t	6	PRO	5.6
41	2j	75	ILE	5.6
45	2n	13	THR	5.6
1	1A	1088	A	5.5
1	1A	1078	U	5.5
1	1A	1090	U	5.5
40	2i	102	LEU	5.5
1	1A	1089	G	5.4
1	2A	2147	G	5.3
51	1t	103	GLY	5.3
1	1A	1080	C	5.2
1	2A	1536	C	5.2
41	2j	34	VAL	5.2
23	11	2	SER	5.1
1	1A	1086	A	5.1
1	2A	2139	C	5.1
40	2i	126	SER	5.1
45	2n	5	ALA	5.0
52	2u	16	GLY	5.0
1	2A	2602	A	5.0
40	2i	10	ARG	5.0
1	1A	1072	C	5.0
26	14	59	PHE	5.0
45	2n	17	LYS	4.9
40	1i	106	ALA	4.9
1	1A	1091	G	4.9
1	2A	1091	G	4.9
1	2A	2106	G	4.9
1	2A	2125	G	4.9
1	1A	1065	U	4.9
34	1c	2	GLY	4.9
1	2A	34	C	4.8
1	2A	1076	C	4.8
1	2A	2136	C	4.8
20	2Y	1	MET	4.8
1	1A	2145	C	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	9	VAL	4.7
32	2a	1532	U	4.7
1	1A	2143	C	4.7
1	2A	2145	C	4.7
1	1A	1063	G	4.7
32	2a	1030(A)	G	4.7
45	2n	18	VAL	4.7
1	2A	2133	G	4.7
40	2i	125	TYR	4.7
52	2u	14	TRP	4.6
1	2A	2172	U	4.6
1	1A	1075	C	4.6
6	2G	76	SER	4.6
50	2s	2	PRO	4.6
35	1d	179	GLU	4.6
15	1T	131	ALA	4.6
53	1y	98	ALA	4.6
1	1A	1066	U	4.6
44	2m	102	ARG	4.6
15	1T	130	ALA	4.6
1	2A	2155	G	4.6
33	2b	165	VAL	4.5
47	1p	82	GLN	4.5
1	2A	2130	U	4.5
45	2n	14	PRO	4.5
1	1A	34	C	4.4
1	2A	2107	C	4.4
40	1i	126	SER	4.4
32	2a	1036	G	4.4
1	2A	2142	C	4.4
1	2A	2143	C	4.4
1	2A	2162	G	4.4
32	2a	1030(B)	C	4.4
1	2A	2173	A	4.4
40	2i	109	VAL	4.4
35	2d	5	ILE	4.4
32	2a	1257	U	4.3
1	2A	2134	A	4.3
41	2j	38	ILE	4.3
1	2A	2154	G	4.3
41	2j	36	GLY	4.3
39	2h	2	LEU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1079	C	4.3
1	2A	2168	G	4.3
51	2t	103	GLY	4.3
23	2l	2	SER	4.3
33	1b	131	PRO	4.3
40	2i	18	PHE	4.3
1	1A	1102	C	4.3
1	2A	2159	G	4.3
32	2a	1001(A)	G	4.3
32	2a	1003	G	4.3
8	2l	146	ALA	4.2
32	1a	1030	C	4.2
1	2A	2135	A	4.2
47	2p	82	GLN	4.2
2	1B	1	U	4.2
53	2y	97	ALA	4.2
32	2a	1031	G	4.2
40	2i	2	GLU	4.2
41	2j	72	VAL	4.2
6	2G	77	ILE	4.2
1	1A	1074	G	4.2
44	1m	2	ALA	4.1
1	2A	2140	C	4.1
1	2A	2146	C	4.1
1	2A	2116	G	4.1
1	2A	2206	G	4.1
44	2m	116	THR	4.1
45	2n	33	VAL	4.1
6	2G	146	TYR	4.1
1	1A	1081	U	4.1
1	2A	2126	A	4.1
33	1b	17	PHE	4.1
52	2u	23	PRO	4.0
1	2A	2150	U	4.0
12	2Q	59	ARG	4.0
15	1T	37	GLY	4.0
45	2n	55	GLY	4.0
32	1a	1286	A	4.0
40	2i	11	LYS	4.0
52	2u	2	GLY	4.0
41	2j	55	LYS	4.0
1	2A	1085	A	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	888	C	4.0
1	1A	1104	C	4.0
1	1A	2144	U	4.0
35	1d	166	LYS	4.0
1	1A	1103	A	4.0
1	2A	2158	A	4.0
44	1m	4	ILE	4.0
41	2j	44	VAL	4.0
40	2i	45	ALA	3.9
50	2s	71	LEU	3.9
1	2A	1046	A	3.9
1	1A	2108	C	3.9
1	1A	2142	C	3.9
1	2A	1092	C	3.9
50	1s	13	ASP	3.9
34	2c	207	VAL	3.9
1	2A	2144	U	3.9
1	1A	2147	G	3.9
3	1D	275	LYS	3.9
40	1i	56	LEU	3.9
26	24	54	GLY	3.9
26	14	63	TYR	3.9
1	1A	1071	G	3.9
1	2A	2127	G	3.9
1	2A	2157	G	3.9
40	2i	66	ARG	3.9
1	1A	2111	C	3.9
2	2B	1	U	3.9
40	2i	67	GLY	3.9
44	2m	106	ASN	3.8
26	14	55	ARG	3.8
40	2i	9	ARG	3.8
32	1a	1036	G	3.8
40	2i	6	GLY	3.8
1	1A	1092	C	3.8
29	27	48	LYS	3.8
1	2A	2149	G	3.8
26	14	54	GLY	3.8
32	1a	1030(A)	G	3.8
7	2H	45	VAL	3.8
1	1A	1026	U	3.8
1	2A	645	C	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2129	C	3.8
40	2i	21	PRO	3.8
40	2i	127	LYS	3.8
1	2A	2124	G	3.8
1	2A	2160	G	3.8
32	2a	1286	A	3.8
40	2i	49	PRO	3.8
41	2j	67	THR	3.8
1	2A	2132	U	3.8
1	2A	1509	C	3.8
33	2b	44	LEU	3.8
41	1j	4	ILE	3.7
32	1a	1532	U	3.7
6	1G	76	SER	3.7
1	2A	2138	C	3.7
21	2Z	191	VAL	3.7
41	2j	77	PRO	3.7
50	2s	63	THR	3.7
45	2n	21	TYR	3.7
35	1d	167	GLY	3.7
1	1A	1062	G	3.7
1	1A	1093	G	3.7
1	2A	2141	G	3.7
26	24	49	PHE	3.7
26	24	50	VAL	3.7
51	1t	18	GLN	3.7
41	2j	46	ARG	3.7
45	2n	30	ALA	3.7
45	2n	59	ALA	3.7
34	1c	90	GLU	3.7
1	2A	2111	C	3.7
1	2A	2137	C	3.7
48	1q	100	LYS	3.7
41	2j	33	GLN	3.7
1	2A	1090	U	3.6
41	2j	78	ASN	3.6
32	2a	1033	G	3.6
40	1i	128	ARG	3.6
1	2A	2175	C	3.6
32	1a	1030(B)	C	3.6
6	2G	20	ILE	3.6
1	1A	1073	A	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	2T	131	ALA	3.6
32	1a	1024	G	3.6
32	1a	1026	G	3.6
8	1I	147	GLN	3.6
33	1b	129	GLU	3.6
33	1b	165	VAL	3.6
52	2u	6	ARG	3.6
40	2i	13	ALA	3.6
41	2j	91	PRO	3.6
40	2i	14	VAL	3.6
1	2A	2165	G	3.6
41	2j	42	THR	3.6
1	2A	2167	U	3.6
1	1A	1067	A	3.6
41	2j	65	LEU	3.6
45	2n	29	ARG	3.5
1	1A	2146	C	3.5
32	2a	1030	C	3.5
41	1j	76	ASN	3.5
1	2A	2151	G	3.5
32	1a	1023	G	3.5
32	2a	1030(C)	G	3.5
26	14	50	VAL	3.5
44	2m	100	GLY	3.5
1	1A	1509	C	3.5
1	1A	2112	G	3.5
1	2A	1087	G	3.5
1	2A	1089	G	3.5
1	2A	2148	G	3.5
1	2A	2207	G	3.5
52	2u	24	ARG	3.5
35	1d	2	GLY	3.5
33	2b	131	PRO	3.5
34	2c	90	GLU	3.5
24	12	70	GLN	3.5
41	2j	71	LEU	3.5
1	2A	1075	C	3.5
1	2A	2128	C	3.5
1	2A	2179	C	3.5
40	2i	88	TYR	3.5
52	2u	9	ARG	3.5
1	2A	2131	G	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1021	G	3.5
1	1A	2117	A	3.5
35	2d	164	ALA	3.5
33	2b	7	VAL	3.5
34	2c	77	ILE	3.4
41	2j	30	SER	3.4
1	2A	2105	C	3.4
1	1A	1082	U	3.4
1	2A	1074	G	3.4
41	2j	32	ALA	3.4
45	2n	38	GLY	3.4
46	2o	86	GLY	3.4
38	2g	16	LEU	3.4
33	2b	15	VAL	3.4
33	2b	136	VAL	3.4
50	2s	41	VAL	3.4
41	2j	6	ILE	3.4
44	1m	59	TYR	3.4
45	2n	34	TYR	3.4
1	1A	2107	C	3.4
7	2H	128	PRO	3.4
34	2c	159	GLY	3.4
41	2j	93	GLY	3.4
1	2A	2109	U	3.4
32	1a	1257	U	3.4
1	1A	275	G	3.4
32	1a	1030(C)	G	3.4
32	2a	1002	G	3.4
33	2b	97	TRP	3.4
1	1A	1057	A	3.4
1	2A	2117	A	3.4
32	2a	1030(D)	A	3.4
22	10	84	LEU	3.4
33	1b	36	ARG	3.4
38	2g	5	ARG	3.4
41	2j	47	PHE	3.4
1	1A	2132	U	3.4
7	2H	136	ILE	3.4
45	2n	7	ILE	3.4
52	2u	13	ILE	3.4
40	2i	5	TYR	3.4
1	2A	2121	G	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1026	G	3.4
1	1A	6	A	3.4
32	2a	1357	A	3.4
7	2H	165	ALA	3.4
40	2i	46	ALA	3.4
45	2n	3	ARG	3.4
26	14	51	ASP	3.4
41	2j	76	ASN	3.4
33	2b	122	PHE	3.4
14	2S	35	ILE	3.3
1	2A	1064	C	3.3
1	2A	1097	U	3.3
33	2b	67	THR	3.3
50	2s	42	PRO	3.3
1	2A	2119	A	3.3
32	1a	1447	A	3.3
32	1a	1531	A	3.3
26	14	49	PHE	3.3
40	2i	17	VAL	3.3
1	2A	2118	U	3.3
26	24	44	THR	3.3
47	1p	69	THR	3.3
1	2A	2183	C	3.3
14	2S	3	ARG	3.3
40	1i	19	LEU	3.3
40	1i	102	LEU	3.3
40	2i	16	ARG	3.3
40	2i	83	ARG	3.3
38	2g	84	ASN	3.3
40	2i	105	ASP	3.3
1	1A	887	A	3.3
41	1j	75	ILE	3.3
1	1A	2805	G	3.3
32	1a	1031	G	3.3
32	1a	1032	G	3.3
32	2a	1032	G	3.3
32	2a	1124	G	3.3
26	24	67	TYR	3.3
41	2j	48	THR	3.3
50	2s	3	ARG	3.3
52	2u	17	THR	3.3
34	2c	32	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	39	LEU	3.3
34	2c	189	ALA	3.3
32	2a	1037	C	3.3
26	24	59	PHE	3.3
32	2a	1035	A	3.3
32	2a	1256	A	3.3
41	2j	45	ARG	3.3
1	2A	1071	G	3.3
41	2j	15	THR	3.3
44	1m	56	LEU	3.3
48	2q	98	LEU	3.3
34	1c	193	TYR	3.3
53	2y	33	HIS	3.3
43	2l	17	LYS	3.3
1	1A	2804	C	3.2
32	1a	1029	C	3.2
1	1A	548	A	3.2
32	2a	1001	A	3.2
33	2b	121	LEU	3.2
34	2c	94	LEU	3.2
44	2m	113	PRO	3.2
50	2s	69	HIS	3.2
33	1b	33	TYR	3.2
52	2u	11	GLY	3.2
44	1m	51	ALA	3.2
1	2A	2110	G	3.2
41	1j	74	ILE	3.2
32	1a	1025	U	3.2
23	2l	26	ARG	3.2
1	2A	1079	C	3.2
1	2A	2108	C	3.2
32	1a	1028	C	3.2
41	2j	88	LEU	3.2
53	2y	38	HIS	3.2
53	2y	45	PRO	3.2
1	1A	229	A	3.2
1	2A	2169	A	3.2
15	2T	130	ALA	3.2
40	2i	86	VAL	3.2
45	2n	25	VAL	3.2
32	1a	1033	G	3.2
40	2i	42	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	32	LEU	3.2
19	1X	95	LEU	3.2
33	1b	97	TRP	3.2
33	1b	38	GLY	3.2
1	2A	2185	C	3.2
4	2E	204	ALA	3.2
1	1A	2119	A	3.2
1	2A	1070	A	3.2
1	2A	2171	A	3.2
32	1a	1030(D)	A	3.2
32	2a	1005	A	3.2
53	1y	95	ARG	3.2
50	2s	66	MET	3.2
1	1A	2159	G	3.2
1	2A	2793	G	3.2
40	2i	69	GLY	3.2
50	2s	4	SER	3.2
33	1b	236	TYR	3.2
34	2c	128	PHE	3.2
41	2j	24	VAL	3.2
50	2s	11	VAL	3.2
32	1a	63	C	3.1
32	1a	1533	C	3.1
52	2u	15	ARG	3.1
14	2S	33	LYS	3.1
33	1b	133	LYS	3.1
32	2a	532	A	3.1
32	2a	1004	A	3.1
51	1t	99	LEU	3.1
47	1p	46	PRO	3.1
41	1j	87	THR	3.1
53	1y	2	THR	3.1
1	1A	2167	U	3.1
32	1a	841	U	3.1
40	2i	53	VAL	3.1
1	2A	2318	G	3.1
32	1a	1001(A)	G	3.1
32	1a	1003	G	3.1
42	1k	25	TYR	3.1
40	2i	104	ARG	3.1
1	1A	2129	C	3.1
6	2G	139	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1028	C	3.1
33	2b	10	LEU	3.1
34	2c	52	LEU	3.1
40	2i	96	LEU	3.1
7	2H	21	PRO	3.1
45	2n	49	HIS	3.1
1	1A	1085	A	3.1
36	2e	22	GLY	3.1
38	2g	128	ALA	3.1
40	2i	81	ILE	3.1
44	2m	84	ILE	3.1
40	2i	101	PHE	3.1
32	2a	1025	U	3.1
33	1b	130	ARG	3.1
7	2H	71	LEU	3.1
1	1A	2174	C	3.1
32	1a	1027	C	3.1
41	2j	87	THR	3.1
7	2H	82	GLY	3.1
33	2b	123	ALA	3.1
1	1A	2158	A	3.1
1	2A	1096	A	3.1
1	2A	2114	A	3.1
3	2D	276	LYS	3.1
33	2b	21	ARG	3.1
34	2c	68	VAL	3.1
34	2c	190	ARG	3.1
40	2i	36	TYR	3.1
40	2i	114	TYR	3.1
1	1A	1094	U	3.1
1	1A	1101	U	3.1
1	1A	2109	U	3.1
51	1t	10	LEU	3.1
1	1A	2125	G	3.1
32	2a	1034	G	3.1
3	1D	276	LYS	3.1
33	1b	237	ALA	3.1
40	2i	63	ILE	3.1
40	1i	42	ARG	3.1
41	2j	43	ARG	3.1
53	2y	7	SER	3.1
32	1a	1001	A	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1183	A	3.0
32	2a	1531	A	3.0
41	2j	8	LEU	3.0
47	1p	17	TYR	3.0
34	2c	129	ALA	3.0
1	2A	1171	G	3.0
1	2A	2156	G	3.0
41	2j	59	SER	3.0
6	2G	175	LEU	3.0
41	2j	40	LEU	3.0
1	1A	2803	C	3.0
32	1a	1037	C	3.0
32	2a	1029	C	3.0
25	23	2	PRO	3.0
1	2A	1088	A	3.0
32	2a	1447	A	3.0
33	1b	132	LYS	3.0
1	1A	1963	U	3.0
1	1A	2150	U	3.0
1	2A	2113	U	3.0
34	2c	192	THR	3.0
48	1q	68	ARG	3.0
52	1u	24	ARG	3.0
34	2c	60	ALA	3.0
44	2m	98	VAL	3.0
26	24	66	SER	3.0
50	2s	30	LEU	3.0
42	2k	117	ASN	3.0
46	2o	75	PRO	3.0
1	1A	1099	G	3.0
1	1A	2115	G	3.0
1	2A	2166	G	3.0
1	2A	2319	G	3.0
26	24	28	LYS	3.0
52	2u	20	LYS	3.0
32	2a	1149	C	3.0
1	2A	652(B)	A	3.0
41	2j	79	ARG	3.0
21	2Z	51	ALA	3.0
8	1I	107	VAL	3.0
9	2N	9	VAL	3.0
50	1s	9	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	12	GLU	3.0
41	2j	62	HIS	3.0
33	1b	37	ASN	3.0
33	2b	236	TYR	3.0
41	2j	96	ILE	3.0
41	1j	31	GLY	3.0
44	2m	105	THR	3.0
40	2i	55	ALA	3.0
45	2n	20	ALA	3.0
1	2A	1086	A	3.0
1	2A	2176	A	3.0
1	2A	2320	A	3.0
32	1a	162	A	3.0
43	2l	18	VAL	3.0
1	2A	2180	U	2.9
40	1i	127	LYS	2.9
53	2y	4	ASN	2.9
26	24	63	TYR	2.9
14	2S	17	ARG	2.9
40	2i	75	ASP	2.9
38	2g	34	GLY	2.9
12	2Q	65	PHE	2.9
33	2b	152	PHE	2.9
34	1c	87	LEU	2.9
1	1A	1176	G	2.9
32	2a	1027	C	2.9
32	2a	1249	C	2.9
32	2a	1260	C	2.9
1	2A	1067	A	2.9
1	2A	2123	G	2.9
6	2G	87	PRO	2.9
38	2g	14	PRO	2.9
44	1m	113	PRO	2.9
1	1A	271(K)	U	2.9
1	2A	1026	U	2.9
1	2A	1083	U	2.9
32	1a	182	U	2.9
47	1p	1	MET	2.9
34	2c	57	ILE	2.9
40	2i	68	GLY	2.9
33	2b	230	VAL	2.9
33	2b	138	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	1d	157	LEU	2.9
47	1p	6	LEU	2.9
1	1A	2114	A	2.9
1	2A	1080	C	2.9
1	2A	1084	A	2.9
32	1a	1492	A	2.9
38	2g	32	ARG	2.9
41	1j	46	ARG	2.9
32	2a	1202	G	2.9
34	2c	23	TYR	2.9
38	2g	85	TYR	2.9
44	2m	87	TYR	2.9
35	2d	166	LYS	2.9
41	2j	90	LEU	2.9
29	27	47	ARG	2.9
1	1A	2170	A	2.9
1	2A	2170	A	2.9
26	24	45	GLY	2.9
32	1a	163	C	2.9
32	2a	1038	C	2.9
32	2a	1119	C	2.9
32	2a	1183	A	2.9
32	2a	1354	C	2.9
41	1j	42	THR	2.9
1	2A	352	G	2.9
1	2A	2321	G	2.9
6	2G	62	LEU	2.9
50	2s	15	LEU	2.9
45	2n	16	PHE	2.9
41	2j	68	HIS	2.9
36	2e	10	MET	2.8
6	1G	83	ARG	2.8
6	2G	118	ARG	2.8
38	2g	41	ARG	2.8
41	2j	70	ARG	2.8
52	1u	6	ARG	2.8
6	2G	78	SER	2.8
33	2b	201	ILE	2.8
34	1c	62	ASP	2.8
44	2m	59	TYR	2.8
6	2G	90	LEU	2.8
45	2n	10	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	54	PHE	2.8
1	2A	6	A	2.8
1	2A	229	A	2.8
32	1a	1005	A	2.8
32	2a	1040	U	2.8
1	2A	2161	C	2.8
1	1A	2141	G	2.8
41	2j	28	ARG	2.8
47	1p	81	ARG	2.8
36	2e	20	GLN	2.8
50	2s	34	TRP	2.8
33	2b	37	ASN	2.8
45	2n	11	LYS	2.8
33	2b	72	GLY	2.8
40	1i	64	THR	2.8
40	2i	92	TYR	2.8
33	1b	7	VAL	2.8
34	1c	86	VAL	2.8
1	1A	1083	U	2.8
32	2a	1118	C	2.8
40	2i	97	LYS	2.8
47	1p	19	ILE	2.8
1	1A	2116	G	2.8
1	1A	2133	G	2.8
1	1A	2153	G	2.8
34	2c	87	LEU	2.8
44	2m	90	LEU	2.8
7	2H	114	VAL	2.8
33	1b	15	VAL	2.8
34	2c	99	VAL	2.8
34	2c	184	TYR	2.8
40	1i	15	ALA	2.8
41	1j	32	ALA	2.8
41	1j	34	VAL	2.8
41	1j	64	GLU	2.8
41	2j	83	GLU	2.8
1	1A	2130	U	2.8
33	2b	132	LYS	2.8
1	2A	1073	A	2.8
33	1b	127	ILE	2.8
40	2i	29	ASN	2.8
35	1d	155	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	1h	2	LEU	2.8
50	2s	5	LEU	2.8
6	2G	147	ASP	2.8
33	2b	164	VAL	2.8
41	2j	63	PHE	2.8
44	2m	17	VAL	2.8
32	2a	1356	G	2.8
32	2a	1373	G	2.8
42	2k	25	TYR	2.8
44	1m	3	ARG	2.8
41	1j	77	PRO	2.7
32	2a	1020	U	2.7
15	1T	104	ASN	2.7
38	1g	16	LEU	2.7
47	2p	48	TRP	2.7
51	1t	24	LEU	2.7
1	1A	1095	A	2.7
50	2s	68	GLY	2.7
1	2A	1104	C	2.7
26	24	55	ARG	2.7
32	2a	1362	C	2.7
33	1b	229	VAL	2.7
34	1c	10	PHE	2.7
34	1c	76	VAL	2.7
34	2c	53	ALA	2.7
35	1d	178	VAL	2.7
44	1m	102	ARG	2.7
34	2c	48	TYR	2.7
40	2i	62	TYR	2.7
40	2i	123	PRO	2.7
53	2y	46	GLN	2.7
34	2c	26	LYS	2.7
1	2A	2186	G	2.7
32	2a	1021	G	2.7
32	2a	1255	G	2.7
44	2m	64	TRP	2.7
46	2o	89	GLY	2.7
32	1a	723	U	2.7
32	2a	1125	U	2.7
32	2a	1150	U	2.7
33	1b	19	HIS	2.7
44	1m	50	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	24	52	THR	2.7
38	2g	83	ALA	2.7
40	2i	64	THR	2.7
40	2i	76	ALA	2.7
50	2s	79	THR	2.7
1	1A	1084	A	2.7
1	1A	1177	A	2.7
32	2a	1123	A	2.7
32	2a	1363(A)	A	2.7
50	2s	59	PRO	2.7
6	1G	182	LYS	2.7
40	2i	116	LYS	2.7
52	2u	3	LYS	2.7
1	1A	2161	C	2.7
32	1a	1007	C	2.7
33	2b	11	LEU	2.7
40	2i	40	LEU	2.7
1	1A	1058	G	2.7
1	2A	171	G	2.7
1	2A	2182	G	2.7
32	2a	630	G	2.7
19	2X	68	ARG	2.7
26	14	48	ARG	2.7
45	2n	12	ARG	2.7
50	2s	35	SER	2.7
33	2b	12	GLU	2.7
51	1t	83	ARG	2.7
12	2Q	104	PHE	2.7
33	2b	57	PHE	2.7
47	1p	22	THR	2.7
50	2s	33	THR	2.7
51	1t	95	ALA	2.7
1	2A	271(K)	U	2.7
6	2G	122	PRO	2.7
35	1d	169	LYS	2.7
40	1i	125	TYR	2.7
40	2i	4	TYR	2.7
44	1m	87	TYR	2.7
48	2q	65	ILE	2.7
51	2t	100	ILE	2.7
32	2a	1006	C	2.7
40	2i	79	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	14	HIS	2.7
18	2W	112	GLY	2.7
43	2l	19	ARG	2.7
51	2t	25	ARG	2.7
52	1u	16	GLY	2.7
6	2G	50	ALA	2.7
6	2G	149	VAL	2.7
34	1c	207	VAL	2.7
34	2c	92	ALA	2.7
40	2i	122	ALA	2.7
41	2j	94	VAL	2.7
45	1n	5	ALA	2.7
41	2j	39	PRO	2.7
1	1A	2166	G	2.6
2	2B	118	G	2.6
32	1a	204	U	2.6
38	2g	154	TYR	2.6
31	19	17	ILE	2.6
33	1b	200	ILE	2.6
41	2j	74	ILE	2.6
53	2y	5	ILE	2.6
6	2G	82	LEU	2.6
6	2G	133	LEU	2.6
34	2c	196	LEU	2.6
40	2i	99	LEU	2.6
26	24	58	ARG	2.6
48	1q	63	ARG	2.6
52	2u	7	ARG	2.6
44	2m	85	GLY	2.6
50	2s	26	GLY	2.6
6	2G	123	ASN	2.6
34	2c	135	LYS	2.6
47	1p	50	LYS	2.6
51	1t	74	LYS	2.6
14	2S	29	PHE	2.6
34	2c	65	ALA	2.6
40	2i	43	ALA	2.6
45	2n	36	PHE	2.6
46	2o	19	PRO	2.6
50	2s	39	THR	2.6
26	24	65	ASP	2.6
14	2S	36	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	214	ILE	2.6
34	2c	29	TYR	2.6
1	1A	614(B)	G	2.6
20	1Y	1	MET	2.6
1	1A	2113	U	2.6
1	1A	2206	G	2.6
1	2A	2104	G	2.6
1	2A	2802	G	2.6
1	2A	2894	G	2.6
18	1W	111	HIS	2.6
7	2H	120	GLY	2.6
26	14	53	GLU	2.6
33	2b	22	LYS	2.6
33	2b	133	LYS	2.6
51	2t	102	GLY	2.6
14	2S	46	VAL	2.6
8	1I	108	THR	2.6
33	1b	125	PRO	2.6
34	2c	200	ALA	2.6
40	2i	65	VAL	2.6
39	2h	3	THR	2.6
50	2s	76	PRO	2.6
1	1A	1100	C	2.6
1	2A	2789	C	2.6
6	2G	88	ILE	2.6
34	2c	124	ILE	2.6
34	1c	94	LEU	2.6
40	2i	58	HIS	2.6
49	1r	87	ARG	2.6
50	2s	78	ARG	2.6
1	2A	12	U	2.6
7	2H	85	LYS	2.6
32	2a	1148	U	2.6
45	2n	4	LYS	2.6
45	2n	15	LYS	2.6
26	24	30	GLU	2.6
1	1A	2110	G	2.6
1	1A	2148	G	2.6
1	2A	1533	G	2.6
1	2A	2100	G	2.6
1	2A	2112	G	2.6
32	1a	1034	G	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	976	G	2.6
21	2Z	68	PRO	2.6
22	20	69	PHE	2.6
33	2b	70	PHE	2.6
34	2c	100	ALA	2.6
35	2d	154	ASN	2.6
38	2g	80	VAL	2.6
40	1i	13	ALA	2.6
40	1i	108	VAL	2.6
41	1j	49	VAL	2.6
50	2s	74	PHE	2.6
6	2G	29	TRP	2.6
41	2j	92	THR	2.6
1	1A	2173	A	2.6
1	2A	1847	A	2.6
32	2a	994	A	2.6
34	2c	152	ILE	2.6
53	2y	40	ILE	2.6
1	1A	2128	C	2.6
32	2a	1363	C	2.6
44	2m	66	LEU	2.6
7	1H	3	ARG	2.6
30	18	46	ARG	2.6
35	1d	153	ARG	2.6
41	2j	64	GLU	2.6
1	1A	1061	U	2.6
1	1A	2118	U	2.6
1	2A	2122	U	2.6
26	24	39	CYS	2.6
6	2G	70	VAL	2.6
8	1I	63	ALA	2.6
34	2c	130	VAL	2.6
33	2b	163	PHE	2.6
36	1e	21	ALA	2.6
14	2S	5	THR	2.5
1	1A	2149	G	2.5
32	1a	380	G	2.5
44	2m	82	MET	2.5
33	2b	68	ILE	2.5
36	2e	13	ILE	2.5
38	2g	42	ILE	2.5
44	2m	4	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	529	A	2.5
1	2A	1057	A	2.5
6	1G	82	LEU	2.5
19	2X	92	LEU	2.5
7	2H	3	ARG	2.5
20	2Y	34	LYS	2.5
34	2c	79	ARG	2.5
53	2y	66	LYS	2.5
53	2y	95	ARG	2.5
33	2b	92	TYR	2.5
52	2u	21	TYR	2.5
1	1A	889	C	2.5
32	1a	1038	C	2.5
5	1F	208	GLY	2.5
14	2S	45	GLY	2.5
44	2m	24	GLY	2.5
40	1i	109	VAL	2.5
50	2s	60	VAL	2.5
38	2g	2	ALA	2.5
38	2g	152	ALA	2.5
41	1j	33	GLN	2.5
53	2y	9	GLN	2.5
47	1p	44	THR	2.5
1	1A	1097	U	2.5
1	1A	1175	U	2.5
26	24	51	ASP	2.5
6	2G	52	ILE	2.5
26	24	5	ILE	2.5
34	1c	84	ILE	2.5
36	2e	109	ILE	2.5
53	2y	35	ILE	2.5
19	2X	95	LEU	2.5
35	1d	194	LEU	2.5
40	2i	85	LEU	2.5
41	1j	85	LEU	2.5
53	2y	24	LEU	2.5
47	1p	16	HIS	2.5
1	2A	2805	G	2.5
2	2B	120	A	2.5
32	1a	1493	A	2.5
32	2a	1349	A	2.5
40	1i	35	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	23	TYR	2.5
51	2t	69	GLY	2.5
7	2H	39	PRO	2.5
6	2G	159	VAL	2.5
33	2b	237	ALA	2.5
40	1i	101	PHE	2.5
50	2s	10	PHE	2.5
32	2a	1007	C	2.5
32	2a	1039	C	2.5
53	2y	3	MET	2.5
46	1o	22	THR	2.5
21	2Z	16	SER	2.5
33	2b	127	ILE	2.5
38	2g	156	TRP	2.5
40	2i	118	LYS	2.5
41	2j	14	LYS	2.5
33	1b	187	LEU	2.5
33	2b	130	ARG	2.5
41	2j	58	ASP	2.5
50	2s	31	ILE	2.5
26	24	57	GLU	2.5
33	1b	12	GLU	2.5
53	1y	68	GLU	2.5
53	2y	71	TYR	2.5
6	1G	89	GLY	2.5
12	2Q	30	GLY	2.5
17	2V	63	GLY	2.5
33	1b	14	GLY	2.5
44	1m	6	GLY	2.5
47	1p	37	GLY	2.5
26	24	29	PRO	2.5
40	1i	49	PRO	2.5
1	1A	1046	A	2.5
1	2A	529	A	2.5
1	2A	614(B)	G	2.5
1	2A	1816	G	2.5
1	2A	2751	G	2.5
2	2B	119	G	2.5
27	15	60	VAL	2.5
32	2a	1022	G	2.5
32	2a	1248	A	2.5
33	1b	29	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	163	ALA	2.5
40	1i	94	ALA	2.5
40	2i	106	ALA	2.5
41	2j	26	ALA	2.5
26	14	52	THR	2.5
34	2c	95	THR	2.5
41	2j	69	ASN	2.5
50	2s	65	ASN	2.5
6	2G	157	ILE	2.5
34	2c	14	ILE	2.5
34	2c	47	LEU	2.5
34	2c	175	LEU	2.5
35	1d	3	ARG	2.5
40	2i	19	LEU	2.5
45	1n	3	ARG	2.5
50	2s	40	ILE	2.5
53	2y	64	SER	2.5
1	1A	886	C	2.5
1	1A	2794	C	2.5
1	2A	2103	C	2.5
34	2c	62	ASP	2.5
40	1i	105	ASP	2.5
1	2A	1082	U	2.5
32	2a	1000	U	2.5
31	29	21	GLY	2.5
33	2b	227	GLY	2.5
35	2d	2	GLY	2.5
41	1j	44	VAL	2.5
45	1n	25	VAL	2.5
19	2X	91	ALA	2.5
33	1b	122	PHE	2.5
33	2b	17	PHE	2.5
35	1d	110	PHE	2.5
40	1i	18	PHE	2.5
44	2m	31	LYS	2.4
44	2m	20	THR	2.4
1	1A	1045	A	2.4
21	2Z	82	ARG	2.4
32	1a	1035	A	2.4
32	2a	975	A	2.4
40	1i	9	ARG	2.4
45	2n	35	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	118	LEU	2.4
34	2c	91	LEU	2.4
1	1A	2127	G	2.4
1	2A	1099	G	2.4
1	2A	2120	G	2.4
14	2S	53	SER	2.4
32	1a	1002	G	2.4
32	2a	1190	G	2.4
33	2b	40	HIS	2.4
38	2g	33	ASP	2.4
40	1i	2	GLU	2.4
32	1a	840	C	2.4
32	2a	980	C	2.4
32	2a	1019	C	2.4
32	2a	1116	C	2.4
32	2a	1128	C	2.4
1	2A	1094	U	2.4
40	2i	72	GLY	2.4
52	2u	4	GLY	2.4
23	21	78	LYS	2.4
29	17	48	LYS	2.4
7	2H	156	ALA	2.4
33	1b	62	ALA	2.4
40	1i	46	ALA	2.4
40	2i	119	ALA	2.4
7	1H	6	ARG	2.4
30	28	46	ARG	2.4
34	1c	165	THR	2.4
39	2h	30	ARG	2.4
41	1j	88	LEU	2.4
48	1q	98	LEU	2.4
51	1t	100	ILE	2.4
45	2n	60	SER	2.4
1	2A	2208	A	2.4
53	2y	51	ASP	2.4
1	1A	2207	G	2.4
1	2A	1537	G	2.4
1	2A	2115	G	2.4
1	2A	2181	G	2.4
32	2a	1323	G	2.4
33	2b	38	GLY	2.4
35	2d	167	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	22	LYS	2.4
33	2b	8	LYS	2.4
