



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:06 am BST

PDB ID : 6ND5
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with chloramphenicol and bound to mRNA and A-, P-, and E-site tRNAs at 2.60Å resolution
Authors : Svetlov, M.S.; Plessa, E.; Chen, C.-W.; Bougas, A.; Krokidis, M.G.; Dinos, G.P.; Polikanov, Y.S.
Deposited on : 2018-12-13
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

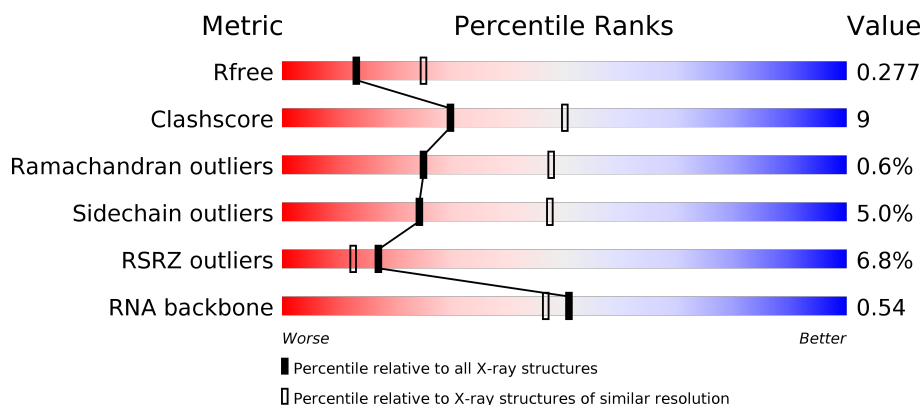
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 on 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	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>31%</div> <div>7%</div> <div></div> </div> <div></div> </div>
1	2A	2915	<div> <div>2%</div> <div> <div></div> <div>54%</div> <div>35%</div> <div>7%</div> <div></div> </div> <div></div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>74%</div> <div>21%</div> <div></div> </div> <div></div> </div>
2	2B	121	<div> <div></div> <div> <div></div> <div>42%</div> <div>45%</div> <div>12%</div> <div></div> </div> <div></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1D	276	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
3	2D	276	<div> <div>4%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
4	1E	206	<div> <div>%</div> <div>78%</div> <div>17%</div> <div>..</div> </div>
4	2E	206	<div> <div>3%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
5	1F	210	<div> <div>64%</div> <div>29%</div> <div>.</div> <div>.</div> </div>
5	2F	210	<div> <div>3%</div> <div>68%</div> <div>25%</div> <div>.</div> <div>.</div> </div>
6	1G	182	<div> <div>%</div> <div>73%</div> <div>24%</div> <div>...</div> </div>
6	2G	182	<div> <div>13%</div> <div>64%</div> <div>32%</div> <div>.</div> <div>..</div> </div>
7	1H	180	<div> <div>72%</div> <div>24%</div> <div>.</div> <div>.</div> </div>
7	2H	180	<div> <div>26%</div> <div>64%</div> <div>32%</div> <div>.</div> <div>.</div> </div>
8	1I	148	<div> <div>%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>
8	2I	148	<div> <div>7%</div> <div>73%</div> <div>22%</div> <div>..</div> </div>
9	1N	140	<div> <div>%</div> <div>81%</div> <div>19%</div> <div>.</div> </div>
9	2N	140	<div> <div>21%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>
10	1O	122	<div> <div>84%</div> <div>16%</div> <div>.</div> </div>
10	2O	122	<div> <div>4%</div> <div>65%</div> <div>34%</div> <div>.</div> </div>
11	1P	150	<div> <div>3%</div> <div>68%</div> <div>30%</div> <div>..</div> </div>
11	2P	150	<div> <div>30%</div> <div>75%</div> <div>23%</div> <div>..</div> </div>
12	1Q	141	<div> <div>%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
12	2Q	141	<div> <div>11%</div> <div>77%</div> <div>23%</div> <div>.</div> </div>
13	1R	118	<div> <div>70%</div> <div>25%</div> <div>.</div> </div>
13	2R	118	<div> <div>69%</div> <div>26%</div> <div>.</div> </div>
14	1S	112	<div> <div>80%</div> <div>15%</div> <div>..</div> </div>
14	2S	112	<div> <div>9%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
15	1T	146	<div> <div>69%</div> <div>20%</div> <div>10%</div> <div>.</div> </div>



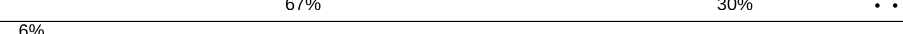


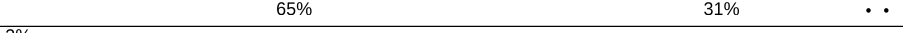

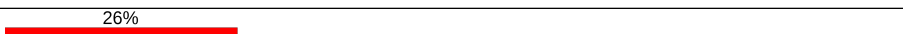





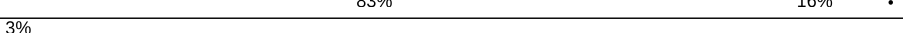


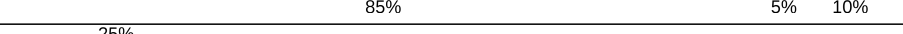




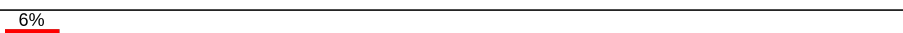


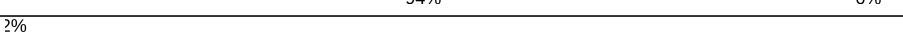
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	PSU	2y	55	-	-	-	X
56	MG	1A	3411	-	-	-	X
56	MG	1A	3489	-	-	-	X
56	MG	1A	3503	-	-	-	X
56	MG	2A	3040	-	-	-	X
56	MG	2A	3243	-	-	-	X
56	MG	2A	3382	-	-	-	X
56	MG	2A	3812	-	-	-	X
56	MG	2a	3031	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300833 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total 1592	C 713	N 285	O 518	P 74	S 2	0	0	0
54	1y	74	Total 1585	C 707	N 285	O 518	P 74	S 1	0	0	0
54	2w	72	Total 1544	C 690	N 278	O 502	P 72	S 2	0	0	0
54	2y	73	Total 1565	C 698	N 283	O 510	P 73	S 1	0	0	0

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	4	Total	Mg	0	0
			4	4		
56	17	8	Total	Mg	0	0
			8	8		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	4	Total	Mg	0	0
			4	4		
56	1N	6	Total	Mg	0	0
			6	6		
56	20	3	Total	Mg	0	0
			3	3		
56	18	7	Total	Mg	0	0
			7	7		
56	2W	3	Total	Mg	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	3	Total 3	Mg 3	0	0
56	13	3	Total 3	Mg 3	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1P	9	Total 9	Mg 9	0	0
56	2B	20	Total 20	Mg 20	0	0
56	23	3	Total 3	Mg 3	0	0
56	1E	15	Total 15	Mg 15	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	4	Total 4	Mg 4	0	0
56	2F	6	Total 6	Mg 6	0	0
56	16	3	Total 3	Mg 3	0	0
56	28	3	Total 3	Mg 3	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1A	1101	Total 1101	Mg 1101	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	2P	4	Total 4	Mg 4	0	0
56	1X	5	Total 5	Mg 5	0	0
56	2q	2	Total 2	Mg 2	0	0
56	12	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2i	1	Total Mg 1 1	0	0
56	1S	3	Total Mg 3 3	0	0
56	25	5	Total Mg 5 5	0	0
56	2T	4	Total Mg 4 4	0	0
56	1D	13	Total Mg 13 13	0	0
56	2N	1	Total Mg 1 1	0	0
56	1e	2	Total Mg 2 2	0	0
56	2m	1	Total Mg 1 1	0	0
56	2G	1	Total Mg 1 1	0	0
56	1I	1	Total Mg 1 1	0	0
56	2f	2	Total Mg 2 2	0	0
56	1V	7	Total Mg 7 7	0	0
56	2X	1	Total Mg 1 1	0	0
56	1w	12	Total Mg 12 12	0	0
56	1a	233	Total Mg 233 233	0	0
56	2Q	4	Total Mg 4 4	0	0
56	15	5	Total Mg 5 5	0	0
56	1x	18	Total Mg 18 18	0	0
56	2j	1	Total Mg 1 1	0	0
56	1R	3	Total Mg 3 3	0	0
56	1s	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

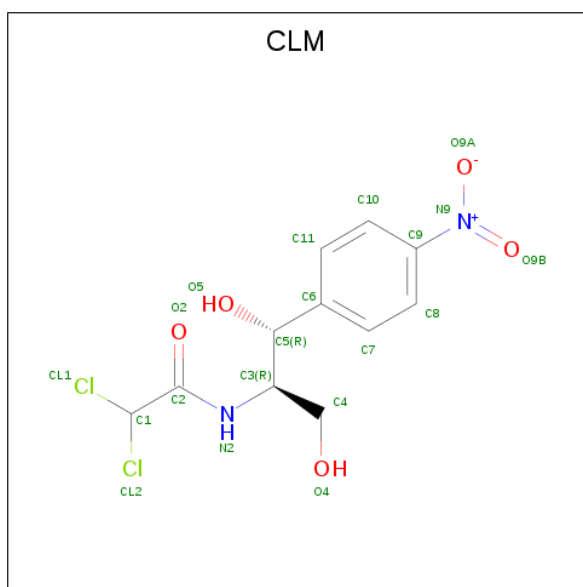
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1m	2	Total 2	Mg 2	0	0
56	2U	3	Total 3	Mg 3	0	0
56	1G	4	Total 4	Mg 4	0	0
56	2O	1	Total 1	Mg 1	0	0
56	1l	5	Total 5	Mg 5	0	0
56	1d	1	Total 1	Mg 1	0	0
56	2r	1	Total 1	Mg 1	0	0
56	2l	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2x	5	Total 5	Mg 5	0	0
56	2R	2	Total 2	Mg 2	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	2D	10	Total 10	Mg 10	0	0
56	14	1	Total 1	Mg 1	0	0
56	2k	1	Total 1	Mg 1	0	0
56	1U	12	Total 12	Mg 12	0	0
56	1O	5	Total 5	Mg 5	0	0
56	27	2	Total 2	Mg 2	0	0
56	19	1	Total 1	Mg 1	0	0
56	1l	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2V	3	Total 3	Mg 3	0	0
56	1F	10	Total 10	Mg 10	0	0
56	10	6	Total 6	Mg 6	0	0
56	2t	1	Total 1	Mg 1	0	0
56	1Q	8	Total 8	Mg 8	0	0
56	2A	887	Total 887	Mg 887	0	0
56	2v	1	Total 1	Mg 1	0	0
56	1h	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	1B	39	Total 39	Mg 39	0	0
56	2y	6	Total 6	Mg 6	0	0
56	2w	4	Total 4	Mg 4	0	0
56	2a	241	Total 241	Mg 241	0	0

- Molecule 57 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
57	1A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
57	2A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1	Total	K	0	0
			1	1		
58	2A	1	Total	K	0	0
			1	1		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

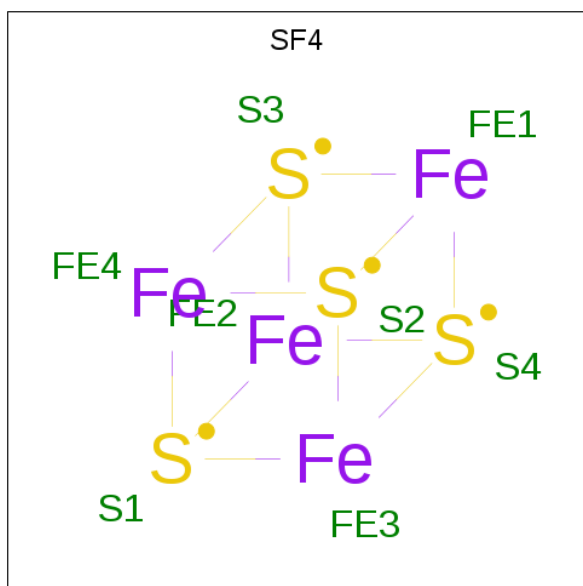
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	4	Total	O	0	0
			4	4		
61	1A	1	Total	O	0	0
			1	1		
61	1A	5	Total	O	0	0
			5	5		
61	1A	1	Total	O	0	0
			1	1		
61	1A	4	Total	O	0	0
			4	4		
61	1A	1	Total	O	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2	Total	O	0	0
			2	2		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	6	Total	O	0	0
			6	6		
61	1A	3	Total	O	0	0
			3	3		
61	1A	4	Total	O	0	0
			4	4		
61	1A	1	Total	O	0	0
			1	1		
61	1A	5	Total	O	0	0
			5	5		
61	1A	2	Total	O	0	0
			2	2		
61	1A	2	Total	O	0	0
			2	2		
61	1A	4	Total	O	0	0
			4	4		
61	1A	2	Total	O	0	0
			2	2		
61	1A	1	Total	O	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	5	Total 5	O 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	3	Total	O	0	0
			3	3		
61	1A	3	Total	O	0	0
			3	3		
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	3	Total	O	0	0
			3	3		
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	4	Total	O	0	0
			4	4		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	6	Total	O	0	0
			6	6		
61	1A	4	Total	O	0	0
			4	4		
61	1A	5	Total	O	0	0
			5	5		
61	1A	5	Total	O	0	0
			5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	4	Total 4	O 4	0	0
61	1A	3	Total 3	O 3	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	5	Total 5	O 5	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1	Total 1	O 1	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	2	Total 2	O 2	0	0
61	1A	1	Total 1	O 1	0	0
61	1A	6	Total 6	O 6	0	0
61	1A	500	Total 500	O 500	0	0
61	1B	3	Total 3	O 3	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	5	Total 5	O 5	0	0
61	1B	4	Total 4	O 4	0	0
61	1B	3	Total 3	O 3	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1B	1	Total 1	O 1	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	6	Total 6	O 6	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	3	Total 3	O 3	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	2	Total 2	O 2	0	0
61	1B	1	Total 1	O 1	0	0
61	1B	3	Total 3	O 3	0	0
61	1B	5	Total 5	O 5	0	0
61	1B	16	Total 16	O 16	0	0
61	1D	5	Total 5	O 5	0	0
61	1D	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1D	1	Total 1	O 1	0	0
61	1D	1	Total 1	O 1	0	0
61	1D	15	Total 15	O 15	0	0
61	1E	2	Total 2	O 2	0	0
61	1E	2	Total 2	O 2	0	0
61	1E	2	Total 2	O 2	0	0
61	1E	2	Total 2	O 2	0	0
61	1E	6	Total 6	O 6	0	0
61	1E	13	Total 13	O 13	0	0
61	1F	1	Total 1	O 1	0	0
61	1F	8	Total 8	O 8	0	0
61	1G	2	Total 2	O 2	0	0
61	1G	3	Total 3	O 3	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	2	Total 2	O 2	0	0
61	1N	4	Total 4	O 4	0	0
61	1O	2	Total 2	O 2	0	0
61	1O	1	Total 1	O 1	0	0
61	1O	4	Total 4	O 4	0	0
61	1P	5	Total 5	O 5	0	0
61	1P	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1P	2	Total 2	O 2	0	0
61	1P	1	Total 1	O 1	0	0
61	1P	6	Total 6	O 6	0	0
61	1P	5	Total 5	O 5	0	0
61	1Q	6	Total 6	O 6	0	0
61	1Q	1	Total 1	O 1	0	0
61	1Q	4	Total 4	O 4	0	0
61	1R	1	Total 1	O 1	0	0
61	1R	7	Total 7	O 7	0	0
61	1S	2	Total 2	O 2	0	0
61	1S	2	Total 2	O 2	0	0
61	1T	1	Total 1	O 1	0	0
61	1T	1	Total 1	O 1	0	0
61	1T	4	Total 4	O 4	0	0
61	1U	9	Total 9	O 9	0	0
61	1V	1	Total 1	O 1	0	0
61	1V	6	Total 6	O 6	0	0
61	1W	9	Total 9	O 9	0	0
61	1X	4	Total 4	O 4	0	0
61	1X	3	Total 3	O 3	0	0
61	1Y	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1Z	1	Total 1	O 1	0	0
61	10	3	Total 3	O 3	0	0
61	10	2	Total 2	O 2	0	0
61	10	7	Total 7	O 7	0	0
61	11	1	Total 1	O 1	0	0
61	11	1	Total 1	O 1	0	0
61	11	8	Total 8	O 8	0	0
61	12	4	Total 4	O 4	0	0
61	13	1	Total 1	O 1	0	0
61	13	3	Total 3	O 3	0	0
61	14	2	Total 2	O 2	0	0
61	15	2	Total 2	O 2	0	0
61	15	5	Total 5	O 5	0	0
61	16	1	Total 1	O 1	0	0
61	17	2	Total 2	O 2	0	0
61	17	5	Total 5	O 5	0	0
61	18	5	Total 5	O 5	0	0
61	18	2	Total 2	O 2	0	0
61	18	1	Total 1	O 1	0	0
61	18	2	Total 2	O 2	0	0
61	18	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	18	3	Total 3	O 3	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	5	Total 5	O 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1a	6	Total 6	O 6	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1a	3	Total 3	O 3	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	3	Total 3	O 3	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	4	Total 4	O 4	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1a	4	Total 4	O 4	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	5	Total 5	O 5	0	0
61	1a	6	Total 6	O 6	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	2	Total 2	O 2	0	0
61	1a	1	Total 1	O 1	0	0
61	1a	78	Total 78	O 78	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1l	6	Total 6	O 6	0	0
61	1l	1	Total 1	O 1	0	0
61	1q	4	Total 4	O 4	0	0
61	1w	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1w	1	Total 1	O 1	0	0
61	1w	9	Total 9	O 9	0	0
61	1x	3	Total 3	O 3	0	0
61	1x	2	Total 2	O 2	0	0
61	1x	1	Total 1	O 1	0	0
61	1x	2	Total 2	O 2	0	0
61	1x	1	Total 1	O 1	0	0
61	1x	1	Total 1	O 1	0	0
61	1x	5	Total 5	O 5	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	6	Total 6	O 6	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	2	Total 2	O 2	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	2	Total 2	O 2	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	4	Total 4	O 4	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	6	Total 6	O 6	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	5	Total 5	O 5	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	6	Total	O	0	0
			6	6		
61	2A	6	Total	O	0	0
			6	6		
61	2A	6	Total	O	0	0
			6	6		
61	2A	4	Total	O	0	0
			4	4		
61	2A	6	Total	O	0	0
			6	6		
61	2A	5	Total	O	0	0
			5	5		
61	2A	4	Total	O	0	0
			4	4		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	4	Total	O	0	0
			4	4		
61	2A	6	Total	O	0	0
			6	6		
61	2A	6	Total	O	0	0
			6	6		
61	2A	6	Total	O	0	0
			6	6		
61	2A	6	Total	O	0	0
			6	6		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	5	Total	O	0	0
			5	5		
61	2A	6	Total	O	0	0
			6	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	5	Total 5	O 5	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	6	Total 6	O 6	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	4	Total 4	O 4	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	3	Total 3	O 3	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	1	Total 1	O 1	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0
61	2A	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	6	Total 6	O 6	0	0
61	2A	222	Total 222	O 222	0	0
61	2B	2	Total 2	O 2	0	0
61	2B	3	Total 3	O 3	0	0
61	2B	3	Total 3	O 3	0	0
61	2B	1	Total 1	O 1	0	0
61	2B	2	Total 2	O 2	0	0
61	2B	1	Total 1	O 1	0	0
61	2B	1	Total 1	O 1	0	0
61	2B	12	Total 12	O 12	0	0
61	2D	5	Total 5	O 5	0	0
61	2D	3	Total 3	O 3	0	0
61	2D	2	Total 2	O 2	0	0
61	2D	7	Total 7	O 7	0	0
61	2E	3	Total 3	O 3	0	0
61	2F	6	Total 6	O 6	0	0
61	2I	3	Total 3	O 3	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	5	Total 5	O 5	0	0
61	2P	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2P	4	Total 4	O 4	0	0
61	2Q	1	Total 1	O 1	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	1	Total 1	O 1	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	2	Total 2	O 2	0	0
61	2T	3	Total 3	O 3	0	0
61	2U	2	Total 2	O 2	0	0
61	2W	3	Total 3	O 3	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	6	Total 6	O 6	0	0
61	20	2	Total 2	O 2	0	0
61	20	2	Total 2	O 2	0	0
61	21	6	Total 6	O 6	0	0
61	22	1	Total 1	O 1	0	0
61	25	4	Total 4	O 4	0	0
61	27	1	Total 1	O 1	0	0
61	27	1	Total 1	O 1	0	0
61	28	4	Total 4	O 4	0	0
61	28	1	Total 1	O 1	0	0
61	28	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	29	1	Total	O	0	0
			1	1		
61	2a	6	Total	O	0	0
			6	6		
61	2a	6	Total	O	0	0
			6	6		
61	2a	5	Total	O	0	0
			5	5		
61	2a	5	Total	O	0	0
			5	5		
61	2a	4	Total	O	0	0
			4	4		
61	2a	6	Total	O	0	0
			6	6		
61	2a	6	Total	O	0	0
			6	6		
61	2a	6	Total	O	0	0
			6	6		
61	2a	5	Total	O	0	0
			5	5		
61	2a	5	Total	O	0	0
			5	5		
61	2a	3	Total	O	0	0
			3	3		
61	2a	5	Total	O	0	0
			5	5		
61	2a	4	Total	O	0	0
			4	4		
61	2a	6	Total	O	0	0
			6	6		
61	2a	3	Total	O	0	0
			3	3		
61	2a	5	Total	O	0	0
			5	5		
61	2a	6	Total	O	0	0
			6	6		
61	2a	4	Total	O	0	0
			4	4		
61	2a	4	Total	O	0	0
			4	4		
61	2a	2	Total	O	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	6	Total 6	O 6	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	4	Total 4	O 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	5	Total 5	O 5	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	6	Total 6	O 6	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	5	Total 5	O 5	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	2	Total 2	O 2	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	3	Total 3	O 3	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	1	Total 1	O 1	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	4	Total 4	O 4	0	0
61	2a	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	2	Total	O	0	0
			2	2		
61	2a	2	Total	O	0	0
			2	2		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	1	Total	O	0	0
			1	1		
61	2a	2	Total	O	0	0
			2	2		
61	2a	2	Total	O	0	0
			2	2		
61	2a	2	Total	O	0	0
			2	2		
61	2a	1	Total	O	0	0
			1	1		
61	2a	2	Total	O	0	0
			2	2		
61	2a	1	Total	O	0	0
			1	1		
61	2a	2	Total	O	0	0
			2	2		