40	1i	95	LYS	2.4
40	2i	25	LYS	2.4
45	2n	9	LYS	2.4
1	2A	2177	C	2.4
1	2A	2803	C	2.4
32	2a	1158	C	2.4
40	2i	108	VAL	2.4
3	1D	2	ALA	2.4
9	1N	115	ARG	2.4
21	2Z	192	ALA	2.4
29	17	45	ALA	2.4
39	1h	110	ALA	2.4
41	1j	54	PHE	2.4
40	1i	10	ARG	2.4
51	1t	94	ALA	2.4
51	1t	97	ALA	2.4
52	2u	10	ARG	2.4
33	2b	154	LEU	2.4
47	2p	19	ILE	2.4
53	2y	6	THR	2.4
7	2H	40	GLU	2.4
20	2Y	91	GLU	2.4
26	14	57	GLU	2.4
33	1b	134	GLU	2.4
1	1A	2169	A	2.4
1	2A	1111	A	2.4
40	1i	6	GLY	2.4
41	2j	10	GLY	2.4
47	1p	66	PRO	2.4
26	14	60	GLN	2.4
34	2c	28	GLN	2.4
42	2k	13	GLN	2.4
50	2s	67	VAL	2.4
1	1A	2793	G	2.4
1	2A	1047	G	2.4
6	2G	80	PHE	2.4
14	2S	79	ALA	2.4
19	1X	68	ARG	2.4
21	1Z	51	ALA	2.4
26	24	61	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	376	G	2.4
32	2a	1023	G	2.4
32	2a	1371	G	2.4
33	1b	70	PHE	2.4
42	2k	75	TYR	2.4
43	1l	64	TYR	2.4
51	1t	12	ALA	2.4
6	2G	152	LEU	2.4
7	2H	98	LEU	2.4
1	1A	362	U	2.4
33	1b	39	ILE	2.4
45	1n	7	ILE	2.4
50	1s	5	LEU	2.4
50	2s	16	LEU	2.4
1	1A	2139	C	2.4
1	2A	1049	C	2.4
32	2a	1369	C	2.4
32	2a	1397	C	2.4
33	2b	16	HIS	2.4
40	2i	23	ASN	2.4
23	2l	83	GLU	2.4
41	2j	35	SER	2.4
21	2Z	93	ASP	2.4
29	27	1	MET	2.4
46	1o	89	GLY	2.4
8	2I	3	VAL	2.4
33	1b	175	ARG	2.4
35	1d	168	ARG	2.4
53	2y	60	VAL	2.4
1	2A	1508	A	2.4
32	2a	1289	A	2.4
4	1E	204	ALA	2.4
34	2c	50	ALA	2.4
34	2c	71	ALA	2.4
40	2i	33	PHE	2.4
7	2H	87	LEU	2.3
45	2n	53	LEU	2.3
50	2s	80	TYR	2.3
33	2b	214	ILE	2.3
32	2a	951	G	2.3
32	2a	1351	U	2.3
32	2a	1446	U	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	2d	24	GLU	2.3
1	1A	1584	C	2.3
1	1A	2137	C	2.3
1	2A	1040	C	2.3
39	2h	4	ASP	2.3
51	1t	98	PRO	2.3
33	2b	18	GLY	2.3
38	1g	32	ARG	2.3
40	2i	20	ARG	2.3
50	2s	29	ARG	2.3
25	23	59	VAL	2.3
41	2j	49	VAL	2.3
14	2S	80	LEU	2.3
22	20	84	LEU	2.3
33	1b	213	LEU	2.3
45	2n	6	LEU	2.3
47	1p	7	ALA	2.3
51	1t	66	ALA	2.3
7	2H	89	ILE	2.3
1	1A	2790	A	2.3
1	2A	1050	A	2.3
32	1a	1004	A	2.3
32	2a	968	A	2.3
33	2b	168	THR	2.3
41	1j	100	THR	2.3
4	1E	163	GLU	2.3
33	2b	101	MET	2.3
32	1a	839	U	2.3
32	2a	1281	U	2.3
41	2j	17	ASP	2.3
1	1A	1106	G	2.3
1	1A	1117	G	2.3
1	1A	2168	G	2.3
1	2A	1056	G	2.3
32	1a	630	G	2.3
32	2a	1024	G	2.3
1	1A	2136	C	2.3
1	1A	2175	C	2.3
1	2A	1072	C	2.3
22	20	55	ARG	2.3
32	2a	979	C	2.3
32	2a	1097	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1259	C	2.3
34	2c	171	GLY	2.3
40	1i	107	ARG	2.3
42	2k	126	ARG	2.3
44	2m	101	GLN	2.3
35	2d	8	VAL	2.3
14	2S	58	LEU	2.3
38	2g	99	LEU	2.3
39	1h	112	LEU	2.3
40	2i	37	PHE	2.3
41	2j	16	LEU	2.3
50	2s	24	ALA	2.3
31	29	17	ILE	2.3
26	14	32	TYR	2.3
35	2d	20	TYR	2.3
52	2u	18	TYR	2.3
3	2D	275	LYS	2.3
6	2G	155	MET	2.3
21	1Z	1	MET	2.3
44	2m	65	LYS	2.3
50	2s	25	LYS	2.3
53	2y	58	ASN	2.3
1	1A	2062	A	2.3
1	2A	2062	A	2.3
32	2a	949	A	2.3
7	2H	10	PRO	2.3
26	14	68	ARG	2.3
33	1b	234	PRO	2.3
33	2b	232	PRO	2.3
44	1m	55	ARG	2.3
44	2m	3	ARG	2.3
44	2m	88	ARG	2.3
51	1t	8	ARG	2.3
35	2d	6	GLY	2.3
1	1A	12	U	2.3
1	1A	1105	U	2.3
1	1A	1420	U	2.3
32	1a	1020	U	2.3
32	1a	1446	U	2.3
40	1i	14	VAL	2.3
45	2n	56	VAL	2.3
47	1p	53	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
53	2y	49	VAL	2.3
40	2i	59	PHE	2.3
53	2y	48	PHE	2.3
21	2Z	113	ALA	2.3
35	1d	149	ALA	2.3
1	1A	545	G	2.3
1	1A	2140	C	2.3
1	1A	2157	G	2.3
1	1A	2187	G	2.3
2	2B	88	C	2.3
32	2a	1018	C	2.3
32	2a	1063	C	2.3
32	2a	1353	G	2.3
9	2N	2	LYS	2.3
41	2j	100	THR	2.3
43	2l	13	LYS	2.3
45	2n	22	THR	2.3
47	2p	39	TYR	2.3
52	1u	18	TYR	2.3
44	2m	12	ASN	2.3
26	24	41	PRO	2.3
33	1b	23	ARG	2.3
40	1i	75	ASP	2.3
41	2j	19	SER	2.3
41	2j	41	PRO	2.3
41	2j	84	GLN	2.3
12	2Q	100	GLY	2.3
32	2a	1151	A	2.3
32	2a	1493	A	2.3
33	1b	228	GLY	2.3
34	2c	81	GLY	2.3
35	2d	87	GLY	2.3
44	2m	95	GLY	2.3
50	1s	84	GLY	2.3
51	1t	101	GLY	2.3
4	2E	182	LEU	2.3
33	1b	230	VAL	2.3
41	2j	85	LEU	2.3
43	1l	18	VAL	2.3
44	1m	60	VAL	2.3
44	1m	117	VAL	2.3
53	2y	34	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	614(A)	U	2.2
6	2G	46	ALA	2.2
29	27	45	ALA	2.2
33	1b	188	ALA	2.2
39	1h	134	ILE	2.2
41	1j	27	ALA	2.2
41	1j	98	ILE	2.2
50	2s	75	ALA	2.2
7	2H	13	LYS	2.2
41	1j	86	MET	2.2
41	2j	7	LYS	2.2
42	2k	124	LYS	2.2
34	2c	191	THR	2.2
52	1u	17	THR	2.2
6	1G	48	GLU	2.2
26	14	67	TYR	2.2
1	2A	2164	C	2.2
32	2a	1277	C	2.2
8	1I	11	ASN	2.2
7	2H	101	ARG	2.2
15	1T	129	ARG	2.2
43	2l	89	ARG	2.2
40	2i	90	PRO	2.2
40	2i	91	ASP	2.2
50	2s	12	ASP	2.2
17	2V	42	GLY	2.2
34	2c	2	GLY	2.2
35	2d	183	GLY	2.2
40	2i	39	GLY	2.2
14	2S	54	LEU	2.2
33	1b	136	VAL	2.2
34	1c	52	LEU	2.2
35	1d	133	VAL	2.2
40	2i	44	VAL	2.2
40	2i	47	LEU	2.2
1	1A	1098	A	2.2
1	1A	1460	A	2.2
1	1A	2176	A	2.2
1	2A	1045	A	2.2
1	2A	1098	A	2.2
6	2G	141	PHE	2.2
14	2S	82	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	2Y	4	LYS	2.2
21	2Z	7	ALA	2.2
26	14	69	LYS	2.2
26	24	40	HIS	2.2
33	2b	200	ILE	2.2
41	2j	98	ILE	2.2
44	1m	5	ALA	2.2
21	1Z	203	GLU	2.2
35	1d	150	GLU	2.2
44	1m	43	THR	2.2
44	1m	116	THR	2.2
6	2G	181	ARG	2.2
38	1g	5	ARG	2.2
41	1j	66	ARG	2.2
41	1j	78	ASN	2.2
46	1o	88	ARG	2.2
53	2y	96	ARG	2.2
32	1a	1039	C	2.2
32	2a	1254	C	2.2
35	2d	74	GLN	2.2
6	2G	116	ASP	2.2
7	2H	166	GLY	2.2
14	2S	60	GLY	2.2
21	2Z	166	SER	2.2
21	2Z	179	ASP	2.2
50	1s	26	GLY	2.2
50	1s	68	GLY	2.2
6	2G	3	LEU	2.2
32	1a	306	G	2.2
32	2a	1216	G	2.2
32	2a	1283	G	2.2
7	2H	15	VAL	2.2
14	2S	57	LYS	2.2
29	17	46	VAL	2.2
33	1b	71	VAL	2.2
35	1d	170	VAL	2.2
6	2G	178	PHE	2.2
35	1d	165	MET	2.2
38	2g	120	ILE	2.2
41	2j	82	ILE	2.2
6	1G	50	ALA	2.2
40	2i	82	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	27	ALA	2.2
49	2r	20	ALA	2.2
1	1A	1069	A	2.2
1	1A	2126	A	2.2
1	1A	2171	A	2.2
40	2i	27	THR	2.2
32	1a	1135	U	2.2
41	2j	5	ARG	2.2
44	1m	114	ARG	2.2
47	2p	25	ARG	2.2
40	1i	62	TYR	2.2
33	1b	232	PRO	2.2
6	2G	24	GLY	2.2
22	20	8	GLY	2.2
33	2b	228	GLY	2.2
34	2c	41	GLY	2.2
38	2g	81	GLY	2.2
43	1l	63	GLY	2.2
51	1t	13	LEU	2.2
7	2H	17	VAL	2.2
8	1I	3	VAL	2.2
21	2Z	1	MET	2.2
34	1c	99	VAL	2.2
37	1f	90	VAL	2.2
40	2i	41	VAL	2.2
1	1A	645	C	2.2
1	2A	277	C	2.2
32	1a	1008	C	2.2
32	2a	1267	C	2.2
32	2a	1359	C	2.2
33	1b	28	PHE	2.2
33	1b	140	HIS	2.2
33	1b	222	ILE	2.2
34	2c	6	HIS	2.2
34	2c	69	HIS	2.2
36	1e	113	ALA	2.2
36	2e	17	ALA	2.2
1	1A	2155	G	2.2
1	2A	11	G	2.2
1	2A	883	G	2.2
1	2A	1062	G	2.2
32	2a	1042	G	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	60	ARG	2.2
12	2Q	60	ARG	2.2
34	1c	79	ARG	2.2
1	2A	2801(A)	A	2.2
34	2c	109	PRO	2.2
35	2d	54	TYR	2.2
42	2k	115	PRO	2.2
1	1A	272(A)	U	2.2
20	2Y	94	LYS	2.2
32	1a	90	U	2.2
53	2y	43	LYS	2.2
19	2X	66	LEU	2.2
22	20	75	LEU	2.2
33	2b	99	GLY	2.2
40	2i	30	GLY	2.2
50	2s	8	GLY	2.2
8	1I	14	ASP	2.2
8	1I	20	ASP	2.2
7	2H	169	VAL	2.2
38	2g	77	SER	2.2
44	1m	54	VAL	2.2
47	1p	2	VAL	2.2
50	1s	4	SER	2.2
33	1b	41	ILE	2.2
53	2y	54	ILE	2.2
45	2n	37	PHE	2.2
47	1p	80	PHE	2.2
50	1s	74	PHE	2.2
42	2k	15	ALA	2.1
44	2m	42	ALA	2.1
1	1A	2138	C	2.1
29	17	23	ARG	2.1
32	2a	1147	C	2.1
33	1b	137	ARG	2.1
34	2c	67	THR	2.1
50	2s	77	THR	2.1
26	14	18	CYS	2.1
1	1A	2124	G	2.1
1	1A	2893	G	2.1
1	2A	2187	G	2.1
32	1a	79	G	2.1
32	1a	102	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1009	G	2.1
32	2a	1224	G	2.1
32	2a	1258	G	2.1
32	2a	1361	G	2.1
33	2b	95	GLN	2.1
41	2j	80	LYS	2.1
43	1l	47	LYS	2.1
50	2s	55	LYS	2.1
51	1t	9	ASN	2.1
7	2H	171	LEU	2.1
34	2c	34	LEU	2.1
1	2A	1069	A	2.1
34	2c	13	GLY	2.1
50	2s	82	GLY	2.1
53	1y	47	GLY	2.1
53	1y	92	GLY	2.1
6	1G	52	ILE	2.1
6	2G	160	VAL	2.1
7	2H	9	ILE	2.1
32	2a	723	U	2.1
33	1b	42	ILE	2.1
34	2c	55	VAL	2.1
34	2c	202	ILE	2.1
48	1q	99	SER	2.1
33	2b	225	ALA	2.1
34	2c	121	ALA	2.1
35	2d	149	ALA	2.1
38	2g	116	ALA	2.1
51	1t	67	ALA	2.1
47	1p	48	TRP	2.1
47	1p	59	TRP	2.1
18	2W	92	ARG	2.1
34	2c	131	ARG	2.1
34	2c	140	ARG	2.1
35	2d	47	ARG	2.1
40	1i	20	ARG	2.1
46	2o	72	ARG	2.1
52	1u	15	ARG	2.1
8	1I	86	THR	2.1
26	24	27	THR	2.1
33	2b	125	PRO	2.1
33	2b	156	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1053	C	2.1
1	1A	2103	C	2.1
1	2A	888	C	2.1
1	2A	2178	C	2.1
32	2a	999	C	2.1
32	2a	1325	C	2.1
36	1e	20	GLN	2.1
7	2H	41	MET	2.1
30	28	25	MET	2.1
14	2S	92	TYR	2.1
21	2Z	9	TYR	2.1
21	2Z	33	LEU	2.1
33	2b	31	TYR	2.1
33	2b	142	LEU	2.1
33	2b	148	TYR	2.1
6	1G	44	GLY	2.1
11	2P	116	GLY	2.1
20	2Y	80	GLY	2.1
34	2c	51	GLY	2.1
35	2d	44	GLY	2.1
42	2k	118	GLY	2.1
40	2i	117	HIS	2.1
1	1A	1056	G	2.1
1	1A	1068	G	2.1
1	2A	545	G	2.1
1	2A	2184	G	2.1
1	2A	2893	G	2.1
6	2G	39	ILE	2.1
8	2I	79	ILE	2.1
21	2Z	86	VAL	2.1
32	1a	156	G	2.1
32	2a	1178	G	2.1
32	2a	1220	G	2.1
33	2b	93	VAL	2.1
36	2e	33	VAL	2.1
42	2k	36	ASP	2.1
44	2m	7	VAL	2.1
44	2m	74	VAL	2.1
33	1b	192	SER	2.1
35	2d	75	PHE	2.1
50	2s	38	SER	2.1
1	1A	1762	A	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	1060	U	2.1
1	2A	1077	A	2.1
1	2A	2099	U	2.1
33	1b	207	ALA	2.1
34	2c	149	ALA	2.1
36	2e	94	ALA	2.1
42	1k	60	ALA	2.1
53	2y	63	ALA	2.1
6	2G	45	GLU	2.1
17	2V	93	GLU	2.1
32	1a	1136	U	2.1
33	2b	134	GLU	2.1
44	2m	69	GLU	2.1
7	1H	59	ARG	2.1
35	1d	132	ARG	2.1
35	2d	115	ARG	2.1
38	2g	155	ARG	2.1
45	2n	61	TRP	2.1
23	2l	81	LYS	2.1
48	2q	100	LYS	2.1
8	2I	134	PRO	2.1
35	2d	39	PRO	2.1
39	2h	70	GLN	2.1
5	2F	181	LEU	2.1
39	2h	135	CYS	2.1
50	1s	23	ASN	2.1
6	2G	131	TYR	2.1
18	1W	112	GLY	2.1
19	2X	94	GLY	2.1
33	1b	40	HIS	2.1
33	2b	89	GLY	2.1
36	1e	133	TYR	2.1
41	1j	68	HIS	2.1
1	2A	884	C	2.1
32	1a	1019	C	2.1
38	1g	50	ILE	2.1
41	2j	23	ILE	2.1
6	2G	180	PHE	2.1
14	2S	12	PHE	2.1
21	2Z	80	ARG	2.1
33	2b	13	ALA	2.1
33	2b	186	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	38	ARG	2.1
38	2g	147	ALA	2.1
49	2r	24	ALA	2.1
51	1t	11	SER	2.1
53	2y	15	ALA	2.1
1	1A	11	G	2.1
1	1A	2106	G	2.1
1	1A	2123	G	2.1
1	1A	2154	G	2.1
1	2A	1039	G	2.1
1	2A	1093	G	2.1
1	2A	1095	A	2.1
2	1B	120	A	2.1
14	2S	93	LYS	2.1
21	2Z	201	LYS	2.1
32	1a	220	G	2.1
7	2H	122	THR	2.1
22	20	43	THR	2.1
32	2a	983	A	2.1
32	2a	1219	U	2.1
32	2a	1287	A	2.1
47	1p	45	THR	2.1
7	2H	168	PRO	2.1
39	1h	72	PRO	2.1
45	2n	54	PRO	2.1
7	2H	7	LEU	2.1
34	2c	33	LEU	2.1
35	1d	174	LEU	2.1
35	2d	108	LEU	2.1
34	1c	3	ASN	2.1
26	14	45	GLY	2.1
26	14	64	GLY	2.1
31	29	20	HIS	2.1
34	2c	31	HIS	2.1
34	2c	158	GLY	2.1
35	2d	180	GLY	2.1
41	1j	10	GLY	2.1
7	1H	92	ILE	2.1
33	2b	39	ILE	2.1
33	2b	58	ILE	2.1
40	1i	36	TYR	2.1
40	2i	77	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	2I	92	VAL	2.1
38	2g	62	PHE	2.1
4	1E	73	GLU	2.0
11	2P	15	ARG	2.0
34	1c	83	ARG	2.0
5	1F	15	SER	2.0
40	1i	84	ALA	2.0
41	1j	26	ALA	2.0
1	2A	652(T)	C	2.0
34	2c	93	LYS	2.0
43	1l	126	LYS	2.0
44	2m	115	LYS	2.0
6	1G	86	MET	2.0
1	2A	895	U	2.0
1	2A	958	U	2.0
6	2G	41	GLN	2.0
7	2H	103	LEU	2.0
32	1a	1000	U	2.0
35	2d	11	LEU	2.0
38	2g	38	LEU	2.0
39	1h	133	LEU	2.0
41	1j	84	GLN	2.0
1	1A	1042	G	2.0
1	1A	1537	G	2.0
1	1A	2160	G	2.0
1	1A	2162	G	2.0
1	1A	2165	G	2.0
1	2A	1103	A	2.0
32	1a	181	G	2.0
32	2a	965	A	2.0
6	2G	127	GLY	2.0
6	2G	144	ILE	2.0
8	1I	109	ILE	2.0
33	1b	99	GLY	2.0
35	1d	23	GLY	2.0
44	2m	68	GLY	2.0
50	1s	8	GLY	2.0
33	2b	71	VAL	2.0
34	1c	201	TYR	2.0
38	1g	154	TYR	2.0
40	1i	28	VAL	2.0
44	2m	60	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	1G	80	PHE	2.0
7	1H	101	ARG	2.0
14	1S	3	ARG	2.0
33	2b	30	ARG	2.0
34	1c	38	ARG	2.0
41	2j	66	ARG	2.0
44	2m	71	ARG	2.0
44	2m	114	ARG	2.0
46	2o	68	ARG	2.0
51	2t	86	ARG	2.0
25	23	60	GLU	2.0
33	1b	20	GLU	2.0
33	2b	86	GLU	2.0
6	1G	46	ALA	2.0
34	1c	24	ALA	2.0
40	2i	60	ASP	2.0
40	2i	78	LYS	2.0
40	2i	94	ALA	2.0
40	2i	95	LYS	2.0
49	1r	24	ALA	2.0
53	2y	80	LYS	2.0
21	1Z	166	SER	2.0
38	2g	125	MET	2.0
4	2E	74	PRO	2.0
6	2G	165	THR	2.0
40	1i	90	PRO	2.0
43	2l	5	PRO	2.0
53	2y	14	PRO	2.0
1	2A	2896	C	2.0
2	2B	4	C	2.0
6	1G	53	LEU	2.0
11	1P	99	LEU	2.0
32	1a	1115	C	2.0
32	2a	990	C	2.0
32	2a	1129	C	2.0
34	2c	107	GLN	2.0
35	2d	160	GLN	2.0
42	1k	13	GLN	2.0
7	1H	174	GLY	2.0
33	2b	41	ILE	2.0
34	1c	80	GLY	2.0
34	2c	80	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	1k	117	ASN	2.0
45	2n	28	GLY	2.0
46	2o	87	ILE	2.0
53	2y	78	ILE	2.0
1	1A	1847	A	2.0
1	2A	887	A	2.0
3	1D	142	VAL	2.0
6	2G	28	VAL	2.0
9	2N	74	ARG	2.0
24	22	51	ARG	2.0
29	27	46	VAL	2.0
32	2a	969	A	2.0
37	1f	88	VAL	2.0
40	1i	66	ARG	2.0
52	2u	22	ARG	2.0
6	2G	25	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	5MU	2A	1915	21/22	0.84	0.11	80,89,96,109	0
1	PSU	2A	1917	20/21	0.86	0.10	78,83,98,100	0
32	2MG	2a	1207	24/25	0.86	0.13	89,94,98,101	0
43	0TD	2l	92	10/11	0.86	0.16	65,71,73,93	0
32	M2G	2a	966	25/26	0.87	0.16	65,72,87,92	0
1	PSU	2A	1911	20/21	0.88	0.09	69,77,90,92	0
1	5MU	1A	1915	21/22	0.88	0.12	73,81,86,90	0
43	0TD	1l	92	10/11	0.89	0.13	56,60,66,80	0
32	5MC	2a	967	21/22	0.89	0.14	71,78,88,88	0
1	PSU	1A	1917	20/21	0.90	0.10	70,75,86,86	0
32	2MG	1a	1207	24/25	0.90	0.12	72,78,83,86	0
1	PSU	1A	1911	20/21	0.92	0.09	63,70,72,72	0
32	PSU	2a	516	20/21	0.93	0.09	79,81,87,87	0
32	5MC	2a	1404	21/22	0.93	0.10	58,64,70,70	0
32	5MC	2a	1407	21/22	0.93	0.11	62,68,74,77	0
32	G7M	2a	527	24/25	0.93	0.12	68,73,75,77	0
1	OMC	2A	1920	21/22	0.94	0.09	63,73,78,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	1a	967	21/22	0.94	0.11	66,72,80,82	0
32	UR3	2a	1498	21/22	0.94	0.10	58,65,71,74	0
32	MA6	2a	1518	24/25	0.94	0.12	57,67,73,75	0
32	4OC	2a	1402	22/23	0.94	0.11	61,69,73,74	0
32	M2G	1a	966	25/26	0.95	0.11	60,66,73,78	0
32	5MC	2a	1400	21/22	0.95	0.13	72,76,80,83	0
32	PSU	1a	516	20/21	0.95	0.08	63,68,74,75	0
32	MA6	2a	1519	24/25	0.95	0.12	61,67,71,74	0
32	G7M	1a	527	24/25	0.95	0.11	49,58,62,67	0
32	5MC	1a	1404	21/22	0.96	0.09	51,54,60,64	0
32	5MC	1a	1407	21/22	0.96	0.10	48,56,61,63	0
1	5MC	2A	1942	21/22	0.96	0.08	46,56,60,61	0
32	UR3	1a	1498	21/22	0.96	0.09	48,54,60,70	0
32	MA6	1a	1519	24/25	0.96	0.10	44,52,58,60	0
1	OMC	1A	1920	21/22	0.96	0.10	53,58,63,66	0
32	5MC	1a	1400	21/22	0.96	0.10	53,60,64,67	0
32	4OC	1a	1402	22/23	0.96	0.09	48,57,60,64	0
1	OMG	2A	2251	24/25	0.97	0.09	37,41,44,48	0
1	2MA	2A	2503	23/24	0.97	0.08	30,38,42,44	0
1	OMU	2A	2552	21/22	0.97	0.08	36,42,46,50	0
32	MA6	1a	1518	24/25	0.97	0.10	46,52,57,59	0
1	5MC	1A	1962	21/22	0.97	0.07	29,37,43,45	0
1	2MA	1A	2503	23/24	0.97	0.08	20,28,31,31	0
1	5MC	1A	1942	21/22	0.97	0.08	34,38,42,43	0
1	5MC	2A	1962	21/22	0.97	0.09	44,50,54,63	0
1	OMU	1A	2552	21/22	0.98	0.06	27,33,35,38	0
1	PSU	1A	2605	20/21	0.98	0.07	26,30,36,37	0
1	OMG	1A	2251	24/25	0.98	0.06	26,30,33,35	0
1	5MU	2A	1939	21/22	0.98	0.07	36,41,45,46	0
1	PSU	2A	2605	20/21	0.98	0.07	35,41,44,44	0
1	5MU	1A	1939	21/22	0.98	0.07	26,32,36,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3986	1/1	0.48	0.27	43,43,43,43	0
54	MG	2a	3041	1/1	0.59	0.24	86,86,86,86	0
54	MG	1a	1743	1/1	0.60	0.21	87,87,87,87	0
54	MG	1a	1836	1/1	0.60	0.20	84,84,84,84	0
54	MG	2A	3380	1/1	0.60	0.23	59,59,59,59	0
54	MG	1A	3872	1/1	0.60	0.20	75,75,75,75	0
54	MG	1A	3213	1/1	0.62	0.26	73,73,73,73	0
54	MG	2A	3208	1/1	0.63	0.28	77,77,77,77	0
54	MG	2A	3034	1/1	0.65	0.29	87,87,87,87	0
54	MG	1A	3581	1/1	0.65	0.20	53,53,53,53	0
54	MG	2A	3343	1/1	0.65	0.25	85,85,85,85	0
54	MG	1a	1676	1/1	0.65	0.20	85,85,85,85	0
54	MG	2G	202	1/1	0.65	0.23	80,80,80,80	0
54	MG	1a	1874	1/1	0.65	0.39	84,84,84,84	0
54	MG	2A	3116	1/1	0.66	0.21	82,82,82,82	0
54	MG	1G	202	1/1	0.67	0.20	71,71,71,71	0
54	MG	1a	1855	1/1	0.67	0.25	86,86,86,86	0
54	MG	2A	3461	1/1	0.67	0.25	72,72,72,72	0
54	MG	1a	1796	1/1	0.67	0.21	86,86,86,86	0
54	MG	2A	3235	1/1	0.67	0.24	83,83,83,83	0
54	MG	2A	3604	1/1	0.68	0.19	46,46,46,46	0
54	MG	1A	3835	1/1	0.68	0.17	63,63,63,63	0
54	MG	2A	3579	1/1	0.68	0.18	62,62,62,62	0
54	MG	2a	3097	1/1	0.68	0.36	86,86,86,86	0
54	MG	2a	3174	1/1	0.68	0.20	86,86,86,86	0
54	MG	2A	3421	1/1	0.69	0.16	69,69,69,69	0
54	MG	1A	3781	1/1	0.69	0.18	33,33,33,33	0
54	MG	14	101	1/1	0.69	0.14	81,81,81,81	0
54	MG	1A	3812	1/1	0.69	0.17	78,78,78,78	0
54	MG	2A	3736	1/1	0.69	0.24	86,86,86,86	0
54	MG	1A	3261	1/1	0.69	0.30	86,86,86,86	0
54	MG	1A	3641	1/1	0.69	0.41	48,48,48,48	0
54	MG	1A	3983	1/1	0.69	0.18	81,81,81,81	0
54	MG	1A	3699	1/1	0.69	0.22	73,73,73,73	0
54	MG	1a	1795	1/1	0.70	0.16	84,84,84,84	0
54	MG	1A	3849	1/1	0.70	0.18	71,71,71,71	0
54	MG	2A	3610	1/1	0.70	0.17	82,82,82,82	0
54	MG	1a	1865	1/1	0.70	0.20	76,76,76,76	0
56	MPD	1O	202	8/8	0.70	0.24	67,75,81,81	0
54	MG	1A	3756	1/1	0.71	0.23	67,67,67,67	0
54	MG	1A	3891	1/1	0.71	0.23	60,60,60,60	0
54	MG	1a	1818	1/1	0.71	0.24	86,86,86,86	0
54	MG	1a	1754	1/1	0.71	0.20	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3194	1/1	0.71	0.20	86,86,86,86	0
54	MG	1a	1837	1/1	0.71	0.22	89,89,89,89	0
54	MG	1A	3796	1/1	0.72	0.31	74,74,74,74	0
54	MG	2A	3364	1/1	0.72	0.21	84,84,84,84	0
54	MG	1A	3924	1/1	0.72	0.20	37,37,37,37	0
54	MG	1a	1671	1/1	0.72	0.17	73,73,73,73	0
54	MG	1a	1765	1/1	0.72	0.20	81,81,81,81	0
54	MG	2a	3062	1/1	0.73	0.21	85,85,85,85	0
54	MG	2a	3092	1/1	0.73	0.15	80,80,80,80	0
54	MG	1a	1794	1/1	0.73	0.44	92,92,92,92	0
54	MG	2A	3420	1/1	0.73	0.28	76,76,76,76	0
54	MG	2a	3002	1/1	0.73	0.19	81,81,81,81	0
54	MG	2j	201	1/1	0.73	0.13	82,82,82,82	0
54	MG	2A	3525	1/1	0.73	0.16	63,63,63,63	0
54	MG	1g	202	1/1	0.74	0.14	73,73,73,73	0
54	MG	2B	201	1/1	0.74	0.15	85,85,85,85	0
54	MG	1A	3686	1/1	0.74	0.15	77,77,77,77	0
54	MG	2O	202	1/1	0.74	0.19	80,80,80,80	0
54	MG	1A	3930	1/1	0.74	0.21	63,63,63,63	0
54	MG	2a	3016	1/1	0.74	0.18	89,89,89,89	0
54	MG	2A	3441	1/1	0.74	0.19	67,67,67,67	0
54	MG	1A	4034	1/1	0.74	0.28	59,59,59,59	0
54	MG	2A	3507	1/1	0.74	0.20	42,42,42,42	0
54	MG	1a	1675	1/1	0.74	0.31	84,84,84,84	0
54	MG	2A	3558	1/1	0.74	0.17	45,45,45,45	0
54	MG	2A	3266	1/1	0.74	0.35	74,74,74,74	0
54	MG	1A	4040	1/1	0.74	0.20	63,63,63,63	0
54	MG	1a	1684	1/1	0.74	0.36	78,78,78,78	0
54	MG	1a	1857	1/1	0.75	0.25	81,81,81,81	0
54	MG	1A	3703	1/1	0.75	0.24	59,59,59,59	0
54	MG	2A	3729	1/1	0.75	0.33	82,82,82,82	0
54	MG	1A	4037	1/1	0.75	0.27	71,71,71,71	0
54	MG	2A	3409	1/1	0.75	0.40	84,84,84,84	0
54	MG	1A	3860	1/1	0.75	0.18	85,85,85,85	0
54	MG	1a	1808	1/1	0.75	0.17	92,92,92,92	0
54	MG	1A	3964	1/1	0.75	0.25	66,66,66,66	0
54	MG	2A	3460	1/1	0.75	0.22	64,64,64,64	0
54	MG	2A	3193	1/1	0.75	0.20	68,68,68,68	0
54	MG	2A	3474	1/1	0.75	0.19	58,58,58,58	0
54	MG	1A	3362	1/1	0.75	0.18	70,70,70,70	0
54	MG	1a	1761	1/1	0.75	0.20	70,70,70,70	0
54	MG	2A	3540	1/1	0.75	0.17	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3520	1/1	0.75	0.14	61,61,61,61	0
54	MG	2A	3561	1/1	0.75	0.24	54,54,54,54	0
54	MG	2A	3300	1/1	0.75	0.21	71,71,71,71	0
56	MPD	2B	219	8/8	0.75	0.30	66,74,79,84	0
54	MG	1A	3531	1/1	0.76	0.23	68,68,68,68	0
54	MG	1A	3996	1/1	0.76	0.43	62,62,62,62	0
54	MG	1a	1860	1/1	0.76	0.17	79,79,79,79	0
54	MG	15	105	1/1	0.76	0.17	56,56,56,56	0
54	MG	15	107	1/1	0.76	0.19	77,77,77,77	0
54	MG	2A	3433	1/1	0.76	0.20	62,62,62,62	0
54	MG	1A	3565	1/1	0.76	0.26	63,63,63,63	0
54	MG	1A	3511	1/1	0.76	0.22	54,54,54,54	0
54	MG	2a	3040	1/1	0.76	0.37	78,78,78,78	0
54	MG	1a	1800	1/1	0.76	0.23	71,71,71,71	0
54	MG	2a	3052	1/1	0.76	0.32	87,87,87,87	0
54	MG	2A	3185	1/1	0.76	0.31	86,86,86,86	0
54	MG	1a	1802	1/1	0.76	0.25	90,90,90,90	0
54	MG	1A	3483	1/1	0.76	0.14	31,31,31,31	0
54	MG	1B	220	1/1	0.76	0.18	50,50,50,50	0
54	MG	1a	1826	1/1	0.76	0.20	82,82,82,82	0
54	MG	2A	3272	1/1	0.76	0.26	76,76,76,76	0
54	MG	1a	1690	1/1	0.76	0.30	73,73,73,73	0
54	MG	1E	306	1/1	0.76	0.30	70,70,70,70	0
54	MG	2A	3299	1/1	0.77	0.26	70,70,70,70	0
54	MG	2G	201	1/1	0.77	0.14	84,84,84,84	0
54	MG	1a	1828	1/1	0.77	0.21	84,84,84,84	0
54	MG	2A	3493	1/1	0.77	0.21	73,73,73,73	0
54	MG	1A	3984	1/1	0.77	0.20	65,65,65,65	0
54	MG	2A	3509	1/1	0.77	0.23	65,65,65,65	0
54	MG	2a	3035	1/1	0.77	0.30	72,72,72,72	0
54	MG	2A	3053	1/1	0.77	0.28	77,77,77,77	0
54	MG	1B	217	1/1	0.77	0.17	67,67,67,67	0
54	MG	1A	3437	1/1	0.77	0.20	59,59,59,59	0
54	MG	1A	3677	1/1	0.77	0.21	67,67,67,67	0
54	MG	1A	3683	1/1	0.77	0.16	68,68,68,68	0
54	MG	2A	3584	1/1	0.77	0.23	69,69,69,69	0
54	MG	2a	3156	1/1	0.77	0.21	73,73,73,73	0
54	MG	2a	3173	1/1	0.77	0.21	83,83,83,83	0
54	MG	2A	3426	1/1	0.77	0.23	59,59,59,59	0
54	MG	1a	1783	1/1	0.77	0.18	80,80,80,80	0
54	MG	2f	202	1/1	0.77	0.13	69,69,69,69	0
54	MG	2A	3698	1/1	0.77	0.26	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1866	1/1	0.77	0.18	80,80,80,80	0
54	MG	1A	3892	1/1	0.77	0.18	59,59,59,59	0
54	MG	2A	3276	1/1	0.78	0.20	87,87,87,87	0
54	MG	2B	214	1/1	0.78	0.15	70,70,70,70	0
54	MG	1a	1820	1/1	0.78	0.19	68,68,68,68	0
54	MG	2A	3489	1/1	0.78	0.20	72,72,72,72	0
54	MG	1a	1825	1/1	0.78	0.18	51,51,51,51	0
54	MG	1a	1777	1/1	0.78	0.18	82,82,82,82	0
54	MG	2A	3345	1/1	0.78	0.16	80,80,80,80	0
54	MG	2a	3019	1/1	0.78	0.18	78,78,78,78	0
54	MG	2A	3515	1/1	0.78	0.26	75,75,75,75	0
54	MG	1A	3878	1/1	0.78	0.22	40,40,40,40	0
54	MG	1A	3624	1/1	0.78	0.20	34,34,34,34	0
54	MG	2a	3049	1/1	0.78	0.26	84,84,84,84	0
54	MG	2A	3153	1/1	0.78	0.14	71,71,71,71	0
54	MG	2A	3410	1/1	0.78	0.23	71,71,71,71	0
54	MG	2a	3074	1/1	0.78	0.24	70,70,70,70	0
54	MG	2a	3077	1/1	0.78	0.21	75,75,75,75	0
54	MG	1a	1715	1/1	0.78	0.22	86,86,86,86	0
54	MG	1A	4017	1/1	0.78	0.24	54,54,54,54	0
54	MG	2a	3149	1/1	0.78	0.21	71,71,71,71	0
54	MG	2A	3598	1/1	0.78	0.24	62,62,62,62	0
54	MG	1A	3505	1/1	0.78	0.15	63,63,63,63	0
54	MG	1A	3357	1/1	0.78	0.14	49,49,49,49	0
54	MG	2A	3614	1/1	0.78	0.13	71,71,71,71	0
54	MG	1T	204	1/1	0.78	0.11	81,81,81,81	0
54	MG	2A	3707	1/1	0.78	0.36	56,56,56,56	0
54	MG	2A	3442	1/1	0.78	0.13	69,69,69,69	0
54	MG	1a	1771	1/1	0.78	0.18	77,77,77,77	0
57	ARG	1F	320	12/12	0.78	0.20	58,76,81,84	0
54	MG	2A	3400	1/1	0.79	0.17	83,83,83,83	0
54	MG	1a	1641	1/1	0.79	0.25	81,81,81,81	0
54	MG	1a	1833	1/1	0.79	0.27	72,72,72,72	0
54	MG	2a	3038	1/1	0.79	0.18	89,89,89,89	0
54	MG	1A	3910	1/1	0.79	0.15	27,27,27,27	0
54	MG	1A	3611	1/1	0.79	0.16	72,72,72,72	0
54	MG	1A	3441	1/1	0.79	0.22	71,71,71,71	0
54	MG	1A	3284	1/1	0.79	0.21	77,77,77,77	0
54	MG	1A	3859	1/1	0.79	0.17	34,34,34,34	0
54	MG	2A	3270	1/1	0.79	0.30	83,83,83,83	0
54	MG	2A	3657	1/1	0.79	0.17	45,45,45,45	0
54	MG	2a	3079	1/1	0.79	0.56	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3693	1/1	0.79	0.27	60,60,60,60	0
54	MG	1a	1863	1/1	0.79	0.16	78,78,78,78	0
54	MG	1A	3704	1/1	0.79	0.22	53,53,53,53	0
54	MG	1A	3738	1/1	0.79	0.12	54,54,54,54	0
54	MG	2a	3160	1/1	0.79	0.47	82,82,82,82	0
54	MG	1A	3646	1/1	0.79	0.15	78,78,78,78	0
54	MG	1A	3497	1/1	0.79	0.18	48,48,48,48	0
54	MG	1A	3591	1/1	0.79	0.19	53,53,53,53	0
54	MG	2A	3052	1/1	0.79	0.28	72,72,72,72	0
54	MG	2A	3368	1/1	0.79	0.23	79,79,79,79	0
54	MG	2A	3524	1/1	0.79	0.16	85,85,85,85	0
54	MG	2I	101	1/1	0.79	0.33	84,84,84,84	0
54	MG	19	102	1/1	0.79	0.17	79,79,79,79	0
54	MG	2A	3557	1/1	0.80	0.20	43,43,43,43	0
54	MG	2A	3190	1/1	0.80	0.43	75,75,75,75	0
54	MG	1a	1780	1/1	0.80	0.21	85,85,85,85	0
54	MG	2A	3565	1/1	0.80	0.20	72,72,72,72	0
54	MG	1a	1655	1/1	0.80	0.12	76,76,76,76	0
54	MG	1A	3870	1/1	0.80	0.14	46,46,46,46	0
54	MG	1A	3305	1/1	0.80	0.16	48,48,48,48	0
54	MG	2A	3600	1/1	0.80	0.15	44,44,44,44	0
54	MG	1A	3456	1/1	0.80	0.19	64,64,64,64	0
54	MG	2a	3050	1/1	0.80	0.28	69,69,69,69	0
54	MG	2A	3606	1/1	0.80	0.20	62,62,62,62	0
54	MG	1D	309	1/1	0.80	0.40	57,57,57,57	0
54	MG	2A	3611	1/1	0.80	0.20	37,37,37,37	0
54	MG	2A	3273	1/1	0.80	0.21	61,61,61,61	0
54	MG	2A	3618	1/1	0.80	0.09	88,88,88,88	0
54	MG	1A	3888	1/1	0.80	0.12	38,38,38,38	0
54	MG	1A	3480	1/1	0.80	0.13	25,25,25,25	0
54	MG	1A	3379	1/1	0.80	0.18	74,74,74,74	0
54	MG	1a	1746	1/1	0.80	0.17	80,80,80,80	0
54	MG	2A	3501	1/1	0.80	0.12	85,85,85,85	0
54	MG	1A	3909	1/1	0.80	0.12	19,19,19,19	0
54	MG	1A	4026	1/1	0.80	0.17	56,56,56,56	0
54	MG	2B	202	1/1	0.80	0.13	82,82,82,82	0
54	MG	2B	213	1/1	0.80	0.19	78,78,78,78	0
54	MG	2A	3093	1/1	0.80	0.18	76,76,76,76	0
54	MG	1A	4033	1/1	0.80	0.22	75,75,75,75	0
54	MG	1A	3188	1/1	0.80	0.17	68,68,68,68	0
54	MG	1A	3790	1/1	0.80	0.24	61,61,61,61	0
54	MG	1a	1867	1/1	0.81	0.27	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1694	1/1	0.81	0.17	69,69,69,69	0
54	MG	1d	305	1/1	0.81	0.12	94,94,94,94	0
54	MG	1A	3537	1/1	0.81	0.15	51,51,51,51	0
54	MG	1a	1726	1/1	0.81	0.12	82,82,82,82	0
54	MG	2A	3366	1/1	0.81	0.14	43,43,43,43	0
54	MG	1a	1813	1/1	0.81	0.19	69,69,69,69	0
54	MG	2A	3379	1/1	0.81	0.20	58,58,58,58	0
54	MG	1a	1735	1/1	0.81	0.22	70,70,70,70	0
54	MG	2A	3072	1/1	0.81	0.23	70,70,70,70	0
54	MG	2A	3089	1/1	0.81	0.22	70,70,70,70	0
54	MG	2A	3090	1/1	0.81	0.16	72,72,72,72	0
54	MG	1A	3235	1/1	0.81	0.17	79,79,79,79	0
54	MG	1A	3364	1/1	0.81	0.12	48,48,48,48	0
54	MG	1A	3585	1/1	0.81	0.25	45,45,45,45	0
54	MG	1a	1611	1/1	0.81	0.27	69,69,69,69	0
54	MG	1A	3516	1/1	0.81	0.14	29,29,29,29	0
54	MG	1A	3367	1/1	0.81	0.13	26,26,26,26	0
54	MG	2A	3443	1/1	0.81	0.27	61,61,61,61	0
54	MG	2A	3677	1/1	0.81	0.24	74,74,74,74	0
54	MG	1A	3840	1/1	0.81	0.12	59,59,59,59	0
54	MG	1A	3450	1/1	0.81	0.19	74,74,74,74	0
54	MG	2A	3253	1/1	0.81	0.21	72,72,72,72	0
54	MG	2A	3486	1/1	0.81	0.23	70,70,70,70	0
54	MG	1a	1781	1/1	0.81	0.14	90,90,90,90	0
54	MG	1A	4024	1/1	0.81	0.16	65,65,65,65	0
54	MG	2A	3499	1/1	0.81	0.12	78,78,78,78	0
54	MG	2n	101	1/1	0.81	0.32	81,81,81,81	0
54	MG	1A	3534	1/1	0.81	0.15	55,55,55,55	0
54	MG	1a	1689	1/1	0.81	0.26	70,70,70,70	0
54	MG	10	106	1/1	0.81	0.11	60,60,60,60	0
54	MG	2E	304	1/1	0.82	0.17	41,41,41,41	0
54	MG	1A	3320	1/1	0.82	0.29	77,77,77,77	0
54	MG	2A	3538	1/1	0.82	0.12	58,58,58,58	0
54	MG	1a	1696	1/1	0.82	0.23	66,66,66,66	0
54	MG	1A	3471	1/1	0.82	0.16	58,58,58,58	0
54	MG	1A	4044	1/1	0.82	0.39	46,46,46,46	0
54	MG	1B	205	1/1	0.82	0.10	59,59,59,59	0
54	MG	1A	3642	1/1	0.82	0.17	67,67,67,67	0
54	MG	2a	3031	1/1	0.82	0.11	80,80,80,80	0
54	MG	2A	3416	1/1	0.82	0.18	58,58,58,58	0
54	MG	1A	3555	1/1	0.82	0.12	44,44,44,44	0
54	MG	2A	3250	1/1	0.82	0.27	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1749	1/1	0.82	0.11	61,61,61,61	0
54	MG	1A	3671	1/1	0.82	0.14	65,65,65,65	0
54	MG	1D	318	1/1	0.82	0.19	59,59,59,59	0
54	MG	2A	3608	1/1	0.82	0.26	84,84,84,84	0
54	MG	1a	1764	1/1	0.82	0.14	82,82,82,82	0
54	MG	2a	3064	1/1	0.82	0.35	78,78,78,78	0
54	MG	2A	3036	1/1	0.82	0.26	78,78,78,78	0
54	MG	2A	3046	1/1	0.82	0.14	65,65,65,65	0
54	MG	2A	3297	1/1	0.82	0.13	49,49,49,49	0
54	MG	1A	3489	1/1	0.82	0.11	26,26,26,26	0
54	MG	2A	3675	1/1	0.82	0.12	60,60,60,60	0
54	MG	2a	3119	1/1	0.82	0.18	86,86,86,86	0
54	MG	2A	3477	1/1	0.82	0.14	75,75,75,75	0
54	MG	2A	3684	1/1	0.82	0.15	51,51,51,51	0
54	MG	1A	3940	1/1	0.82	0.18	54,54,54,54	0
54	MG	2A	3301	1/1	0.82	0.14	60,60,60,60	0
54	MG	2A	3333	1/1	0.82	0.24	62,62,62,62	0
54	MG	2A	3339	1/1	0.82	0.13	37,37,37,37	0
54	MG	2a	3195	1/1	0.82	0.18	81,81,81,81	0
54	MG	1Q	204	1/1	0.82	0.18	48,48,48,48	0
54	MG	1A	3962	1/1	0.82	0.15	53,53,53,53	0
54	MG	2A	3354	1/1	0.82	0.23	78,78,78,78	0
54	MG	1A	3749	1/1	0.82	0.17	68,68,68,68	0
54	MG	1a	1850	1/1	0.82	0.15	66,66,66,66	0
54	MG	2D	308	1/1	0.82	0.20	77,77,77,77	0
54	MG	1A	3389	1/1	0.83	0.12	33,33,33,33	0
54	MG	1A	4000	1/1	0.83	0.20	84,84,84,84	0
54	MG	1A	3785	1/1	0.83	0.13	41,41,41,41	0
54	MG	1A	3688	1/1	0.83	0.26	70,70,70,70	0
54	MG	1A	3435	1/1	0.83	0.13	39,39,39,39	0
54	MG	1A	3900	1/1	0.83	0.13	59,59,59,59	0
54	MG	1A	3543	1/1	0.83	0.17	65,65,65,65	0
54	MG	1a	1774	1/1	0.83	0.18	78,78,78,78	0
54	MG	1A	3833	1/1	0.83	0.24	63,63,63,63	0
54	MG	1A	3667	1/1	0.83	0.14	31,31,31,31	0
54	MG	1a	1657	1/1	0.83	0.41	77,77,77,77	0
54	MG	1a	1871	1/1	0.83	0.18	78,78,78,78	0
54	MG	1a	1669	1/1	0.83	0.32	66,66,66,66	0
54	MG	1A	3722	1/1	0.83	0.12	40,40,40,40	0
54	MG	1A	4047	1/1	0.83	0.14	55,55,55,55	0
54	MG	2A	3316	1/1	0.83	0.14	53,53,53,53	0
54	MG	2A	3328	1/1	0.83	0.13	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1i	201	1/1	0.83	0.20	77,77,77,77	0
54	MG	2A	3012	1/1	0.83	0.20	68,68,68,68	0
54	MG	2a	3039	1/1	0.83	0.25	70,70,70,70	0
54	MG	1A	4051	1/1	0.83	0.27	49,49,49,49	0
54	MG	1a	1799	1/1	0.83	0.15	67,67,67,67	0
54	MG	2A	3350	1/1	0.83	0.22	55,55,55,55	0
54	MG	1A	4057	1/1	0.83	0.16	44,44,44,44	0
54	MG	2A	3570	1/1	0.83	0.13	56,56,56,56	0
54	MG	2a	3054	1/1	0.83	0.26	83,83,83,83	0
54	MG	1a	1801	1/1	0.83	0.19	71,71,71,71	0
54	MG	1A	3735	1/1	0.83	0.13	63,63,63,63	0
54	MG	1A	3593	1/1	0.83	0.18	66,66,66,66	0
54	MG	2A	3086	1/1	0.83	0.31	80,80,80,80	0
54	MG	1A	3216	1/1	0.83	0.29	50,50,50,50	0
54	MG	2A	3384	1/1	0.83	0.16	60,60,60,60	0
54	MG	1A	3975	1/1	0.83	0.18	56,56,56,56	0
54	MG	2A	3405	1/1	0.83	0.13	49,49,49,49	0
54	MG	2a	3142	1/1	0.83	0.17	66,66,66,66	0
54	MG	1A	3282	1/1	0.83	0.08	84,84,84,84	0
54	MG	2A	3109	1/1	0.83	0.09	73,73,73,73	0
54	MG	2A	3615	1/1	0.83	0.20	71,71,71,71	0
54	MG	1A	3778	1/1	0.83	0.13	28,28,28,28	0
54	MG	2A	3619	1/1	0.83	0.34	53,53,53,53	0
54	MG	1A	3874	1/1	0.83	0.13	53,53,53,53	0
54	MG	2A	3162	1/1	0.83	0.17	68,68,68,68	0
54	MG	2A	3182	1/1	0.83	0.20	60,60,60,60	0
54	MG	2A	3681	1/1	0.83	0.12	78,78,78,78	0
54	MG	2A	3683	1/1	0.83	0.16	78,78,78,78	0
54	MG	2A	3429	1/1	0.83	0.22	43,43,43,43	0
54	MG	1A	3988	1/1	0.83	0.09	75,75,75,75	0
54	MG	2A	3440	1/1	0.83	0.14	68,68,68,68	0
54	MG	1A	4008	1/1	0.84	0.16	49,49,49,49	0
54	MG	1A	3782	1/1	0.84	0.15	45,45,45,45	0
54	MG	2A	3503	1/1	0.84	0.18	73,73,73,73	0
54	MG	2A	3042	1/1	0.84	0.31	81,81,81,81	0
54	MG	10	105	1/1	0.84	0.14	57,57,57,57	0
54	MG	1a	1741	1/1	0.84	0.25	68,68,68,68	0
54	MG	2A	3517	1/1	0.84	0.18	70,70,70,70	0
54	MG	2G	203	1/1	0.84	0.17	78,78,78,78	0
54	MG	2A	3521	1/1	0.84	0.16	74,74,74,74	0
54	MG	1a	1821	1/1	0.84	0.14	78,78,78,78	0
54	MG	2A	3061	1/1	0.84	0.27	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3647	1/1	0.84	0.29	68,68,68,68	0
54	MG	1A	3662	1/1	0.84	0.12	45,45,45,45	0
54	MG	1a	1827	1/1	0.84	0.18	86,86,86,86	0
54	MG	1A	3182	1/1	0.84	0.19	76,76,76,76	0
54	MG	1A	3803	1/1	0.84	0.22	63,63,63,63	0
54	MG	2A	3098	1/1	0.84	0.26	67,67,67,67	0
54	MG	1A	3719	1/1	0.84	0.13	74,74,74,74	0
54	MG	2A	3574	1/1	0.84	0.14	60,60,60,60	0
54	MG	2A	3577	1/1	0.84	0.19	59,59,59,59	0
54	MG	1A	3821	1/1	0.84	0.18	77,77,77,77	0
54	MG	2A	3391	1/1	0.84	0.29	75,75,75,75	0
54	MG	1a	1637	1/1	0.84	0.24	72,72,72,72	0
54	MG	1A	3670	1/1	0.84	0.29	37,37,37,37	0
54	MG	2A	3406	1/1	0.84	0.15	66,66,66,66	0
54	MG	1A	3478	1/1	0.84	0.14	32,32,32,32	0
54	MG	1a	1859	1/1	0.84	0.19	78,78,78,78	0
54	MG	1A	3673	1/1	0.84	0.12	65,65,65,65	0
54	MG	1a	1664	1/1	0.84	0.15	83,83,83,83	0
54	MG	2A	3202	1/1	0.84	0.24	74,74,74,74	0
54	MG	1A	3739	1/1	0.84	0.16	52,52,52,52	0
54	MG	2a	3134	1/1	0.84	0.17	69,69,69,69	0
54	MG	2A	3216	1/1	0.84	0.13	67,67,67,67	0
54	MG	1A	3271	1/1	0.84	0.11	48,48,48,48	0
54	MG	2a	3154	1/1	0.84	0.12	67,67,67,67	0
54	MG	1B	210	1/1	0.84	0.38	84,84,84,84	0
54	MG	1A	3753	1/1	0.84	0.12	27,27,27,27	0
54	MG	1A	3404	1/1	0.84	0.15	30,30,30,30	0
54	MG	1a	1876	1/1	0.84	0.24	74,74,74,74	0
54	MG	2a	3181	1/1	0.84	0.20	78,78,78,78	0
54	MG	2A	3457	1/1	0.84	0.10	84,84,84,84	0
54	MG	1A	3760	1/1	0.84	0.17	63,63,63,63	0
54	MG	1A	3645	1/1	0.84	0.28	49,49,49,49	0
54	MG	2A	3275	1/1	0.84	0.15	59,59,59,59	0
54	MG	1A	3374	1/1	0.84	0.12	67,67,67,67	0
54	MG	1l	202	1/1	0.84	0.18	83,83,83,83	0
54	MG	1A	3882	1/1	0.84	0.11	40,40,40,40	0
54	MG	2A	3024	1/1	0.84	0.20	67,67,67,67	0
54	MG	1a	1699	1/1	0.85	0.13	64,64,64,64	0
54	MG	1a	1712	1/1	0.85	0.14	64,64,64,64	0
54	MG	1P	206	1/1	0.85	0.12	48,48,48,48	0
54	MG	1A	3082	1/1	0.85	0.15	57,57,57,57	0
54	MG	1A	3764	1/1	0.85	0.19	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3688	1/1	0.85	0.11	75,75,75,75	0
54	MG	1A	3131	1/1	0.85	0.14	59,59,59,59	0
54	MG	1A	3947	1/1	0.85	0.15	52,52,52,52	0
54	MG	2A	3148	1/1	0.85	0.25	66,66,66,66	0
54	MG	1A	3959	1/1	0.85	0.12	59,59,59,59	0
54	MG	2A	3161	1/1	0.85	0.22	84,84,84,84	0
54	MG	2A	3737	1/1	0.85	0.30	72,72,72,72	0
54	MG	1A	3536	1/1	0.85	0.16	44,44,44,44	0
54	MG	1A	3416	1/1	0.85	0.16	68,68,68,68	0
54	MG	2B	204	1/1	0.85	0.11	75,75,75,75	0
54	MG	2B	207	1/1	0.85	0.16	81,81,81,81	0
54	MG	1a	1755	1/1	0.85	0.22	74,74,74,74	0
54	MG	1A	3967	1/1	0.85	0.18	75,75,75,75	0
54	MG	2B	217	1/1	0.85	0.11	83,83,83,83	0
54	MG	1A	3297	1/1	0.85	0.11	53,53,53,53	0
54	MG	2A	3444	1/1	0.85	0.17	66,66,66,66	0
54	MG	2A	3451	1/1	0.85	0.17	70,70,70,70	0
54	MG	2A	3196	1/1	0.85	0.15	63,63,63,63	0
54	MG	1A	3979	1/1	0.85	0.11	50,50,50,50	0
54	MG	1a	1861	1/1	0.85	0.16	71,71,71,71	0
54	MG	2A	3210	1/1	0.85	0.15	62,62,62,62	0
54	MG	1a	1766	1/1	0.85	0.25	84,84,84,84	0
54	MG	2A	3227	1/1	0.85	0.14	65,65,65,65	0
54	MG	2A	3229	1/1	0.85	0.21	67,67,67,67	0
54	MG	1a	1638	1/1	0.85	0.41	80,80,80,80	0
54	MG	1A	3202	1/1	0.85	0.18	66,66,66,66	0
54	MG	2a	3037	1/1	0.85	0.21	74,74,74,74	0
54	MG	1a	1775	1/1	0.85	0.12	86,86,86,86	0
54	MG	1a	1870	1/1	0.85	0.29	72,72,72,72	0
54	MG	1a	1654	1/1	0.85	0.14	80,80,80,80	0
54	MG	1A	3370	1/1	0.85	0.11	47,47,47,47	0
54	MG	1A	3157	1/1	0.85	0.35	73,73,73,73	0
54	MG	1A	3376	1/1	0.85	0.10	43,43,43,43	0
54	MG	2a	3051	1/1	0.85	0.30	77,77,77,77	0
54	MG	1a	1787	1/1	0.85	0.15	72,72,72,72	0
54	MG	2A	3277	1/1	0.85	0.14	34,34,34,34	0
54	MG	2a	3056	1/1	0.85	0.23	76,76,76,76	0
54	MG	2a	3058	1/1	0.85	0.23	77,77,77,77	0
54	MG	1h	201	1/1	0.85	0.27	59,59,59,59	0
54	MG	1B	224	1/1	0.85	0.20	72,72,72,72	0
54	MG	1B	226	1/1	0.85	0.11	73,73,73,73	0
54	MG	1n	101	1/1	0.85	0.46	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3313	1/1	0.85	0.23	63,63,63,63	0
54	MG	1t	201	1/1	0.85	0.13	74,74,74,74	0
54	MG	2a	3093	1/1	0.85	0.19	76,76,76,76	0
54	MG	1A	3587	1/1	0.85	0.18	64,64,64,64	0
54	MG	2A	3023	1/1	0.85	0.19	69,69,69,69	0
54	MG	1D	315	1/1	0.85	0.17	73,73,73,73	0
54	MG	2A	3028	1/1	0.85	0.15	61,61,61,61	0
54	MG	1A	3519	1/1	0.85	0.12	27,27,27,27	0
54	MG	1E	303	1/1	0.85	0.13	29,29,29,29	0
54	MG	1A	3332	1/1	0.85	0.14	29,29,29,29	0
54	MG	2A	3356	1/1	0.85	0.14	72,72,72,72	0
54	MG	2A	3361	1/1	0.85	0.22	63,63,63,63	0
54	MG	2A	3363	1/1	0.85	0.20	71,71,71,71	0
54	MG	1a	1805	1/1	0.85	0.12	70,70,70,70	0
54	MG	1a	1691	1/1	0.85	0.15	59,59,59,59	0
54	MG	1a	1810	1/1	0.85	0.19	76,76,76,76	0
54	MG	2A	3054	1/1	0.85	0.32	76,76,76,76	0
54	MG	2A	3056	1/1	0.85	0.30	59,59,59,59	0
54	MG	2A	3383	1/1	0.85	0.17	52,52,52,52	0
54	MG	1F	312	1/1	0.85	0.15	39,39,39,39	0
56	MPD	1a	1878	8/8	0.85	0.15	55,70,73,73	0
56	MPD	2A	3743	8/8	0.85	0.28	46,57,62,63	0
56	MPD	2A	3744	8/8	0.85	0.25	63,68,74,74	0
54	MG	2A	3623	1/1	0.85	0.21	62,62,62,62	0
54	MG	1A	3522	1/1	0.85	0.13	58,58,58,58	0
54	MG	1a	1811	1/1	0.86	0.11	71,71,71,71	0
54	MG	2A	3385	1/1	0.86	0.20	65,65,65,65	0
54	MG	2A	3682	1/1	0.86	0.10	74,74,74,74	0
54	MG	1A	3281	1/1	0.86	0.09	77,77,77,77	0
54	MG	2A	3091	1/1	0.86	0.27	68,68,68,68	0
54	MG	1A	3452	1/1	0.86	0.12	53,53,53,53	0
54	MG	1A	3605	1/1	0.86	0.10	42,42,42,42	0
54	MG	2A	3695	1/1	0.86	0.12	53,53,53,53	0
54	MG	1A	3823	1/1	0.86	0.20	42,42,42,42	0
54	MG	2A	3706	1/1	0.86	0.17	65,65,65,65	0
54	MG	1A	3702	1/1	0.86	0.20	43,43,43,43	0
54	MG	2A	3724	1/1	0.86	0.26	71,71,71,71	0
54	MG	1A	3340	1/1	0.86	0.11	65,65,65,65	0
54	MG	1A	3837	1/1	0.86	0.13	44,44,44,44	0
54	MG	2A	3160	1/1	0.86	0.20	75,75,75,75	0
54	MG	2A	3742	1/1	0.86	0.14	50,50,50,50	0
54	MG	1A	3380	1/1	0.86	0.13	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1829	1/1	0.86	0.14	83,83,83,83	0
54	MG	1A	3627	1/1	0.86	0.17	39,39,39,39	0
54	MG	1A	3628	1/1	0.86	0.12	65,65,65,65	0
54	MG	2B	208	1/1	0.86	0.26	66,66,66,66	0
54	MG	2B	209	1/1	0.86	0.19	70,70,70,70	0
54	MG	1E	309	1/1	0.86	0.22	58,58,58,58	0
54	MG	1a	1730	1/1	0.86	0.27	75,75,75,75	0
54	MG	2B	215	1/1	0.86	0.09	75,75,75,75	0
54	MG	1A	3987	1/1	0.86	0.14	53,53,53,53	0
54	MG	1a	1740	1/1	0.86	0.14	65,65,65,65	0
54	MG	2A	3450	1/1	0.86	0.13	70,70,70,70	0
54	MG	2A	3207	1/1	0.86	0.17	74,74,74,74	0
54	MG	2A	3453	1/1	0.86	0.12	74,74,74,74	0
54	MG	1G	201	1/1	0.86	0.11	77,77,77,77	0
54	MG	1A	3636	1/1	0.86	0.18	68,68,68,68	0
54	MG	20	103	1/1	0.86	0.19	72,72,72,72	0
54	MG	1A	3993	1/1	0.86	0.28	52,52,52,52	0
54	MG	1A	3036	1/1	0.86	0.30	62,62,62,62	0
54	MG	2a	3003	1/1	0.86	0.15	70,70,70,70	0
54	MG	1a	1752	1/1	0.86	0.19	75,75,75,75	0
54	MG	2A	3230	1/1	0.86	0.33	68,68,68,68	0
54	MG	2a	3026	1/1	0.86	0.20	78,78,78,78	0
54	MG	2A	3234	1/1	0.86	0.18	75,75,75,75	0
54	MG	1A	3027	1/1	0.86	0.16	65,65,65,65	0
54	MG	2A	3249	1/1	0.86	0.27	68,68,68,68	0
54	MG	1Z	301	1/1	0.86	0.18	69,69,69,69	0
54	MG	1a	1868	1/1	0.86	0.21	65,65,65,65	0
54	MG	2A	3261	1/1	0.86	0.18	62,62,62,62	0
54	MG	1a	1759	1/1	0.86	0.13	76,76,76,76	0
54	MG	1A	4004	1/1	0.86	0.16	86,86,86,86	0
54	MG	1a	1763	1/1	0.86	0.15	68,68,68,68	0
54	MG	1A	3034	1/1	0.86	0.12	63,63,63,63	0
54	MG	1A	3486	1/1	0.86	0.10	32,32,32,32	0
54	MG	1A	3550	1/1	0.86	0.11	47,47,47,47	0
54	MG	1A	3886	1/1	0.86	0.10	31,31,31,31	0
54	MG	2A	3290	1/1	0.86	0.12	62,62,62,62	0
54	MG	2A	3554	1/1	0.86	0.11	77,77,77,77	0
54	MG	18	101	1/1	0.86	0.21	77,77,77,77	0
54	MG	2a	3072	1/1	0.86	0.16	82,82,82,82	0
54	MG	1A	3654	1/1	0.86	0.14	69,69,69,69	0
54	MG	1A	3554	1/1	0.86	0.24	44,44,44,44	0
54	MG	1a	1778	1/1	0.86	0.20	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3567	1/1	0.86	0.15	54,54,54,54	0
54	MG	1a	1630	1/1	0.86	0.23	68,68,68,68	0
54	MG	1a	1632	1/1	0.86	0.08	42,42,42,42	0
54	MG	1a	1635	1/1	0.86	0.37	65,65,65,65	0
54	MG	1A	3768	1/1	0.86	0.20	55,55,55,55	0
54	MG	2A	3031	1/1	0.86	0.19	77,77,77,77	0
54	MG	2a	3145	1/1	0.86	0.11	82,82,82,82	0
54	MG	2A	3595	1/1	0.86	0.12	65,65,65,65	0
54	MG	1a	1791	1/1	0.86	0.18	75,75,75,75	0
54	MG	1A	3426	1/1	0.86	0.15	40,40,40,40	0