Continued on next page...

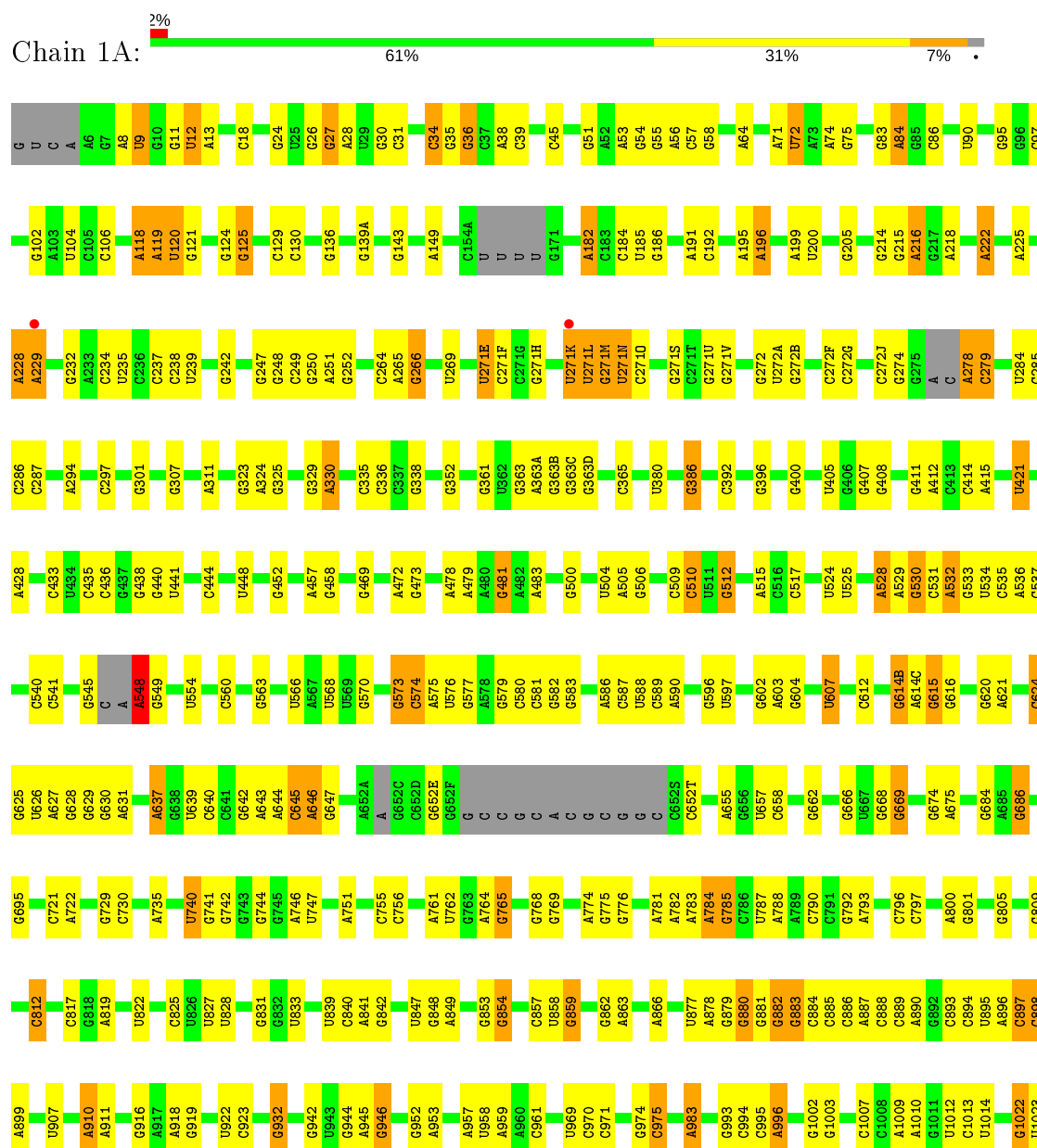
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2a	2	Total 2	O 2	0	0
61	2a	2	Total 2	O 2	0	0
61	2a	40	Total 40	O 40	0	0
61	2d	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2j	1	Total 1	O 1	0	0
61	2l	1	Total 1	O 1	0	0
61	2l	1	Total 1	O 1	0	0
61	2p	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	2	Total 2	O 2	0	0
61	2x	2	Total 2	O 2	0	0
61	2x	2	Total 2	O 2	0	0
61	2x	3	Total 3	O 3	0	0
61	2y	6	Total 6	O 6	0	0
61	2y	1	Total 1	O 1	0	0
61	2y	6	Total 6	O 6	0	0

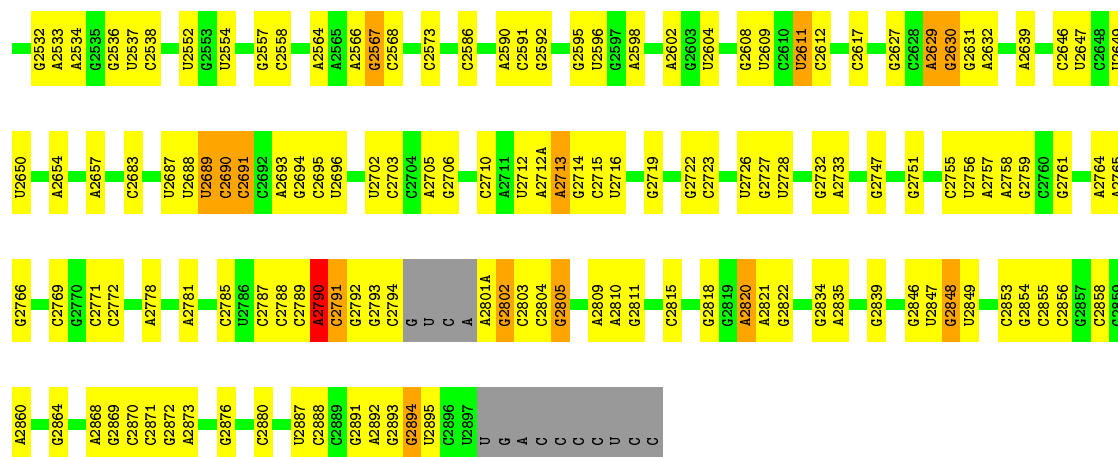
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