54	MG	1A	3434	1/1	0.86	0.20	65,65,65,65	0
54	MG	2a	3164	1/1	0.86	0.11	69,69,69,69	0
54	MG	2A	3043	1/1	0.86	0.15	56,56,56,56	0
54	MG	1A	3576	1/1	0.86	0.18	52,52,52,52	0
54	MG	1A	3189	1/1	0.86	0.13	68,68,68,68	0
54	MG	2a	3186	1/1	0.86	0.23	78,78,78,78	0
54	MG	1A	4053	1/1	0.86	0.13	53,53,53,53	0
54	MG	1a	1659	1/1	0.86	0.23	64,64,64,64	0
54	MG	1A	3142	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3059	1/1	0.86	0.17	73,73,73,73	0
54	MG	2A	3377	1/1	0.86	0.13	58,58,58,58	0
54	MG	2o	101	1/1	0.86	0.16	69,69,69,69	0
54	MG	2A	3622	1/1	0.86	0.14	66,66,66,66	0
54	MG	1B	203	1/1	0.86	0.26	69,69,69,69	0
54	MG	2A	3624	1/1	0.86	0.17	76,76,76,76	0
54	MG	1A	3331	1/1	0.86	0.10	30,30,30,30	0
54	MG	2A	3660	1/1	0.86	0.09	31,31,31,31	0
54	MG	1B	206	1/1	0.86	0.19	64,64,64,64	0
54	MG	1A	3754	1/1	0.87	0.20	48,48,48,48	0
54	MG	1A	3973	1/1	0.87	0.12	44,44,44,44	0
54	MG	2A	3470	1/1	0.87	0.14	84,84,84,84	0
54	MG	1a	1674	1/1	0.87	0.20	76,76,76,76	0
54	MG	1A	3144	1/1	0.87	0.14	69,69,69,69	0
54	MG	1A	3584	1/1	0.87	0.19	53,53,53,53	0
54	MG	1A	3763	1/1	0.87	0.19	65,65,65,65	0
54	MG	1D	314	1/1	0.87	0.11	60,60,60,60	0
54	MG	1A	3124	1/1	0.87	0.14	39,39,39,39	0
54	MG	1A	3873	1/1	0.87	0.10	47,47,47,47	0
54	MG	2A	3502	1/1	0.87	0.14	69,69,69,69	0
54	MG	1A	3548	1/1	0.87	0.10	38,38,38,38	0
54	MG	2A	3298	1/1	0.87	0.16	64,64,64,64	0
54	MG	1A	3875	1/1	0.87	0.13	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3989	1/1	0.87	0.14	53,53,53,53	0
54	MG	1A	3694	1/1	0.87	0.09	71,71,71,71	0
54	MG	2A	3520	1/1	0.87	0.14	62,62,62,62	0
54	MG	1a	1713	1/1	0.87	0.10	94,94,94,94	0
54	MG	2A	3057	1/1	0.87	0.20	58,58,58,58	0
54	MG	1A	3428	1/1	0.87	0.18	47,47,47,47	0
54	MG	1a	1822	1/1	0.87	0.13	71,71,71,71	0
54	MG	2a	3004	1/1	0.87	0.21	73,73,73,73	0
54	MG	1a	1722	1/1	0.87	0.17	61,61,61,61	0
54	MG	2A	3546	1/1	0.87	0.09	74,74,74,74	0
54	MG	2A	3342	1/1	0.87	0.13	40,40,40,40	0
54	MG	2a	3027	1/1	0.87	0.31	74,74,74,74	0
54	MG	2A	3083	1/1	0.87	0.15	48,48,48,48	0
54	MG	1A	3884	1/1	0.87	0.14	65,65,65,65	0
54	MG	1A	3308	1/1	0.87	0.36	49,49,49,49	0
54	MG	1a	1731	1/1	0.87	0.17	59,59,59,59	0
54	MG	1a	1734	1/1	0.87	0.28	69,69,69,69	0
54	MG	1A	3650	1/1	0.87	0.11	53,53,53,53	0
54	MG	1A	4012	1/1	0.87	0.21	69,69,69,69	0
54	MG	2a	3043	1/1	0.87	0.28	63,63,63,63	0
54	MG	2a	3045	1/1	0.87	0.22	84,84,84,84	0
54	MG	2A	3576	1/1	0.87	0.10	66,66,66,66	0
54	MG	2A	3100	1/1	0.87	0.28	63,63,63,63	0
54	MG	1A	4015	1/1	0.87	0.25	48,48,48,48	0
54	MG	1A	3468	1/1	0.87	0.14	60,60,60,60	0
54	MG	2A	3593	1/1	0.87	0.10	72,72,72,72	0
54	MG	2A	3137	1/1	0.87	0.15	51,51,51,51	0
54	MG	1a	1853	1/1	0.87	0.12	66,66,66,66	0
54	MG	1A	3792	1/1	0.87	0.13	35,35,35,35	0
54	MG	2A	3381	1/1	0.87	0.14	47,47,47,47	0
54	MG	10	107	1/1	0.87	0.14	73,73,73,73	0
54	MG	1A	3716	1/1	0.87	0.18	29,29,29,29	0
54	MG	2a	3075	1/1	0.87	0.17	70,70,70,70	0
54	MG	1A	4030	1/1	0.87	0.18	75,75,75,75	0
54	MG	1A	3606	1/1	0.87	0.18	50,50,50,50	0
54	MG	15	108	1/1	0.87	0.31	42,42,42,42	0
54	MG	2A	3189	1/1	0.87	0.25	66,66,66,66	0
54	MG	1A	3665	1/1	0.87	0.07	22,22,22,22	0
54	MG	2a	3110	1/1	0.87	0.23	77,77,77,77	0
54	MG	2a	3112	1/1	0.87	0.15	55,55,55,55	0
54	MG	1A	3561	1/1	0.87	0.12	54,54,54,54	0
54	MG	1A	3925	1/1	0.87	0.13	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3414	1/1	0.87	0.15	91,91,91,91	0
54	MG	2a	3143	1/1	0.87	0.12	55,55,55,55	0
54	MG	2A	3198	1/1	0.87	0.29	77,77,77,77	0
54	MG	2A	3654	1/1	0.87	0.10	85,85,85,85	0
54	MG	2A	3417	1/1	0.87	0.19	68,68,68,68	0
54	MG	1a	1616	1/1	0.87	0.15	73,73,73,73	0
54	MG	2A	3663	1/1	0.87	0.16	85,85,85,85	0
54	MG	1A	3354	1/1	0.87	0.16	60,60,60,60	0
54	MG	1A	4045	1/1	0.87	0.16	64,64,64,64	0
54	MG	1A	3935	1/1	0.87	0.14	53,53,53,53	0
54	MG	2a	3179	1/1	0.87	0.18	69,69,69,69	0
54	MG	2A	3213	1/1	0.87	0.26	64,64,64,64	0
54	MG	2A	3434	1/1	0.87	0.11	63,63,63,63	0
54	MG	2a	3191	1/1	0.87	0.12	88,88,88,88	0
54	MG	2A	3438	1/1	0.87	0.12	54,54,54,54	0
54	MG	1A	3567	1/1	0.87	0.16	64,64,64,64	0
54	MG	1b	301	1/1	0.87	0.15	80,80,80,80	0
54	MG	1A	3834	1/1	0.87	0.15	59,59,59,59	0
54	MG	1A	3950	1/1	0.87	0.17	51,51,51,51	0
54	MG	2A	3701	1/1	0.87	0.15	65,65,65,65	0
54	MG	2p	101	1/1	0.87	0.44	67,67,67,67	0
54	MG	2t	201	1/1	0.87	0.15	54,54,54,54	0
54	MG	1B	202	1/1	0.87	0.14	74,74,74,74	0
54	MG	2A	3449	1/1	0.87	0.21	58,58,58,58	0
54	MG	1A	3952	1/1	0.87	0.07	68,68,68,68	0
54	MG	1A	3746	1/1	0.87	0.21	57,57,57,57	0
54	MG	1A	3164	1/1	0.87	0.18	51,51,51,51	0
54	MG	1A	3676	1/1	0.87	0.11	44,44,44,44	0
54	MG	1A	3916	1/1	0.88	0.11	39,39,39,39	0
54	MG	1A	4023	1/1	0.88	0.09	28,28,28,28	0
54	MG	1a	1804	1/1	0.88	0.10	71,71,71,71	0
54	MG	1A	3918	1/1	0.88	0.16	51,51,51,51	0
54	MG	1A	3484	1/1	0.88	0.10	30,30,30,30	0
54	MG	1A	3092	1/1	0.88	0.12	62,62,62,62	0
54	MG	2B	210	1/1	0.88	0.20	82,82,82,82	0
54	MG	1A	3538	1/1	0.88	0.17	63,63,63,63	0
54	MG	2A	3494	1/1	0.88	0.10	53,53,53,53	0
54	MG	1A	3600	1/1	0.88	0.16	44,44,44,44	0
54	MG	1a	1814	1/1	0.88	0.12	64,64,64,64	0
54	MG	1A	3601	1/1	0.88	0.12	66,66,66,66	0
54	MG	2D	310	1/1	0.88	0.10	31,31,31,31	0
54	MG	1A	4038	1/1	0.88	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
54	MG	2F	303	1/1	0.88	0.17	59,59,59,59	0
54	MG	1A	3487	1/1	0.88	0.14	34,34,34,34	0
54	MG	1A	3839	1/1	0.88	0.12	39,39,39,39	0
54	MG	2A	3308	1/1	0.88	0.16	67,67,67,67	0
54	MG	1A	3208	1/1	0.88	0.26	73,73,73,73	0
54	MG	1A	3462	1/1	0.88	0.17	43,43,43,43	0
54	MG	2A	3319	1/1	0.88	0.12	53,53,53,53	0
54	MG	28	102	1/1	0.88	0.20	60,60,60,60	0
54	MG	1a	1737	1/1	0.88	0.32	79,79,79,79	0
54	MG	1A	3463	1/1	0.88	0.11	27,27,27,27	0
54	MG	1a	1601	1/1	0.88	0.26	78,78,78,78	0
54	MG	2a	3008	1/1	0.88	0.43	75,75,75,75	0
54	MG	1A	3685	1/1	0.88	0.10	70,70,70,70	0
54	MG	1A	3508	1/1	0.88	0.10	47,47,47,47	0
54	MG	2A	3552	1/1	0.88	0.11	80,80,80,80	0
54	MG	2A	3553	1/1	0.88	0.09	75,75,75,75	0
54	MG	2A	3344	1/1	0.88	0.11	40,40,40,40	0
54	MG	2a	3033	1/1	0.88	0.20	65,65,65,65	0
54	MG	1a	1628	1/1	0.88	0.23	77,77,77,77	0
54	MG	2A	3347	1/1	0.88	0.12	48,48,48,48	0
54	MG	2A	3099	1/1	0.88	0.13	65,65,65,65	0
54	MG	1a	1846	1/1	0.88	0.12	80,80,80,80	0
54	MG	1a	1751	1/1	0.88	0.20	64,64,64,64	0
54	MG	2A	3113	1/1	0.88	0.27	76,76,76,76	0
54	MG	1A	3560	1/1	0.88	0.12	42,42,42,42	0
54	MG	2A	3121	1/1	0.88	0.24	72,72,72,72	0
54	MG	2A	3124	1/1	0.88	0.17	76,76,76,76	0
54	MG	1a	1631	1/1	0.88	0.23	74,74,74,74	0
54	MG	2A	3370	1/1	0.88	0.24	73,73,73,73	0
54	MG	2A	3375	1/1	0.88	0.11	40,40,40,40	0
54	MG	2A	3142	1/1	0.88	0.18	68,68,68,68	0
54	MG	2a	3055	1/1	0.88	0.26	74,74,74,74	0
54	MG	1A	3689	1/1	0.88	0.15	47,47,47,47	0
54	MG	1a	1756	1/1	0.88	0.18	66,66,66,66	0
54	MG	1A	3976	1/1	0.88	0.15	53,53,53,53	0
54	MG	2A	3605	1/1	0.88	0.12	68,68,68,68	0
54	MG	1A	3394	1/1	0.88	0.11	37,37,37,37	0
54	MG	1A	3469	1/1	0.88	0.10	57,57,57,57	0
54	MG	2A	3170	1/1	0.88	0.20	67,67,67,67	0
54	MG	2a	3076	1/1	0.88	0.09	72,72,72,72	0
54	MG	2A	3388	1/1	0.88	0.20	72,72,72,72	0
54	MG	2A	3176	1/1	0.88	0.16	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3784	1/1	0.88	0.12	49,49,49,49	0
54	MG	1a	1644	1/1	0.88	0.29	61,61,61,61	0
54	MG	2A	3186	1/1	0.88	0.25	54,54,54,54	0
54	MG	2a	3107	1/1	0.88	0.13	75,75,75,75	0
54	MG	1a	1645	1/1	0.88	0.29	74,74,74,74	0
54	MG	1a	1770	1/1	0.88	0.14	68,68,68,68	0
54	MG	1a	1653	1/1	0.88	0.21	59,59,59,59	0
54	MG	2a	3125	1/1	0.88	0.16	82,82,82,82	0
54	MG	2A	3628	1/1	0.88	0.16	90,90,90,90	0
54	MG	2a	3137	1/1	0.88	0.14	68,68,68,68	0
54	MG	2A	3195	1/1	0.88	0.23	67,67,67,67	0
54	MG	1a	1772	1/1	0.88	0.29	71,71,71,71	0
54	MG	2A	3658	1/1	0.88	0.11	42,42,42,42	0
54	MG	1B	218	1/1	0.88	0.10	59,59,59,59	0
54	MG	2a	3151	1/1	0.88	0.22	68,68,68,68	0
54	MG	1A	3265	1/1	0.88	0.17	62,62,62,62	0
54	MG	2A	3205	1/1	0.88	0.14	63,63,63,63	0
54	MG	2a	3157	1/1	0.88	0.14	93,93,93,93	0
54	MG	1a	1656	1/1	0.88	0.19	50,50,50,50	0
54	MG	2A	3680	1/1	0.88	0.12	42,42,42,42	0
54	MG	2A	3430	1/1	0.88	0.12	60,60,60,60	0
54	MG	1A	3409	1/1	0.88	0.21	59,59,59,59	0
54	MG	2a	3176	1/1	0.88	0.23	63,63,63,63	0
54	MG	1A	3580	1/1	0.88	0.10	24,24,24,24	0
54	MG	2A	3437	1/1	0.88	0.12	69,69,69,69	0
54	MG	2a	3182	1/1	0.88	0.12	66,66,66,66	0
54	MG	1A	3411	1/1	0.88	0.23	73,73,73,73	0
54	MG	1h	202	1/1	0.88	0.14	64,64,64,64	0
54	MG	2a	3193	1/1	0.88	0.26	76,76,76,76	0
54	MG	2A	3218	1/1	0.88	0.29	72,72,72,72	0
54	MG	1A	3799	1/1	0.88	0.20	70,70,70,70	0
54	MG	1A	3481	1/1	0.88	0.14	40,40,40,40	0
54	MG	1A	3270	1/1	0.88	0.12	65,65,65,65	0
54	MG	1n	102	1/1	0.88	0.14	67,67,67,67	0
54	MG	2A	3720	1/1	0.88	0.13	57,57,57,57	0
54	MG	2A	3723	1/1	0.88	0.22	67,67,67,67	0
54	MG	2r	101	1/1	0.88	0.13	68,68,68,68	0
54	MG	1A	3904	1/1	0.88	0.10	69,69,69,69	0
56	MPD	1A	4058	8/8	0.88	0.20	51,55,64,66	0
54	MG	1A	3813	1/1	0.88	0.19	38,38,38,38	0
54	MG	2A	3730	1/1	0.88	0.24	74,74,74,74	0
54	MG	2A	3735	1/1	0.88	0.09	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3820	1/1	0.88	0.15	53,53,53,53	0
54	MG	1A	4014	1/1	0.88	0.09	67,67,67,67	0
54	MG	1A	3913	1/1	0.88	0.10	29,29,29,29	0
58	ZN	24	501	1/1	0.88	0.20	157,157,157,157	0
54	MG	1B	228	1/1	0.89	0.09	68,68,68,68	0
54	MG	1A	3562	1/1	0.89	0.19	71,71,71,71	0
54	MG	1D	311	1/1	0.89	0.19	49,49,49,49	0
54	MG	1A	3889	1/1	0.89	0.11	45,45,45,45	0
54	MG	2A	3731	1/1	0.89	0.18	72,72,72,72	0
54	MG	2A	3732	1/1	0.89	0.09	74,74,74,74	0
54	MG	1a	1779	1/1	0.89	0.11	55,55,55,55	0
54	MG	2A	3221	1/1	0.89	0.12	65,65,65,65	0
54	MG	2A	3446	1/1	0.89	0.18	64,64,64,64	0
54	MG	2A	3448	1/1	0.89	0.14	56,56,56,56	0
54	MG	1A	3692	1/1	0.89	0.11	65,65,65,65	0
54	MG	1A	3693	1/1	0.89	0.17	69,69,69,69	0
54	MG	1A	3563	1/1	0.89	0.11	51,51,51,51	0
54	MG	1y	204	1/1	0.89	0.11	86,86,86,86	0
54	MG	2A	3455	1/1	0.89	0.13	42,42,42,42	0
54	MG	2A	3003	1/1	0.89	0.09	66,66,66,66	0
54	MG	2A	3242	1/1	0.89	0.16	66,66,66,66	0
54	MG	2A	3010	1/1	0.89	0.16	73,73,73,73	0
54	MG	1a	1784	1/1	0.89	0.14	66,66,66,66	0
54	MG	2A	3471	1/1	0.89	0.10	55,55,55,55	0
54	MG	2A	3252	1/1	0.89	0.15	65,65,65,65	0
54	MG	2D	304	1/1	0.89	0.38	52,52,52,52	0
54	MG	2A	3016	1/1	0.89	0.28	74,74,74,74	0
54	MG	2D	309	1/1	0.89	0.27	42,42,42,42	0
54	MG	2A	3480	1/1	0.89	0.20	61,61,61,61	0
54	MG	2E	301	1/1	0.89	0.15	73,73,73,73	0
54	MG	2A	3482	1/1	0.89	0.09	64,64,64,64	0
54	MG	1A	3250	1/1	0.89	0.12	64,64,64,64	0
54	MG	2A	3488	1/1	0.89	0.09	73,73,73,73	0
54	MG	1a	1789	1/1	0.89	0.15	66,66,66,66	0
54	MG	1E	307	1/1	0.89	0.12	34,34,34,34	0
54	MG	1A	3907	1/1	0.89	0.09	53,53,53,53	0
54	MG	2R	203	1/1	0.89	0.22	60,60,60,60	0
54	MG	2W	203	1/1	0.89	0.15	64,64,64,64	0
54	MG	1A	3801	1/1	0.89	0.10	49,49,49,49	0
54	MG	1a	1677	1/1	0.89	0.14	63,63,63,63	0
54	MG	1F	315	1/1	0.89	0.13	47,47,47,47	0
54	MG	1a	1687	1/1	0.89	0.14	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3286	1/1	0.89	0.17	52,52,52,52	0
54	MG	2A	3508	1/1	0.89	0.13	67,67,67,67	0
54	MG	1A	3369	1/1	0.89	0.17	65,65,65,65	0
54	MG	2a	3009	1/1	0.89	0.17	70,70,70,70	0
54	MG	2A	3294	1/1	0.89	0.09	43,43,43,43	0
54	MG	1A	3074	1/1	0.89	0.20	53,53,53,53	0
54	MG	2a	3021	1/1	0.89	0.20	71,71,71,71	0
54	MG	2a	3023	1/1	0.89	0.15	62,62,62,62	0
54	MG	2a	3025	1/1	0.89	0.23	70,70,70,70	0
54	MG	1N	203	1/1	0.89	0.12	63,63,63,63	0
54	MG	1N	205	1/1	0.89	0.15	60,60,60,60	0
54	MG	1A	3578	1/1	0.89	0.15	72,72,72,72	0
54	MG	1a	1809	1/1	0.89	0.10	72,72,72,72	0
54	MG	2A	3528	1/1	0.89	0.11	42,42,42,42	0
54	MG	2A	3535	1/1	0.89	0.09	67,67,67,67	0
54	MG	2A	3304	1/1	0.89	0.12	77,77,77,77	0
54	MG	1A	3299	1/1	0.89	0.21	67,67,67,67	0
54	MG	2A	3543	1/1	0.89	0.18	56,56,56,56	0
54	MG	1a	1706	1/1	0.89	0.19	60,60,60,60	0
54	MG	2A	3067	1/1	0.89	0.21	58,58,58,58	0
54	MG	1a	1709	1/1	0.89	0.15	56,56,56,56	0
54	MG	2A	3321	1/1	0.89	0.12	48,48,48,48	0
54	MG	1a	1711	1/1	0.89	0.14	74,74,74,74	0
54	MG	2A	3330	1/1	0.89	0.10	35,35,35,35	0
54	MG	2A	3560	1/1	0.89	0.11	44,44,44,44	0
54	MG	1A	3278	1/1	0.89	0.43	56,56,56,56	0
54	MG	1A	4028	1/1	0.89	0.12	51,51,51,51	0
54	MG	10	102	1/1	0.89	0.25	56,56,56,56	0
54	MG	1a	1720	1/1	0.89	0.19	70,70,70,70	0
54	MG	1A	3485	1/1	0.89	0.10	46,46,46,46	0
54	MG	1A	3829	1/1	0.89	0.17	45,45,45,45	0
54	MG	2a	3069	1/1	0.89	0.25	68,68,68,68	0
54	MG	2A	3346	1/1	0.89	0.14	42,42,42,42	0
54	MG	2a	3073	1/1	0.89	0.15	75,75,75,75	0
54	MG	1A	3421	1/1	0.89	0.12	29,29,29,29	0
54	MG	11	104	1/1	0.89	0.12	55,55,55,55	0
54	MG	1A	3424	1/1	0.89	0.12	69,69,69,69	0
54	MG	1A	3946	1/1	0.89	0.09	31,31,31,31	0
54	MG	1A	3181	1/1	0.89	0.17	58,58,58,58	0
54	MG	2a	3084	1/1	0.89	0.10	41,41,41,41	0
54	MG	2A	3118	1/1	0.89	0.29	45,45,45,45	0
54	MG	1A	3664	1/1	0.89	0.12	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3096	1/1	0.89	0.13	65,65,65,65	0
54	MG	1A	3465	1/1	0.89	0.17	73,73,73,73	0
54	MG	2a	3102	1/1	0.89	0.28	66,66,66,66	0
54	MG	2a	3103	1/1	0.89	0.18	70,70,70,70	0
54	MG	2A	3125	1/1	0.89	0.24	66,66,66,66	0
54	MG	2a	3109	1/1	0.89	0.18	78,78,78,78	0
54	MG	2A	3132	1/1	0.89	0.10	54,54,54,54	0
54	MG	1A	3595	1/1	0.89	0.15	60,60,60,60	0
54	MG	2a	3113	1/1	0.89	0.14	69,69,69,69	0
54	MG	2A	3376	1/1	0.89	0.11	37,37,37,37	0
54	MG	2A	3613	1/1	0.89	0.13	61,61,61,61	0
54	MG	2a	3126	1/1	0.89	0.15	75,75,75,75	0
54	MG	1A	4049	1/1	0.89	0.12	62,62,62,62	0
54	MG	2A	3378	1/1	0.89	0.14	74,74,74,74	0
54	MG	1a	1605	1/1	0.89	0.20	67,67,67,67	0
54	MG	2A	3152	1/1	0.89	0.13	52,52,52,52	0
54	MG	2A	3621	1/1	0.89	0.22	64,64,64,64	0
54	MG	1A	3427	1/1	0.89	0.14	59,59,59,59	0
54	MG	1a	1858	1/1	0.89	0.11	61,61,61,61	0
54	MG	1A	3269	1/1	0.89	0.13	59,59,59,59	0
54	MG	2a	3155	1/1	0.89	0.17	54,54,54,54	0
54	MG	2A	3625	1/1	0.89	0.12	74,74,74,74	0
54	MG	1A	3603	1/1	0.89	0.10	45,45,45,45	0
54	MG	2A	3642	1/1	0.89	0.12	80,80,80,80	0
54	MG	2a	3161	1/1	0.89	0.18	64,64,64,64	0
54	MG	1A	3509	1/1	0.89	0.10	32,32,32,32	0
54	MG	2A	3656	1/1	0.89	0.16	33,33,33,33	0
54	MG	2A	3174	1/1	0.89	0.14	70,70,70,70	0
54	MG	1A	3325	1/1	0.89	0.08	39,39,39,39	0
54	MG	2A	3178	1/1	0.89	0.10	61,61,61,61	0
54	MG	2a	3180	1/1	0.89	0.10	76,76,76,76	0
54	MG	1A	3767	1/1	0.89	0.15	67,67,67,67	0
54	MG	2A	3670	1/1	0.89	0.10	71,71,71,71	0
54	MG	2a	3185	1/1	0.89	0.15	77,77,77,77	0
54	MG	2A	3672	1/1	0.89	0.10	48,48,48,48	0
54	MG	2a	3189	1/1	0.89	0.13	60,60,60,60	0
54	MG	1A	3679	1/1	0.89	0.11	70,70,70,70	0
54	MG	2a	3192	1/1	0.89	0.15	82,82,82,82	0
54	MG	1A	3610	1/1	0.89	0.37	41,41,41,41	0
54	MG	2A	3411	1/1	0.89	0.24	49,49,49,49	0
54	MG	2A	3412	1/1	0.89	0.11	50,50,50,50	0
54	MG	2A	3188	1/1	0.89	0.17	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3476	1/1	0.89	0.12	51,51,51,51	0
54	MG	1A	3985	1/1	0.89	0.08	54,54,54,54	0
54	MG	1A	3616	1/1	0.89	0.22	38,38,38,38	0
54	MG	1a	1767	1/1	0.89	0.16	79,79,79,79	0
54	MG	1A	3783	1/1	0.89	0.14	43,43,43,43	0
54	MG	1a	1652	1/1	0.89	0.24	60,60,60,60	0
54	MG	2A	3700	1/1	0.89	0.14	61,61,61,61	0
54	MG	1d	303	1/1	0.89	0.24	74,74,74,74	0
54	MG	2A	3702	1/1	0.89	0.10	60,60,60,60	0
54	MG	2A	3705	1/1	0.89	0.13	51,51,51,51	0
54	MG	2A	3203	1/1	0.89	0.18	56,56,56,56	0
54	MG	1A	3622	1/1	0.89	0.20	69,69,69,69	0
54	MG	2A	3715	1/1	0.89	0.13	67,67,67,67	0
54	MG	1f	201	1/1	0.89	0.23	71,71,71,71	0
54	MG	2A	3462	1/1	0.90	0.11	56,56,56,56	0
54	MG	2A	3464	1/1	0.90	0.11	70,70,70,70	0
54	MG	1P	203	1/1	0.90	0.15	39,39,39,39	0
54	MG	1A	3353	1/1	0.90	0.12	47,47,47,47	0
54	MG	2A	3220	1/1	0.90	0.10	61,61,61,61	0
54	MG	1a	1877	1/1	0.90	0.16	69,69,69,69	0
54	MG	2A	3479	1/1	0.90	0.12	42,42,42,42	0
54	MG	1A	3991	1/1	0.90	0.08	50,50,50,50	0
54	MG	1A	3853	1/1	0.90	0.12	50,50,50,50	0
54	MG	1A	3994	1/1	0.90	0.15	49,49,49,49	0
54	MG	1A	3995	1/1	0.90	0.21	46,46,46,46	0
54	MG	1g	201	1/1	0.90	0.23	67,67,67,67	0
54	MG	1a	1742	1/1	0.90	0.14	80,80,80,80	0
54	MG	2A	3245	1/1	0.90	0.21	62,62,62,62	0
54	MG	2A	3495	1/1	0.90	0.26	70,70,70,70	0
54	MG	1A	3575	1/1	0.90	0.14	47,47,47,47	0
54	MG	1A	3997	1/1	0.90	0.21	43,43,43,43	0
54	MG	1A	3010	1/1	0.90	0.14	58,58,58,58	0
54	MG	2N	201	1/1	0.90	0.09	77,77,77,77	0
54	MG	1A	4002	1/1	0.90	0.13	56,56,56,56	0
54	MG	13	103	1/1	0.90	0.10	69,69,69,69	0
54	MG	1A	4003	1/1	0.90	0.15	62,62,62,62	0
54	MG	2A	3269	1/1	0.90	0.30	66,66,66,66	0
54	MG	15	104	1/1	0.90	0.22	31,31,31,31	0
54	MG	25	101	1/1	0.90	0.22	70,70,70,70	0
54	MG	1y	203	1/1	0.90	0.24	80,80,80,80	0
54	MG	2A	3519	1/1	0.90	0.10	72,72,72,72	0
54	MG	1A	3262	1/1	0.90	0.18	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3001	1/1	0.90	0.24	70,70,70,70	0
54	MG	2A	3002	1/1	0.90	0.15	50,50,50,50	0
54	MG	1A	3748	1/1	0.90	0.30	67,67,67,67	0
54	MG	1A	3579	1/1	0.90	0.10	62,62,62,62	0
54	MG	17	106	1/1	0.90	0.21	59,59,59,59	0
54	MG	1A	3649	1/1	0.90	0.20	40,40,40,40	0
54	MG	2a	3022	1/1	0.90	0.17	77,77,77,77	0
54	MG	1A	3196	1/1	0.90	0.32	67,67,67,67	0
54	MG	1A	3755	1/1	0.90	0.12	62,62,62,62	0
54	MG	2A	3545	1/1	0.90	0.18	77,77,77,77	0
54	MG	1A	3518	1/1	0.90	0.11	60,60,60,60	0
54	MG	1A	3757	1/1	0.90	0.14	46,46,46,46	0
54	MG	2A	3032	1/1	0.90	0.14	58,58,58,58	0
54	MG	2a	3034	1/1	0.90	0.18	73,73,73,73	0
54	MG	1A	3656	1/1	0.90	0.13	55,55,55,55	0
54	MG	1a	1618	1/1	0.90	0.11	65,65,65,65	0
54	MG	2A	3311	1/1	0.90	0.16	56,56,56,56	0
54	MG	1a	1620	1/1	0.90	0.11	64,64,64,64	0
54	MG	1A	3467	1/1	0.90	0.09	49,49,49,49	0
54	MG	2A	3564	1/1	0.90	0.10	61,61,61,61	0
54	MG	1a	1776	1/1	0.90	0.21	71,71,71,71	0
54	MG	1A	3414	1/1	0.90	0.25	59,59,59,59	0
54	MG	1A	3765	1/1	0.90	0.15	47,47,47,47	0
54	MG	2A	3329	1/1	0.90	0.11	51,51,51,51	0
54	MG	1A	3586	1/1	0.90	0.25	58,58,58,58	0
54	MG	2A	3332	1/1	0.90	0.18	67,67,67,67	0
54	MG	1a	1634	1/1	0.90	0.26	75,75,75,75	0
54	MG	1A	3300	1/1	0.90	0.20	68,68,68,68	0
54	MG	1A	3163	1/1	0.90	0.11	44,44,44,44	0
54	MG	1A	3133	1/1	0.90	0.40	51,51,51,51	0
54	MG	2a	3060	1/1	0.90	0.10	67,67,67,67	0
54	MG	1a	1640	1/1	0.90	0.14	83,83,83,83	0
54	MG	2a	3063	1/1	0.90	0.10	68,68,68,68	0
54	MG	1A	4043	1/1	0.90	0.10	62,62,62,62	0
54	MG	2A	3602	1/1	0.90	0.10	48,48,48,48	0
54	MG	2a	3071	1/1	0.90	0.28	69,69,69,69	0
54	MG	2A	3081	1/1	0.90	0.16	48,48,48,48	0
54	MG	1A	3908	1/1	0.90	0.23	40,40,40,40	0
54	MG	1A	3594	1/1	0.90	0.18	75,75,75,75	0
54	MG	1a	1650	1/1	0.90	0.21	69,69,69,69	0
54	MG	1A	3310	1/1	0.90	0.18	64,64,64,64	0
54	MG	1A	3598	1/1	0.90	0.13	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3092	1/1	0.90	0.19	65,65,65,65	0
54	MG	1A	3678	1/1	0.90	0.19	42,42,42,42	0
54	MG	2a	3085	1/1	0.90	0.21	68,68,68,68	0
54	MG	2A	3094	1/1	0.90	0.09	55,55,55,55	0
54	MG	1A	3139	1/1	0.90	0.29	67,67,67,67	0
54	MG	2a	3095	1/1	0.90	0.09	58,58,58,58	0
54	MG	1A	3071	1/1	0.90	0.23	49,49,49,49	0
54	MG	1A	3429	1/1	0.90	0.09	29,29,29,29	0
54	MG	2A	3106	1/1	0.90	0.12	54,54,54,54	0
54	MG	2A	3107	1/1	0.90	0.18	58,58,58,58	0
54	MG	2a	3105	1/1	0.90	0.14	72,72,72,72	0
54	MG	1A	3378	1/1	0.90	0.11	46,46,46,46	0
54	MG	1a	1660	1/1	0.90	0.13	71,71,71,71	0
54	MG	1A	3187	1/1	0.90	0.12	59,59,59,59	0
54	MG	2A	3630	1/1	0.90	0.12	61,61,61,61	0
54	MG	2A	3640	1/1	0.90	0.14	74,74,74,74	0
54	MG	2a	3117	1/1	0.90	0.14	71,71,71,71	0
54	MG	1a	1665	1/1	0.90	0.27	77,77,77,77	0
54	MG	2A	3649	1/1	0.90	0.09	76,76,76,76	0
54	MG	2A	3652	1/1	0.90	0.10	59,59,59,59	0
54	MG	1a	1667	1/1	0.90	0.17	64,64,64,64	0
54	MG	1A	3014	1/1	0.90	0.31	65,65,65,65	0
54	MG	1A	3804	1/1	0.90	0.09	57,57,57,57	0
54	MG	1A	3386	1/1	0.90	0.15	67,67,67,67	0
54	MG	2a	3144	1/1	0.90	0.21	47,47,47,47	0
54	MG	2A	3134	1/1	0.90	0.17	70,70,70,70	0
54	MG	2A	3392	1/1	0.90	0.32	62,62,62,62	0
54	MG	1A	3558	1/1	0.90	0.16	64,64,64,64	0
54	MG	2a	3153	1/1	0.90	0.09	78,78,78,78	0
54	MG	1A	3283	1/1	0.90	0.11	49,49,49,49	0
54	MG	2A	3674	1/1	0.90	0.09	72,72,72,72	0
54	MG	2A	3146	1/1	0.90	0.17	56,56,56,56	0
54	MG	1A	3451	1/1	0.90	0.12	57,57,57,57	0
54	MG	1a	1680	1/1	0.90	0.37	75,75,75,75	0
54	MG	1A	3960	1/1	0.90	0.08	65,65,65,65	0
54	MG	1A	3501	1/1	0.90	0.08	67,67,67,67	0
54	MG	1A	3504	1/1	0.90	0.13	61,61,61,61	0
54	MG	1A	3965	1/1	0.90	0.12	59,59,59,59	0
54	MG	1A	3831	1/1	0.90	0.08	26,26,26,26	0
54	MG	2a	3177	1/1	0.90	0.23	72,72,72,72	0
54	MG	1a	1835	1/1	0.90	0.08	64,64,64,64	0
54	MG	2A	3694	1/1	0.90	0.13	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3968	1/1	0.90	0.25	51,51,51,51	0
54	MG	2A	3696	1/1	0.90	0.13	63,63,63,63	0
54	MG	1A	3969	1/1	0.90	0.16	60,60,60,60	0
54	MG	2A	3180	1/1	0.90	0.21	69,69,69,69	0
54	MG	1a	1698	1/1	0.90	0.13	60,60,60,60	0
54	MG	1a	1847	1/1	0.90	0.21	73,73,73,73	0
54	MG	1A	3832	1/1	0.90	0.11	52,52,52,52	0
54	MG	1a	1702	1/1	0.90	0.16	56,56,56,56	0
54	MG	1a	1703	1/1	0.90	0.09	39,39,39,39	0
54	MG	1a	1705	1/1	0.90	0.11	78,78,78,78	0
54	MG	2d	301	1/1	0.90	0.18	67,67,67,67	0
54	MG	2e	201	1/1	0.90	0.16	65,65,65,65	0
54	MG	2A	3716	1/1	0.90	0.12	40,40,40,40	0
54	MG	2A	3192	1/1	0.90	0.25	65,65,65,65	0
54	MG	1A	3630	1/1	0.90	0.11	27,27,27,27	0
54	MG	1A	3709	1/1	0.90	0.15	66,66,66,66	0
54	MG	1A	3710	1/1	0.90	0.10	52,52,52,52	0
54	MG	1A	3390	1/1	0.90	0.12	28,28,28,28	0
54	MG	1A	3838	1/1	0.90	0.09	60,60,60,60	0
54	MG	1A	3638	1/1	0.90	0.23	58,58,58,58	0
54	MG	2A	3204	1/1	0.90	0.16	68,68,68,68	0
54	MG	1A	3639	1/1	0.90	0.11	46,46,46,46	0
54	MG	1A	3845	1/1	0.90	0.30	60,60,60,60	0
54	MG	1A	3848	1/1	0.90	0.17	53,53,53,53	0
54	MG	1a	1727	1/1	0.90	0.20	46,46,46,46	0
54	MG	1O	201	1/1	0.90	0.12	59,59,59,59	0
54	MG	2A	3215	1/1	0.90	0.14	63,63,63,63	0
54	MG	1A	3459	1/1	0.91	0.10	52,52,52,52	0
54	MG	1a	1869	1/1	0.91	0.15	66,66,66,66	0
54	MG	1A	3766	1/1	0.91	0.07	31,31,31,31	0
54	MG	1A	3326	1/1	0.91	0.17	44,44,44,44	0
54	MG	1a	1872	1/1	0.91	0.14	65,65,65,65	0
54	MG	1a	1873	1/1	0.91	0.21	61,61,61,61	0
54	MG	2A	3206	1/1	0.91	0.30	55,55,55,55	0
54	MG	2B	206	1/1	0.91	0.18	69,69,69,69	0
54	MG	1A	3244	1/1	0.91	0.37	45,45,45,45	0
54	MG	1a	1875	1/1	0.91	0.12	87,87,87,87	0
54	MG	1A	3772	1/1	0.91	0.09	34,34,34,34	0
54	MG	2A	3211	1/1	0.91	0.23	64,64,64,64	0
54	MG	2A	3465	1/1	0.91	0.10	60,60,60,60	0
54	MG	1A	3061	1/1	0.91	0.13	55,55,55,55	0
54	MG	1a	1733	1/1	0.91	0.20	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3472	1/1	0.91	0.17	62,62,62,62	0
54	MG	1A	3392	1/1	0.91	0.10	37,37,37,37	0
54	MG	1I	105	1/1	0.91	0.10	44,44,44,44	0
54	MG	1A	4005	1/1	0.91	0.25	38,38,38,38	0
54	MG	1A	3260	1/1	0.91	0.13	62,62,62,62	0
54	MG	2A	3225	1/1	0.91	0.22	49,49,49,49	0
54	MG	2A	3483	1/1	0.91	0.08	61,61,61,61	0
54	MG	1A	3541	1/1	0.91	0.19	63,63,63,63	0
54	MG	2A	3487	1/1	0.91	0.12	52,52,52,52	0
54	MG	1A	3398	1/1	0.91	0.11	34,34,34,34	0
54	MG	1A	3893	1/1	0.91	0.13	60,60,60,60	0
54	MG	1A	4016	1/1	0.91	0.10	63,63,63,63	0
54	MG	1A	3895	1/1	0.91	0.21	39,39,39,39	0
54	MG	2Q	202	1/1	0.91	0.11	66,66,66,66	0
54	MG	1A	4020	1/1	0.91	0.15	61,61,61,61	0
54	MG	2T	201	1/1	0.91	0.25	68,68,68,68	0
54	MG	2A	3498	1/1	0.91	0.10	73,73,73,73	0
54	MG	2Y	201	1/1	0.91	0.18	60,60,60,60	0
54	MG	20	102	1/1	0.91	0.08	71,71,71,71	0
54	MG	2A	3244	1/1	0.91	0.09	63,63,63,63	0
54	MG	1A	4022	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3896	1/1	0.91	0.13	49,49,49,49	0
54	MG	1y	201	1/1	0.91	0.09	76,76,76,76	0
54	MG	1a	1602	1/1	0.91	0.16	78,78,78,78	0
54	MG	1A	3343	1/1	0.91	0.09	43,43,43,43	0
54	MG	1A	3346	1/1	0.91	0.10	40,40,40,40	0
54	MG	2A	3513	1/1	0.91	0.12	56,56,56,56	0
54	MG	1a	1760	1/1	0.91	0.24	68,68,68,68	0
54	MG	2A	3268	1/1	0.91	0.22	58,58,58,58	0
54	MG	1a	1614	1/1	0.91	0.19	68,68,68,68	0
54	MG	1a	1615	1/1	0.91	0.11	57,57,57,57	0
54	MG	1A	3551	1/1	0.91	0.17	46,46,46,46	0
54	MG	2A	3522	1/1	0.91	0.18	64,64,64,64	0
54	MG	1A	3793	1/1	0.91	0.12	64,64,64,64	0
54	MG	2A	3017	1/1	0.91	0.12	61,61,61,61	0
54	MG	2A	3526	1/1	0.91	0.10	58,58,58,58	0
54	MG	2a	3030	1/1	0.91	0.15	73,73,73,73	0
54	MG	2A	3019	1/1	0.91	0.29	51,51,51,51	0
54	MG	1A	3795	1/1	0.91	0.14	70,70,70,70	0
54	MG	2A	3278	1/1	0.91	0.21	60,60,60,60	0
54	MG	1a	1621	1/1	0.91	0.14	58,58,58,58	0
54	MG	2a	3036	1/1	0.91	0.23	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3287	1/1	0.91	0.18	65,65,65,65	0
54	MG	1A	3199	1/1	0.91	0.14	48,48,48,48	0
54	MG	1A	4036	1/1	0.91	0.09	65,65,65,65	0
54	MG	2A	3547	1/1	0.91	0.09	38,38,38,38	0
54	MG	1A	3288	1/1	0.91	0.14	46,46,46,46	0
54	MG	2a	3042	1/1	0.91	0.29	74,74,74,74	0
54	MG	1A	3625	1/1	0.91	0.10	30,30,30,30	0
54	MG	2A	3035	1/1	0.91	0.26	68,68,68,68	0
54	MG	1A	3093	1/1	0.91	0.13	64,64,64,64	0
54	MG	1A	3700	1/1	0.91	0.10	49,49,49,49	0
54	MG	1A	3359	1/1	0.91	0.12	41,41,41,41	0
54	MG	2A	3045	1/1	0.91	0.15	67,67,67,67	0
54	MG	1A	3423	1/1	0.91	0.09	32,32,32,32	0
54	MG	1A	3264	1/1	0.91	0.27	30,30,30,30	0
54	MG	1A	3938	1/1	0.91	0.08	59,59,59,59	0
54	MG	1a	1642	1/1	0.91	0.25	68,68,68,68	0
54	MG	1A	3637	1/1	0.91	0.08	46,46,46,46	0
54	MG	2a	3061	1/1	0.91	0.14	68,68,68,68	0
54	MG	2A	3327	1/1	0.91	0.10	42,42,42,42	0
54	MG	1A	4052	1/1	0.91	0.15	64,64,64,64	0
54	MG	1a	1785	1/1	0.91	0.12	79,79,79,79	0
54	MG	1A	3941	1/1	0.91	0.09	50,50,50,50	0
54	MG	2A	3589	1/1	0.91	0.09	66,66,66,66	0
54	MG	2A	3064	1/1	0.91	0.08	55,55,55,55	0
54	MG	1a	1788	1/1	0.91	0.11	73,73,73,73	0
54	MG	2A	3071	1/1	0.91	0.14	50,50,50,50	0
54	MG	1A	3943	1/1	0.91	0.12	65,65,65,65	0
54	MG	1a	1790	1/1	0.91	0.27	74,74,74,74	0
54	MG	1A	3822	1/1	0.91	0.11	31,31,31,31	0
54	MG	2a	3078	1/1	0.91	0.25	70,70,70,70	0
54	MG	1A	3425	1/1	0.91	0.12	32,32,32,32	0
54	MG	2a	3083	1/1	0.91	0.13	82,82,82,82	0
54	MG	1A	3949	1/1	0.91	0.09	60,60,60,60	0
54	MG	1A	3828	1/1	0.91	0.09	18,18,18,18	0
54	MG	2a	3086	1/1	0.91	0.15	62,62,62,62	0
54	MG	2a	3090	1/1	0.91	0.13	58,58,58,58	0
54	MG	1A	3715	1/1	0.91	0.14	28,28,28,28	0
54	MG	2A	3351	1/1	0.91	0.29	61,61,61,61	0
54	MG	1B	214	1/1	0.91	0.08	49,49,49,49	0
54	MG	1A	3956	1/1	0.91	0.12	67,67,67,67	0
54	MG	1a	1662	1/1	0.91	0.23	67,67,67,67	0
54	MG	2a	3098	1/1	0.91	0.11	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3099	1/1	0.91	0.12	74,74,74,74	0
54	MG	2A	3616	1/1	0.91	0.09	58,58,58,58	0
54	MG	1A	3119	1/1	0.91	0.30	54,54,54,54	0
54	MG	1A	3718	1/1	0.91	0.18	53,53,53,53	0
54	MG	2A	3620	1/1	0.91	0.14	58,58,58,58	0
54	MG	1B	221	1/1	0.91	0.20	66,66,66,66	0
54	MG	2A	3367	1/1	0.91	0.09	66,66,66,66	0
54	MG	1a	1668	1/1	0.91	0.18	60,60,60,60	0
54	MG	1A	3961	1/1	0.91	0.12	69,69,69,69	0
54	MG	1A	3366	1/1	0.91	0.09	54,54,54,54	0
54	MG	2A	3111	1/1	0.91	0.14	51,51,51,51	0
54	MG	2A	3629	1/1	0.91	0.12	73,73,73,73	0
54	MG	1A	3963	1/1	0.91	0.10	66,66,66,66	0
54	MG	2a	3127	1/1	0.91	0.23	74,74,74,74	0
54	MG	2a	3131	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3574	1/1	0.91	0.12	65,65,65,65	0
54	MG	1A	3643	1/1	0.91	0.23	38,38,38,38	0
54	MG	2a	3139	1/1	0.91	0.10	73,73,73,73	0
54	MG	2A	3647	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3266	1/1	0.91	0.36	73,73,73,73	0
54	MG	1a	1679	1/1	0.91	0.28	72,72,72,72	0
54	MG	1A	3368	1/1	0.91	0.11	24,24,24,24	0
54	MG	2a	3148	1/1	0.91	0.12	67,67,67,67	0
54	MG	2A	3126	1/1	0.91	0.19	67,67,67,67	0
54	MG	1a	1823	1/1	0.91	0.10	65,65,65,65	0
54	MG	1D	316	1/1	0.91	0.15	53,53,53,53	0
54	MG	1A	3011	1/1	0.91	0.16	66,66,66,66	0
54	MG	2A	3138	1/1	0.91	0.33	62,62,62,62	0
54	MG	2A	3666	1/1	0.91	0.08	62,62,62,62	0
54	MG	1A	3309	1/1	0.91	0.34	41,41,41,41	0
54	MG	2a	3158	1/1	0.91	0.09	68,68,68,68	0
54	MG	2A	3402	1/1	0.91	0.09	45,45,45,45	0
54	MG	2A	3403	1/1	0.91	0.11	39,39,39,39	0
54	MG	1A	3214	1/1	0.91	0.13	58,58,58,58	0
54	MG	2A	3676	1/1	0.91	0.08	55,55,55,55	0
54	MG	2A	3147	1/1	0.91	0.33	79,79,79,79	0
54	MG	1A	3653	1/1	0.91	0.09	54,54,54,54	0
54	MG	1A	3317	1/1	0.91	0.32	54,54,54,54	0
54	MG	1a	1834	1/1	0.91	0.10	51,51,51,51	0
54	MG	2A	3158	1/1	0.91	0.20	44,44,44,44	0
54	MG	1a	1695	1/1	0.91	0.23	65,65,65,65	0
54	MG	2A	3686	1/1	0.91	0.13	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3851	1/1	0.91	0.10	54,54,54,54	0
54	MG	1a	1697	1/1	0.91	0.29	68,68,68,68	0
54	MG	1F	314	1/1	0.91	0.31	43,43,43,43	0
54	MG	1A	3319	1/1	0.91	0.14	60,60,60,60	0
54	MG	2A	3422	1/1	0.91	0.15	61,61,61,61	0
54	MG	1a	1700	1/1	0.91	0.21	64,64,64,64	0
54	MG	1A	3515	1/1	0.91	0.12	28,28,28,28	0
54	MG	1A	3172	1/1	0.91	0.14	67,67,67,67	0
54	MG	2A	3432	1/1	0.91	0.23	78,78,78,78	0
54	MG	1A	3863	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3864	1/1	0.91	0.09	51,51,51,51	0
54	MG	2A	3436	1/1	0.91	0.07	49,49,49,49	0
54	MG	2A	3709	1/1	0.91	0.20	74,74,74,74	0
54	MG	2A	3711	1/1	0.91	0.08	74,74,74,74	0
54	MG	1A	3867	1/1	0.91	0.18	45,45,45,45	0
54	MG	1a	1710	1/1	0.91	0.13	67,67,67,67	0
54	MG	1A	3193	1/1	0.91	0.11	64,64,64,64	0
54	MG	2A	3722	1/1	0.91	0.15	48,48,48,48	0
54	MG	1A	3383	1/1	0.91	0.11	54,54,54,54	0
54	MG	2A	3191	1/1	0.91	0.26	57,57,57,57	0
54	MG	2A	3727	1/1	0.91	0.18	62,62,62,62	0
54	MG	1A	3458	1/1	0.91	0.12	55,55,55,55	0
54	MG	1T	201	1/1	0.91	0.12	52,52,52,52	0
54	MG	1a	1717	1/1	0.91	0.12	70,70,70,70	0
54	MG	2A	3447	1/1	0.91	0.10	44,44,44,44	0
54	MG	2A	3038	1/1	0.92	0.16	67,67,67,67	0
54	MG	1A	3255	1/1	0.92	0.17	47,47,47,47	0
54	MG	1A	3635	1/1	0.92	0.11	31,31,31,31	0
54	MG	1A	3566	1/1	0.92	0.08	61,61,61,61	0
54	MG	1A	3510	1/1	0.92	0.10	73,73,73,73	0
54	MG	1a	1792	1/1	0.92	0.12	66,66,66,66	0
54	MG	2A	3281	1/1	0.92	0.11	24,24,24,24	0
54	MG	2A	3285	1/1	0.92	0.12	54,54,54,54	0
54	MG	1A	3460	1/1	0.92	0.11	63,63,63,63	0
54	MG	2E	305	1/1	0.92	0.09	57,57,57,57	0
54	MG	2E	307	1/1	0.92	0.19	67,67,67,67	0
54	MG	1A	3512	1/1	0.92	0.11	60,60,60,60	0
54	MG	1A	3150	1/1	0.92	0.48	45,45,45,45	0
54	MG	1A	3713	1/1	0.92	0.11	54,54,54,54	0
54	MG	1F	316	1/1	0.92	0.12	57,57,57,57	0
54	MG	1a	1678	1/1	0.92	0.08	65,65,65,65	0
54	MG	2O	201	1/1	0.92	0.14	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3210	1/1	0.92	0.10	55,55,55,55	0
54	MG	1A	3905	1/1	0.92	0.10	75,75,75,75	0
54	MG	1a	1682	1/1	0.92	0.20	59,59,59,59	0
54	MG	2A	3302	1/1	0.92	0.13	55,55,55,55	0
54	MG	2T	203	1/1	0.92	0.09	63,63,63,63	0
54	MG	2V	203	1/1	0.92	0.13	69,69,69,69	0
54	MG	2W	202	1/1	0.92	0.13	52,52,52,52	0
54	MG	1a	1807	1/1	0.92	0.19	60,60,60,60	0
54	MG	2A	3307	1/1	0.92	0.11	45,45,45,45	0
54	MG	1a	1683	1/1	0.92	0.18	78,78,78,78	0
54	MG	1A	3811	1/1	0.92	0.32	47,47,47,47	0
54	MG	2A	3533	1/1	0.92	0.13	57,57,57,57	0
54	MG	2A	3085	1/1	0.92	0.21	75,75,75,75	0
54	MG	1a	1686	1/1	0.92	0.13	66,66,66,66	0
54	MG	1A	3464	1/1	0.92	0.09	46,46,46,46	0
54	MG	2A	3320	1/1	0.92	0.14	69,69,69,69	0
54	MG	1A	3330	1/1	0.92	0.10	65,65,65,65	0
54	MG	1A	4006	1/1	0.92	0.12	18,18,18,18	0
54	MG	1a	1817	1/1	0.92	0.15	76,76,76,76	0
54	MG	2a	3010	1/1	0.92	0.14	68,68,68,68	0
54	MG	2A	3548	1/1	0.92	0.12	72,72,72,72	0
54	MG	1A	4007	1/1	0.92	0.12	42,42,42,42	0
54	MG	2a	3020	1/1	0.92	0.18	63,63,63,63	0
54	MG	1A	3817	1/1	0.92	0.10	41,41,41,41	0
54	MG	1R	202	1/1	0.92	0.19	50,50,50,50	0
54	MG	1A	3098	1/1	0.92	0.10	59,59,59,59	0
54	MG	1A	3102	1/1	0.92	0.10	36,36,36,36	0
54	MG	1V	206	1/1	0.92	0.14	59,59,59,59	0
54	MG	1W	201	1/1	0.92	0.14	50,50,50,50	0
54	MG	1A	3725	1/1	0.92	0.07	36,36,36,36	0
54	MG	2A	3110	1/1	0.92	0.23	56,56,56,56	0
54	MG	1A	3728	1/1	0.92	0.12	39,39,39,39	0
54	MG	1A	3648	1/1	0.92	0.13	57,57,57,57	0
54	MG	1A	3063	1/1	0.92	0.12	42,42,42,42	0
54	MG	1A	3932	1/1	0.92	0.14	61,61,61,61	0
54	MG	2A	3352	1/1	0.92	0.18	65,65,65,65	0
54	MG	1a	1708	1/1	0.92	0.14	72,72,72,72	0
54	MG	2A	3582	1/1	0.92	0.10	60,60,60,60	0
54	MG	1A	3532	1/1	0.92	0.18	55,55,55,55	0
54	MG	1A	3936	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3590	1/1	0.92	0.09	41,41,41,41	0
54	MG	2A	3591	1/1	0.92	0.12	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1844	1/1	0.92	0.09	65,65,65,65	0
54	MG	2a	3048	1/1	0.92	0.14	74,74,74,74	0
54	MG	13	102	1/1	0.92	0.12	46,46,46,46	0
54	MG	2A	3597	1/1	0.92	0.10	41,41,41,41	0
54	MG	2A	3365	1/1	0.92	0.14	65,65,65,65	0
54	MG	1A	3740	1/1	0.92	0.10	31,31,31,31	0
54	MG	1a	1849	1/1	0.92	0.34	72,72,72,72	0
54	MG	1A	3741	1/1	0.92	0.08	51,51,51,51	0
54	MG	1a	1851	1/1	0.92	0.18	72,72,72,72	0
54	MG	2a	3057	1/1	0.92	0.08	88,88,88,88	0
54	MG	2A	3372	1/1	0.92	0.17	71,71,71,71	0
54	MG	2a	3059	1/1	0.92	0.23	75,75,75,75	0
54	MG	1A	3342	1/1	0.92	0.09	48,48,48,48	0
54	MG	1A	3121	1/1	0.92	0.13	49,49,49,49	0
54	MG	1a	1856	1/1	0.92	0.12	63,63,63,63	0
54	MG	2A	3151	1/1	0.92	0.20	67,67,67,67	0
54	MG	1a	1719	1/1	0.92	0.10	75,75,75,75	0
54	MG	2a	3065	1/1	0.92	0.17	64,64,64,64	0
54	MG	15	106	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3945	1/1	0.92	0.07	42,42,42,42	0
54	MG	1A	3344	1/1	0.92	0.09	32,32,32,32	0
54	MG	1A	3303	1/1	0.92	0.15	42,42,42,42	0
54	MG	1A	3236	1/1	0.92	0.24	64,64,64,64	0
54	MG	2A	3166	1/1	0.92	0.10	61,61,61,61	0
54	MG	2A	3167	1/1	0.92	0.14	53,53,53,53	0
54	MG	1A	3237	1/1	0.92	0.28	58,58,58,58	0
54	MG	2A	3397	1/1	0.92	0.11	57,57,57,57	0
54	MG	2A	3172	1/1	0.92	0.15	65,65,65,65	0
54	MG	2A	3401	1/1	0.92	0.10	50,50,50,50	0
54	MG	1a	1732	1/1	0.92	0.08	56,56,56,56	0
54	MG	2A	3175	1/1	0.92	0.26	75,75,75,75	0
54	MG	2A	3636	1/1	0.92	0.07	58,58,58,58	0
54	MG	2A	3637	1/1	0.92	0.07	64,64,64,64	0
54	MG	2A	3404	1/1	0.92	0.16	70,70,70,70	0
54	MG	1A	3951	1/1	0.92	0.10	68,68,68,68	0
54	MG	2A	3643	1/1	0.92	0.08	56,56,56,56	0
54	MG	2A	3177	1/1	0.92	0.10	71,71,71,71	0
54	MG	1A	3546	1/1	0.92	0.10	35,35,35,35	0
54	MG	1A	3955	1/1	0.92	0.09	31,31,31,31	0
54	MG	2A	3653	1/1	0.92	0.11	57,57,57,57	0
54	MG	1A	3039	1/1	0.92	0.14	57,57,57,57	0
54	MG	1a	1612	1/1	0.92	0.18	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	4048	1/1	0.92	0.14	54,54,54,54	0
54	MG	1A	3958	1/1	0.92	0.17	54,54,54,54	0
54	MG	1A	3273	1/1	0.92	0.10	39,39,39,39	0
54	MG	1a	1744	1/1	0.92	0.18	63,63,63,63	0
54	MG	2a	3111	1/1	0.92	0.15	66,66,66,66	0
54	MG	1A	3604	1/1	0.92	0.08	43,43,43,43	0
54	MG	2A	3669	1/1	0.92	0.12	60,60,60,60	0
54	MG	2a	3115	1/1	0.92	0.08	69,69,69,69	0
54	MG	1A	3444	1/1	0.92	0.10	50,50,50,50	0
54	MG	1a	1750	1/1	0.92	0.08	60,60,60,60	0
54	MG	2A	3194	1/1	0.92	0.09	47,47,47,47	0
54	MG	1A	3448	1/1	0.92	0.12	49,49,49,49	0
54	MG	1a	1624	1/1	0.92	0.12	59,59,59,59	0
54	MG	1A	3449	1/1	0.92	0.10	63,63,63,63	0
54	MG	2A	3678	1/1	0.92	0.07	62,62,62,62	0
54	MG	2a	3136	1/1	0.92	0.11	75,75,75,75	0
54	MG	2A	3679	1/1	0.92	0.08	48,48,48,48	0
54	MG	2a	3138	1/1	0.92	0.15	70,70,70,70	0
54	MG	1f	202	1/1	0.92	0.12	49,49,49,49	0
54	MG	1A	3557	1/1	0.92	0.13	56,56,56,56	0
54	MG	1A	3314	1/1	0.92	0.20	39,39,39,39	0
54	MG	1A	3771	1/1	0.92	0.11	54,54,54,54	0
54	MG	2A	3439	1/1	0.92	0.18	52,52,52,52	0
54	MG	2a	3146	1/1	0.92	0.14	70,70,70,70	0
54	MG	1B	207	1/1	0.92	0.30	61,61,61,61	0
54	MG	2A	3687	1/1	0.92	0.11	62,62,62,62	0
54	MG	1A	3868	1/1	0.92	0.08	65,65,65,65	0
54	MG	1l	201	1/1	0.92	0.16	65,65,65,65	0
54	MG	1A	3619	1/1	0.92	0.10	44,44,44,44	0
54	MG	1B	215	1/1	0.92	0.18	56,56,56,56	0
54	MG	2A	3445	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3212	1/1	0.92	0.14	67,67,67,67	0
54	MG	1B	216	1/1	0.92	0.19	69,69,69,69	0
54	MG	1o	3100	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3775	1/1	0.92	0.09	34,34,34,34	0
54	MG	1A	3620	1/1	0.92	0.25	45,45,45,45	0
54	MG	2a	3172	1/1	0.92	0.14	78,78,78,78	0
54	MG	1a	1768	1/1	0.92	0.19	74,74,74,74	0
54	MG	2A	3452	1/1	0.92	0.12	38,38,38,38	0
54	MG	1a	1769	1/1	0.92	0.15	67,67,67,67	0
54	MG	1A	3559	1/1	0.92	0.09	52,52,52,52	0
54	MG	2A	3456	1/1	0.92	0.13	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3399	1/1	0.92	0.08	40,40,40,40	0
54	MG	2A	3718	1/1	0.92	0.12	51,51,51,51	0
54	MG	1a	1649	1/1	0.92	0.23	63,63,63,63	0
54	MG	2A	3721	1/1	0.92	0.10	68,68,68,68	0
54	MG	1A	3980	1/1	0.92	0.12	57,57,57,57	0
54	MG	2A	3232	1/1	0.92	0.09	59,59,59,59	0
54	MG	1A	3981	1/1	0.92	0.10	60,60,60,60	0
54	MG	2A	3725	1/1	0.92	0.09	75,75,75,75	0
54	MG	1A	3982	1/1	0.92	0.13	51,51,51,51	0
54	MG	2A	3728	1/1	0.92	0.09	87,87,87,87	0
54	MG	2A	3466	1/1	0.92	0.10	73,73,73,73	0
54	MG	2A	3468	1/1	0.92	0.12	69,69,69,69	0
54	MG	1B	229	1/1	0.92	0.08	62,62,62,62	0
54	MG	2A	3243	1/1	0.92	0.12	44,44,44,44	0
54	MG	1A	3403	1/1	0.92	0.09	23,23,23,23	0
54	MG	1A	3880	1/1	0.92	0.09	57,57,57,57	0
54	MG	1D	312	1/1	0.92	0.30	44,44,44,44	0
54	MG	1D	313	1/1	0.92	0.12	66,66,66,66	0
54	MG	1a	1782	1/1	0.92	0.12	70,70,70,70	0
54	MG	1A	3245	1/1	0.92	0.22	39,39,39,39	0
54	MG	2A	3033	1/1	0.92	0.17	53,53,53,53	0
54	MG	2A	3485	1/1	0.92	0.08	42,42,42,42	0
54	MG	1A	3145	1/1	0.92	0.17	56,56,56,56	0
54	MG	1a	1663	1/1	0.92	0.09	69,69,69,69	0
54	MG	1A	3788	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3037	1/1	0.92	0.20	52,52,52,52	0
54	MG	2B	211	1/1	0.92	0.12	63,63,63,63	0
58	ZN	14	102	1/1	0.92	0.13	144,144,144,144	0
54	MG	2A	3492	1/1	0.92	0.12	54,54,54,54	0
54	MG	1a	1672	1/1	0.93	0.11	48,48,48,48	0
54	MG	1A	3088	1/1	0.93	0.29	40,40,40,40	0
54	MG	2A	3490	1/1	0.93	0.10	65,65,65,65	0
54	MG	1A	3974	1/1	0.93	0.12	64,64,64,64	0
54	MG	2A	3280	1/1	0.93	0.07	53,53,53,53	0
54	MG	1A	3205	1/1	0.93	0.24	43,43,43,43	0
54	MG	1A	3207	1/1	0.93	0.27	46,46,46,46	0
54	MG	2A	3497	1/1	0.93	0.12	45,45,45,45	0
54	MG	2B	216	1/1	0.93	0.16	69,69,69,69	0
54	MG	1A	3494	1/1	0.93	0.07	67,67,67,67	0
54	MG	2D	303	1/1	0.93	0.33	45,45,45,45	0
54	MG	1A	3495	1/1	0.93	0.09	31,31,31,31	0
54	MG	2A	3289	1/1	0.93	0.19	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3074	1/1	0.93	0.12	58,58,58,58	0
54	MG	2A	3079	1/1	0.93	0.13	61,61,61,61	0
54	MG	2A	3504	1/1	0.93	0.10	63,63,63,63	0