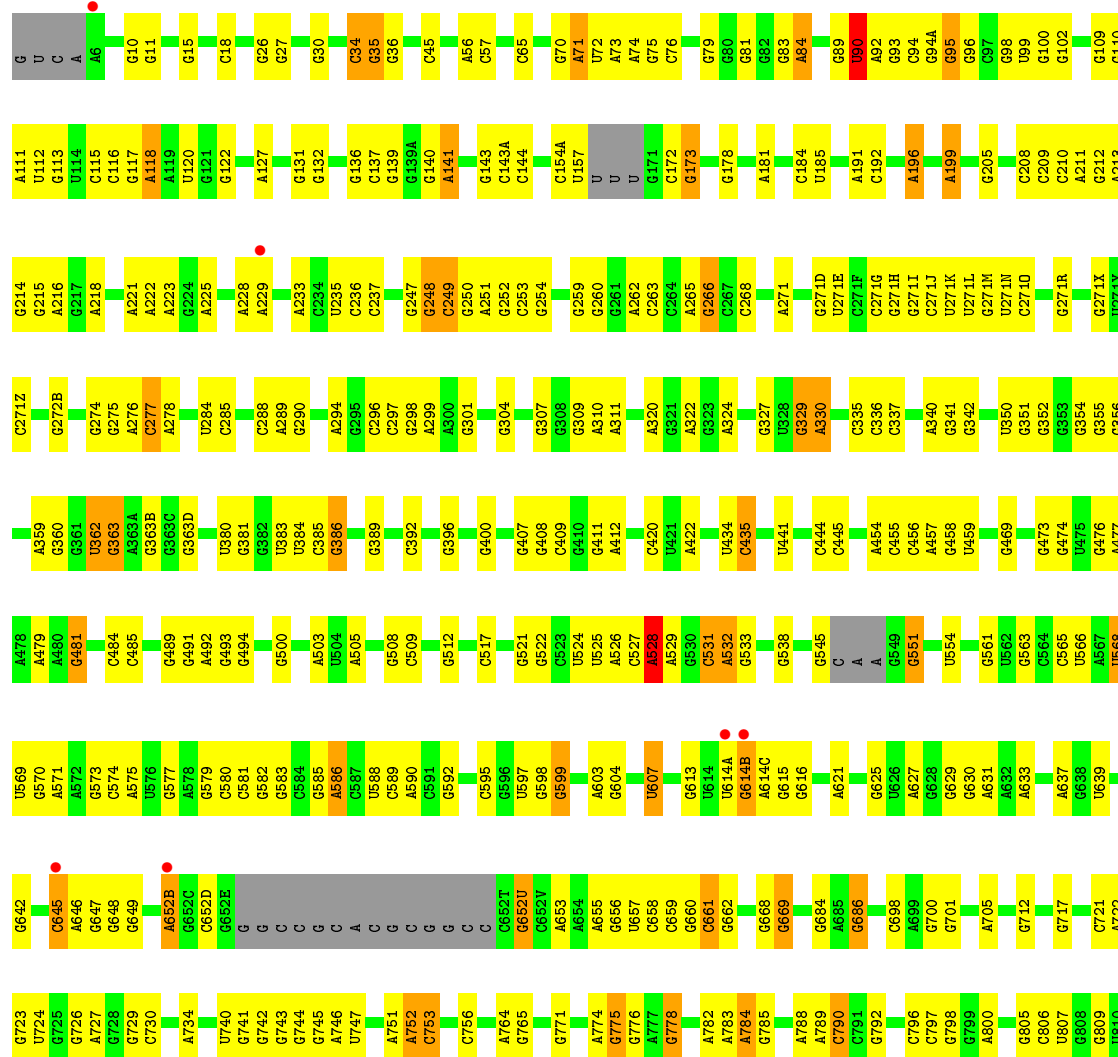
• Molecule 1: 23S Ribosomal RNA



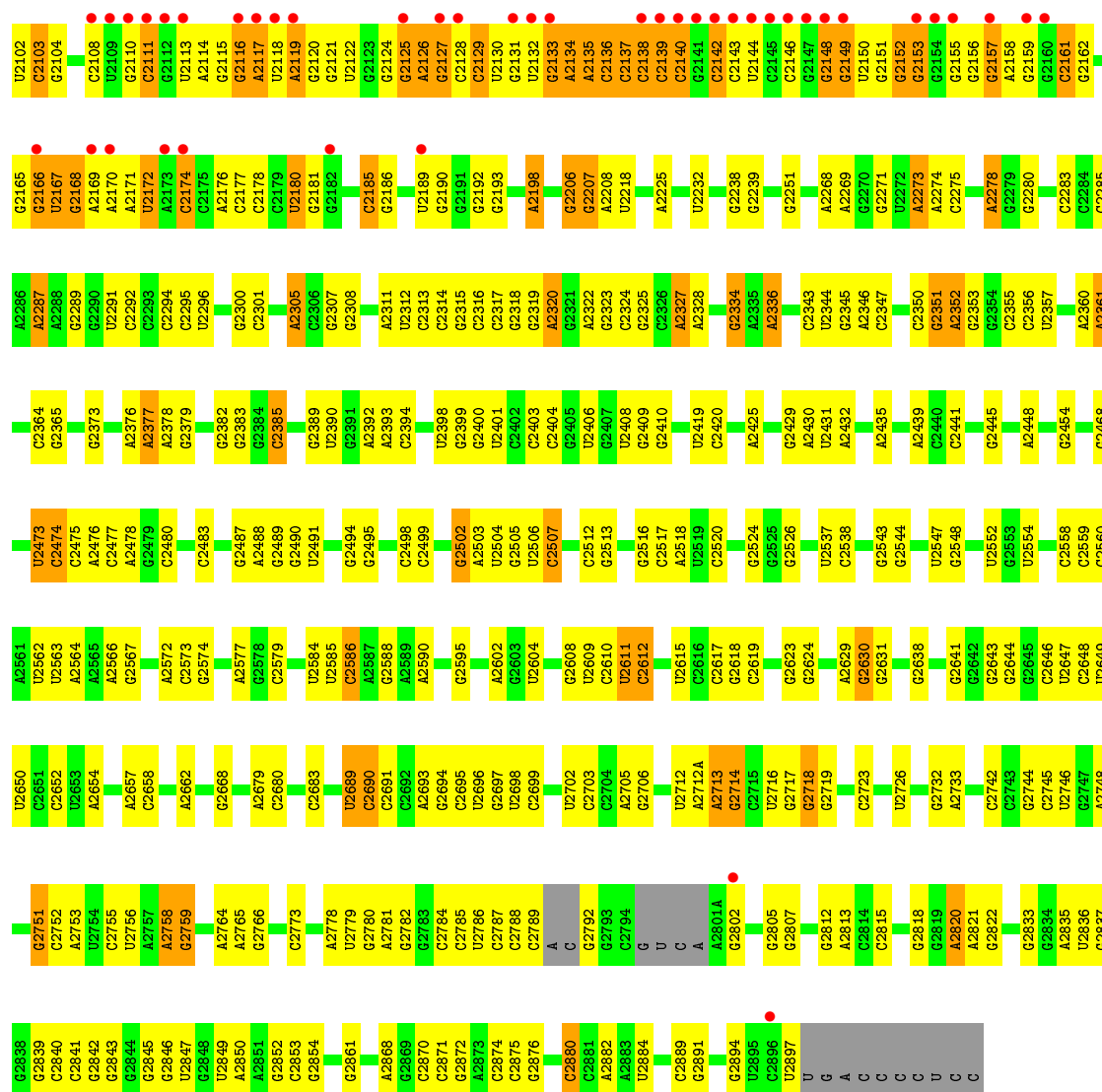
G2400	U2291	G2181	G2120	G2021	A1913	C1782	A1652	C1509	C1408	A1276	C1178	G1089	G1024
U2406	C2292	G2182	G2121	U2022	A1914	A1783	G1653	A1509A	C1409	G1277	C1179	U1090	U1026
G2407	A2305	G2184	U2122	G2023	U1915	A1786	A1654	A1509B	G1410	A1278	G1183	C1092	A1027
U2408	G2308	C2185	G2125	A2030	A1919	A1789	A1655	G1517	G1416	A1286	G1183	U1093	A1028
G2409	G2309	G2187	A2126	A2031	A1919	A1789	A1656	G1520	C1417	A1287	G1187	U1094	A1032
G2410	A2310	G2188	C2128	A2032	C1920	C1790	A1664	G1537	A1418	U1288	U1188	A1095	U1033
A2418	A2311	U2189	G2129	A2033	U1923	A1791	A1665	G1547	A1419	U1292	U1189	A1096	U1033
U2419	U2312	G2190	U2130	G2038	G1924	U1794	G1666	G	U1420	C1293	G1190	U1097	U1034
G2425	C2314	G2191	G2039	G2039	C1924	U1794	G1667	U	G1421	G1293	U1199	U1101	U1035
G2429	G2315	G2192	U2132	C2040	G1929	C1795	A1668	A	G1422	G1297	U1199	G1036	G1036
G2430	G2319	G2193	A2134	U2041	A1930	U1796	A1669	C	G1426	C1297	U1205	G1037	G1037
U2431	A2320	A2198	A2135	A2042	U1931	C1797	C1670	G1537	A1427	U1300	G1206	C1038	C1038
A2432			G2136	C2043	A1932	U1798	C1675	G1537	C1428	U1301	G1206	U1105	G1039
G2435	G2325	G2206	C2137	G2049	G1934	G1799	C1675	A1542	A1429	A1302	A1210	A1106	C1040
G2439	A2326	G2207	G2138	G2053	G1935	G1801	U1688	C1546	C1430	G1303	G1211	G1107	C1041
G2440	G2327	U2218	C2140	A2054	A1936	A1802	A1692	A1542	C1432	G1309	A1213	U1108	G1044
G2441	A2328	G2219	G2141	G2055	A1937	A1803	U1693	A1558	U1433	G1310	G1216	A1110	A1046
G2442	G2329	G2220	C2142	G2056	A1938	A1803	U1693	G1559	C1432	G1311	G1217	A1111	A1047
G2443	G2330	G2223	G2143	G2066	U1956	G1823	U1693	A1572	A1439	U1312	G1218	U1112	A1048
G2444	G2331	G2224	U2144	A2060	C1957	G1826	G1696	A1578	A1441	U1313	G1219	U1113	
G2445	A2225	G2224	C2145	G2061	A1952	U1817	G1696	A1569	G1442	U1329	A1220	G1114	C1052
G2448	A2226	A2227	G2146	G2065	A1953	U1818	A1700	A1570	C1447	U1352	C1230	U1059	C1053
U2449	A2336	G2228	G2148	C2066	G1954	A1821	A1701	A1571	A1448	A1353	G1231	G1060	
G2454	G2347	U2232	U2150	G2069	U1963	G1826	G1702	A1572	A1449	U1352	A1226	G1067	G1062
G2467	C2350	G2233	G2151	G2070	U1963	C1830	G1703	U1578	A1449	A1353	C1230	U1066	U
G2474	A2351	G2234	G2152	A2071	G1964	A1830	A1713	G1581	A1448	A1354	G1231	G1067	G1062
G2475	G2352	G2238	G2153	U2086	C1965	G1840	G1717	C1584	A1452	G1356	G1238	G1068	G1062
A2476	G2359	G2239	G2155	G2087	A1966	G1847	G1718	A1586	U1453	U1357	G1239	G1063	G1063
C2477	A2360	U2243	G2157	G2090	C1967	A1847	A1722	A1587	G1455	G1358	U1240	C1064	C1064
A2478	A2361	U2244	A2158	G2159	G1968	A1853	G1746	C1589	U1466	A1360	G1244	U1065	U1065
G2484	G2364	G2250	G2160	U2096	A1970	A1854	G1750	G1593	C1467	A1360	A1247	A1067	A1067
A2488	G2365	G2251	G2161	U2099	A1971	A1854	G1750	G1593	A1468	A1365	A1247	G1069	G1069
U2491	A2369	G2252	G2162	G2100	G1973	G1858	G1754	G1594	G1470	A1365	G1250	A1070	A1070
G2496	G2372	C2284	C2163	U2101	U1991	G1861	C1754	A1608	G1478	U1372	G1251	G1139	A1070
A2497	A2376	A2268	G2165	U2102	U1991	G1862	A1755	A1609	C1478	A1373	G1252	C1140	C1072
G2498	A2377	G2270	U2167	G2106	U1992	G1863	G1756	A1610	G1482	A1379	A1253	G1153	A1073
G2502	G2379	G2271	A2169	G2107	U1993	A1866	G1758	C1611	U1489	G1380	G1256	A1155	G1074
G2505	A2383	U2272	G2170	C2108	G1997	A1877	A1762	G1619	A1490	A1384	G1264	A1156	C1076
G2518	G2384	A2274	A2171	U2109	G1998	G1878	G1763	C1636	U1489	A1384	A1265	G1164	A1077
G2520	G2385	G2275	U2172	G2110	C1999	A1878	G1764	A1637	C1493	G1386	A1266	U1165	U1078
G2521	A2386	G2276	A2173	C2111	G2000	C1881	U1765	C1638	A1494	U1396	U1267	C1166	C1080
U2522	U2390	C2283	G2174	U2113	A2001	A1889	C1767	A1641	C1498	U1366	A1268	U1167	G1081
G2529	G2396	A2286	G2175	A2114	G2002	A1890	C1767	G1642	U1489	G1401	A1269	U1167	U1082
			C2176	G2115	U2011	A1890	A1773	G1642	A1490	C1402	G1270	G1171	U1083
			G2177	A2014	A1900	G1899	U1779	G1645	C1504	C1402	C1271	G1173	A1084
			C2178	A2014	A1900	G1899	U1779	C1646	C1505	U1405	A1272	A1174	A1085
			G2179	A2020	A1900	G1899	U1779	C1647	C1506	U1406	U1274	A1175	A1086
			U2180	A2020	A1900	G1899	U1779	C1648	A1507	C1407	A1275	G1176	G1087
													A1088



• Molecule 1: 23S Ribosomal RNA

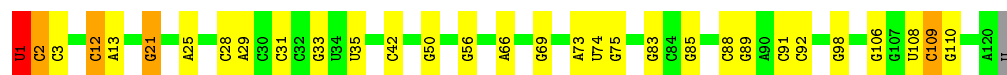


G2010	G1906	C1790	G1581	C1493	U1390	U1273	A	C	G	G968	C885	U811
U2011	G1906	A1791	C1584	A1494	U1391	A1278	C1178	U	A	U969	C886	C812
G2012	G1910	C1588	A1586	A1496	U1405	G1279	C1179	G	G	C970	A887	U813
A2013	G1913	C1795	C1592	C1504	U1406	A1284	G1187	U	A	G972	C889	C814
A2014	C1914	U1796	G1593	C1505	C1409	A1287	U1188	G	A	G974	A890	C817
A2020	U1915	C1797	G1594	C1506	G1410	U1288	G1191	A	A	C975	C892	G818
C2021	U1798	G1696	G1595	C1507	C1411	U1289	G1192	C	C	G	C893	G819
U2022	G1799	A1596	A1597	C1508	A1412	U1292	G1193	C	A	G979	A895	A820
G2023	C1800	A1698	A1598	A1509	G1413	U1293	G1194	A	A	A980	U895	A821
G2027	A1919	G1699	C1598	C1509	G1414	C1293	G1195	C	G	G983	C897	U822
G2030	C1920	A1801	C1599	A1509A	U1415	U1300	G1196	G	G	A983	U898	U827
A2031	G1921	A1803	C1600	A1509B	G1416	A1301	A1204	A	A	A984	U899	U828
A2032	A1927	G1702	C1604	C1511	C1417	U1302	U1205	G	G	C985	A900	G832
G2033	A1928	G1703	C1607	U1514	U1420	G1309	G1206	G	G	G987	C902	U833
U2034	A1929	C1711	C1608	G1515	G1421	G1310	A1210	U	U	G989	C903	C834
G2035	G1930	U1712	A1608	G1516	G1422	U1311	U1211	G	G	C994	C904	U839
G2040	U1931	U1713	A1609	G1517	G1423	U1312	G1212	C	C	C995	A910	C840
C2043	G1932	G1714	A1610	U1518	G1424	C1314	A1214	U	U	G997	C914	G845
C2044	G1933	G1721	A1614	G1519	A1427	C1315	A1127	C	A	A1000	A917	U847
G2045	A1936	U1722	G1619	G1525	C1428	A1316	A1128	G	A	A1001	A918	G848
G2046	A1937	U1739	G1622	U1529	G1429	U1317	U1130	A	A	G1002	G919	A849
C2049	A1938	G1740	C1622	C1530	A1434	U1341	G1131	G	G	G1003	C920	C850
C2050	U1939	G1746	G1630	C1531	C1437	C1345	C1135	C	A	C1004	G921	U851
A2051	G1947	G1747	C1631	C1532	C1437	C1346	G1136	C	A	C1005	U922	G852
G2052	G1947A	G1747A	A1631A	C1533	C1437	C1347	G1137	C	C	C1006	C923	G853
G2053	G1751	C1751	A1632	U	G1442	C1351	G1138	C	C	C1007	C924	G854
A2054	C1754	C1754	C1636	A	G1443	U1352	C1139	C	C	G1011	C925	G855
C2055	A1755	A1755	A1637	C1536	G1444	A1354	C1140	C	A	U1012	A926	C856
G2056	G1756	G1756	G1638	G1538	A1445	C1358	U1141	U	U	C1013	C927	C857
A2059	U1757	U1757	U1639	G1539	G1448	A1359	A1142A	C	C	G1016	G932	G859
A2060	U1758	G1758	C1640	U1540	A1449	A1360	C1147	U	U	G1017	A933	U860
G2061	A1759	A1759	G1645	G1541	G1450	G1364	A1148	C	U	A861	G862	A861
A2062	C1761	C1761	C1646	C1542	G1456	A1365	C1153	C	A	C936	G863	A863
C2065	G1763	G1763	C1648	A1544	G1456	A1366	A1155	A	A	A1020	G864	G864
G2069	G1764	G1764	G1651	C1547	A1460	G1368	A1246	G	G	A1021	C865	C865
G2070	A1652	A1652	A1652	C1557	C1462	G1369	G1248	A	A	U1022	A866	A866
A2071	G1653	G1653	A1654	C1558	C1463	C1370	A1156	C	C	G1023	A941	A941
U2079	A1654	A1654	C1654	A1566	C1467	U1372	U1159	G	G	U1024	G942	G942
U2086	C1657	C1657	C1657	A1567	C1471	A1373	G1255	C	C	G1025	G943	U943
G2087	C1658	C1658	C1658	A1567	A1471	C1376	G1256	U	U	U1026	A945	A945
G2093	U1659	U1659	U1659	A1568	A1477	G1377	C1166	C	G	A1027	G946	G946
C2096	C1660	C1660	C1660	A1569	A1477	G1377	U1167	C	U	A1028	G947	G947
U2098	G1661	G1661	G1661	A1570	G1478	U1378	G1168	A	A	G1031	G948	G948
G2099	A1662	A1662	C1663	A1571	G1478	A1379	G1169	C	C	A1032	A953	C876
A2099	C1663	C1663	C1663	A1571	U1481	G1380	G1170	U	U	U1033	U958	U877
G2100	C1670	C1670	C1670	U1576	G1482	C1383	G1171	A	A	G1037	A959	G879
G2101	A1785	A1785	C1674	C1577	G1482	A1384	G	C	C	C1038	A960	G880
	A1786	A1786	G1674	U1578	A1490	G1385	U	C	C	G1039	C961	G881
				A1580	G1491	G1386	A	U	U	A	G882	G882
					G1492		G	C	C	C1043	G883	C884



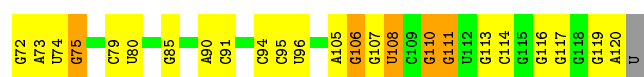
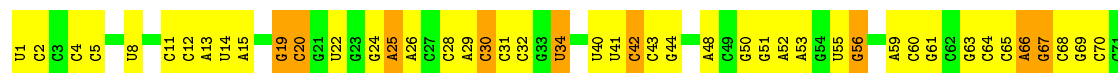
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 74% 21%

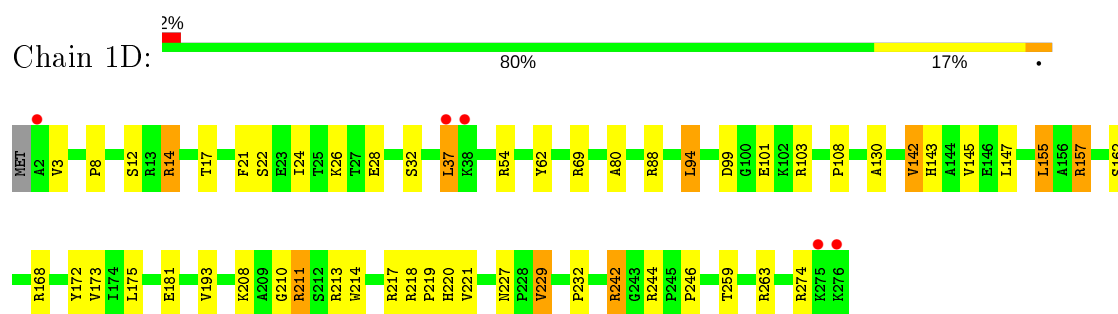


• Molecule 2: 5S Ribosomal RNA

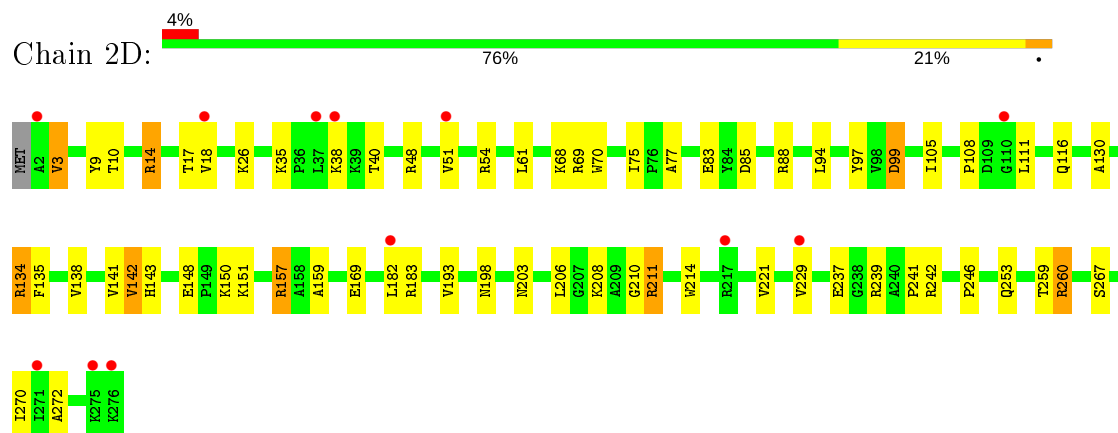
Chain 2B: 42% 45% 12%



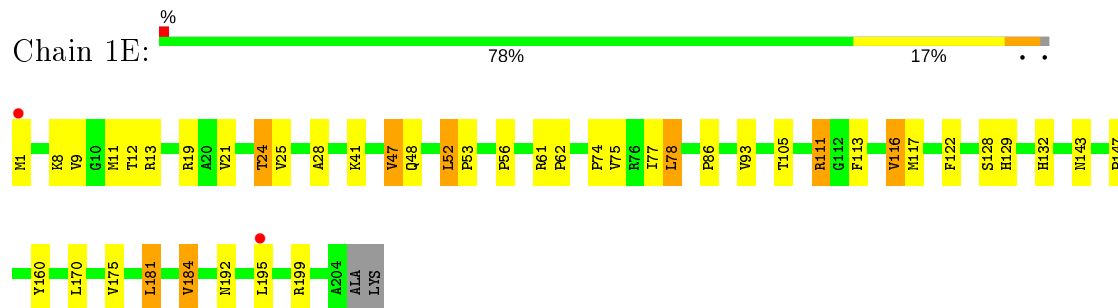
• Molecule 3: 50S ribosomal protein L2



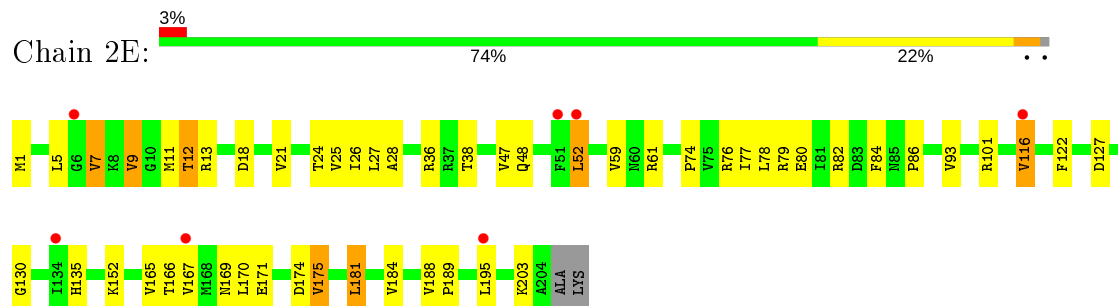
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3

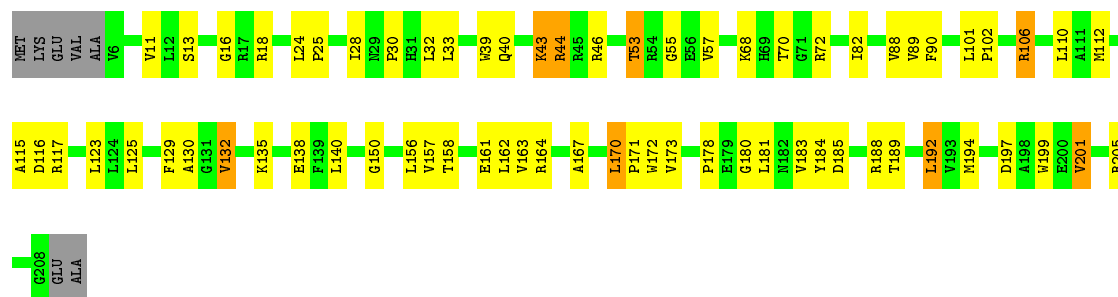


- Molecule 4: 50S ribosomal protein L3

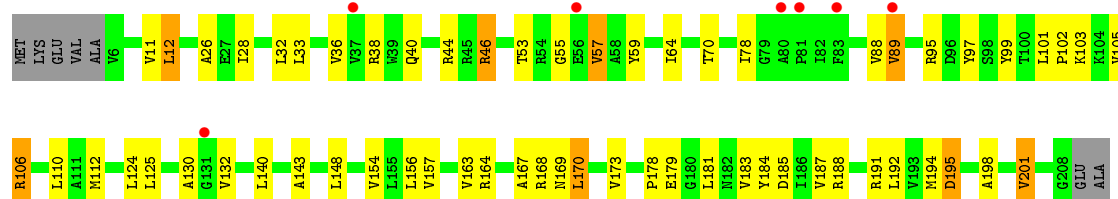


- Molecule 5: 50S ribosomal protein L4

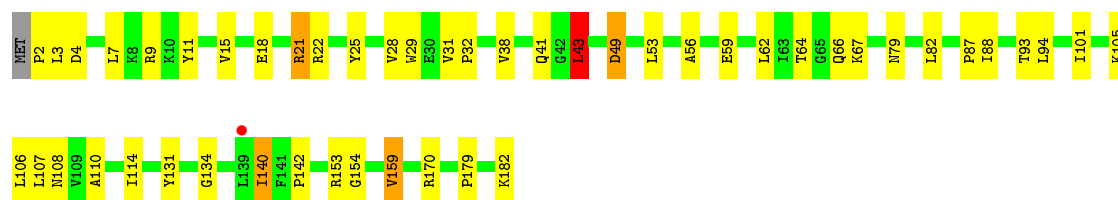




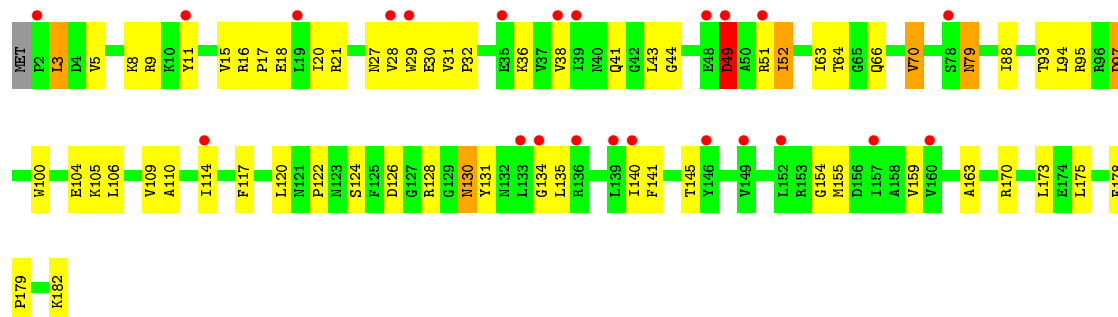
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5