54	MG	1E	304	1/1	0.93	0.09	52,52,52,52	0
54	MG	1a	1681	1/1	0.93	0.16	59,59,59,59	0
54	MG	1A	3854	1/1	0.93	0.12	48,48,48,48	0
54	MG	2A	3510	1/1	0.93	0.08	38,38,38,38	0
54	MG	2A	3511	1/1	0.93	0.15	66,66,66,66	0
54	MG	1A	3856	1/1	0.93	0.07	47,47,47,47	0
54	MG	1A	3747	1/1	0.93	0.08	65,65,65,65	0
54	MG	1A	3496	1/1	0.93	0.07	28,28,28,28	0
54	MG	2A	3518	1/1	0.93	0.07	61,61,61,61	0
54	MG	1A	3173	1/1	0.93	0.23	46,46,46,46	0
54	MG	1a	1688	1/1	0.93	0.29	77,77,77,77	0
54	MG	1A	3570	1/1	0.93	0.10	57,57,57,57	0
54	MG	2A	3309	1/1	0.93	0.10	55,55,55,55	0
54	MG	2A	3523	1/1	0.93	0.14	51,51,51,51	0
54	MG	2A	3310	1/1	0.93	0.11	67,67,67,67	0
54	MG	1A	3866	1/1	0.93	0.09	46,46,46,46	0
54	MG	2A	3096	1/1	0.93	0.11	48,48,48,48	0
54	MG	2A	3315	1/1	0.93	0.11	30,30,30,30	0
54	MG	2A	3530	1/1	0.93	0.10	44,44,44,44	0
54	MG	1A	3572	1/1	0.93	0.09	25,25,25,25	0
54	MG	1A	3178	1/1	0.93	0.18	52,52,52,52	0
54	MG	1G	204	1/1	0.93	0.14	60,60,60,60	0
54	MG	2A	3539	1/1	0.93	0.06	56,56,56,56	0
54	MG	2a	3001	1/1	0.93	0.09	49,49,49,49	0
54	MG	1A	3990	1/1	0.93	0.16	61,61,61,61	0
54	MG	2A	3542	1/1	0.93	0.16	69,69,69,69	0
54	MG	1A	3371	1/1	0.93	0.08	34,34,34,34	0
54	MG	1a	1831	1/1	0.93	0.14	66,66,66,66	0
54	MG	1A	3438	1/1	0.93	0.13	61,61,61,61	0
54	MG	1A	3758	1/1	0.93	0.10	52,52,52,52	0
54	MG	2a	3014	1/1	0.93	0.16	63,63,63,63	0
54	MG	2A	3112	1/1	0.93	0.15	58,58,58,58	0
54	MG	2A	3551	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3651	1/1	0.93	0.11	43,43,43,43	0
54	MG	1Q	202	1/1	0.93	0.07	36,36,36,36	0
54	MG	2A	3341	1/1	0.93	0.15	53,53,53,53	0
54	MG	2A	3556	1/1	0.93	0.10	65,65,65,65	0
54	MG	1Q	203	1/1	0.93	0.12	56,56,56,56	0
54	MG	1a	1838	1/1	0.93	0.13	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3123	1/1	0.93	0.23	42,42,42,42	0
54	MG	2a	3028	1/1	0.93	0.29	67,67,67,67	0
54	MG	1a	1842	1/1	0.93	0.09	67,67,67,67	0
54	MG	1A	3577	1/1	0.93	0.12	46,46,46,46	0
54	MG	2a	3032	1/1	0.93	0.08	92,92,92,92	0
54	MG	1A	3507	1/1	0.93	0.10	46,46,46,46	0
54	MG	2A	3349	1/1	0.93	0.09	34,34,34,34	0
54	MG	2A	3569	1/1	0.93	0.11	71,71,71,71	0
54	MG	1A	3440	1/1	0.93	0.11	72,72,72,72	0
54	MG	1a	1848	1/1	0.93	0.15	66,66,66,66	0
54	MG	1A	4001	1/1	0.93	0.14	81,81,81,81	0
54	MG	1V	201	1/1	0.93	0.24	38,38,38,38	0
54	MG	1A	3267	1/1	0.93	0.29	55,55,55,55	0
54	MG	2A	3580	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3360	1/1	0.93	0.17	50,50,50,50	0
54	MG	1A	3101	1/1	0.93	0.20	43,43,43,43	0
54	MG	2A	3362	1/1	0.93	0.12	62,62,62,62	0
54	MG	2a	3046	1/1	0.93	0.12	61,61,61,61	0
54	MG	1A	3147	1/1	0.93	0.16	45,45,45,45	0
54	MG	1A	3770	1/1	0.93	0.15	62,62,62,62	0
54	MG	2A	3150	1/1	0.93	0.13	68,68,68,68	0
54	MG	1A	3186	1/1	0.93	0.10	60,60,60,60	0
54	MG	1A	3890	1/1	0.93	0.08	50,50,50,50	0
54	MG	1A	3328	1/1	0.93	0.13	65,65,65,65	0
54	MG	2A	3599	1/1	0.93	0.06	56,56,56,56	0
54	MG	2A	3154	1/1	0.93	0.16	59,59,59,59	0
54	MG	2A	3371	1/1	0.93	0.08	74,74,74,74	0
54	MG	1l	101	1/1	0.93	0.13	45,45,45,45	0
54	MG	1a	1724	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	4009	1/1	0.93	0.16	64,64,64,64	0
54	MG	1A	4011	1/1	0.93	0.11	53,53,53,53	0
54	MG	2A	3163	1/1	0.93	0.10	63,63,63,63	0
54	MG	1a	1729	1/1	0.93	0.11	69,69,69,69	0
54	MG	2A	3612	1/1	0.93	0.14	57,57,57,57	0
54	MG	1A	3329	1/1	0.93	0.13	31,31,31,31	0
54	MG	1A	3517	1/1	0.93	0.08	44,44,44,44	0
54	MG	2a	3070	1/1	0.93	0.14	54,54,54,54	0
54	MG	1A	3675	1/1	0.93	0.17	55,55,55,55	0
54	MG	1A	3232	1/1	0.93	0.13	41,41,41,41	0
54	MG	1A	3387	1/1	0.93	0.13	41,41,41,41	0
54	MG	2A	3387	1/1	0.93	0.17	72,72,72,72	0
54	MG	1A	3070	1/1	0.93	0.08	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3112	1/1	0.93	0.32	42,42,42,42	0
54	MG	1A	3681	1/1	0.93	0.12	56,56,56,56	0
54	MG	2A	3393	1/1	0.93	0.07	34,34,34,34	0
54	MG	2A	3394	1/1	0.93	0.19	64,64,64,64	0
54	MG	2A	3396	1/1	0.93	0.09	37,37,37,37	0
54	MG	1A	3682	1/1	0.93	0.12	56,56,56,56	0
54	MG	2A	3399	1/1	0.93	0.11	39,39,39,39	0
54	MG	1A	3791	1/1	0.93	0.17	65,65,65,65	0
54	MG	2a	3088	1/1	0.93	0.23	49,49,49,49	0
54	MG	2A	3631	1/1	0.93	0.10	71,71,71,71	0
54	MG	2A	3632	1/1	0.93	0.11	86,86,86,86	0
54	MG	2A	3633	1/1	0.93	0.14	61,61,61,61	0
54	MG	2a	3094	1/1	0.93	0.09	62,62,62,62	0
54	MG	2A	3635	1/1	0.93	0.09	59,59,59,59	0
54	MG	1A	3599	1/1	0.93	0.07	47,47,47,47	0
54	MG	1A	3335	1/1	0.93	0.08	32,32,32,32	0
54	MG	2A	3187	1/1	0.93	0.14	58,58,58,58	0
54	MG	1a	1745	1/1	0.93	0.08	57,57,57,57	0
54	MG	1A	4031	1/1	0.93	0.07	66,66,66,66	0
54	MG	2A	3645	1/1	0.93	0.07	64,64,64,64	0
54	MG	1a	1603	1/1	0.93	0.13	72,72,72,72	0
54	MG	2A	3407	1/1	0.93	0.20	70,70,70,70	0
54	MG	2A	3408	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3914	1/1	0.93	0.07	38,38,38,38	0
54	MG	1A	3794	1/1	0.93	0.10	39,39,39,39	0
54	MG	1A	4035	1/1	0.93	0.11	62,62,62,62	0
54	MG	1A	3158	1/1	0.93	0.16	64,64,64,64	0
54	MG	1A	3243	1/1	0.93	0.11	46,46,46,46	0
54	MG	2A	3415	1/1	0.93	0.10	47,47,47,47	0
54	MG	1A	3798	1/1	0.93	0.13	65,65,65,65	0
54	MG	2a	3120	1/1	0.93	0.07	55,55,55,55	0
54	MG	2a	3122	1/1	0.93	0.11	78,78,78,78	0
54	MG	2a	3123	1/1	0.93	0.07	64,64,64,64	0
54	MG	1A	3161	1/1	0.93	0.10	43,43,43,43	0
54	MG	2A	3200	1/1	0.93	0.13	42,42,42,42	0
54	MG	1A	4042	1/1	0.93	0.11	67,67,67,67	0
54	MG	1A	3195	1/1	0.93	0.10	52,52,52,52	0
54	MG	1A	3934	1/1	0.93	0.08	63,63,63,63	0
54	MG	1A	3466	1/1	0.93	0.09	57,57,57,57	0
54	MG	1A	3608	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3805	1/1	0.93	0.09	44,44,44,44	0
54	MG	1y	202	1/1	0.93	0.09	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3141	1/1	0.93	0.09	64,64,64,64	0
54	MG	2A	3209	1/1	0.93	0.10	58,58,58,58	0
54	MG	1A	3806	1/1	0.93	0.26	42,42,42,42	0
54	MG	1A	3808	1/1	0.93	0.10	62,62,62,62	0
54	MG	1A	3810	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3539	1/1	0.93	0.09	64,64,64,64	0
54	MG	2a	3147	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	4054	1/1	0.93	0.13	64,64,64,64	0
54	MG	1a	1639	1/1	0.93	0.14	68,68,68,68	0
54	MG	1A	3540	1/1	0.93	0.10	57,57,57,57	0
54	MG	1A	3701	1/1	0.93	0.30	41,41,41,41	0
54	MG	2A	3692	1/1	0.93	0.07	44,44,44,44	0
54	MG	1A	3615	1/1	0.93	0.19	38,38,38,38	0
54	MG	2A	3018	1/1	0.93	0.40	54,54,54,54	0
54	MG	1A	3289	1/1	0.93	0.18	58,58,58,58	0
54	MG	2A	3228	1/1	0.93	0.17	71,71,71,71	0
54	MG	1A	3408	1/1	0.93	0.19	57,57,57,57	0
54	MG	1A	3347	1/1	0.93	0.10	55,55,55,55	0
54	MG	1B	209	1/1	0.93	0.09	62,62,62,62	0
54	MG	1A	3953	1/1	0.93	0.07	26,26,26,26	0
54	MG	1A	3290	1/1	0.93	0.13	56,56,56,56	0
54	MG	2A	3237	1/1	0.93	0.14	48,48,48,48	0
54	MG	2A	3241	1/1	0.93	0.19	54,54,54,54	0
54	MG	1A	3826	1/1	0.93	0.18	35,35,35,35	0
54	MG	2A	3710	1/1	0.93	0.09	63,63,63,63	0
54	MG	1A	3064	1/1	0.93	0.27	43,43,43,43	0
54	MG	2A	3712	1/1	0.93	0.12	61,61,61,61	0
54	MG	2A	3458	1/1	0.93	0.17	64,64,64,64	0
54	MG	2a	3183	1/1	0.93	0.11	70,70,70,70	0
54	MG	1A	3355	1/1	0.93	0.07	38,38,38,38	0
54	MG	1A	3251	1/1	0.93	0.28	76,76,76,76	0
54	MG	1A	3254	1/1	0.93	0.09	76,76,76,76	0
54	MG	2A	3463	1/1	0.93	0.11	56,56,56,56	0
54	MG	1A	3360	1/1	0.93	0.07	26,26,26,26	0
54	MG	1A	3720	1/1	0.93	0.25	43,43,43,43	0
54	MG	1A	3632	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3467	1/1	0.93	0.11	34,34,34,34	0
54	MG	2A	3255	1/1	0.93	0.15	51,51,51,51	0
54	MG	2A	3259	1/1	0.93	0.10	49,49,49,49	0
54	MG	2A	3260	1/1	0.93	0.10	31,31,31,31	0
54	MG	2A	3044	1/1	0.93	0.20	65,65,65,65	0
54	MG	2A	3473	1/1	0.93	0.20	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
54	MG	2A	3264	1/1	0.93	0.24	73,73,73,73	0
54	MG	2A	3734	1/1	0.93	0.11	51,51,51,51	0
54	MG	1A	3724	1/1	0.93	0.12	54,54,54,54	0
54	MG	1A	3634	1/1	0.93	0.09	35,35,35,35	0
54	MG	1D	303	1/1	0.93	0.10	41,41,41,41	0
54	MG	2A	3738	1/1	0.93	0.12	81,81,81,81	0
54	MG	2A	3740	1/1	0.93	0.14	69,69,69,69	0
54	MG	1A	3197	1/1	0.93	0.10	56,56,56,56	0
54	MG	1A	3120	1/1	0.93	0.20	52,52,52,52	0
54	MG	2A	3055	1/1	0.93	0.12	43,43,43,43	0
54	MG	2B	203	1/1	0.93	0.22	70,70,70,70	0
54	MG	2A	3274	1/1	0.93	0.07	43,43,43,43	0
54	MG	1A	3970	1/1	0.93	0.10	70,70,70,70	0
54	MG	1A	3253	1/1	0.94	0.09	46,46,46,46	0
54	MG	1H	201	1/1	0.94	0.16	66,66,66,66	0
54	MG	1H	203	1/1	0.94	0.11	66,66,66,66	0
54	MG	1A	3589	1/1	0.94	0.17	69,69,69,69	0
54	MG	1A	3492	1/1	0.94	0.08	24,24,24,24	0
54	MG	1A	3047	1/1	0.94	0.32	48,48,48,48	0
54	MG	2A	3197	1/1	0.94	0.11	63,63,63,63	0
54	MG	1A	3402	1/1	0.94	0.12	29,29,29,29	0
54	MG	1A	3836	1/1	0.94	0.07	53,53,53,53	0
54	MG	1A	3048	1/1	0.94	0.24	47,47,47,47	0
54	MG	1A	3327	1/1	0.94	0.10	56,56,56,56	0
54	MG	1a	1714	1/1	0.94	0.14	73,73,73,73	0
54	MG	1A	3406	1/1	0.94	0.08	28,28,28,28	0
54	MG	1A	3711	1/1	0.94	0.07	39,39,39,39	0
54	MG	1d	301	1/1	0.94	0.26	75,75,75,75	0
54	MG	1R	204	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	3712	1/1	0.94	0.10	66,66,66,66	0
54	MG	1A	3846	1/1	0.94	0.09	55,55,55,55	0
54	MG	2A	3739	1/1	0.94	0.15	60,60,60,60	0
54	MG	2A	3459	1/1	0.94	0.09	73,73,73,73	0
54	MG	1T	205	1/1	0.94	0.10	62,62,62,62	0
54	MG	1U	201	1/1	0.94	0.15	41,41,41,41	0
54	MG	1A	3503	1/1	0.94	0.10	43,43,43,43	0
54	MG	1a	1728	1/1	0.94	0.11	56,56,56,56	0
54	MG	1V	204	1/1	0.94	0.14	54,54,54,54	0
54	MG	1V	205	1/1	0.94	0.12	63,63,63,63	0
54	MG	1A	3258	1/1	0.94	0.18	38,38,38,38	0
54	MG	1A	3602	1/1	0.94	0.09	53,53,53,53	0
54	MG	1m	201	1/1	0.94	0.07	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3469	1/1	0.94	0.08	64,64,64,64	0
54	MG	2A	3226	1/1	0.94	0.24	57,57,57,57	0
54	MG	1A	3259	1/1	0.94	0.15	45,45,45,45	0
54	MG	1A	3506	1/1	0.94	0.10	53,53,53,53	0
54	MG	1n	103	1/1	0.94	0.20	73,73,73,73	0
54	MG	1A	3123	1/1	0.94	0.05	35,35,35,35	0
54	MG	2A	3476	1/1	0.94	0.10	61,61,61,61	0
54	MG	1A	3857	1/1	0.94	0.07	62,62,62,62	0
54	MG	2A	3478	1/1	0.94	0.14	34,34,34,34	0
54	MG	2D	306	1/1	0.94	0.15	47,47,47,47	0
54	MG	1A	3075	1/1	0.94	0.21	45,45,45,45	0
54	MG	1A	3607	1/1	0.94	0.08	49,49,49,49	0
54	MG	1A	3190	1/1	0.94	0.28	72,72,72,72	0
54	MG	2D	311	1/1	0.94	0.10	65,65,65,65	0
54	MG	2D	312	1/1	0.94	0.14	56,56,56,56	0
54	MG	1A	3420	1/1	0.94	0.10	29,29,29,29	0
54	MG	2E	302	1/1	0.94	0.23	52,52,52,52	0
54	MG	1A	3731	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3076	1/1	0.94	0.19	44,44,44,44	0
54	MG	13	104	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3008	1/1	0.94	0.10	53,53,53,53	0
54	MG	2A	3247	1/1	0.94	0.07	60,60,60,60	0
54	MG	2A	3009	1/1	0.94	0.15	56,56,56,56	0
54	MG	1a	1748	1/1	0.94	0.14	67,67,67,67	0
54	MG	1A	3613	1/1	0.94	0.22	40,40,40,40	0
54	MG	1A	3869	1/1	0.94	0.09	39,39,39,39	0
54	MG	2A	3254	1/1	0.94	0.18	46,46,46,46	0
54	MG	2A	3496	1/1	0.94	0.10	72,72,72,72	0
54	MG	2R	202	1/1	0.94	0.12	46,46,46,46	0
54	MG	1A	3422	1/1	0.94	0.11	62,62,62,62	0
54	MG	2A	3256	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3871	1/1	0.94	0.09	46,46,46,46	0
54	MG	2A	3500	1/1	0.94	0.10	61,61,61,61	0
54	MG	1a	1753	1/1	0.94	0.14	59,59,59,59	0
54	MG	2A	3022	1/1	0.94	0.18	51,51,51,51	0
54	MG	2A	3262	1/1	0.94	0.34	52,52,52,52	0
54	MG	1A	3513	1/1	0.94	0.07	23,23,23,23	0
54	MG	2A	3505	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	3617	1/1	0.94	0.12	48,48,48,48	0
54	MG	2A	3026	1/1	0.94	0.09	58,58,58,58	0
54	MG	27	101	1/1	0.94	0.28	45,45,45,45	0
54	MG	17	103	1/1	0.94	0.29	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1757	1/1	0.94	0.19	56,56,56,56	0
54	MG	1a	1758	1/1	0.94	0.18	66,66,66,66	0
54	MG	2A	3512	1/1	0.94	0.21	45,45,45,45	0
54	MG	1A	3745	1/1	0.94	0.10	42,42,42,42	0
54	MG	2a	3005	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3618	1/1	0.94	0.16	36,36,36,36	0
54	MG	18	102	1/1	0.94	0.12	45,45,45,45	0
54	MG	1a	1762	1/1	0.94	0.06	57,57,57,57	0
54	MG	2a	3012	1/1	0.94	0.14	68,68,68,68	0
54	MG	18	103	1/1	0.94	0.21	42,42,42,42	0
54	MG	1A	3876	1/1	0.94	0.07	29,29,29,29	0
54	MG	2a	3018	1/1	0.94	0.09	57,57,57,57	0
54	MG	2A	3279	1/1	0.94	0.07	32,32,32,32	0
54	MG	2A	3039	1/1	0.94	0.16	57,57,57,57	0
54	MG	2A	3041	1/1	0.94	0.06	34,34,34,34	0
54	MG	2A	3283	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3284	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	4019	1/1	0.94	0.15	39,39,39,39	0
54	MG	1A	3337	1/1	0.94	0.10	18,18,18,18	0
54	MG	2A	3529	1/1	0.94	0.08	49,49,49,49	0
54	MG	1A	3194	1/1	0.94	0.09	54,54,54,54	0
54	MG	2A	3531	1/1	0.94	0.11	32,32,32,32	0
54	MG	2A	3532	1/1	0.94	0.07	54,54,54,54	0
54	MG	1a	1604	1/1	0.94	0.24	76,76,76,76	0
54	MG	1A	3079	1/1	0.94	0.31	45,45,45,45	0
54	MG	2A	3536	1/1	0.94	0.07	65,65,65,65	0
54	MG	2A	3291	1/1	0.94	0.09	50,50,50,50	0
54	MG	2A	3293	1/1	0.94	0.06	39,39,39,39	0
54	MG	2A	3047	1/1	0.94	0.08	59,59,59,59	0
54	MG	2A	3048	1/1	0.94	0.13	55,55,55,55	0
54	MG	2A	3050	1/1	0.94	0.09	42,42,42,42	0
54	MG	2A	3544	1/1	0.94	0.14	60,60,60,60	0
54	MG	1a	1607	1/1	0.94	0.09	67,67,67,67	0
54	MG	1a	1608	1/1	0.94	0.09	67,67,67,67	0
54	MG	1A	3883	1/1	0.94	0.08	28,28,28,28	0
54	MG	1a	1773	1/1	0.94	0.12	74,74,74,74	0
54	MG	2A	3550	1/1	0.94	0.12	55,55,55,55	0
54	MG	1A	4025	1/1	0.94	0.10	55,55,55,55	0
54	MG	2A	3305	1/1	0.94	0.12	69,69,69,69	0
54	MG	2A	3306	1/1	0.94	0.21	60,60,60,60	0
54	MG	1A	3052	1/1	0.94	0.09	44,44,44,44	0
54	MG	1A	3054	1/1	0.94	0.16	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2a	3053	1/1	0.94	0.17	64,64,64,64	0
54	MG	1A	3058	1/1	0.94	0.10	45,45,45,45	0
54	MG	2A	3062	1/1	0.94	0.12	61,61,61,61	0
54	MG	2A	3559	1/1	0.94	0.10	62,62,62,62	0
54	MG	2A	3063	1/1	0.94	0.09	48,48,48,48	0
54	MG	1a	1617	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3314	1/1	0.94	0.07	49,49,49,49	0
54	MG	2A	3065	1/1	0.94	0.11	51,51,51,51	0
54	MG	1A	3059	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3568	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3318	1/1	0.94	0.09	40,40,40,40	0
54	MG	1A	3523	1/1	0.94	0.07	24,24,24,24	0
54	MG	1A	3631	1/1	0.94	0.10	59,59,59,59	0
54	MG	2a	3067	1/1	0.94	0.19	66,66,66,66	0
54	MG	2a	3068	1/1	0.94	0.15	72,72,72,72	0
54	MG	2A	3575	1/1	0.94	0.07	55,55,55,55	0
54	MG	1a	1623	1/1	0.94	0.20	58,58,58,58	0
54	MG	2A	3322	1/1	0.94	0.09	55,55,55,55	0
54	MG	2A	3578	1/1	0.94	0.06	50,50,50,50	0
54	MG	2A	3326	1/1	0.94	0.18	63,63,63,63	0
54	MG	2A	3075	1/1	0.94	0.12	58,58,58,58	0
54	MG	2A	3076	1/1	0.94	0.10	54,54,54,54	0
54	MG	1A	3430	1/1	0.94	0.09	29,29,29,29	0
54	MG	2A	3080	1/1	0.94	0.17	68,68,68,68	0
54	MG	1A	3432	1/1	0.94	0.07	18,18,18,18	0
54	MG	1A	3433	1/1	0.94	0.08	40,40,40,40	0
54	MG	2A	3336	1/1	0.94	0.08	49,49,49,49	0
54	MG	2A	3337	1/1	0.94	0.21	67,67,67,67	0
54	MG	2A	3596	1/1	0.94	0.08	49,49,49,49	0
54	MG	1A	3351	1/1	0.94	0.09	52,52,52,52	0
54	MG	2A	3340	1/1	0.94	0.18	79,79,79,79	0
54	MG	1A	3095	1/1	0.94	0.11	51,51,51,51	0
54	MG	2a	3091	1/1	0.94	0.25	69,69,69,69	0
54	MG	2A	3087	1/1	0.94	0.11	49,49,49,49	0
54	MG	1A	3277	1/1	0.94	0.33	36,36,36,36	0
54	MG	1A	3148	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3096	1/1	0.94	0.24	49,49,49,49	0
54	MG	1A	3035	1/1	0.94	0.12	53,53,53,53	0
54	MG	1A	3443	1/1	0.94	0.17	62,62,62,62	0
54	MG	1A	3544	1/1	0.94	0.06	24,24,24,24	0
54	MG	1A	3911	1/1	0.94	0.06	39,39,39,39	0
54	MG	2a	3100	1/1	0.94	0.12	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3097	1/1	0.94	0.19	54,54,54,54	0
54	MG	1A	3777	1/1	0.94	0.07	38,38,38,38	0
54	MG	1A	3030	1/1	0.94	0.05	35,35,35,35	0
54	MG	1A	3022	1/1	0.94	0.08	45,45,45,45	0
54	MG	2a	3108	1/1	0.94	0.16	71,71,71,71	0
54	MG	1A	3549	1/1	0.94	0.12	51,51,51,51	0
54	MG	1A	3103	1/1	0.94	0.10	45,45,45,45	0
54	MG	2A	3108	1/1	0.94	0.06	57,57,57,57	0
54	MG	1A	3365	1/1	0.94	0.07	24,24,24,24	0
54	MG	1a	1806	1/1	0.94	0.10	74,74,74,74	0
54	MG	2a	3114	1/1	0.94	0.10	79,79,79,79	0
54	MG	1A	3221	1/1	0.94	0.23	41,41,41,41	0
54	MG	1B	204	1/1	0.94	0.08	52,52,52,52	0
54	MG	1A	3787	1/1	0.94	0.11	50,50,50,50	0
54	MG	2A	3115	1/1	0.94	0.15	56,56,56,56	0
54	MG	2A	3627	1/1	0.94	0.08	71,71,71,71	0
54	MG	1A	3230	1/1	0.94	0.34	47,47,47,47	0
54	MG	1A	3294	1/1	0.94	0.16	57,57,57,57	0
54	MG	1A	3105	1/1	0.94	0.10	70,70,70,70	0
54	MG	1A	3937	1/1	0.94	0.12	46,46,46,46	0
54	MG	1a	1815	1/1	0.94	0.15	67,67,67,67	0
54	MG	1a	1816	1/1	0.94	0.16	65,65,65,65	0
54	MG	1A	3657	1/1	0.94	0.20	56,56,56,56	0
54	MG	2A	3127	1/1	0.94	0.11	65,65,65,65	0
54	MG	1A	3170	1/1	0.94	0.20	54,54,54,54	0
54	MG	1A	3109	1/1	0.94	0.20	38,38,38,38	0
54	MG	2A	3136	1/1	0.94	0.15	62,62,62,62	0
54	MG	1A	3372	1/1	0.94	0.08	34,34,34,34	0
54	MG	2A	3644	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3944	1/1	0.94	0.07	64,64,64,64	0
54	MG	2A	3386	1/1	0.94	0.10	40,40,40,40	0
54	MG	2A	3648	1/1	0.94	0.08	65,65,65,65	0
54	MG	1A	3066	1/1	0.94	0.19	39,39,39,39	0
54	MG	1A	3669	1/1	0.94	0.13	65,65,65,65	0
54	MG	2A	3389	1/1	0.94	0.11	40,40,40,40	0
54	MG	2A	3390	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3655	1/1	0.94	0.09	49,49,49,49	0
54	MG	1a	1670	1/1	0.94	0.10	69,69,69,69	0
54	MG	1B	222	1/1	0.94	0.09	58,58,58,58	0
54	MG	2A	3149	1/1	0.94	0.09	40,40,40,40	0
54	MG	1A	3238	1/1	0.94	0.31	42,42,42,42	0
54	MG	2A	3661	1/1	0.94	0.08	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1a	1673	1/1	0.94	0.17	63,63,63,63	0
54	MG	2A	3664	1/1	0.94	0.07	62,62,62,62	0
54	MG	1A	3800	1/1	0.94	0.07	82,82,82,82	0
54	MG	2a	3165	1/1	0.94	0.12	79,79,79,79	0
54	MG	2a	3166	1/1	0.94	0.15	68,68,68,68	0
54	MG	2a	3169	1/1	0.94	0.09	73,73,73,73	0
54	MG	1A	3564	1/1	0.94	0.08	44,44,44,44	0
54	MG	1A	3672	1/1	0.94	0.08	50,50,50,50	0
54	MG	2A	3155	1/1	0.94	0.12	67,67,67,67	0
54	MG	1A	3377	1/1	0.94	0.07	32,32,32,32	0
54	MG	2A	3159	1/1	0.94	0.15	71,71,71,71	0
54	MG	2a	3178	1/1	0.94	0.11	58,58,58,58	0
54	MG	1A	3113	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3179	1/1	0.94	0.16	40,40,40,40	0
54	MG	1A	3118	1/1	0.94	0.11	41,41,41,41	0
54	MG	1A	3809	1/1	0.94	0.11	61,61,61,61	0
54	MG	1A	3381	1/1	0.94	0.10	41,41,41,41	0
54	MG	1A	3312	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3168	1/1	0.94	0.08	51,51,51,51	0
54	MG	2a	3187	1/1	0.94	0.19	74,74,74,74	0
54	MG	2a	3188	1/1	0.94	0.20	65,65,65,65	0
54	MG	1A	3475	1/1	0.94	0.12	51,51,51,51	0
54	MG	2A	3171	1/1	0.94	0.08	51,51,51,51	0
54	MG	2A	3413	1/1	0.94	0.26	59,59,59,59	0
54	MG	1A	3384	1/1	0.94	0.14	53,53,53,53	0
54	MG	2A	3173	1/1	0.94	0.11	62,62,62,62	0
54	MG	1A	3815	1/1	0.94	0.11	42,42,42,42	0
54	MG	1A	3313	1/1	0.94	0.17	52,52,52,52	0
54	MG	2A	3418	1/1	0.94	0.06	31,31,31,31	0
54	MG	2f	201	1/1	0.94	0.10	56,56,56,56	0
54	MG	1A	3249	1/1	0.94	0.18	56,56,56,56	0
54	MG	1A	3316	1/1	0.94	0.22	53,53,53,53	0
54	MG	1A	3045	1/1	0.94	0.24	56,56,56,56	0
54	MG	2A	3425	1/1	0.94	0.13	70,70,70,70	0
54	MG	2A	3179	1/1	0.94	0.11	52,52,52,52	0