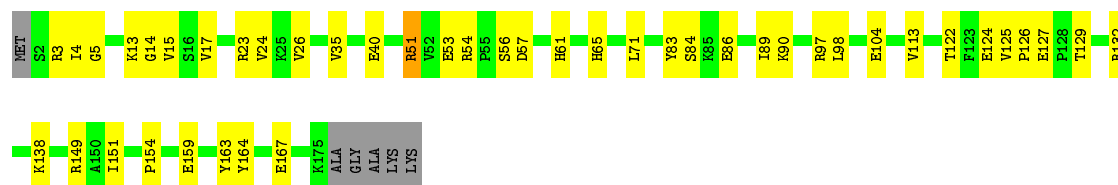


- Molecule 6: 50S ribosomal protein L5

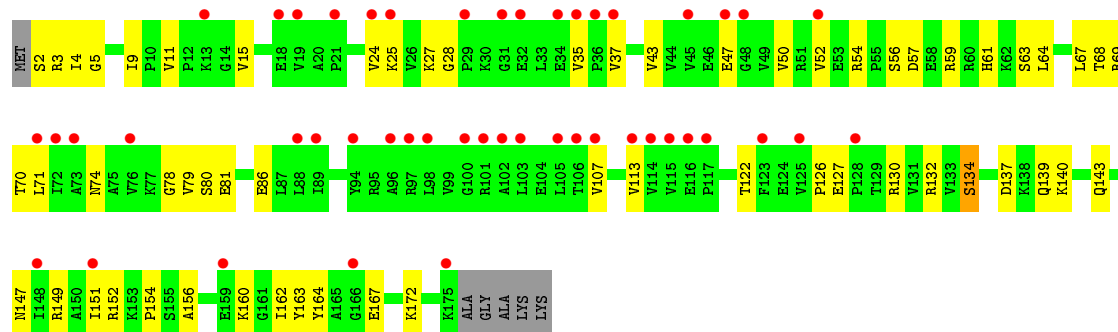


- Molecule 7: 50S ribosomal protein L6

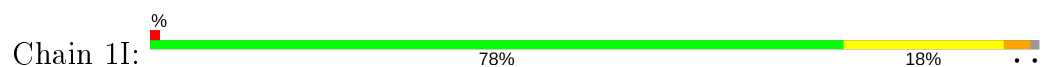




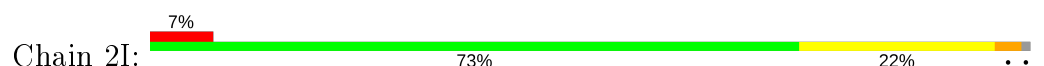
• Molecule 7: 50S ribosomal protein L6



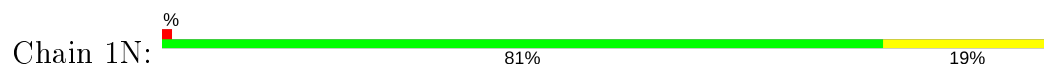
• Molecule 8: 50S ribosomal protein L9



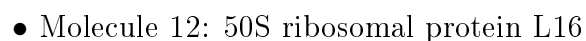
• Molecule 8: 50S ribosomal protein L9

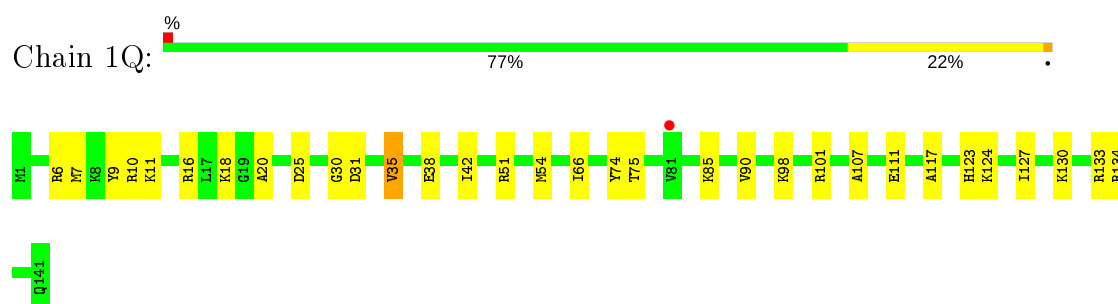


• Molecule 9: 50S ribosomal protein L13

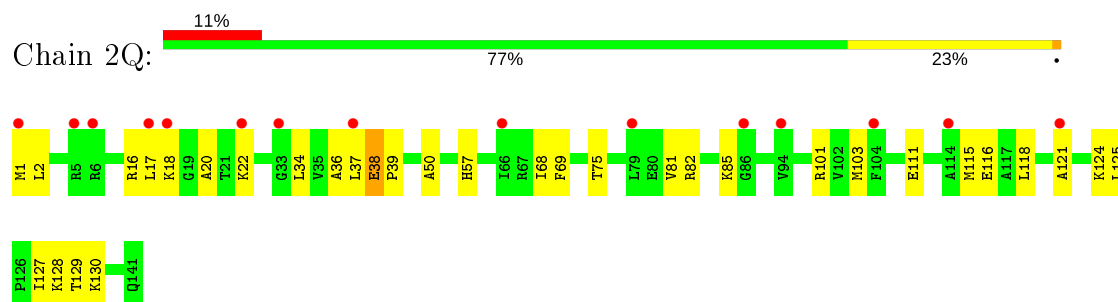


• Molecule 9: 50S ribosomal protein L13

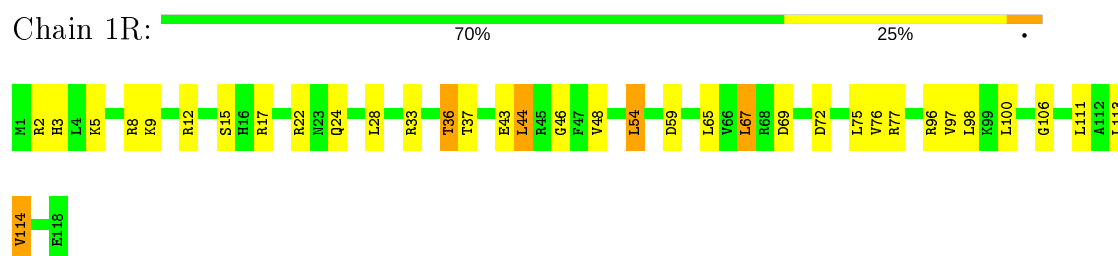




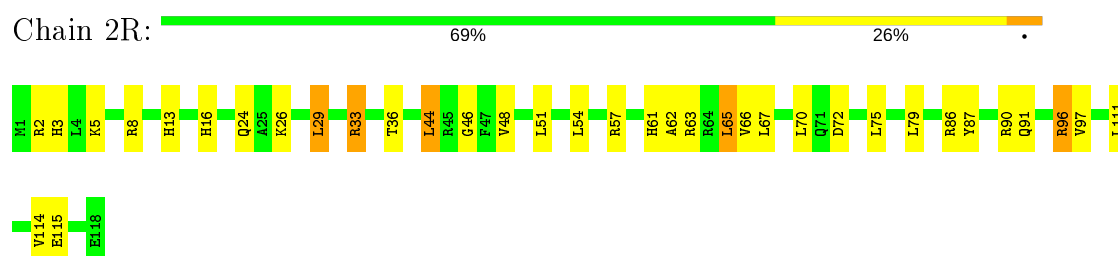
- Molecule 12: 50S ribosomal protein L16



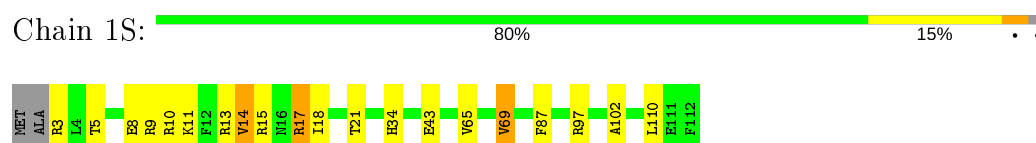
- Molecule 13: 50S ribosomal protein L17



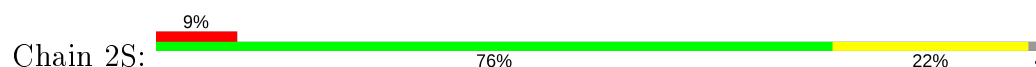
- Molecule 13: 50S ribosomal protein L17

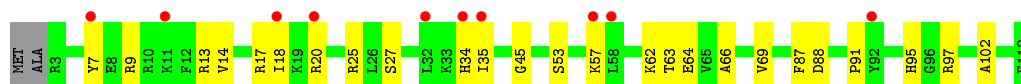


- Molecule 14: 50S ribosomal protein L18



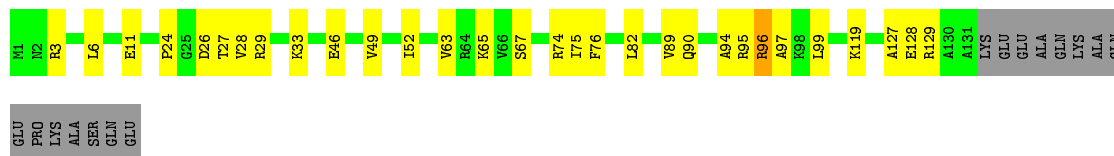
- Molecule 14: 50S ribosomal protein L18





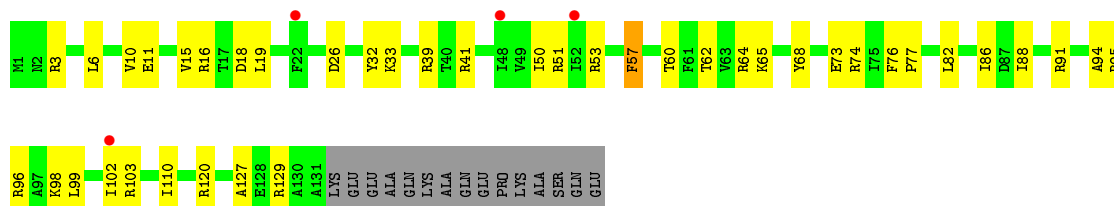
- Molecule 15: 50S ribosomal protein L19

Chain 1T: 69% 20% 10%



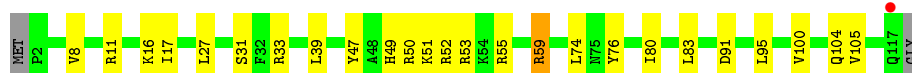
- Molecule 15: 50S ribosomal protein L19

Chain 2T: 3% 62% 27% 10%



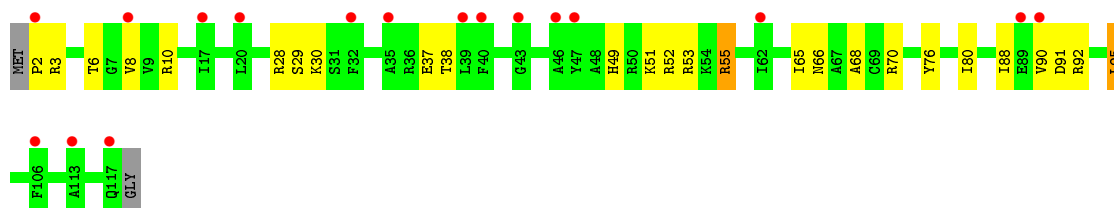
- Molecule 16: 50S ribosomal protein L20

Chain 1U: % 77% 20% ..



- Molecule 16: 50S ribosomal protein L20

Chain 2U: 14% 76% 20% ..

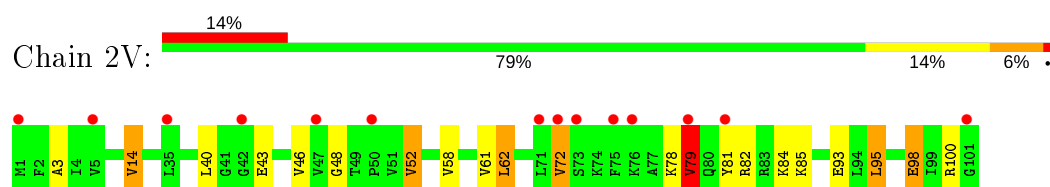


- Molecule 17: 50S ribosomal protein L21

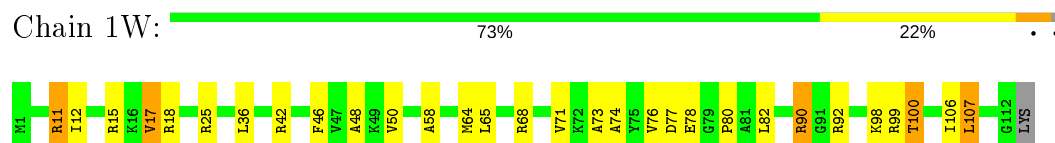
Chain 1V: 77% 21% ..



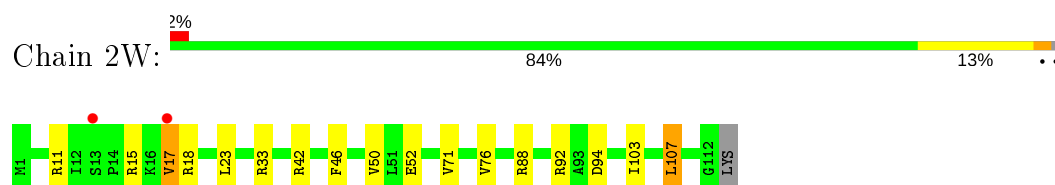
- Molecule 17: 50S ribosomal protein L21



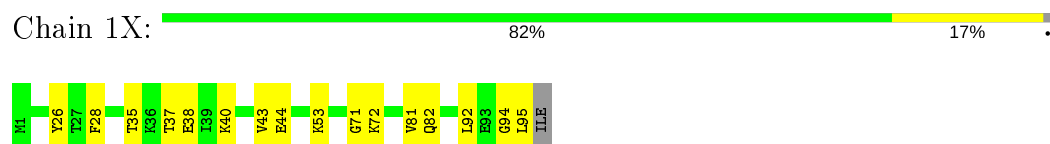
- Molecule 18: 50S ribosomal protein L22



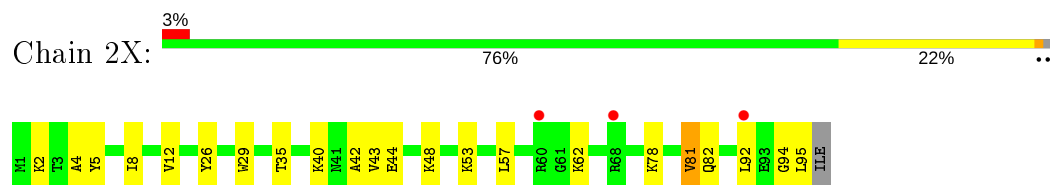
- Molecule 18: 50S ribosomal protein L22



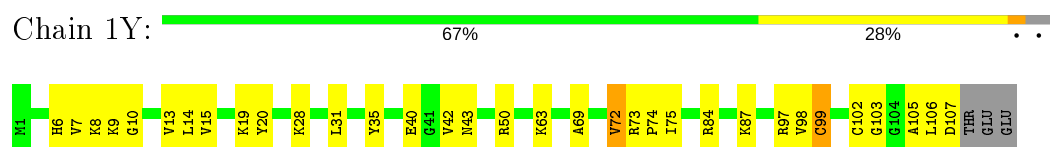
- Molecule 19: 50S ribosomal protein L23



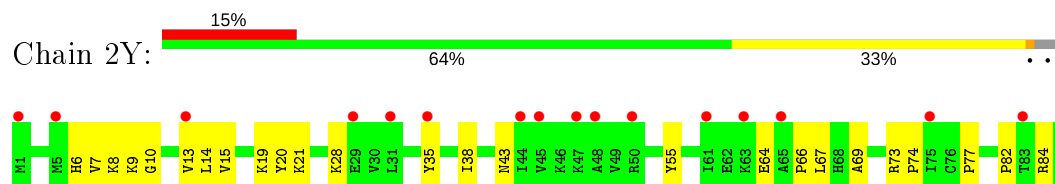
- Molecule 19: 50S ribosomal protein L23

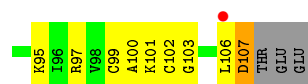


- Molecule 20: 50S ribosomal protein L24

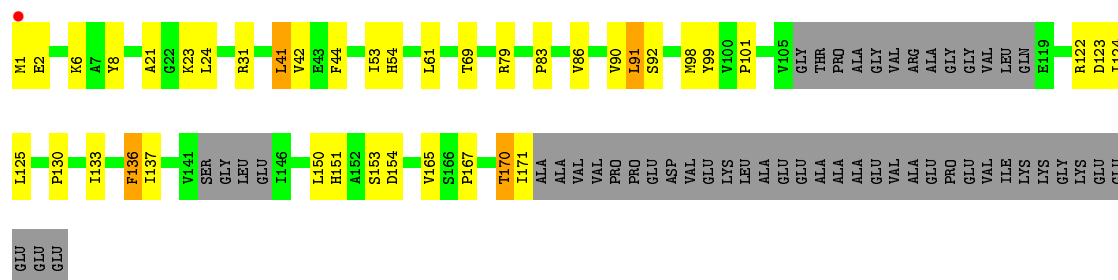


- Molecule 20: 50S ribosomal protein L24

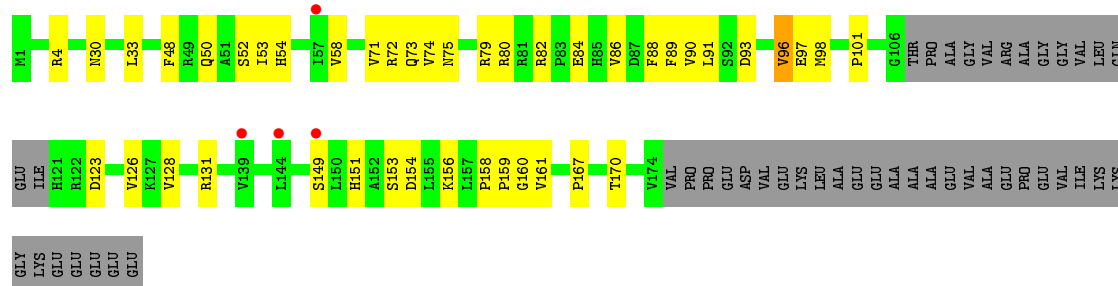




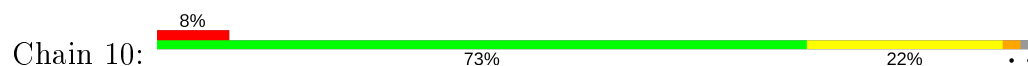
- Molecule 21: 50S ribosomal protein L25



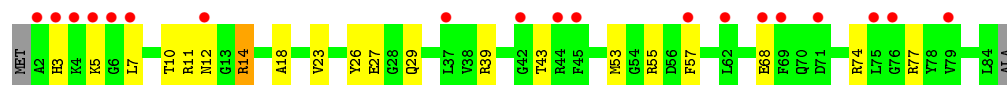
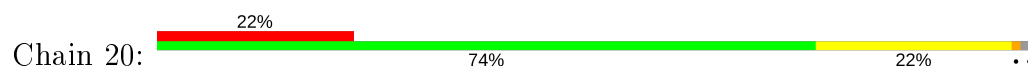
- Molecule 21: 50S ribosomal protein L25



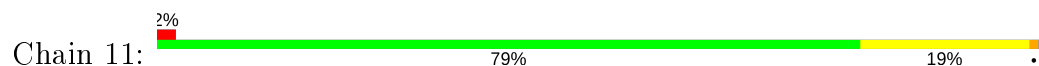
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27

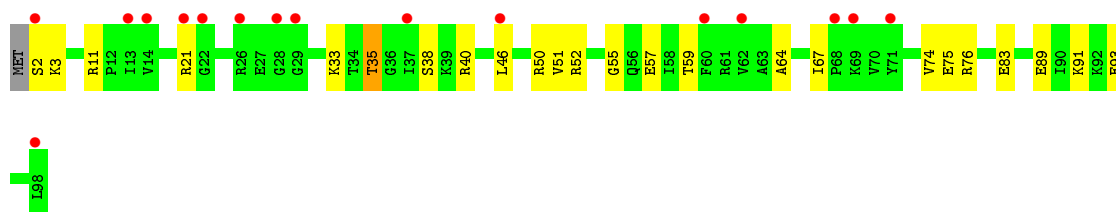
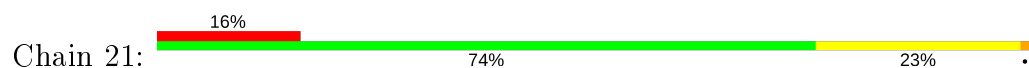


- Molecule 23: 50S ribosomal protein L28

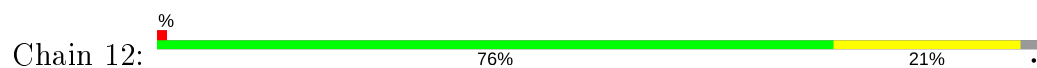




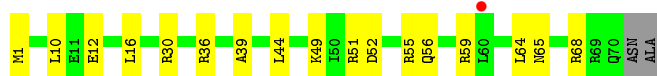
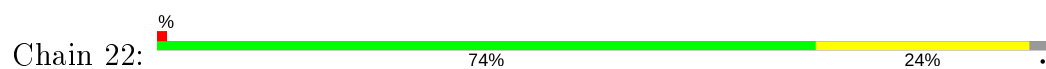
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



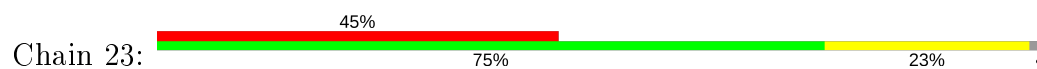
- Molecule 24: 50S ribosomal protein L29



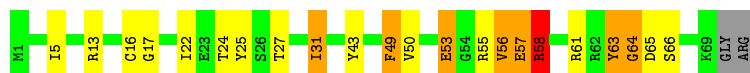
- Molecule 25: 50S ribosomal protein L30



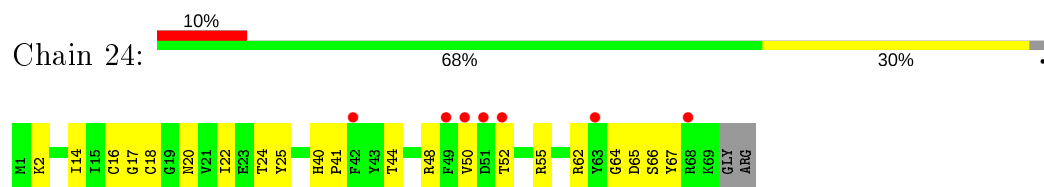
- Molecule 25: 50S ribosomal protein L30



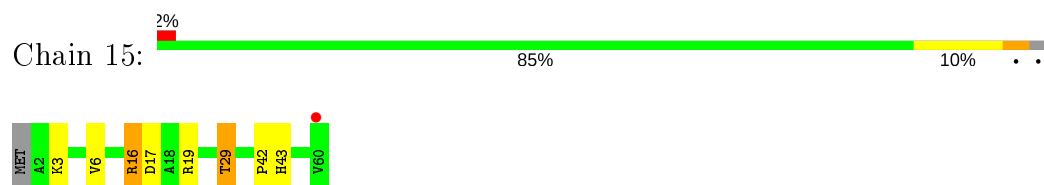
- Molecule 26: 50S ribosomal protein L31



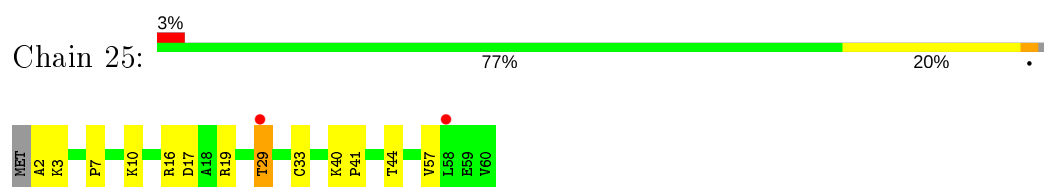
- Molecule 26: 50S ribosomal protein L31



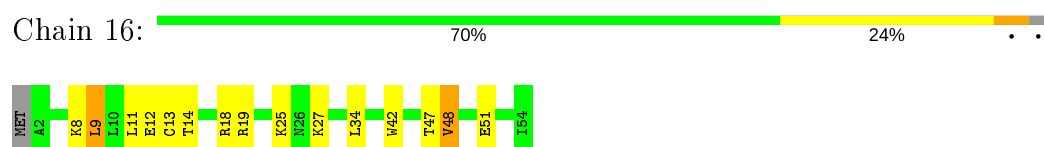
- Molecule 27: 50S ribosomal protein L32



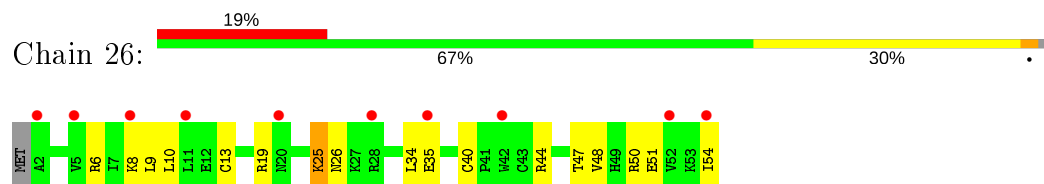
- Molecule 27: 50S ribosomal protein L32



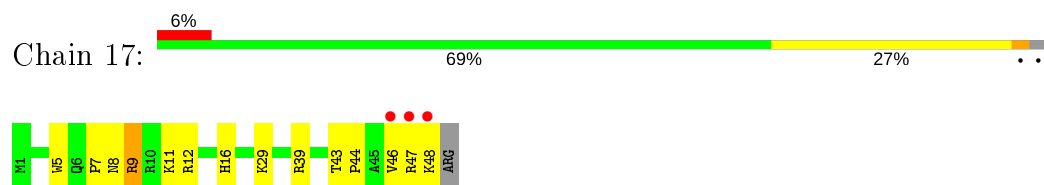
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

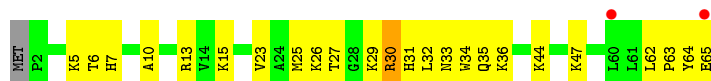


- Molecule 29: 50S ribosomal protein L34

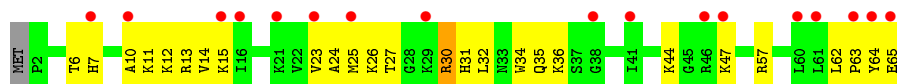




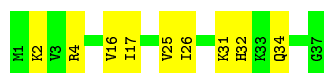
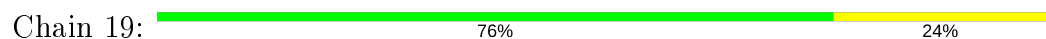
- Molecule 30: 50S ribosomal protein L35



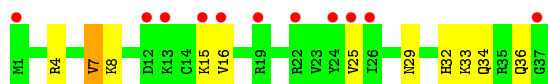
- Molecule 30: 50S ribosomal protein L35



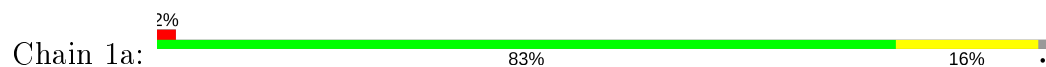
- Molecule 31: 50S ribosomal protein L36

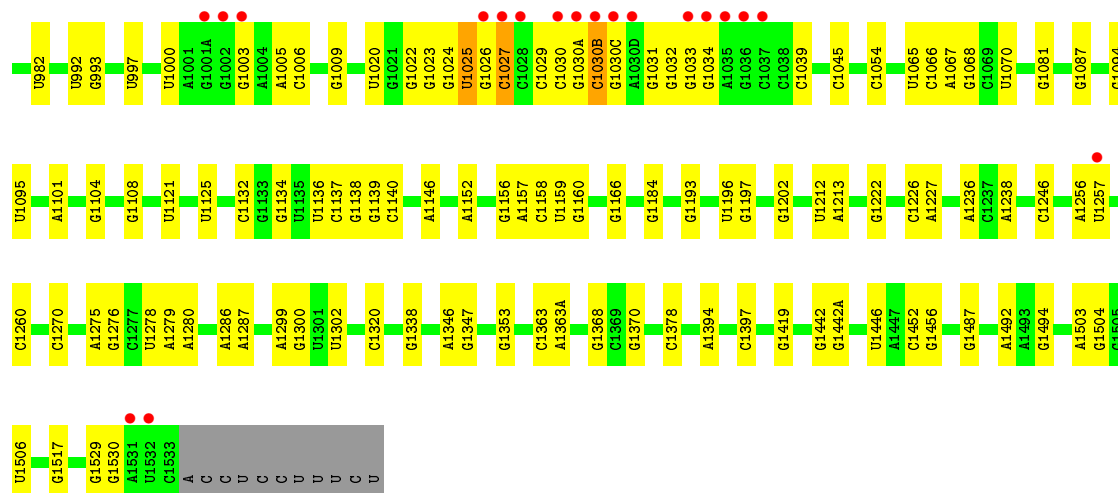


- Molecule 31: 50S ribosomal protein L36

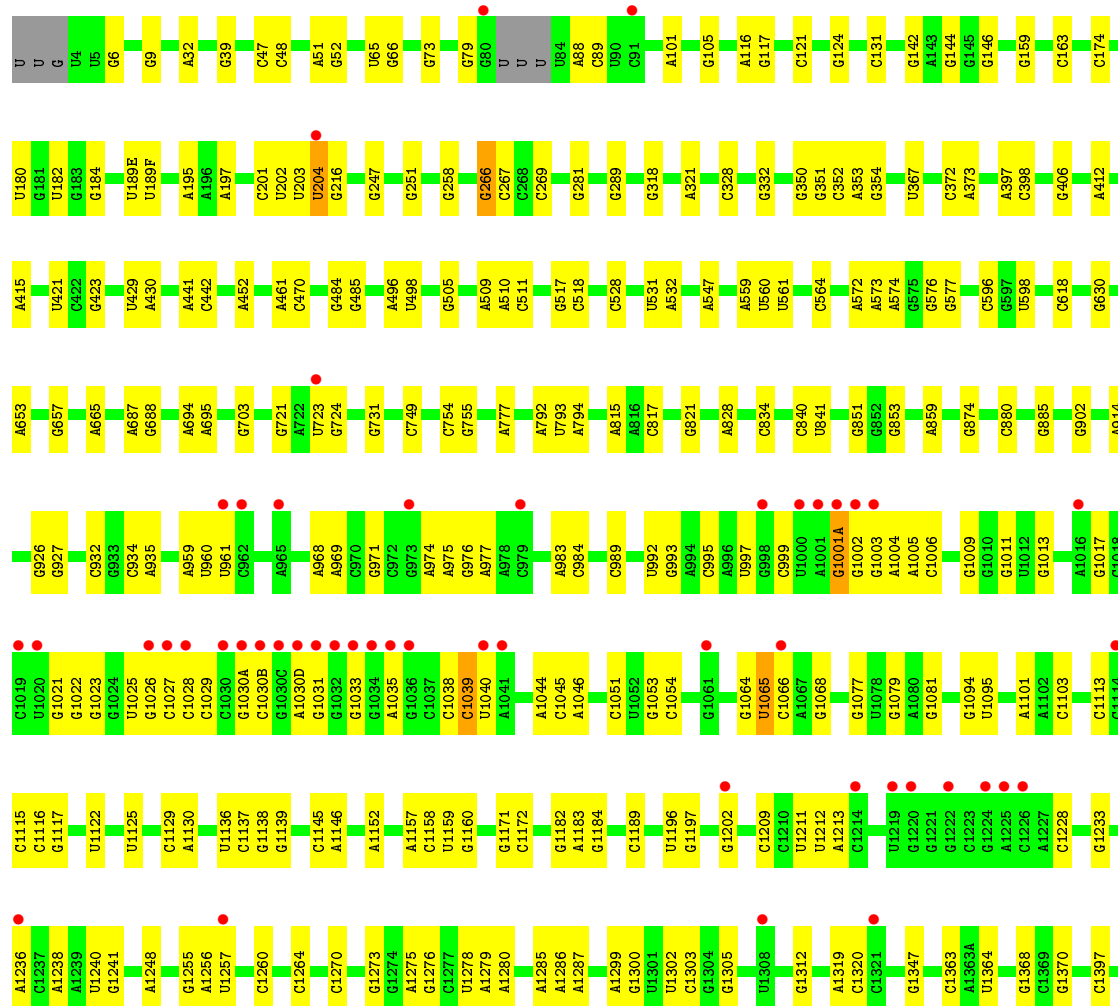
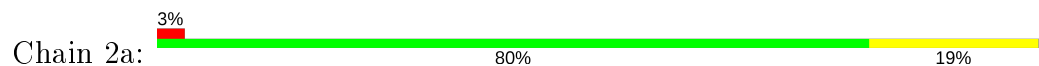


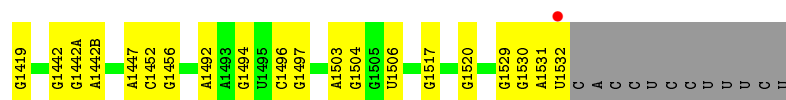
- Molecule 32: 16S Ribosomal RNA



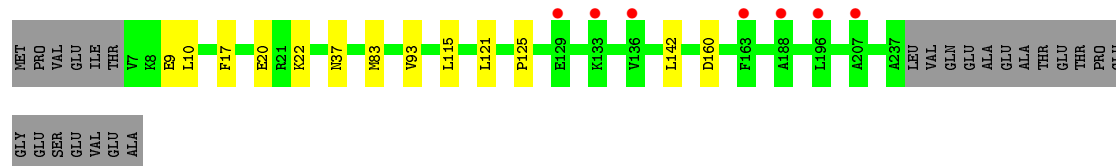
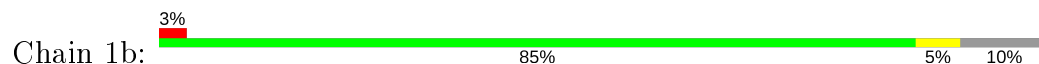


• Molecule 32: 16S Ribosomal RNA

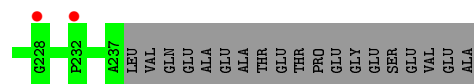
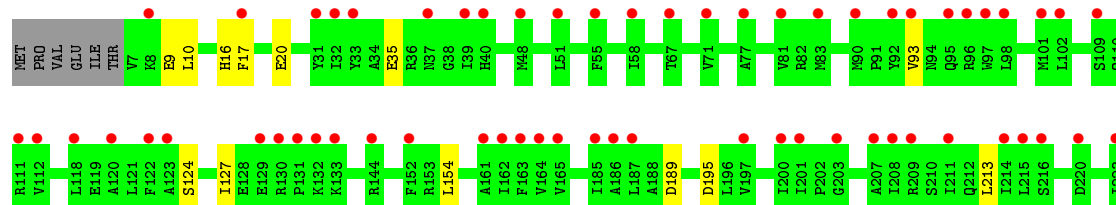
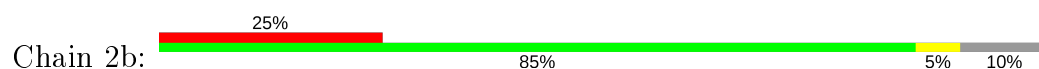