54	MG	2A	3428	1/1	0.94	0.14	62,62,62,62	0
54	MG	1a	1693	1/1	0.94	0.22	68,68,68,68	0
55	CPF	1A	4056	24/24	0.94	0.13	34,46,55,61	0
55	CPF	2A	3741	24/24	0.94	0.12	39,44,56,58	0
54	MG	1A	3391	1/1	0.94	0.07	30,30,30,30	0
54	MG	2A	3184	1/1	0.94	0.17	66,66,66,66	0
54	MG	1A	3825	1/1	0.94	0.34	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
54	MG	1A	3318	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3827	1/1	0.94	0.12	59,59,59,59	0
54	MG	1F	317	1/1	0.94	0.11	43,43,43,43	0
54	MG	1A	3183	1/1	0.94	0.18	34,34,34,34	0
54	MG	1A	3395	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3717	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	3921	1/1	0.95	0.24	44,44,44,44	0
54	MG	2V	201	1/1	0.95	0.13	60,60,60,60	0
54	MG	1A	3612	1/1	0.95	0.10	62,62,62,62	0
54	MG	1A	4039	1/1	0.95	0.17	63,63,63,63	0
54	MG	1A	3128	1/1	0.95	0.06	44,44,44,44	0
54	MG	2A	3571	1/1	0.95	0.09	53,53,53,53	0
54	MG	20	101	1/1	0.95	0.13	65,65,65,65	0
54	MG	2A	3183	1/1	0.95	0.10	61,61,61,61	0
54	MG	2A	3382	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	4041	1/1	0.95	0.31	45,45,45,45	0
54	MG	23	101	1/1	0.95	0.17	59,59,59,59	0
54	MG	1A	3180	1/1	0.95	0.07	57,57,57,57	0
54	MG	1A	3279	1/1	0.95	0.07	51,51,51,51	0
54	MG	28	101	1/1	0.95	0.10	58,58,58,58	0
54	MG	1A	3707	1/1	0.95	0.17	50,50,50,50	0
54	MG	1A	3393	1/1	0.95	0.07	44,44,44,44	0
54	MG	1A	4046	1/1	0.95	0.13	69,69,69,69	0
54	MG	1A	3339	1/1	0.95	0.12	37,37,37,37	0
54	MG	2A	3588	1/1	0.95	0.06	38,38,38,38	0
54	MG	1A	3056	1/1	0.95	0.18	36,36,36,36	0
54	MG	2a	3006	1/1	0.95	0.25	58,58,58,58	0
54	MG	2a	3007	1/1	0.95	0.09	71,71,71,71	0
54	MG	2A	3006	1/1	0.95	0.15	54,54,54,54	0
54	MG	1A	3816	1/1	0.95	0.09	53,53,53,53	0
54	MG	1A	4050	1/1	0.95	0.15	76,76,76,76	0
54	MG	1A	3396	1/1	0.95	0.07	24,24,24,24	0
54	MG	2A	3395	1/1	0.95	0.06	61,61,61,61	0
54	MG	2a	3015	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3818	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3942	1/1	0.95	0.06	48,48,48,48	0
54	MG	1A	3621	1/1	0.95	0.11	34,34,34,34	0
54	MG	2A	3199	1/1	0.95	0.06	53,53,53,53	0
54	MG	1A	4055	1/1	0.95	0.10	57,57,57,57	0
54	MG	2A	3603	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3072	1/1	0.95	0.27	32,32,32,32	0
54	MG	1a	1619	1/1	0.95	0.06	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
54	MG	1B	201	1/1	0.95	0.14	54,54,54,54	0
54	MG	2A	3607	1/1	0.95	0.10	54,54,54,54	0
54	MG	1A	3002	1/1	0.95	0.11	53,53,53,53	0
54	MG	2A	3025	1/1	0.95	0.10	52,52,52,52	0
54	MG	1A	3547	1/1	0.95	0.08	41,41,41,41	0
54	MG	2A	3027	1/1	0.95	0.14	39,39,39,39	0
54	MG	1A	3401	1/1	0.95	0.11	26,26,26,26	0
54	MG	1a	1626	1/1	0.95	0.12	64,64,64,64	0
54	MG	1A	3140	1/1	0.95	0.18	41,41,41,41	0
54	MG	1a	1629	1/1	0.95	0.14	51,51,51,51	0
54	MG	1A	3629	1/1	0.95	0.15	60,60,60,60	0
54	MG	1A	3723	1/1	0.95	0.07	32,32,32,32	0
54	MG	1A	3032	1/1	0.95	0.21	51,51,51,51	0
54	MG	1A	3474	1/1	0.95	0.09	45,45,45,45	0
54	MG	1A	3954	1/1	0.95	0.05	31,31,31,31	0
54	MG	1A	3241	1/1	0.95	0.13	48,48,48,48	0
54	MG	2A	3224	1/1	0.95	0.12	56,56,56,56	0
54	MG	1A	3730	1/1	0.95	0.10	67,67,67,67	0
54	MG	1A	3957	1/1	0.95	0.10	55,55,55,55	0
54	MG	2a	3047	1/1	0.95	0.09	57,57,57,57	0
54	MG	1A	3023	1/1	0.95	0.11	30,30,30,30	0
54	MG	1B	219	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3477	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	3736	1/1	0.95	0.09	46,46,46,46	0
54	MG	1A	3291	1/1	0.95	0.15	36,36,36,36	0
54	MG	2A	3233	1/1	0.95	0.10	72,72,72,72	0
54	MG	2A	3634	1/1	0.95	0.07	62,62,62,62	0
54	MG	1a	1646	1/1	0.95	0.23	58,58,58,58	0
54	MG	1a	1647	1/1	0.95	0.15	51,51,51,51	0
54	MG	2A	3236	1/1	0.95	0.19	62,62,62,62	0
54	MG	1A	3077	1/1	0.95	0.21	35,35,35,35	0
54	MG	2A	3238	1/1	0.95	0.07	61,61,61,61	0
54	MG	1A	3410	1/1	0.95	0.10	32,32,32,32	0
54	MG	1B	227	1/1	0.95	0.06	61,61,61,61	0
54	MG	1A	3078	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	3843	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3640	1/1	0.95	0.23	48,48,48,48	0
54	MG	2A	3058	1/1	0.95	0.08	56,56,56,56	0
54	MG	2a	3066	1/1	0.95	0.09	63,63,63,63	0
54	MG	1A	3412	1/1	0.95	0.07	25,25,25,25	0
54	MG	2A	3060	1/1	0.95	0.14	44,44,44,44	0
54	MG	2A	3251	1/1	0.95	0.19	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3356	1/1	0.95	0.07	27,27,27,27	0
54	MG	1A	3246	1/1	0.95	0.30	48,48,48,48	0
54	MG	1a	1803	1/1	0.95	0.07	50,50,50,50	0
54	MG	1A	3972	1/1	0.95	0.06	33,33,33,33	0
54	MG	2A	3659	1/1	0.95	0.07	34,34,34,34	0
54	MG	1A	3644	1/1	0.95	0.13	49,49,49,49	0
54	MG	2A	3258	1/1	0.95	0.35	44,44,44,44	0
54	MG	2A	3066	1/1	0.95	0.13	61,61,61,61	0
54	MG	1A	3751	1/1	0.95	0.06	32,32,32,32	0
54	MG	1A	3418	1/1	0.95	0.07	42,42,42,42	0
54	MG	2A	3667	1/1	0.95	0.07	62,62,62,62	0
54	MG	1D	317	1/1	0.95	0.09	52,52,52,52	0
54	MG	2A	3073	1/1	0.95	0.26	49,49,49,49	0
54	MG	1A	3247	1/1	0.95	0.10	42,42,42,42	0
54	MG	2A	3673	1/1	0.95	0.07	41,41,41,41	0
54	MG	2a	3089	1/1	0.95	0.05	60,60,60,60	0
54	MG	1A	3491	1/1	0.95	0.12	28,28,28,28	0
54	MG	1A	3248	1/1	0.95	0.12	45,45,45,45	0
54	MG	2A	3077	1/1	0.95	0.12	61,61,61,61	0
54	MG	2A	3271	1/1	0.95	0.06	77,77,77,77	0
54	MG	2A	3078	1/1	0.95	0.07	53,53,53,53	0
54	MG	1a	1812	1/1	0.95	0.08	63,63,63,63	0
54	MG	1A	3192	1/1	0.95	0.22	45,45,45,45	0
54	MG	1A	3862	1/1	0.95	0.06	45,45,45,45	0
54	MG	1A	3363	1/1	0.95	0.13	63,63,63,63	0
54	MG	1A	3759	1/1	0.95	0.06	48,48,48,48	0
54	MG	1F	313	1/1	0.95	0.28	48,48,48,48	0
54	MG	2a	3101	1/1	0.95	0.09	66,66,66,66	0
54	MG	1A	3025	1/1	0.95	0.20	41,41,41,41	0
54	MG	2A	3088	1/1	0.95	0.24	57,57,57,57	0
54	MG	1A	3761	1/1	0.95	0.08	51,51,51,51	0
54	MG	2A	3689	1/1	0.95	0.08	59,59,59,59	0
54	MG	2A	3690	1/1	0.95	0.07	56,56,56,56	0
54	MG	1A	3081	1/1	0.95	0.51	47,47,47,47	0
54	MG	1A	3500	1/1	0.95	0.06	24,24,24,24	0
54	MG	1F	318	1/1	0.95	0.08	66,66,66,66	0
54	MG	1F	319	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3020	1/1	0.95	0.31	41,41,41,41	0
54	MG	1A	3115	1/1	0.95	0.20	35,35,35,35	0
54	MG	1G	203	1/1	0.95	0.11	64,64,64,64	0
54	MG	1A	3660	1/1	0.95	0.23	53,53,53,53	0
54	MG	2A	3292	1/1	0.95	0.07	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3992	1/1	0.95	0.06	19,19,19,19	0
54	MG	1A	3160	1/1	0.95	0.13	56,56,56,56	0
54	MG	2A	3295	1/1	0.95	0.10	44,44,44,44	0
54	MG	2A	3101	1/1	0.95	0.12	78,78,78,78	0
54	MG	1A	3769	1/1	0.95	0.06	29,29,29,29	0
54	MG	1A	3084	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3583	1/1	0.95	0.11	37,37,37,37	0
54	MG	2A	3714	1/1	0.95	0.12	65,65,65,65	0
54	MG	2a	3135	1/1	0.95	0.08	69,69,69,69	0
54	MG	1A	3666	1/1	0.95	0.08	48,48,48,48	0
54	MG	1P	205	1/1	0.95	0.08	74,74,74,74	0
54	MG	1A	3201	1/1	0.95	0.21	49,49,49,49	0
54	MG	1A	3087	1/1	0.95	0.17	39,39,39,39	0
54	MG	1a	1845	1/1	0.95	0.19	60,60,60,60	0
54	MG	1A	3204	1/1	0.95	0.19	50,50,50,50	0
54	MG	1A	3779	1/1	0.95	0.11	51,51,51,51	0
54	MG	2A	3117	1/1	0.95	0.09	44,44,44,44	0
54	MG	1Q	205	1/1	0.95	0.12	54,54,54,54	0
54	MG	2A	3120	1/1	0.95	0.18	53,53,53,53	0
54	MG	1A	3053	1/1	0.95	0.10	48,48,48,48	0
54	MG	2A	3122	1/1	0.95	0.36	45,45,45,45	0
54	MG	1A	3887	1/1	0.95	0.06	68,68,68,68	0
54	MG	1a	1701	1/1	0.95	0.11	66,66,66,66	0
54	MG	1R	206	1/1	0.95	0.19	58,58,58,58	0
54	MG	1A	3166	1/1	0.95	0.09	41,41,41,41	0
54	MG	1a	1704	1/1	0.95	0.08	46,46,46,46	0
54	MG	2A	3128	1/1	0.95	0.24	62,62,62,62	0
54	MG	2A	3130	1/1	0.95	0.13	64,64,64,64	0
54	MG	2A	3516	1/1	0.95	0.12	67,67,67,67	0
54	MG	2A	3131	1/1	0.95	0.18	64,64,64,64	0
54	MG	1A	3321	1/1	0.95	0.14	55,55,55,55	0
54	MG	1A	3323	1/1	0.95	0.21	37,37,37,37	0
54	MG	1A	3324	1/1	0.95	0.08	33,33,33,33	0
54	MG	1U	203	1/1	0.95	0.34	40,40,40,40	0
54	MG	2a	3168	1/1	0.95	0.08	71,71,71,71	0
54	MG	1U	205	1/1	0.95	0.33	33,33,33,33	0
54	MG	2a	3170	1/1	0.95	0.11	68,68,68,68	0
54	MG	1U	206	1/1	0.95	0.23	43,43,43,43	0
54	MG	2A	3143	1/1	0.95	0.13	42,42,42,42	0
54	MG	2B	205	1/1	0.95	0.15	53,53,53,53	0
54	MG	2a	3175	1/1	0.95	0.10	75,75,75,75	0
54	MG	2A	3145	1/1	0.95	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
54	MG	1A	3067	1/1	0.95	0.08	53,53,53,53	0
54	MG	1V	203	1/1	0.95	0.14	44,44,44,44	0
54	MG	1A	3596	1/1	0.95	0.08	19,19,19,19	0
54	MG	1A	3894	1/1	0.95	0.12	38,38,38,38	0
54	MG	1A	3209	1/1	0.95	0.31	43,43,43,43	0
54	MG	2B	212	1/1	0.95	0.17	72,72,72,72	0
54	MG	1A	3171	1/1	0.95	0.20	36,36,36,36	0
54	MG	1W	203	1/1	0.95	0.17	35,35,35,35	0
54	MG	1A	3037	1/1	0.95	0.09	53,53,53,53	0
54	MG	1A	3903	1/1	0.95	0.06	42,42,42,42	0
54	MG	1A	3385	1/1	0.95	0.12	58,58,58,58	0
54	MG	2A	3156	1/1	0.95	0.20	46,46,46,46	0
54	MG	1A	3094	1/1	0.95	0.11	38,38,38,38	0
54	MG	2D	305	1/1	0.95	0.39	48,48,48,48	0
54	MG	1A	3521	1/1	0.95	0.06	64,64,64,64	0
54	MG	2D	307	1/1	0.95	0.25	51,51,51,51	0
54	MG	1A	3215	1/1	0.95	0.15	38,38,38,38	0
54	MG	2A	3355	1/1	0.95	0.09	53,53,53,53	0
54	MG	1I	103	1/1	0.95	0.09	55,55,55,55	0
54	MG	2A	3359	1/1	0.95	0.09	60,60,60,60	0
54	MG	1A	3388	1/1	0.95	0.07	31,31,31,31	0
54	MG	1A	3525	1/1	0.95	0.10	63,63,63,63	0
54	MG	2A	3164	1/1	0.95	0.12	55,55,55,55	0
54	MG	1A	4027	1/1	0.95	0.10	59,59,59,59	0
54	MG	1A	3527	1/1	0.95	0.10	60,60,60,60	0
54	MG	1A	4029	1/1	0.95	0.09	46,46,46,46	0
54	MG	2F	301	1/1	0.95	0.32	48,48,48,48	0
54	MG	1A	3453	1/1	0.95	0.11	55,55,55,55	0
54	MG	2A	3555	1/1	0.95	0.08	72,72,72,72	0
54	MG	1a	1739	1/1	0.95	0.12	66,66,66,66	0
54	MG	15	101	1/1	0.95	0.13	41,41,41,41	0
54	MG	1A	3696	1/1	0.95	0.08	56,56,56,56	0
54	MG	1A	3915	1/1	0.95	0.15	25,25,25,25	0
54	MG	1A	3126	1/1	0.95	0.13	40,40,40,40	0
54	MG	2A	3374	1/1	0.95	0.07	54,54,54,54	0
57	ARG	1B	230	12/12	0.95	0.10	37,56,63,63	0
54	MG	2A	3563	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3917	1/1	0.95	0.12	29,29,29,29	0
54	MG	1A	3457	1/1	0.95	0.09	64,64,64,64	0
54	MG	2A	3617	1/1	0.96	0.08	68,68,68,68	0
54	MG	1A	3780	1/1	0.96	0.12	48,48,48,48	0
54	MG	2A	3240	1/1	0.96	0.32	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
54	MG	1A	3024	1/1	0.96	0.15	26,26,26,26	0
54	MG	2A	3068	1/1	0.96	0.25	41,41,41,41	0
54	MG	1A	3358	1/1	0.96	0.09	34,34,34,34	0
54	MG	1A	3498	1/1	0.96	0.12	58,58,58,58	0
54	MG	1A	3499	1/1	0.96	0.10	51,51,51,51	0
54	MG	2A	3246	1/1	0.96	0.10	60,60,60,60	0
54	MG	1P	202	1/1	0.96	0.18	38,38,38,38	0
54	MG	1A	3674	1/1	0.96	0.17	48,48,48,48	0
54	MG	1A	3786	1/1	0.96	0.08	51,51,51,51	0
54	MG	1A	4013	1/1	0.96	0.08	47,47,47,47	0
54	MG	1A	3111	1/1	0.96	0.17	39,39,39,39	0
54	MG	1A	3086	1/1	0.96	0.06	49,49,49,49	0
54	MG	1A	3502	1/1	0.96	0.07	41,41,41,41	0
54	MG	1A	3361	1/1	0.96	0.09	50,50,50,50	0
54	MG	1A	3015	1/1	0.96	0.06	35,35,35,35	0
54	MG	2A	3084	1/1	0.96	0.08	42,42,42,42	0
54	MG	1a	1824	1/1	0.96	0.08	55,55,55,55	0
54	MG	1R	203	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3906	1/1	0.96	0.07	64,64,64,64	0
54	MG	1a	1685	1/1	0.96	0.15	59,59,59,59	0
54	MG	1R	205	1/1	0.96	0.15	45,45,45,45	0
54	MG	1A	3295	1/1	0.96	0.11	41,41,41,41	0
54	MG	1A	3242	1/1	0.96	0.33	43,43,43,43	0
54	MG	1a	1832	1/1	0.96	0.06	75,75,75,75	0
54	MG	1T	203	1/1	0.96	0.15	65,65,65,65	0
54	MG	2A	3651	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3017	1/1	0.96	0.18	34,34,34,34	0
54	MG	2A	3095	1/1	0.96	0.12	51,51,51,51	0
54	MG	1A	3191	1/1	0.96	0.19	38,38,38,38	0
54	MG	1A	3797	1/1	0.96	0.07	77,77,77,77	0
54	MG	1A	3152	1/1	0.96	0.22	33,33,33,33	0
54	MG	1A	3431	1/1	0.96	0.08	31,31,31,31	0
54	MG	1A	3304	1/1	0.96	0.22	39,39,39,39	0
54	MG	1a	1843	1/1	0.96	0.07	58,58,58,58	0
54	MG	2A	3102	1/1	0.96	0.11	56,56,56,56	0
54	MG	2A	3104	1/1	0.96	0.09	72,72,72,72	0
54	MG	2A	3105	1/1	0.96	0.18	55,55,55,55	0
54	MG	1A	3154	1/1	0.96	0.32	38,38,38,38	0
54	MG	1A	3306	1/1	0.96	0.14	24,24,24,24	0
54	MG	1A	4032	1/1	0.96	0.07	59,59,59,59	0
54	MG	1A	3155	1/1	0.96	0.18	42,42,42,42	0
54	MG	1A	3920	1/1	0.96	0.07	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3116	1/1	0.96	0.08	39,39,39,39	0
54	MG	1W	202	1/1	0.96	0.11	54,54,54,54	0
54	MG	1A	3922	1/1	0.96	0.07	52,52,52,52	0
54	MG	2A	3114	1/1	0.96	0.10	49,49,49,49	0
54	MG	1A	3117	1/1	0.96	0.11	41,41,41,41	0
54	MG	10	101	1/1	0.96	0.13	47,47,47,47	0
54	MG	1A	3439	1/1	0.96	0.10	56,56,56,56	0
54	MG	1A	3159	1/1	0.96	0.10	38,38,38,38	0
54	MG	2A	3119	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3198	1/1	0.96	0.19	45,45,45,45	0
54	MG	2A	3484	1/1	0.96	0.07	58,58,58,58	0
54	MG	1A	3933	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3038	1/1	0.96	0.16	49,49,49,49	0
54	MG	1A	3029	1/1	0.96	0.11	40,40,40,40	0
54	MG	1A	3446	1/1	0.96	0.07	58,58,58,58	0
54	MG	1A	3524	1/1	0.96	0.14	51,51,51,51	0
54	MG	13	101	1/1	0.96	0.15	36,36,36,36	0
54	MG	1A	3043	1/1	0.96	0.12	17,17,17,17	0
54	MG	1A	3526	1/1	0.96	0.11	27,27,27,27	0
54	MG	1A	3614	1/1	0.96	0.26	39,39,39,39	0
54	MG	1a	1723	1/1	0.96	0.06	60,60,60,60	0
54	MG	1A	3819	1/1	0.96	0.09	48,48,48,48	0
54	MG	2a	3080	1/1	0.96	0.06	75,75,75,75	0
54	MG	1A	3256	1/1	0.96	0.08	44,44,44,44	0
54	MG	15	102	1/1	0.96	0.18	39,39,39,39	0
54	MG	2A	3699	1/1	0.96	0.06	66,66,66,66	0
54	MG	1A	3528	1/1	0.96	0.07	52,52,52,52	0
54	MG	2a	3087	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3530	1/1	0.96	0.28	31,31,31,31	0
54	MG	1A	3060	1/1	0.96	0.07	62,62,62,62	0
54	MG	2A	3704	1/1	0.96	0.11	60,60,60,60	0
54	MG	1A	3824	1/1	0.96	0.08	41,41,41,41	0
54	MG	2A	3144	1/1	0.96	0.14	54,54,54,54	0
54	MG	1A	3008	1/1	0.96	0.05	45,45,45,45	0
54	MG	2A	3708	1/1	0.96	0.06	74,74,74,74	0
54	MG	1A	3206	1/1	0.96	0.13	47,47,47,47	0
54	MG	2A	3324	1/1	0.96	0.09	35,35,35,35	0
54	MG	17	105	1/1	0.96	0.30	49,49,49,49	0
54	MG	1d	304	1/1	0.96	0.17	65,65,65,65	0
54	MG	2A	3713	1/1	0.96	0.06	69,69,69,69	0
54	MG	1A	3721	1/1	0.96	0.17	40,40,40,40	0
54	MG	1A	3535	1/1	0.96	0.07	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3167	1/1	0.96	0.09	51,51,51,51	0
54	MG	2A	3331	1/1	0.96	0.08	37,37,37,37	0
54	MG	1A	3012	1/1	0.96	0.10	44,44,44,44	0
54	MG	2a	3106	1/1	0.96	0.06	66,66,66,66	0
54	MG	19	101	1/1	0.96	0.18	56,56,56,56	0
54	MG	2A	3334	1/1	0.96	0.09	37,37,37,37	0
54	MG	1g	203	1/1	0.96	0.09	66,66,66,66	0
54	MG	1A	3125	1/1	0.96	0.27	46,46,46,46	0
54	MG	1A	3100	1/1	0.96	0.34	38,38,38,38	0
54	MG	1A	3729	1/1	0.96	0.10	52,52,52,52	0
54	MG	2A	3726	1/1	0.96	0.06	61,61,61,61	0
54	MG	1k	201	1/1	0.96	0.10	46,46,46,46	0
54	MG	1B	208	1/1	0.96	0.06	45,45,45,45	0
54	MG	2a	3116	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3211	1/1	0.96	0.21	36,36,36,36	0
54	MG	1A	3005	1/1	0.96	0.10	29,29,29,29	0
54	MG	1a	1606	1/1	0.96	0.19	55,55,55,55	0
54	MG	1B	211	1/1	0.96	0.06	61,61,61,61	0
54	MG	2A	3733	1/1	0.96	0.08	64,64,64,64	0
54	MG	2A	3165	1/1	0.96	0.17	55,55,55,55	0
54	MG	2A	3348	1/1	0.96	0.05	38,38,38,38	0
54	MG	1A	3542	1/1	0.96	0.27	35,35,35,35	0
54	MG	2a	3128	1/1	0.96	0.09	71,71,71,71	0
54	MG	1a	1609	1/1	0.96	0.06	60,60,60,60	0
54	MG	1A	3268	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3737	1/1	0.96	0.21	41,41,41,41	0
54	MG	1a	1613	1/1	0.96	0.11	31,31,31,31	0
54	MG	1A	3080	1/1	0.96	0.33	46,46,46,46	0
54	MG	1A	3633	1/1	0.96	0.08	34,34,34,34	0
54	MG	1A	3065	1/1	0.96	0.22	35,35,35,35	0
54	MG	1A	3136	1/1	0.96	0.06	41,41,41,41	0
54	MG	1A	3272	1/1	0.96	0.32	39,39,39,39	0
54	MG	2A	3005	1/1	0.96	0.10	59,59,59,59	0
54	MG	1A	3397	1/1	0.96	0.10	27,27,27,27	0
54	MG	2A	3007	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3217	1/1	0.96	0.17	42,42,42,42	0
54	MG	1B	225	1/1	0.96	0.05	44,44,44,44	0
54	MG	1A	3852	1/1	0.96	0.12	43,43,43,43	0
54	MG	1A	3274	1/1	0.96	0.10	63,63,63,63	0
54	MG	1a	1625	1/1	0.96	0.12	55,55,55,55	0
54	MG	1A	3552	1/1	0.96	0.08	55,55,55,55	0
54	MG	1A	3750	1/1	0.96	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
54	MG	1A	3400	1/1	0.96	0.07	45,45,45,45	0
54	MG	1D	305	1/1	0.96	0.12	46,46,46,46	0
54	MG	1A	3752	1/1	0.96	0.09	39,39,39,39	0
54	MG	2D	301	1/1	0.96	0.20	48,48,48,48	0
54	MG	2a	3159	1/1	0.96	0.11	59,59,59,59	0
54	MG	2D	302	1/1	0.96	0.13	46,46,46,46	0
54	MG	1A	3275	1/1	0.96	0.08	33,33,33,33	0
54	MG	1A	3050	1/1	0.96	0.21	32,32,32,32	0
54	MG	1A	3222	1/1	0.96	0.29	42,42,42,42	0
54	MG	1a	1636	1/1	0.96	0.07	40,40,40,40	0
54	MG	2a	3167	1/1	0.96	0.06	51,51,51,51	0
54	MG	1A	3224	1/1	0.96	0.25	42,42,42,42	0
54	MG	2A	3030	1/1	0.96	0.14	33,33,33,33	0
54	MG	1A	3405	1/1	0.96	0.05	24,24,24,24	0
54	MG	2a	3171	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3345	1/1	0.96	0.11	50,50,50,50	0
54	MG	1A	3407	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3482	1/1	0.96	0.05	26,26,26,26	0
54	MG	1A	3280	1/1	0.96	0.26	52,52,52,52	0
54	MG	1a	1643	1/1	0.96	0.19	56,56,56,56	0
54	MG	1A	3225	1/1	0.96	0.13	59,59,59,59	0
54	MG	1E	305	1/1	0.96	0.11	27,27,27,27	0
54	MG	1A	3226	1/1	0.96	0.20	34,34,34,34	0
54	MG	1a	1786	1/1	0.96	0.17	60,60,60,60	0
54	MG	1A	3352	1/1	0.96	0.09	29,29,29,29	0
54	MG	1A	3568	1/1	0.96	0.06	52,52,52,52	0
54	MG	1F	304	1/1	0.96	0.12	34,34,34,34	0
54	MG	1F	308	1/1	0.96	0.18	31,31,31,31	0
54	MG	1F	310	1/1	0.96	0.20	54,54,54,54	0
54	MG	2A	3585	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3569	1/1	0.96	0.11	51,51,51,51	0
54	MG	1a	1793	1/1	0.96	0.06	74,74,74,74	0
54	MG	2a	3190	1/1	0.96	0.10	62,62,62,62	0
54	MG	2Q	203	1/1	0.96	0.10	61,61,61,61	0
54	MG	2A	3049	1/1	0.96	0.16	47,47,47,47	0
54	MG	2A	3217	1/1	0.96	0.08	51,51,51,51	0
54	MG	1A	3659	1/1	0.96	0.11	68,68,68,68	0
54	MG	2A	3594	1/1	0.96	0.10	58,58,58,58	0
54	MG	2A	3051	1/1	0.96	0.10	62,62,62,62	0
54	MG	1A	3106	1/1	0.96	0.19	34,34,34,34	0
54	MG	2W	201	1/1	0.96	0.27	49,49,49,49	0
54	MG	2A	3222	1/1	0.96	0.07	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3223	1/1	0.96	0.27	40,40,40,40	0
54	MG	1A	3571	1/1	0.96	0.19	46,46,46,46	0
54	MG	1a	1797	1/1	0.96	0.10	56,56,56,56	0
54	MG	1a	1798	1/1	0.96	0.07	80,80,80,80	0
54	MG	1A	3663	1/1	0.96	0.07	29,29,29,29	0
54	MG	1A	3998	1/1	0.96	0.09	83,83,83,83	0
54	MG	1a	1661	1/1	0.96	0.12	72,72,72,72	0
54	MG	23	102	1/1	0.96	0.10	48,48,48,48	0
54	MG	1A	3999	1/1	0.96	0.09	62,62,62,62	0
54	MG	2A	3231	1/1	0.96	0.09	41,41,41,41	0
56	MPD	18	104	8/8	0.96	0.12	32,39,43,43	0
54	MG	1A	3413	1/1	0.96	0.06	42,42,42,42	0
54	MG	1A	3107	1/1	0.96	0.24	42,42,42,42	0
54	MG	1A	3285	1/1	0.96	0.10	64,64,64,64	0
54	MG	2A	3419	1/1	0.96	0.15	55,55,55,55	0
54	MG	1a	1666	1/1	0.96	0.10	63,63,63,63	0
54	MG	1A	3417	1/1	0.96	0.09	36,36,36,36	0
54	MG	1A	3184	1/1	0.96	0.18	46,46,46,46	0
54	MG	2A	3423	1/1	0.96	0.23	66,66,66,66	0
54	MG	2A	3139	1/1	0.97	0.15	43,43,43,43	0
54	MG	2A	3140	1/1	0.97	0.17	54,54,54,54	0
54	MG	2a	3024	1/1	0.97	0.19	65,65,65,65	0
54	MG	2A	3296	1/1	0.97	0.10	39,39,39,39	0