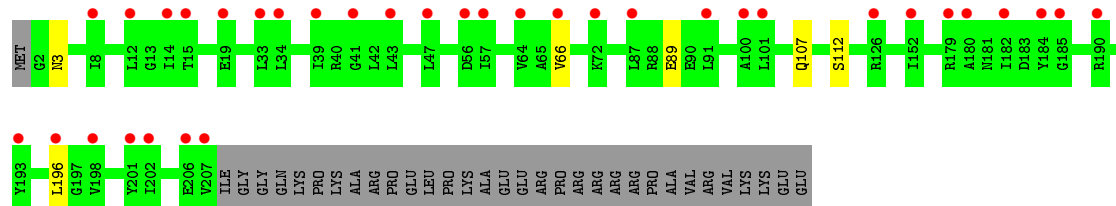
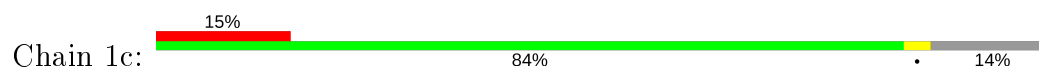
- Molecule 33: 30S ribosomal protein S2



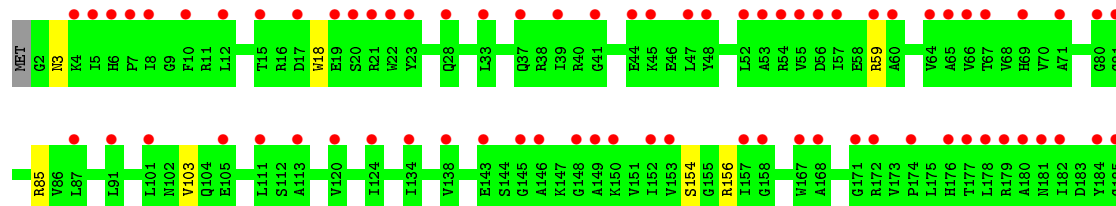
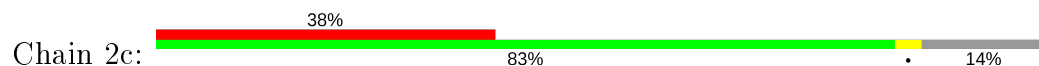
- Molecule 33: 30S ribosomal protein S2

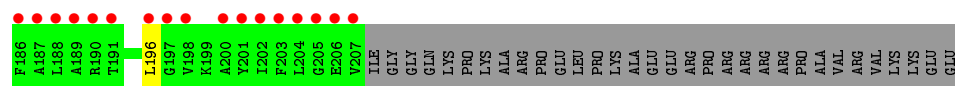


- Molecule 34: 30S ribosomal protein S3

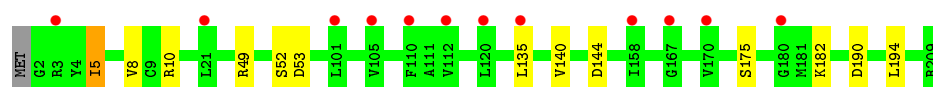


- Molecule 34: 30S ribosomal protein S3

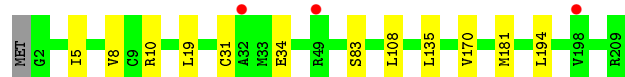




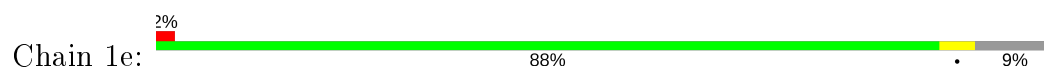
- Molecule 35: 30S ribosomal protein S4



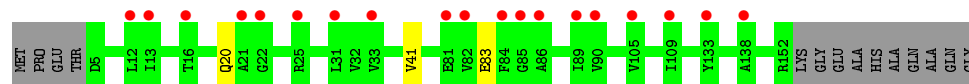
- Molecule 35: 30S ribosomal protein S4



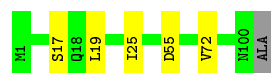
- Molecule 36: 30S ribosomal protein S5



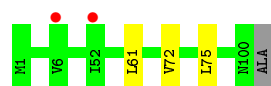
- Molecule 36: 30S ribosomal protein S5



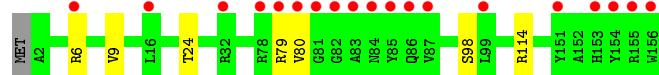
- Molecule 37: 30S ribosomal protein S6



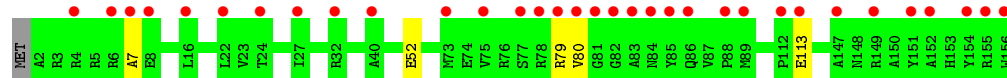
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



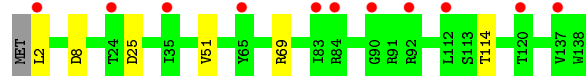
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8



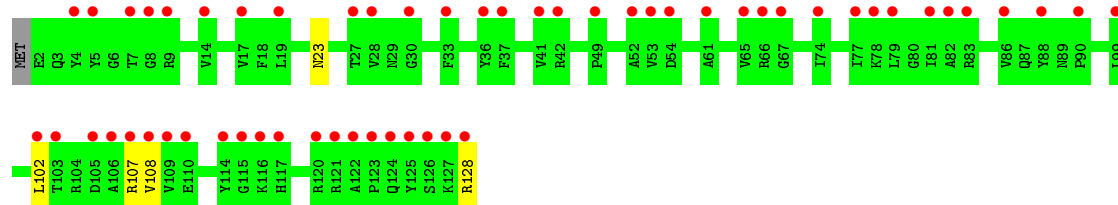
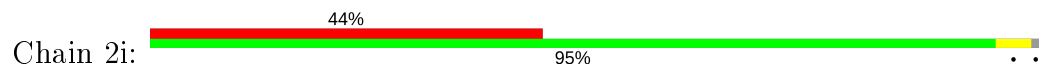
- Molecule 39: 30S ribosomal protein S8



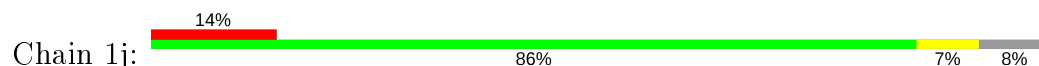
- Molecule 40: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S9

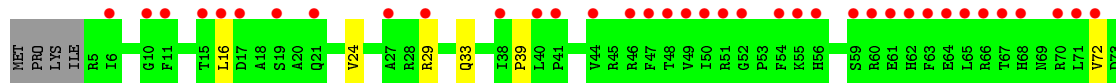
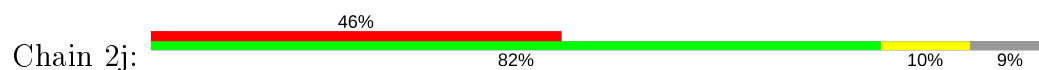


- Molecule 41: 30S ribosomal protein S10

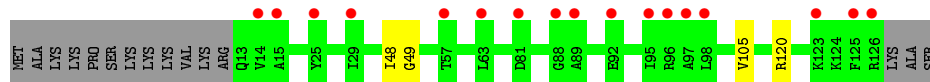
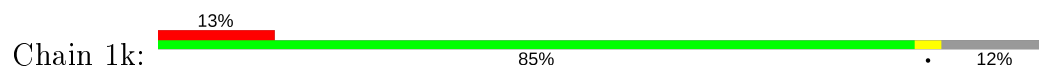




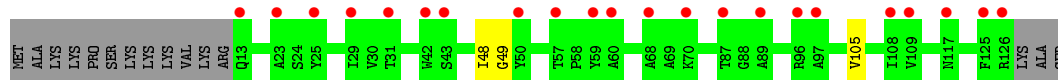
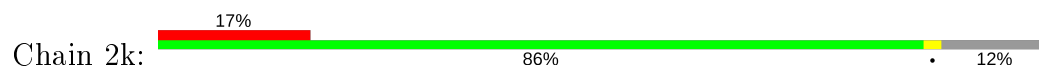
- Molecule 41: 30S ribosomal protein S10



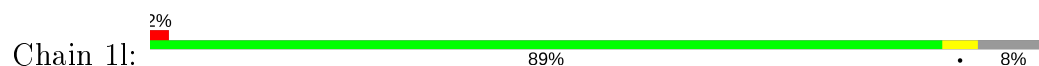
- Molecule 42: 30S ribosomal protein S11



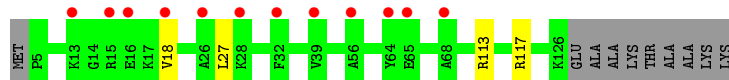
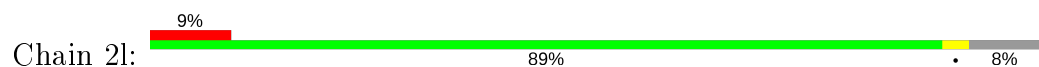
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12

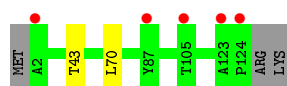


- Molecule 43: 30S ribosomal protein S12

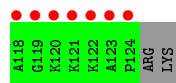


- Molecule 44: 30S ribosomal protein S13

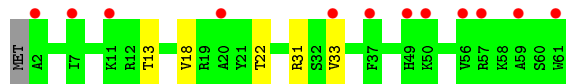
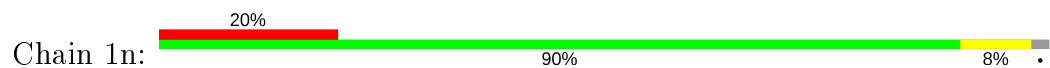




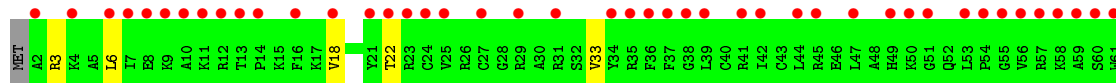
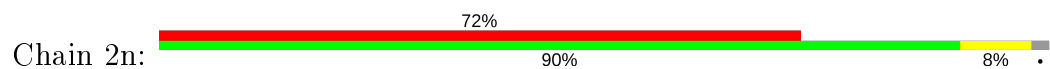
- Molecule 44: 30S ribosomal protein S13



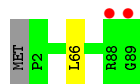
- Molecule 45: 30S ribosomal protein S14 type Z



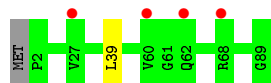
- Molecule 45: 30S ribosomal protein S14 type Z



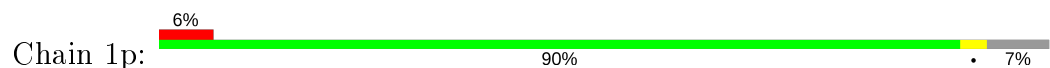
- Molecule 46: 30S ribosomal protein S15

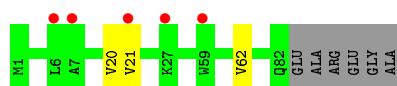


- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16





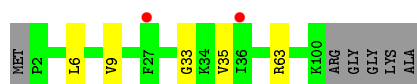
- Molecule 47: 30S ribosomal protein S16

Chain 2p: 89% 5% 7%



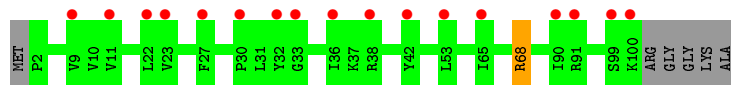
- Molecule 48: 30S ribosomal protein S17

Chain 1q: 2% 90% 5% 6%



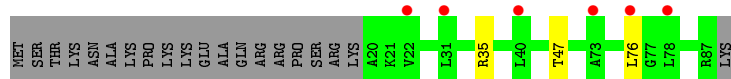
- Molecule 48: 30S ribosomal protein S17

Chain 2q: 16% 93% 6%



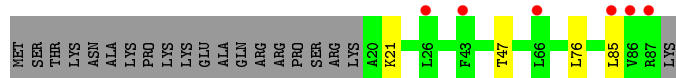
- Molecule 49: 30S ribosomal protein S18

Chain 1r: 7% 74% 23%



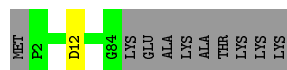
- Molecule 49: 30S ribosomal protein S18

Chain 2r: 7% 73% 5% 23%

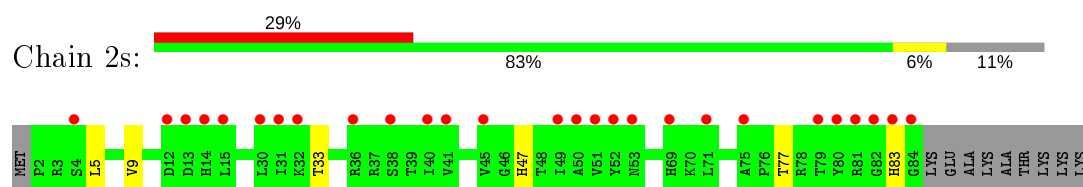


- Molecule 50: 30S ribosomal protein S19

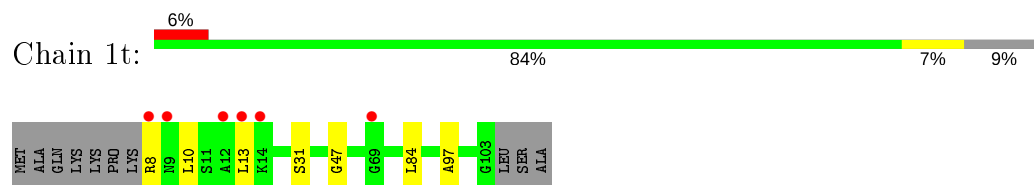
Chain 1s: 88% 11%



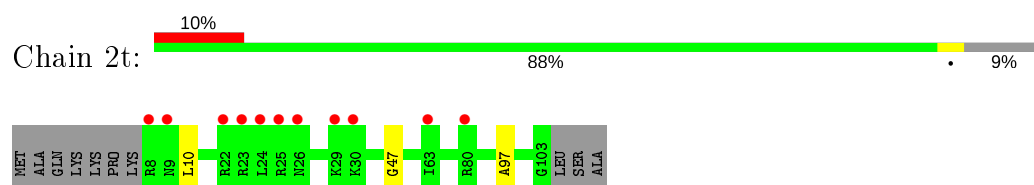
- Molecule 50: 30S ribosomal protein S19



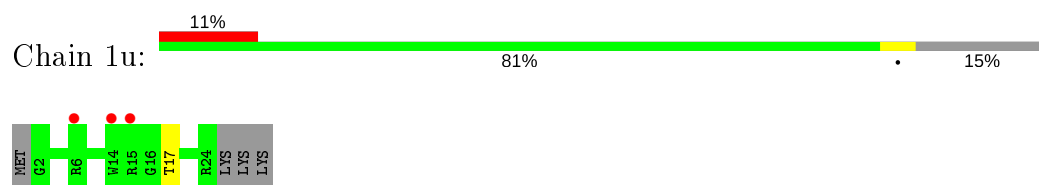
- Molecule 51: 30S ribosomal protein S20



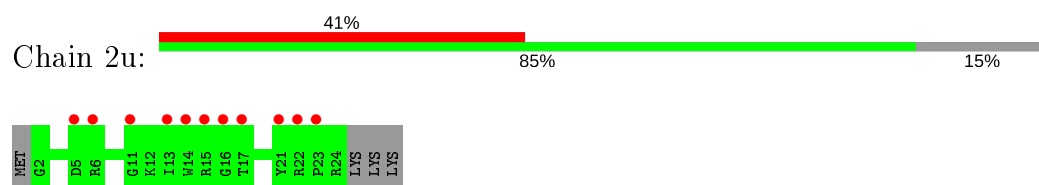
- Molecule 51: 30S ribosomal protein S20



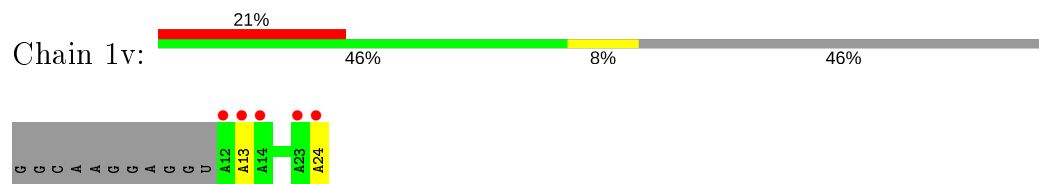
- Molecule 52: 30S ribosomal protein Thx



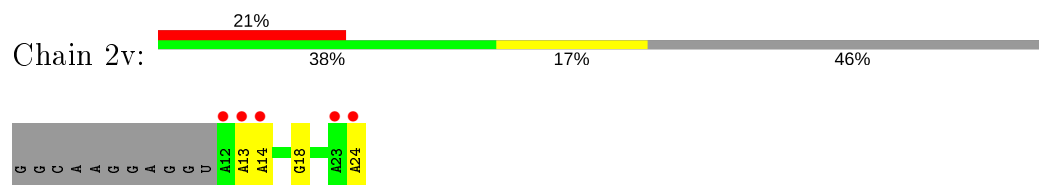
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



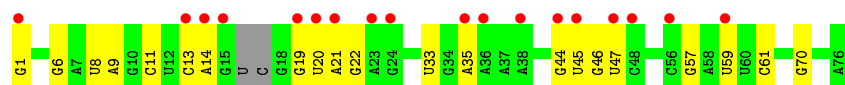
- Molecule 53: mRNA



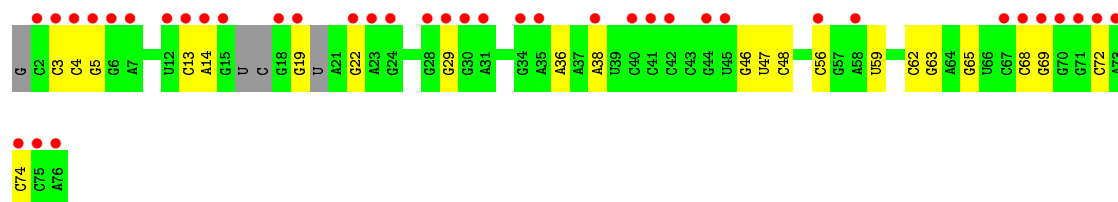
- Molecule 54: A-site and E-site tRNAs



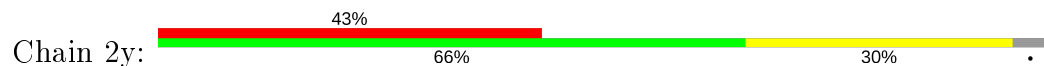
- Molecule 54: A-site and E-site tRNAs



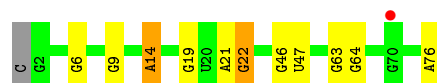
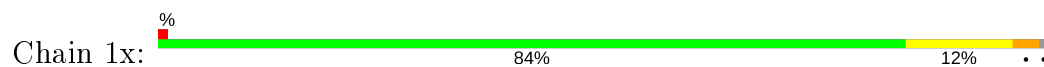
- Molecule 54: A-site and E-site tRNAs



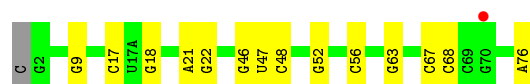
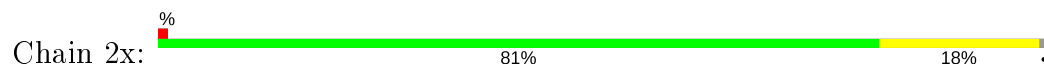
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.99Å 448.29Å 618.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.28 – 2.60 254.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (127.28-2.60) 98.7 (254.56-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.229 , 0.276 0.230 , 0.277	Depositor DCC
R_{free} test set	86986 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	300833	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, CLM, ZN, M2G, OMG, 2MU, MIA, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, K, PSU

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	0.33	0/69009	0.82	39/107712 (0.0%)
1	2A	0.26	0/67293	0.78	15/105034 (0.0%)
2	1B	0.32	1/2882 (0.0%)	0.74	0/4494
2	2B	0.30	1/2879 (0.0%)	0.80	1/4487 (0.0%)
3	1D	0.32	0/2186	0.53	0/2944
3	2D	0.28	0/2186	0.49	0/2944
4	1E	0.28	0/1592	0.49	0/2149
4	2E	0.26	0/1592	0.48	0/2149
5	1F	0.27	0/1619	0.47	0/2193
5	2F	0.26	0/1615	0.44	0/2188
6	1G	0.27	0/1448	0.45	0/1957
6	2G	0.25	0/1453	0.45	0/1963
7	1H	0.27	0/1356	0.45	0/1834
7	2H	0.25	0/1356	0.44	0/1834
8	1I	0.25	0/1112	0.44	0/1514
8	2I	0.25	0/1079	0.47	0/1475
9	1N	0.28	0/1144	0.46	0/1543
9	2N	0.25	0/1144	0.43	0/1543
10	1O	0.30	0/943	0.49	0/1269
10	2O	0.28	0/943	0.48	0/1269
11	1P	0.27	0/1152	0.49	0/1533
11	2P	0.27	0/1152	0.48	0/1533
12	1Q	0.29	0/1143	0.46	0/1527
12	2Q	0.26	0/1143	0.45	0/1527
13	1R	0.26	0/982	0.47	0/1312
13	2R	0.24	0/982	0.44	0/1312
14	1S	0.27	0/883	0.48	0/1176
14	2S	0.25	0/880	0.43	0/1172
15	1T	0.26	0/1105	0.45	0/1477
15	2T	0.24	0/1097	0.44	0/1468
16	1U	0.29	0/977	0.44	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.25	0/977	0.39	0/1301
17	1V	0.30	0/782	0.52	0/1049
17	2V	0.27	0/782	0.49	0/1049
18	1W	0.28	0/897	0.47	0/1205
18	2W	0.26	0/897	0.42	0/1205
19	1X	0.30	0/764	0.50	0/1025
19	2X	0.25	0/764	0.45	0/1025
20	1Y	0.29	0/819	0.48	0/1095
20	2Y	0.27	0/819	0.49	0/1095
21	1Z	0.27	0/1267	0.48	0/1717
21	2Z	0.26	0/1299	0.48	0/1763
22	10	0.29	0/662	0.48	0/881
22	20	0.27	0/662	0.49	0/881
23	11	0.27	0/762	0.47	0/1014
23	21	0.26	0/762	0.46	0/1014
24	12	0.26	0/590	0.41	0/781
24	22	0.24	0/590	0.36	0/781
25	13	0.27	0/474	0.45	0/635
25	23	0.25	0/469	0.41	0/630
26	14	0.29	0/565	0.53	0/761
26	24	0.29	0/545	0.49	0/737
27	15	0.27	0/469	0.52	0/635
27	25	0.27	0/469	0.44	0/635
28	16	0.28	0/460	0.48	0/613
28	26	0.26	0/456	0.44	0/608
29	17	0.26	0/426	0.45	0/561
29	27	0.24	0/426	0.45	0/561
30	18	0.28	0/525	0.49	0/691
30	28	0.25	0/525	0.44	0/691
31	19	0.27	0/310	0.48	0/407
31	29	0.26	0/310	0.50	0/407
32	1a	0.26	0/35795	0.81	24/55864 (0.0%)
32	2a	0.25	0/35886	0.81	20/56005 (0.0%)
33	1b	0.25	0/1881	0.45	0/2542
33	2b	0.26	0/1860	0.45	0/2518
34	1c	0.25	0/1572	0.43	0/2126
34	2c	0.25	0/1566	0.45	0/2119
35	1d	0.25	0/1685	0.42	0/2262
35	2d	0.25	0/1704	0.43	0/2284
36	1e	0.26	0/1145	0.48	0/1543
36	2e	0.25	0/1149	0.47	0/1548
37	1f	0.26	0/823	0.45	0/1115
37	2f	0.26	0/829	0.44	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.24	0/1250	0.41	0/1679
38	2g	0.24	0/1254	0.41	0/1683
39	1h	0.25	0/1108	0.44	0/1494
39	2h	0.24	0/1108	0.43	0/1494
40	1i	0.27	0/1002	0.47	0/1346
40	2i	0.26	0/997	0.47	0/1343
41	1j	0.24	0/722	0.48	0/982
41	2j	0.25	0/727	0.48	0/988
42	1k	0.25	0/844	0.45	0/1145
42	2k	0.25	0/848	0.44	0/1149
43	1l	0.26	0/937	0.49	0/1260
43	2l	0.25	0/937	0.47	0/1260
44	1m	0.26	0/969	0.43	0/1302
44	2m	0.26	0/961	0.47	0/1291
45	1n	0.25	0/501	0.41	0/664
45	2n	0.25	0/501	0.40	0/664
46	1o	0.24	0/739	0.42	0/985
46	2o	0.23	0/739	0.39	0/985
47	1p	0.24	0/697	0.44	0/939
47	2p	0.26	0/693	0.47	0/935
48	1q	0.25	0/836	0.44	0/1117
48	2q	0.25	0/836	0.44	0/1117
49	1r	0.25	0/560	0.42	0/746
49	2r	0.24	0/560	0.42	0/746
50	1s	0.25	0/667	0.50	0/900
50	2s	0.27	0/661	0.53	0/893
51	1t	0.24	0/730	0.41	0/965
51	2t	0.24	0/729	0.40	0/965
52	1u	0.24	0/203	0.44	0/266
52	2u	0.27	0/203	0.46	0/266
53	1v	0.34	0/310	0.88	0/480
53	2v	0.38	0/310	0.89	0/480
54	1w	0.43	1/1606 (0.1%)	1.04	1/2497 (0.0%)
54	1y	0.41	1/1606 (0.1%)	1.00	4/2497 (0.2%)
54	2w	0.34	0/1556	0.99	0/2418
54	2y	0.41	1/1583 (0.1%)	0.98	3/2459 (0.1%)
55	1x	0.39	0/1725	1.02	10/2689 (0.4%)
55	2x	0.31	0/1725	0.92	1/2689 (0.0%)
All	All	0.28	5/316686 (0.0%)	0.73	118/474113 (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
26	14	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	1	G	OP3-P	-10.51	1.48	1.61
54	1w	1	G	OP3-P	-10.46	1.48	1.61
2	2B	1	U	OP3-P	-10.40	1.48	1.61
54	2y	1	G	OP3-P	-10.33	1.48	1.61
2	1B	1	U	OP3-P	-10.31	1.48	1.61

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1075	C	N1-C2-O2	10.47	125.18	118.90
1	1A	801	G	O5'-P-OP2	-9.90	96.79	105.70
1	1A	975	C	N1-C2-O2	-9.05	113.47	118.90
2	2B	80	U	O4'-C1'-N1	8.59	115.07	108.20
1	2A	2473	U	C2-N1-C1'	7.86	127.13	117.70
32	2a	1054	C	C2-N1-C1'	7.79	127.37	118.80
1	1A	975	C	C2-N1-C1'	-7.78	110.24	118.80
54	2y	33	U	C2-N1-C1'	7.74	126.99	117.70
32	1a	1027	C	N3-C4-C5	-7.66	118.83	121.90
55	1x	46	G	C6-N1-C2	-7.57	120.56	125.10
54	1y	33	U	C2-N1-C1'	7.53	126.74	117.70
1	1A	2167	U	C2-N1-C1'	7.48	126.68	117.70
1	1A	1075	C	C2-N3-C4	7.46	123.63	119.90
32	2a	754	C	C2-N1-C1'	7.40	126.94	118.80
1	1A	12	U	C2-N1-C1'	7.37	126.55	117.70
32	1a	1030(B)	C	C2-N1-C1'	7.19	126.71	118.80
55	1x	14	A	C4-C5-C6	7.12	120.56	117.00
32	2a	1054	C	N1-C2-O2	7.11	123.16	118.90
1	2A	2139	C	C2-N1-C1'	7.06	126.57	118.80
32	1a	1034	G	C6-N1-C2	6.95	129.27	125.10
32	1a	1030	C	N1-C2-O2	6.92	123.05	118.90
32	1a	1030(B)	C	N1-C2-O2	6.90	123.04	118.90
32	1a	1027	C	C5-C4-N4	6.88	125.02	120.20
32	1a	1034	G	N3-C2-N2	6.85	124.69	119.90
32	2a	754	C	N1-C2-O2	6.80	122.98	118.90
54	1y	33	U	N1-C2-O2	6.75	127.53	122.80
32	2a	1158	C	N1-C2-O2	6.61	122.86	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1063	G	N3-C2-N2	6.58	124.51	119.90
1	2A	2473	U	N1-C2-O2	6.57	127.39	122.80
32	2a	1158	C	C2-N1-C1'	6.53	125.98	118.80
1	1A	2167	U	N1-C2-O2	6.51	127.36	122.80
32	1a	1025	U	N1-C2-O2	6.40	127.28	122.80
1	1A	2061	G	O5'-P-OP2	-6.40	99.94	105.70
32	1a	841	U	C5-C6-N1	6.37	125.88	122.70
1	1A	1058	G	C5-C6-O6	6.30	132.38	128.60
32	1a	266	G	P-O3'-C3'	6.27	127.22	119.70
54	2y	33	U	N1-C2-O2	6.16	127.11	122.80
1	1A	2167	U	N3-C2-O2	-6.14	117.90	122.20
1	1A	1176	G	OP1-P-O3'	6.14	118.70	105.20
1	1A	1313	U	C2-N1-C1'	6.13	125.06	117.70
55	1x	22	G	C4-C5-C6	-6.12	115.13	118.80
1	1A	889	C	N1-C2-O2	6.08	122.55	118.90
32	1a	1030(B)	C	N3-C2-O2	-6.07	117.65	121.90
1	1A	512	G	O4'-C1'-N9	6.06	113.05	108.20
32	2a	1054	C	N3-C2-O2	-6.06	117.66	121.90
1	1A	624	C	O5'-P-OP1	-6.05	100.25	105.70
32	2a	1028	C	C2-N3-C4	6.04	122.92	119.90
32	1a	754	C	C2-N1-C1'	6.02	125.42	118.80
1	2A	2139	C	C6-N1-C1'	-6.01	113.58	120.80
55	1x	22	G	N1-C6-O6	-5.99	116.31	119.90
55	1x	14	A	C5-N7-C8	5.96	106.88	103.90
1	2A	1313	U	C2-N1-C1'	5.94	124.83	117.70
1	2A	2140	C	C2-N1-C1'	5.93	125.32	118.80
54	2y	33	U	N3-C2-O2	-5.89	118.08	122.20
32	2a	1001(A)	G	N3-C4-N9	5.87	129.52	126.00
1	1A	1075	C	C2-N1-C1'	5.87	125.26	118.80
32	2a	1039	C	N1-C2-O2	5.87	122.42	118.90
32	1a	1027	C	C6-N1-C1'	5.87	127.84	120.80
55	1x	22	G	C8-N9-C1'	5.86	134.62	127.00
1	1A	1075	C	N3-C2-O2	-5.85	117.81	121.90
1	1A	1063	G	C5-C6-O6	5.85	132.11	128.60
32	1a	1034	G	C5-C6-O6	5.81	132.09	128.60
1	2A	2473	U	N3-C2-O2	-5.81	118.13	122.20
32	1a	1030(B)	C	C6-N1-C2	-5.80	117.98	120.30
1	1A	1063	G	C6-N1-C2	5.78	128.57	125.10
54	1w	22	G	N1-C6-O6	5.77	123.36	119.90
55	1x	22	G	N3-C4-N9	-5.72	122.56	126.00
54	1y	33	U	N3-C2-O2	-5.71	118.20	122.20
1	1A	1080	C	N3-C4-C5	-5.70	119.62	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	975	C	C6-N1-C1'	5.69	127.63	120.80
1	1A	1080	C	C2-N3-C4	5.64	122.72	119.90
1	2A	2136	C	N1-C2-O2	5.64	122.28	118.90
1	1A	1102	C	C2-N1-C1'	5.60	124.97	118.80
1	1A	847	U	C2-N1-C1'	5.57	124.38	117.70
32	1a	1158	C	C2-N1-C1'	5.57	124.93	118.80
32	1a	1034	G	N9-C4-C5	-5.52	103.19	105.40
1	2A	2149	G	N3-C4-N9	5.51	129.31	126.00
1	2A	2174	C	N1-C2-O2	5.48	122.19	118.90
1	1A	2790	A	C2-N3-C4	5.44	113.32	110.60
1	1A	1313	U	N3-C2-O2	-5.43	118.40	122.20
32	2a	266	G	P-O3'-C3'	5.41	126.19	119.70
55	1x	22	G	C6-C5-N7	5.40	133.64	130.40
1	1A	2848	G	O4'-C1'-N9	5.39	112.51	108.20
32	2a	1158	C	N3-C2-O2	-5.38	118.13	121.90
32	1a	1025	U	C2-N1-C1'	5.37	124.15	117.70
1	2A	90	U	C2-N1-C1'	5.37	124.14	117.70
32	2a	65	U	P-O3'-C3'	5.36	126.14	119.70
32	2a	1054	C	C6-N1-C1'	-5.35	114.38	120.80
1	2A	528	A	OP1-P-O3'	5.35	116.97	105.20
1	1A	1174	A	P-O3'-C3'	5.34	126.11	119.70
1	1A	975	C	N3-C2-O2	5.34	125.64	121.90
32	2a	754	C	N3-C2-O2	-5.34	118.17	121.90
1	2A	2473	U	C6-N1-C1'	-5.33	113.73	121.20
32	2a	1054	C	C6-N1-C2	-5.33	118.17	120.30
1	1A	1313	U	N1-C2-O2	5.31	126.52	122.80
1	1A	787	U	O5'-P-OP1	-5.24	100.98	105.70
1	1A	1102	C	N1-C2-O2	5.24	122.04	118.90
32	1a	1027	C	N3-C2-O2	-5.23	118.24	121.90
1	1A	12	U	C6-N1-C1'	-5.23	113.88	121.20
55	1x	14	A	C5-C6-N1	-5.20	115.10	117.70
32	1a	98	G	N3-C4-N9	5.19	129.12	126.00
32	1a	1030	C	C2-N3-C4	5.18	122.49	119.90
1	1A	889	C	C2-N1-C1'	5.18	124.50	118.80
1	1A	568	U	C5-C4-O4	-5.17	122.80	125.90
55	1x	22	G	C4-N9-C1'	-5.17	119.78	126.50
32	2a	1028	C	C5-C4-N4	5.15	123.81	120.20
32	2a	754	C	C6-N1-C1'	-5.13	114.64	120.80
1	2A	2152	G	N3-C4-N9	5.12	129.07	126.00
1	1A	548	A	P-O3'-C3'	5.11	125.84	119.70
32	1a	754	C	N1-C2-O2	5.09	121.95	118.90
32	2a	204	U	C2-N1-C1'	5.09	123.81	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1075	C	C5-C6-N1	5.07	123.54	121.00
1	2A	2152	G	C5-C6-O6	-5.07	125.56	128.60
54	1y	33	U	C6-N1-C1'	-5.06	114.12	121.20
32	2a	1065	U	P-O3'-C3'	5.04	125.75	119.70
32	1a	1067	A	P-O3'-C3'	5.01	125.72	119.70
32	1a	841	U	C6-N1-C2	-5.01	117.99	121.00
55	2x	17	C	C2-N1-C1'	5.01	124.31	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	57	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31191	688	0
1	2A	60322	0	30425	795	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	45	0
3	1D	2136	0	2218	45	0
3	2D	2136	0	2218	57	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	37	0
5	1F	1584	0	1625	43	0
5	2F	1580	0	1619	37	0
6	1G	1423	0	1436	33	0
6	2G	1428	0	1438	46	0
7	1H	1330	0	1407	23	0
7	2H	1330	0	1407	40	0
8	1I	1097	0	1140	17	0
8	2I	1064	0	1082	20	0
9	1N	1117	0	1184	17	0
9	2N	1117	0	1184	27	0
10	1O	933	0	996	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	2O	933	0	996	30	0
11	1P	1135	0	1212	40	0
11	2P	1135	0	1212	27	0
12	1Q	1122	0	1179	26	0
12	2Q	1122	0	1179	24	0
13	1R	968	0	1033	27	0
13	2R	968	0	1033	25	0
14	1S	873	0	927	16	0
14	2S	870	0	923	19	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	29	0
16	1U	959	0	1019	22	0
16	2U	959	0	1018	20	0
17	1V	771	0	829	10	0
17	2V	771	0	830	15	0
18	1W	886	0	940	22	0
18	2W	886	0	940	10	0
19	1X	750	0	814	9	0
19	2X	750	0	814	16	0
20	1Y	806	0	881	22	0
20	2Y	806	0	881	25	0
21	1Z	1240	0	1240	26	0
21	2Z	1271	0	1273	29	0
22	10	653	0	674	18	0
22	20	653	0	674	19	0
23	11	755	0	826	13	0
23	21	755	0	826	19	0
24	12	588	0	643	10	0
24	22	588	0	643	13	0
25	13	469	0	518	15	0
25	23	464	0	514	9	0
26	14	552	0	533	18	0
26	24	532	0	503	12	0
27	15	455	0	465	6	0
27	25	455	0	465	13	0
28	16	453	0	473	10	0
28	26	449	0	469	12	0
29	17	418	0	467	9	0
29	27	418	0	467	14	0
30	18	517	0	582	21	0
30	28	517	0	582	23	0
31	19	307	0	335	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	29	307	0	335	9	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16340	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1675	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1184	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	2u	199	0	208	0	0
53	1v	277	0	140	0	0
53	2v	277	0	140	0	0
54	1w	1592	0	819	0	0
54	1y	1585	0	804	0	0
54	2w	1544	0	788	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	829	0	0
55	2x	1625	0	829	0	0
56	10	6	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	3	0	0	0	0
56	14	1	0	0	0	0
56	15	5	0	0	0	0
56	16	3	0	0	0	0
56	17	8	0	0	0	0
56	18	7	0	0	0	0
56	19	1	0	0	0	0
56	1A	1101	0	0	0	0
56	1B	39	0	0	0	0
56	1D	13	0	0	0	0
56	1E	15	0	0	0	0
56	1F	10	0	0	0	0
56	1G	4	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	5	0	0	0	0
56	1P	9	0	0	0	0
56	1Q	8	0	0	0	0
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	4	0	0	0	0
56	1U	12	0	0	0	0
56	1V	7	0	0	0	0
56	1W	5	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	233	0	0	0	0
56	1b	2	0	0	0	0
56	1d	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1h	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	2	0	0	0	0
56	1n	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	12	0	0	0	0
56	1x	18	0	0	0	0
56	20	3	0	0	0	0
56	21	1	0	0	0	0
56	23	3	0	0	0	0
56	25	5	0	0	0	0
56	27	2	0	0	0	0
56	28	3	0	0	0	0
56	2A	887	0	0	0	0
56	2B	20	0	0	0	0
56	2D	10	0	0	0	0
56	2E	4	0	0	0	0
56	2F	6	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	4	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	2	0	0	0	0
56	2T	4	0	0	0	0
56	2U	3	0	0	0	0
56	2V	3	0	0	0	0
56	2W	3	0	0	0	0
56	2X	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	241	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2i	1	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2l	4	0	0	0	0
56	2m	1	0	0	0	0
56	2q	2	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	1	0	0	0	0
56	2w	4	0	0	0	0
56	2x	5	0	0	0	0
56	2y	6	0	0	0	0
57	1A	20	0	11	0	0
57	2A	20	0	11	1	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	12	0	0	1	0
61	11	10	0	0	0	0
61	12	4	0	0	0	0
61	13	4	0	0	0	0
61	14	2	0	0	0	0
61	15	7	0	0	0	0
61	16	1	0	0	1	0
61	17	7	0	0	0	0
61	18	19	0	0	2	0
61	1A	2246	0	0	69	0
61	1B	73	0	0	1	0
61	1D	24	0	0	1	0
61	1E	27	0	0	0	0
61	1F	9	0	0	0	0
61	1G	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1H	1	0	0	0	0
61	1I	2	0	0	0	0
61	1N	4	0	0	0	0
61	1O	7	0	0	0	0
61	1P	21	0	0	0	0
61	1Q	11	0	0	0	0
61	1R	8	0	0	1	0
61	1S	4	0	0	0	0
61	1T	6	0	0	0	0
61	1U	9	0	0	0	0
61	1V	7	0	0	0	0
61	1W	9	0	0	2	0
61	1X	7	0	0	0	0
61	1Y	3	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	430	0	0	0	0
61	1b	1	0	0	0	0
61	1d	1	0	0	0	0
61	1f	1	0	0	0	0
61	1l	7	0	0	0	0
61	1q	4	0	0	0	0
61	1w	16	0	0	0	0
61	1x	15	0	0	0	0
61	1y	1	0	0	0	0
61	20	10	0	0	1	0
61	21	6	0	0	0	0
61	22	1	0	0	0	0
61	25	4	0	0	0	0
61	27	2	0	0	1	0
61	28	6	0	0	0	0
61	29	1	0	0	0	0
61	2A	1405	0	0	58	0
61	2B	25	0	0	1	0
61	2D	17	0	0	0	0
61	2E	3	0	0	0	0
61	2F	6	0	0	0	0
61	2I	3	0	0	0	0
61	2N	1	0	0	0	0
61	2O	1	0	0	0	0
61	2P	11	0	0	1	0
61	2Q	2	0	0	0	0
61	2R	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2T	5	0	0	0	0
61	2U	2	0	0	0	0
61	2W	3	0	0	0	0
61	2Z	1	0	0	0	0
61	2a	380	0	0	0	0
61	2d	1	0	0	0	0
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	3	0	0	0	0
61	2l	2	0	0	0	0
61	2p	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	2	0	0	0	0
61	2x	7	0	0	0	0
61	2y	13	0	0	0	0
All	All	300833	0	196713	2412	0