54	MG	1N	201	1/1	0.97	0.11	46,46,46,46	0
54	MG	1N	202	1/1	0.97	0.10	42,42,42,42	0
54	MG	1A	3003	1/1	0.97	0.05	27,27,27,27	0
54	MG	2a	3029	1/1	0.97	0.08	40,40,40,40	0
54	MG	1A	3926	1/1	0.97	0.04	66,66,66,66	0
54	MG	1A	3928	1/1	0.97	0.07	56,56,56,56	0
54	MG	1P	201	1/1	0.97	0.25	38,38,38,38	0
54	MG	1A	3929	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3293	1/1	0.97	0.17	49,49,49,49	0
54	MG	2A	3004	1/1	0.97	0.07	45,45,45,45	0
54	MG	1P	204	1/1	0.97	0.17	52,52,52,52	0
54	MG	1A	3588	1/1	0.97	0.10	45,45,45,45	0
54	MG	1A	3743	1/1	0.97	0.10	53,53,53,53	0
54	MG	1Q	201	1/1	0.97	0.12	36,36,36,36	0
54	MG	2A	3665	1/1	0.97	0.09	66,66,66,66	0
54	MG	1A	3185	1/1	0.97	0.12	50,50,50,50	0
54	MG	2A	3312	1/1	0.97	0.14	44,44,44,44	0
54	MG	1A	3590	1/1	0.97	0.10	50,50,50,50	0
54	MG	2a	3044	1/1	0.97	0.21	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2A	3011	1/1	0.97	0.07	41,41,41,41	0
54	MG	1a	1658	1/1	0.97	0.08	72,72,72,72	0
54	MG	2A	3014	1/1	0.97	0.08	49,49,49,49	0
54	MG	2A	3317	1/1	0.97	0.10	53,53,53,53	0
54	MG	2A	3015	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3830	1/1	0.97	0.08	36,36,36,36	0
54	MG	1A	3348	1/1	0.97	0.07	56,56,56,56	0
54	MG	1A	3592	1/1	0.97	0.11	54,54,54,54	0
54	MG	2A	3491	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3939	1/1	0.97	0.05	61,61,61,61	0
54	MG	2A	3323	1/1	0.97	0.10	36,36,36,36	0
54	MG	2A	3020	1/1	0.97	0.16	49,49,49,49	0
54	MG	2A	3021	1/1	0.97	0.07	43,43,43,43	0
54	MG	1A	3085	1/1	0.97	0.15	44,44,44,44	0
54	MG	1A	3296	1/1	0.97	0.11	33,33,33,33	0
54	MG	1A	3057	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3298	1/1	0.97	0.21	60,60,60,60	0
54	MG	1T	202	1/1	0.97	0.08	65,65,65,65	0
54	MG	1A	3127	1/1	0.97	0.29	40,40,40,40	0
54	MG	1A	3533	1/1	0.97	0.05	28,28,28,28	0
54	MG	2A	3029	1/1	0.97	0.07	45,45,45,45	0
54	MG	1A	3046	1/1	0.97	0.18	42,42,42,42	0
54	MG	1A	3301	1/1	0.97	0.26	44,44,44,44	0
54	MG	2A	3506	1/1	0.97	0.08	62,62,62,62	0
54	MG	2A	3338	1/1	0.97	0.10	41,41,41,41	0
54	MG	1U	202	1/1	0.97	0.13	33,33,33,33	0
54	MG	1A	3948	1/1	0.97	0.11	62,62,62,62	0
54	MG	2A	3181	1/1	0.97	0.12	58,58,58,58	0
54	MG	1U	204	1/1	0.97	0.25	40,40,40,40	0
54	MG	1A	3841	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3257	1/1	0.97	0.22	39,39,39,39	0
54	MG	2A	3514	1/1	0.97	0.11	62,62,62,62	0
54	MG	1U	207	1/1	0.97	0.24	40,40,40,40	0
54	MG	1A	3844	1/1	0.97	0.08	47,47,47,47	0
54	MG	1A	3218	1/1	0.97	0.06	43,43,43,43	0
54	MG	2A	3040	1/1	0.97	0.11	44,44,44,44	0
54	MG	2a	3082	1/1	0.97	0.06	80,80,80,80	0
54	MG	1A	3219	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3220	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3019	1/1	0.97	0.21	33,33,33,33	0
54	MG	1A	3132	1/1	0.97	0.07	51,51,51,51	0
54	MG	1A	3419	1/1	0.97	0.05	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
54	MG	1A	3609	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3680	1/1	0.97	0.11	57,57,57,57	0
54	MG	1A	3855	1/1	0.97	0.12	50,50,50,50	0
54	MG	2A	3719	1/1	0.97	0.09	66,66,66,66	0
54	MG	1A	3263	1/1	0.97	0.20	38,38,38,38	0
54	MG	10	103	1/1	0.97	0.13	52,52,52,52	0
54	MG	10	104	1/1	0.97	0.09	50,50,50,50	0
54	MG	1A	3311	1/1	0.97	0.17	55,55,55,55	0
54	MG	2A	3201	1/1	0.97	0.20	56,56,56,56	0
54	MG	1a	1692	1/1	0.97	0.11	66,66,66,66	0
54	MG	1a	1819	1/1	0.97	0.07	61,61,61,61	0
54	MG	1A	3223	1/1	0.97	0.16	41,41,41,41	0
54	MG	2A	3537	1/1	0.97	0.06	63,63,63,63	0
54	MG	1A	3016	1/1	0.97	0.26	38,38,38,38	0
54	MG	1A	3488	1/1	0.97	0.09	33,33,33,33	0
54	MG	11	102	1/1	0.97	0.07	59,59,59,59	0
54	MG	2a	3104	1/1	0.97	0.09	81,81,81,81	0
54	MG	2A	3541	1/1	0.97	0.07	64,64,64,64	0
54	MG	1A	3134	1/1	0.97	0.10	38,38,38,38	0
54	MG	2A	3373	1/1	0.97	0.06	62,62,62,62	0
54	MG	1A	3490	1/1	0.97	0.06	63,63,63,63	0
54	MG	1A	3776	1/1	0.97	0.05	45,45,45,45	0
54	MG	1A	3315	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3971	1/1	0.97	0.12	45,45,45,45	0
54	MG	1A	3049	1/1	0.97	0.22	40,40,40,40	0
54	MG	2A	3214	1/1	0.97	0.07	49,49,49,49	0
54	MG	1a	1830	1/1	0.97	0.11	64,64,64,64	0
54	MG	1A	3493	1/1	0.97	0.07	40,40,40,40	0
54	MG	1A	3695	1/1	0.97	0.12	48,48,48,48	0
54	MG	1A	3228	1/1	0.97	0.28	44,44,44,44	0
54	MG	2A	3219	1/1	0.97	0.07	51,51,51,51	0
54	MG	2A	3069	1/1	0.97	0.10	55,55,55,55	0
54	MG	1A	3697	1/1	0.97	0.05	61,61,61,61	0
54	MG	1a	1707	1/1	0.97	0.08	45,45,45,45	0
54	MG	15	103	1/1	0.97	0.30	43,43,43,43	0
54	MG	1A	3698	1/1	0.97	0.19	50,50,50,50	0
54	MG	1A	3556	1/1	0.97	0.09	64,64,64,64	0
54	MG	1a	1839	1/1	0.97	0.09	55,55,55,55	0
54	MG	1a	1840	1/1	0.97	0.05	64,64,64,64	0
54	MG	2a	3132	1/1	0.97	0.08	52,52,52,52	0
54	MG	1A	3229	1/1	0.97	0.23	40,40,40,40	0
54	MG	2A	3566	1/1	0.97	0.10	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3137	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3168	1/1	0.97	0.09	33,33,33,33	0
54	MG	1A	3233	1/1	0.97	0.27	38,38,38,38	0
54	MG	2B	218	1/1	0.97	0.07	55,55,55,55	0
54	MG	2a	3140	1/1	0.97	0.07	72,72,72,72	0
54	MG	2A	3082	1/1	0.97	0.50	49,49,49,49	0
54	MG	2A	3398	1/1	0.97	0.17	66,66,66,66	0
54	MG	17	104	1/1	0.97	0.11	38,38,38,38	0
54	MG	1A	3322	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3705	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3706	1/1	0.97	0.09	53,53,53,53	0
54	MG	1A	3885	1/1	0.97	0.06	44,44,44,44	0
54	MG	1D	301	1/1	0.97	0.29	44,44,44,44	0
54	MG	2A	3239	1/1	0.97	0.48	46,46,46,46	0
54	MG	2a	3150	1/1	0.97	0.06	78,78,78,78	0
54	MG	1A	3062	1/1	0.97	0.12	44,44,44,44	0
54	MG	2a	3152	1/1	0.97	0.10	57,57,57,57	0
54	MG	1a	1854	1/1	0.97	0.06	62,62,62,62	0
54	MG	1A	3031	1/1	0.97	0.08	22,22,22,22	0
54	MG	1A	3051	1/1	0.97	0.33	36,36,36,36	0
54	MG	1A	3382	1/1	0.97	0.06	50,50,50,50	0
54	MG	2E	303	1/1	0.97	0.09	47,47,47,47	0
54	MG	1A	3276	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3097	1/1	0.97	0.19	36,36,36,36	0
54	MG	2E	306	1/1	0.97	0.10	32,32,32,32	0
54	MG	1A	3714	1/1	0.97	0.04	39,39,39,39	0
54	MG	2a	3163	1/1	0.97	0.05	71,71,71,71	0
54	MG	2A	3248	1/1	0.97	0.11	57,57,57,57	0
54	MG	2F	302	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3239	1/1	0.97	0.19	37,37,37,37	0
54	MG	2F	304	1/1	0.97	0.17	46,46,46,46	0
54	MG	1A	3240	1/1	0.97	0.17	64,64,64,64	0
54	MG	1A	3802	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3717	1/1	0.97	0.07	48,48,48,48	0
54	MG	1E	302	1/1	0.97	0.09	41,41,41,41	0
54	MG	1A	3176	1/1	0.97	0.28	46,46,46,46	0
54	MG	1A	3203	1/1	0.97	0.17	40,40,40,40	0
54	MG	2Q	201	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3177	1/1	0.97	0.24	53,53,53,53	0
54	MG	1A	3807	1/1	0.97	0.04	57,57,57,57	0
54	MG	2A	3424	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3333	1/1	0.97	0.14	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3334	1/1	0.97	0.05	28,28,28,28	0
54	MG	2T	202	1/1	0.97	0.19	68,68,68,68	0
54	MG	2A	3427	1/1	0.97	0.11	37,37,37,37	0
54	MG	2A	3609	1/1	0.97	0.14	62,62,62,62	0
54	MG	1F	303	1/1	0.97	0.16	34,34,34,34	0
54	MG	1A	3021	1/1	0.97	0.09	41,41,41,41	0
54	MG	2A	3263	1/1	0.97	0.07	52,52,52,52	0
54	MG	2A	3431	1/1	0.97	0.05	52,52,52,52	0
54	MG	1a	1747	1/1	0.97	0.10	54,54,54,54	0
54	MG	2A	3265	1/1	0.97	0.06	32,32,32,32	0
54	MG	1F	306	1/1	0.97	0.17	38,38,38,38	0
54	MG	2A	3267	1/1	0.97	0.08	52,52,52,52	0
54	MG	1F	307	1/1	0.97	0.06	37,37,37,37	0
54	MG	1a	1622	1/1	0.97	0.04	48,48,48,48	0
54	MG	1A	3336	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3099	1/1	0.97	0.21	36,36,36,36	0
54	MG	1A	3726	1/1	0.97	0.07	52,52,52,52	0
54	MG	1e	201	1/1	0.97	0.08	59,59,59,59	0
54	MG	1e	202	1/1	0.97	0.07	68,68,68,68	0
54	MG	1A	4010	1/1	0.97	0.04	54,54,54,54	0
54	MG	2A	3626	1/1	0.97	0.04	60,60,60,60	0
54	MG	2k	201	1/1	0.97	0.09	57,57,57,57	0
54	MG	1a	1627	1/1	0.97	0.06	52,52,52,52	0
54	MG	1A	3814	1/1	0.97	0.07	44,44,44,44	0
54	MG	1A	3041	1/1	0.97	0.05	23,23,23,23	0
54	MG	1A	3287	1/1	0.97	0.10	18,18,18,18	0
54	MG	1A	3341	1/1	0.97	0.10	34,34,34,34	0
54	MG	1A	3582	1/1	0.97	0.09	28,28,28,28	0
54	MG	1a	1633	1/1	0.97	0.09	47,47,47,47	0
54	MG	1A	3734	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3026	1/1	0.97	0.18	32,32,32,32	0
54	MG	2a	3013	1/1	0.97	0.19	54,54,54,54	0
54	MG	1A	4018	1/1	0.97	0.07	50,50,50,50	0
54	MG	1A	3151	1/1	0.97	0.07	41,41,41,41	0
54	MG	2A	3133	1/1	0.97	0.06	51,51,51,51	0
54	MG	2a	3017	1/1	0.97	0.06	58,58,58,58	0
54	MG	1A	3083	1/1	0.97	0.08	46,46,46,46	0
54	MG	1A	3923	1/1	0.97	0.07	57,57,57,57	0
54	MG	1H	202	1/1	0.97	0.09	59,59,59,59	0
58	ZN	2Y	202	1/1	0.97	0.05	97,97,97,97	0
54	MG	1A	3652	1/1	0.97	0.05	39,39,39,39	0
58	ZN	2n	102	1/1	0.97	0.06	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1D	304	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3252	1/1	0.98	0.17	31,31,31,31	0
54	MG	1D	306	1/1	0.98	0.08	17,17,17,17	0
54	MG	2a	3081	1/1	0.98	0.06	74,74,74,74	0
54	MG	1D	307	1/1	0.98	0.04	40,40,40,40	0
54	MG	1D	308	1/1	0.98	0.10	33,33,33,33	0
54	MG	1A	3661	1/1	0.98	0.06	31,31,31,31	0
54	MG	1D	310	1/1	0.98	0.22	29,29,29,29	0
54	MG	1A	3013	1/1	0.98	0.04	26,26,26,26	0
54	MG	1a	1862	1/1	0.98	0.05	65,65,65,65	0
54	MG	1A	3455	1/1	0.98	0.06	31,31,31,31	0
54	MG	1a	1864	1/1	0.98	0.06	62,62,62,62	0
54	MG	2A	3169	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3861	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3042	1/1	0.98	0.19	29,29,29,29	0
54	MG	2A	3638	1/1	0.98	0.08	40,40,40,40	0
54	MG	1A	3114	1/1	0.98	0.12	33,33,33,33	0
54	MG	2A	3641	1/1	0.98	0.07	63,63,63,63	0
54	MG	1A	3727	1/1	0.98	0.04	71,71,71,71	0
54	MG	1A	3033	1/1	0.98	0.06	48,48,48,48	0
54	MG	1A	3292	1/1	0.98	0.06	51,51,51,51	0
54	MG	1E	301	1/1	0.98	0.18	45,45,45,45	0
54	MG	2A	3646	1/1	0.98	0.11	59,59,59,59	0
54	MG	1A	4021	1/1	0.98	0.07	30,30,30,30	0
54	MG	1A	3668	1/1	0.98	0.04	47,47,47,47	0
54	MG	2A	3070	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3650	1/1	0.98	0.09	57,57,57,57	0
54	MG	2A	3288	1/1	0.98	0.07	35,35,35,35	0
54	MG	1A	3135	1/1	0.98	0.14	26,26,26,26	0
54	MG	1A	3732	1/1	0.98	0.05	57,57,57,57	0
54	MG	1A	3162	1/1	0.98	0.23	42,42,42,42	0
54	MG	1A	3373	1/1	0.98	0.11	36,36,36,36	0
54	MG	1E	308	1/1	0.98	0.07	62,62,62,62	0
54	MG	1A	3514	1/1	0.98	0.07	27,27,27,27	0
54	MG	1d	302	1/1	0.98	0.16	65,65,65,65	0
54	MG	2R	201	1/1	0.98	0.19	49,49,49,49	0
54	MG	1F	301	1/1	0.98	0.13	39,39,39,39	0
54	MG	1A	3415	1/1	0.98	0.04	31,31,31,31	0
54	MG	1A	3055	1/1	0.98	0.09	51,51,51,51	0
54	MG	2A	3662	1/1	0.98	0.04	57,57,57,57	0
54	MG	1F	305	1/1	0.98	0.06	38,38,38,38	0
54	MG	1A	3375	1/1	0.98	0.09	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	2V	202	1/1	0.98	0.12	44,44,44,44	0
54	MG	1A	3877	1/1	0.98	0.05	46,46,46,46	0
54	MG	2A	3534	1/1	0.98	0.04	69,69,69,69	0
54	MG	17	101	1/1	0.98	0.10	38,38,38,38	0
54	MG	2A	3668	1/1	0.98	0.04	44,44,44,44	0
54	MG	2X	101	1/1	0.98	0.07	58,58,58,58	0
54	MG	2a	3129	1/1	0.98	0.05	65,65,65,65	0
54	MG	2a	3130	1/1	0.98	0.06	70,70,70,70	0
54	MG	2A	3303	1/1	0.98	0.06	27,27,27,27	0
54	MG	17	102	1/1	0.98	0.12	43,43,43,43	0
54	MG	2a	3133	1/1	0.98	0.05	76,76,76,76	0
54	MG	2A	3671	1/1	0.98	0.07	64,64,64,64	0
54	MG	1A	3068	1/1	0.98	0.05	31,31,31,31	0
54	MG	1F	309	1/1	0.98	0.15	34,34,34,34	0
54	MG	1A	3227	1/1	0.98	0.11	29,29,29,29	0
54	MG	1F	311	1/1	0.98	0.06	37,37,37,37	0
54	MG	17	107	1/1	0.98	0.06	52,52,52,52	0
54	MG	1A	3881	1/1	0.98	0.05	42,42,42,42	0
54	MG	1A	3742	1/1	0.98	0.04	23,23,23,23	0
54	MG	1A	3165	1/1	0.98	0.06	40,40,40,40	0
54	MG	1A	3744	1/1	0.98	0.09	53,53,53,53	0
54	MG	1A	3138	1/1	0.98	0.17	39,39,39,39	0
54	MG	1A	3623	1/1	0.98	0.06	47,47,47,47	0
54	MG	2A	3549	1/1	0.98	0.04	25,25,25,25	0
54	MG	1A	3044	1/1	0.98	0.05	31,31,31,31	0
54	MG	1A	3966	1/1	0.98	0.09	49,49,49,49	0
54	MG	1A	3573	1/1	0.98	0.06	48,48,48,48	0
54	MG	1A	3231	1/1	0.98	0.20	39,39,39,39	0
54	MG	2A	3435	1/1	0.98	0.05	59,59,59,59	0
54	MG	1A	3009	1/1	0.98	0.05	35,35,35,35	0
54	MG	2a	3011	1/1	0.98	0.08	49,49,49,49	0
54	MG	1A	3169	1/1	0.98	0.15	31,31,31,31	0
54	MG	2A	3103	1/1	0.98	0.06	30,30,30,30	0
54	MG	1A	3687	1/1	0.98	0.14	31,31,31,31	0
54	MG	1A	3234	1/1	0.98	0.12	31,31,31,31	0
54	MG	2A	3325	1/1	0.98	0.10	34,34,34,34	0
54	MG	2A	3697	1/1	0.98	0.05	68,68,68,68	0
54	MG	1a	1610	1/1	0.98	0.33	56,56,56,56	0
54	MG	2A	3562	1/1	0.98	0.05	62,62,62,62	0
54	MG	2a	3162	1/1	0.98	0.07	79,79,79,79	0
54	MG	1A	3141	1/1	0.98	0.15	37,37,37,37	0
54	MG	1A	3690	1/1	0.98	0.05	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3307	1/1	0.98	0.21	40,40,40,40	0
54	MG	2A	3703	1/1	0.98	0.07	55,55,55,55	0
54	MG	1A	3897	1/1	0.98	0.03	32,32,32,32	0
54	MG	1N	204	1/1	0.98	0.04	55,55,55,55	0
54	MG	1A	3977	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3001	1/1	0.98	0.04	40,40,40,40	0
54	MG	1A	3143	1/1	0.98	0.05	40,40,40,40	0
54	MG	2A	3335	1/1	0.98	0.06	37,37,37,37	0
54	MG	2A	3572	1/1	0.98	0.08	41,41,41,41	0
54	MG	2A	3573	1/1	0.98	0.05	58,58,58,58	0
54	MG	1A	3028	1/1	0.98	0.28	33,33,33,33	0
54	MG	1A	3349	1/1	0.98	0.07	28,28,28,28	0
54	MG	2A	3454	1/1	0.98	0.04	47,47,47,47	0
54	MG	2A	3013	1/1	0.98	0.07	26,26,26,26	0
54	MG	1A	3350	1/1	0.98	0.04	37,37,37,37	0
54	MG	1A	3762	1/1	0.98	0.14	38,38,38,38	0
54	MG	1A	3174	1/1	0.98	0.12	36,36,36,36	0
54	MG	1a	1721	1/1	0.98	0.12	63,63,63,63	0
54	MG	2A	3583	1/1	0.98	0.06	71,71,71,71	0
54	MG	2a	3184	1/1	0.98	0.06	58,58,58,58	0
54	MG	1A	3175	1/1	0.98	0.17	36,36,36,36	0
54	MG	1A	3436	1/1	0.98	0.04	34,34,34,34	0
54	MG	2A	3586	1/1	0.98	0.08	73,73,73,73	0
54	MG	1A	3122	1/1	0.98	0.05	67,67,67,67	0
54	MG	1a	1725	1/1	0.98	0.05	62,62,62,62	0
54	MG	1A	3146	1/1	0.98	0.31	39,39,39,39	0
54	MG	1A	3007	1/1	0.98	0.09	43,43,43,43	0
54	MG	1R	201	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3091	1/1	0.98	0.05	24,24,24,24	0
54	MG	1A	3149	1/1	0.98	0.17	50,50,50,50	0
54	MG	1A	3442	1/1	0.98	0.05	18,18,18,18	0
54	MG	1B	212	1/1	0.98	0.08	47,47,47,47	0
54	MG	1A	3004	1/1	0.98	0.06	41,41,41,41	0
54	MG	1A	3919	1/1	0.98	0.04	19,19,19,19	0
54	MG	2A	3358	1/1	0.98	0.07	42,42,42,42	0
54	MG	1A	3708	1/1	0.98	0.04	37,37,37,37	0
54	MG	1a	1736	1/1	0.98	0.06	67,67,67,67	0
54	MG	1A	3545	1/1	0.98	0.07	44,44,44,44	0
54	MG	1a	1738	1/1	0.98	0.05	56,56,56,56	0
54	MG	1A	3842	1/1	0.98	0.04	33,33,33,33	0
54	MG	1A	3108	1/1	0.98	0.07	42,42,42,42	0
54	MG	2A	3481	1/1	0.98	0.07	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
54	MG	1A	3597	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3445	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	3018	1/1	0.98	0.15	28,28,28,28	0
54	MG	1A	3040	1/1	0.98	0.09	35,35,35,35	0
54	MG	1A	3129	1/1	0.98	0.15	35,35,35,35	0
54	MG	1A	3850	1/1	0.98	0.08	44,44,44,44	0
54	MG	1A	3655	1/1	0.98	0.06	39,39,39,39	0
54	MG	2A	3257	1/1	0.98	0.08	21,21,21,21	0
54	MG	1A	3156	1/1	0.98	0.14	39,39,39,39	0
54	MG	1V	202	1/1	0.98	0.15	35,35,35,35	0
54	MG	1A	3286	1/1	0.98	0.07	22,22,22,22	0
58	ZN	1Y	501	1/1	0.98	0.04	58,58,58,58	0
54	MG	1a	1651	1/1	0.98	0.07	46,46,46,46	0
58	ZN	15	109	1/1	0.98	0.04	61,61,61,61	0
54	MG	1A	3658	1/1	0.98	0.05	54,54,54,54	0
54	MG	1A	3553	1/1	0.98	0.17	59,59,59,59	0
58	ZN	26	501	1/1	0.98	0.03	67,67,67,67	0
58	ZN	29	501	1/1	0.98	0.04	76,76,76,76	0
54	MG	2A	3157	1/1	0.98	0.18	54,54,54,54	0
59	SF4	1d	306	8/8	0.98	0.05	60,71,79,80	0
59	SF4	2d	302	8/8	0.98	0.05	71,83,87,87	0
54	MG	2A	3135	1/1	0.99	0.09	43,43,43,43	0
54	MG	2A	3527	1/1	0.99	0.07	54,54,54,54	0
54	MG	2A	3691	1/1	0.99	0.03	51,51,51,51	0
54	MG	1A	3302	1/1	0.99	0.07	47,47,47,47	0
54	MG	1B	223	1/1	0.99	0.06	58,58,58,58	0
54	MG	2A	3581	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3901	1/1	0.99	0.04	43,43,43,43	0
54	MG	1A	3902	1/1	0.99	0.06	28,28,28,28	0
54	MG	2A	3639	1/1	0.99	0.06	42,42,42,42	0
54	MG	1A	3110	1/1	0.99	0.13	35,35,35,35	0
54	MG	2A	3282	1/1	0.99	0.06	53,53,53,53	0
54	MG	2A	3141	1/1	0.99	0.07	61,61,61,61	0
54	MG	2a	3118	1/1	0.99	0.04	56,56,56,56	0
54	MG	2A	3587	1/1	0.99	0.04	46,46,46,46	0
54	MG	1A	3789	1/1	0.99	0.03	29,29,29,29	0
54	MG	2a	3121	1/1	0.99	0.10	67,67,67,67	0
54	MG	1A	3104	1/1	0.99	0.14	37,37,37,37	0
54	MG	1A	3089	1/1	0.99	0.04	42,42,42,42	0
54	MG	2a	3124	1/1	0.99	0.03	80,80,80,80	0
54	MG	1A	3090	1/1	0.99	0.16	26,26,26,26	0
54	MG	2A	3592	1/1	0.99	0.04	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1D	302	1/1	0.99	0.05	55,55,55,55	0
54	MG	1A	3069	1/1	0.99	0.07	35,35,35,35	0
54	MG	1A	3153	1/1	0.99	0.15	38,38,38,38	0
54	MG	1A	3847	1/1	0.99	0.03	26,26,26,26	0
54	MG	1A	3470	1/1	0.99	0.04	48,48,48,48	0
54	MG	1A	3912	1/1	0.99	0.03	49,49,49,49	0
54	MG	1A	3006	1/1	0.99	0.04	25,25,25,25	0
54	MG	1A	3472	1/1	0.99	0.03	57,57,57,57	0
54	MG	2A	3601	1/1	0.99	0.04	46,46,46,46	0
54	MG	1A	3473	1/1	0.99	0.06	39,39,39,39	0
54	MG	1A	3773	1/1	0.99	0.05	43,43,43,43	0
54	MG	1A	3774	1/1	0.99	0.05	43,43,43,43	0
54	MG	1A	3200	1/1	0.99	0.23	39,39,39,39	0
54	MG	1a	1841	1/1	0.99	0.03	63,63,63,63	0
54	MG	1A	3684	1/1	0.99	0.04	61,61,61,61	0
54	MG	1a	1716	1/1	0.99	0.06	46,46,46,46	0
54	MG	1A	3529	1/1	0.99	0.03	25,25,25,25	0
54	MG	1a	1718	1/1	0.99	0.09	40,40,40,40	0
54	MG	2A	3353	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3130	1/1	0.99	0.32	35,35,35,35	0
54	MG	1A	3858	1/1	0.99	0.11	39,39,39,39	0
54	MG	1A	3626	1/1	0.99	0.08	29,29,29,29	0
54	MG	1A	3212	1/1	0.99	0.11	33,33,33,33	0
54	MG	1A	3733	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3073	1/1	0.99	0.06	42,42,42,42	0
54	MG	1a	1852	1/1	0.99	0.08	40,40,40,40	0
54	MG	1B	213	1/1	0.99	0.04	39,39,39,39	0
54	MG	1A	3927	1/1	0.99	0.07	56,56,56,56	0
54	MG	1A	3461	1/1	0.99	0.03	52,52,52,52	0
54	MG	1A	3691	1/1	0.99	0.03	36,36,36,36	0
54	MG	1A	3865	1/1	0.99	0.06	55,55,55,55	0
54	MG	1a	1648	1/1	0.99	0.13	51,51,51,51	0
54	MG	2A	3129	1/1	0.99	0.04	33,33,33,33	0
58	ZN	19	103	1/1	0.99	0.03	50,50,50,50	0
58	ZN	1n	104	1/1	0.99	0.03	77,77,77,77	0
54	MG	2A	3369	1/1	0.99	0.04	51,51,51,51	0
54	MG	1A	3479	1/1	0.99	0.06	42,42,42,42	0
58	ZN	25	102	1/1	0.99	0.03	71,71,71,71	0
54	MG	1A	3447	1/1	0.99	0.04	32,32,32,32	0
54	MG	2A	3685	1/1	0.99	0.04	47,47,47,47	0
54	MG	1F	302	1/1	0.99	0.05	34,34,34,34	0
54	MG	1A	3898	1/1	0.99	0.04	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MG	1A	3899	1/1	0.99	0.07	41,41,41,41	0
54	MG	2A	3357	1/1	1.00	0.05	34,34,34,34	0
54	MG	1A	3978	1/1	1.00	0.04	33,33,33,33	0
54	MG	1A	3879	1/1	1.00	0.07	35,35,35,35	0
54	MG	1A	3931	1/1	1.00	0.04	47,47,47,47	0
54	MG	2A	3475	1/1	1.00	0.08	37,37,37,37	0
58	ZN	16	501	1/1	1.00	0.05	48,48,48,48	0
54	MG	1A	3338	1/1	1.00	0.05	34,34,34,34	0
54	MG	1A	3454	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.