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

All (2412) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2138:C:N4	1:2A:2153:G:H1	1.53	1.07
1:2A:2129:C:N4	1:2A:2159:G:H1	1.55	1.03
1:1A:1058:G:H1	1:1A:1080:C:N4	1.56	1.01
1:2A:1002:G:H1	1:2A:1038:C:N4	42.24	1.01
1:1A:1082:U:O4	1:1A:1086:A:N1	1.96	0.97
1:1A:2100:G:H1	1:1A:2189:U:H3	1.11	0.96
1:1A:2136:C:N4	1:1A:2155:G:H1	1.64	0.95
1:1A:2136:C:H42	1:1A:2155:G:H1	0.97	0.94
1:1A:1059:G:H1	1:1A:1079:C:N4	1.65	0.92
1:2A:2136:C:N4	1:2A:2155:G:H1	1.68	0.92
1:2A:2121:G:H1	1:2A:2177:C:H42	0.99	0.92
1:2A:2099:U:H3	1:2A:2190:G:H1	1.18	0.91
1:2A:1011:G:H1	1:2A:1018:C:N4	18.10	0.91
1:1A:1082:U:H3	1:1A:1086:A:N6	1.68	0.91
1:1A:1059:G:H1	1:1A:1079:C:H42	0.92	0.91
1:1A:1082:U:H3	1:1A:1086:A:H61	0.92	0.91
1:2A:1011:G:H1	1:2A:1018:C:H42	17.82	0.90
1:2A:2096:U:H3	1:2A:2193:G:H1	1.20	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1055:G:H1	1:1A:1104:C:H42	1.21	0.89
1:2A:2127:G:C2	1:2A:2161:C:N3	2.41	0.88
1:2A:2121:G:H1	1:2A:2177:C:N4	1.73	0.87
1:1A:2136:C:N3	1:1A:2155:G:N2	2.23	0.85
1:1A:1054:A:H61	1:1A:1105:U:H3	1.25	0.85
1:2A:2127:G:N1	1:2A:2161:C:C4	2.45	0.85
1:2A:2127:G:N2	1:2A:2161:C:C2	2.44	0.85
1:2A:2127:G:C6	1:2A:2161:C:N4	2.45	0.85
1:2A:2129:C:H42	1:2A:2159:G:H1	0.89	0.84
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.60	0.84
22:10:10:THR:HG22	22:10:12:ASN:H	1.43	0.83
1:1A:1058:G:N2	1:1A:1080:C:N3	2.24	0.83
1:1A:1054:A:N6	1:1A:1105:U:H3	1.76	0.83
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.11	0.83
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.60	0.83
1:2A:2127:G:C2	1:2A:2161:C:C4	2.67	0.83
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.10	0.83
1:2A:1002:G:N2	1:2A:1038:C:N3	41.60	0.83
1:2A:2138:C:N3	1:2A:2153:G:N2	2.26	0.82
1:1A:1065:U:O2	1:1A:1073:A:N6	2.12	0.82
1:2A:878:A:H61	1:2A:899:A:H1'	1.43	0.82
1:2A:1566:A:OP1	3:2D:211:ARG:NH1	2.13	0.81
1:1A:1818:U:OP2	3:1D:157:ARG:NH1	2.13	0.81
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.14	0.81
1:2A:266:G:H5''	1:2A:268:C:H41	11.35	0.81
1:1A:2135:A:H5'	1:1A:2160:G:H4'	1.62	0.81
1:1A:1058:G:H1	1:1A:1080:C:H42	0.82	0.80
1:2A:2167:U:H2'	1:2A:2168:G:H21	1.42	0.80
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.64	0.80
1:2A:2129:C:N3	1:2A:2159:G:N2	2.29	0.80
1:1A:2099:U:H3	1:1A:2190:G:H1	1.27	0.79
1:2A:652(D):C:H42	1:2A:652(U):G:H1	1.28	0.79
1:1A:882:G:H1	1:1A:894:C:H42	1.26	0.79
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.64	0.79
3:2D:69:ARG:HE	3:2D:130:ALA:HB2	1.47	0.79
1:1A:880:G:H2'	1:1A:881:G:H8	1.48	0.78
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.65	0.78
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.16	0.78
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.19	0.77
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.67	0.77
1:1A:1422:G:H5''	10:1O:48:PRO:HB3	100.25	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1689:A:H62	1:2A:1698:A:H2	1.31	0.77
1:2A:2595:G:N7	61:2A:6286:HOH:O	2.17	0.77
8:2I:124:GLY:H	8:2I:144:VAL:HG23	1.50	0.76
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.68	0.76
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.19	0.75
1:2A:1818:U:OP2	3:2D:157:ARG:NH1	2.20	0.75
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.19	0.75
1:1A:1039:G:H1	1:1A:1116:C:H42	1.33	0.75
1:2A:993:G:N7	1:2A:1213:A:N6	48.90	0.75
1:2A:1002:G:H1	1:2A:1038:C:H42	42.52	0.74
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.70	0.74
1:2A:775:G:O3'	61:2A:4892:HOH:O	2.06	0.74
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.21	0.74
1:2A:2127:G:C2	1:2A:2161:C:C2	2.75	0.74
1:1A:2129:C:H42	1:1A:2159:G:H1	1.36	0.74
1:1A:2759:G:N7	61:1A:4924:HOH:O	2.20	0.73
1:1A:510:C:OP1	61:1A:6777:HOH:O	2.05	0.73
1:2A:1007:C:N3	1:2A:1022:G:O6	16.53	0.73
1:2A:2875:C:OP1	15:2T:3:ARG:NH1	2.22	0.73
1:1A:400:G:N7	61:1A:6131:HOH:O	2.20	0.73
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.52	0.73
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.71	0.73
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.21	0.73
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.21	0.73
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.21	0.73
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.21	0.72
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.23	0.72
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.55	0.72
1:2A:89:G:H3'	1:2A:90:U:H5''	1.71	0.72
30:28:32:LEU:O	30:28:36:LYS:NZ	2.21	0.72
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD22	1.70	0.72
4:1E:77:ILE:HG21	4:1E:195:LEU:HD11	1.72	0.72
1:1A:279:C:H42	1:1A:361:G:H1	1.36	0.71
1:2A:698:C:O2'	1:2A:734:A:N6	2.23	0.71
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.38	0.71
1:1A:1783:A:N7	61:1A:6221:HOH:O	2.24	0.71
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.72	0.71
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.73	0.71
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE2	1.56	0.71
1:2A:1011:G:N2	1:2A:1018:C:N3	20.66	0.71
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1059:G:N2	1:1A:1079:C:N3	2.37	0.70
1:2A:1780:A:N7	61:2A:4441:HOH:O	2.24	0.70
1:2A:307:G:N1	1:2A:310:A:OP2	2.24	0.70
1:2A:309:G:N3	1:2A:329:G:O2'	2.24	0.70
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.56	0.70
1:2A:2121:G:N2	1:2A:2177:C:N3	2.33	0.70
1:2A:2502:G:N7	61:2A:5288:HOH:O	2.23	0.70
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.20	0.70
1:1A:1023:U:OP2	61:1A:5955:HOH:O	2.09	0.70
22:20:10:THR:HG22	22:20:12:ASN:H	1.57	0.70
1:2A:2138:C:H42	1:2A:2153:G:H1	0.77	0.70
9:1N:67:LEU:HA	9:1N:87:LEU:HD22	1.74	0.70
1:1A:2722:G:OP2	61:1A:4900:HOH:O	2.10	0.70
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.55	0.70
1:1A:2789:C:O2	1:1A:2894:G:N2	2.17	0.70
1:2A:500:G:N1	1:2A:503:A:OP2	2.25	0.70
6:2G:79:ASN:OD1	6:2G:79:ASN:N	2.25	0.70
1:2A:947:G:OP2	61:2A:5952:HOH:O	2.10	0.70
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.23	0.69
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.72	0.69
1:2A:1204:A:H2	1:2A:1241:A:H62	1.40	0.69
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.24	0.69
1:2A:854:G:H2'	1:2A:855:G:H8	1.57	0.69
9:2N:34:LEU:HD21	9:2N:120:LEU:HB2	1.73	0.69
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.75	0.69
1:2A:962:G:OP1	61:2A:4963:HOH:O	2.11	0.69
28:26:10:LEU:HD13	28:26:19:ARG:HD3	1.75	0.69
17:2V:46:VAL:HG23	17:2V:52:VAL:HG11	1.73	0.69
1:1A:1311:G:H2'	29:17:47:ARG:HH22	1.57	0.69
28:26:34:LEU:H	28:26:51:GLU:HG2	1.58	0.69
1:1A:1055:G:H1	1:1A:1104:C:N4	1.89	0.69
1:2A:630:G:OP2	30:28:15:LYS:NZ	2.24	0.69
1:2A:84:A:N1	1:2A:98:G:O2'	2.24	0.69
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.74	0.68
6:2G:18:GLU:OE1	6:2G:21:ARG:NH1	2.26	0.68
1:1A:1053:C:H42	1:1A:1106:G:H1	1.40	0.68
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.29	0.68
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.27	0.68
1:2A:2136:C:N3	1:2A:2155:G:N2	2.36	0.68
1:2A:2431:U:OP1	61:2A:4426:HOH:O	2.12	0.68
12:1Q:10:ARG:HH12	12:1Q:90:VAL:H	1.40	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:987:G:O2'	1:2A:1000:A:N3	2.24	0.68
1:2A:586:A:N1	1:2A:809:G:O2'	2.25	0.68
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.57	0.68
23:21:59:THR:O	23:21:91:LYS:NZ	2.27	0.68
9:2N:40:PRO:HB3	16:2U:68:ALA:HB2	1.76	0.68
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.40	0.68
1:1A:9:U:H3	1:1A:2629:A:H2	1.40	0.68
1:1A:1773:A:OP2	61:1A:5760:HOH:O	2.12	0.67
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.26	0.67
1:2A:81:G:N7	61:2A:4126:HOH:O	2.27	0.67
1:1A:1026:U:OP1	61:1A:5955:HOH:O	2.11	0.67
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.28	0.67
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.27	0.67
26:24:64:GLY:O	26:24:66:SER:N	2.26	0.67
1:1A:2121:G:H1	1:1A:2177:C:H42	1.42	0.67
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.76	0.67
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	1.76	0.67
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.27	0.67
1:2A:2136:C:N4	1:2A:2155:G:N1	2.41	0.67
1:1A:1077:A:H2'	1:1A:1078:U:H4'	1.75	0.67
1:1A:2022:U:OP1	61:1A:7049:HOH:O	2.12	0.67
1:2A:882:G:H2'	1:2A:883:G:C8	2.29	0.67
1:2A:922:U:O2'	22:20:29:GLN:NE2	2.26	0.67
5:1F:158:THR:O	5:1F:164:ARG:NH1	2.28	0.67
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.22	0.67
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.27	0.67
23:21:50:ARG:NH1	23:21:57:GLU:OE2	2.28	0.67
6:2G:105:LYS:NZ	26:24:25:TYR:O	2.28	0.67
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.77	0.66
25:13:5:LYS:NZ	25:13:34:GLU:OE2	2.28	0.66
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.75	0.66
61:2A:4822:HOH:O	11:2P:42:SER:O	2.13	0.66
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.28	0.66
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.28	0.66
1:1A:2632:A:HO2'	1:1A:2811:G:HO2'	1.39	0.66
1:2A:1771:C:OP1	61:2A:6272:HOH:O	2.14	0.66
1:2A:2049:G:N7	61:2A:6105:HOH:O	2.26	0.66
1:1A:530:G:N1	1:1A:2023:G:OP1	2.25	0.66
1:1A:500:G:N7	61:1A:6883:HOH:O	2.27	0.66
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.61	0.66
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:392:C:H5''	1:2A:409:C:H5''	1.76	0.66
7:2H:59:ARG:O	7:2H:63:SER:OG	2.14	0.66
4:2E:18:ASP:OD2	15:2T:33:LYS:NZ	2.28	0.66
1:1A:1176:G:H1'	1:1A:1177:A:H5''	1.78	0.66
26:24:14:ILE:HB	26:24:22:ILE:HB	1.78	0.66
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.77	0.66
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.61	0.66
1:2A:1119:C:H2'	1:2A:1120:G:C8	3.19	0.66
1:2A:299:A:H5''	20:2Y:86:ARG:HH21	1.60	0.66
1:1A:392:C:OP1	61:1A:6959:HOH:O	2.13	0.65
1:2A:1537:G:H2'	1:2A:1538:G:H8	1.60	0.65
1:2A:2577:A:OP1	61:2A:4831:HOH:O	2.13	0.65
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.78	0.65
1:1A:483:A:H5''	20:1Y:50:ARG:HG2	1.78	0.65
1:1A:2053:G:OP1	61:1A:7036:HOH:O	2.14	0.65
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.78	0.65
1:1A:250:G:OP2	30:18:13:ARG:NH2	2.30	0.65
1:1A:1447:G:N7	61:1A:6819:HOH:O	2.29	0.65
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.61	0.65
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.10	0.65
1:2A:1266:G:N2	1:2A:1269:A:OP2	13.70	0.65
1:2A:72:U:OP1	61:2A:6029:HOH:O	2.14	0.65
61:2A:6386:HOH:O	4:2E:127:ASP:OD2	2.14	0.65
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.77	0.65
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.79	0.65
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.78	0.65
1:1A:1173:G:N1	1:1A:1176:G:OP2	2.30	0.65
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.78	0.65
1:1A:1267:U:OP1	61:1A:6299:HOH:O	2.15	0.65
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.80	0.64
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.62	0.64
1:1A:631:A:OP1	11:1P:65:ARG:NE	2.30	0.64
12:2Q:16:ARG:HG2	12:2Q:18:LYS:HG3	1.78	0.64
1:1A:1469:A:OP2	61:1A:6789:HOH:O	2.13	0.64
1:1A:192:C:OP1	61:1A:4755:HOH:O	2.14	0.64
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.32	0.64
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.80	0.64
1:2A:2127:G:C6	1:2A:2161:C:C4	2.85	0.64
1:1A:2839:G:OP1	61:1A:6632:HOH:O	2.15	0.64
21:1Z:41:LEU:HD11	21:1Z:83:PRO:HG2	1.79	0.64
1:2A:2280:G:N7	61:20:206:HOH:O	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.63	0.64
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.78	0.64
1:2A:307:G:H21	1:2A:330:A:H62	1.46	0.64
1:1A:307:G:N7	61:1A:5169:HOH:O	2.30	0.64
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.78	0.64
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.31	0.64
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.44	0.64
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.78	0.64
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.31	0.64
5:1F:70:THR:HG23	5:1F:72:ARG:H	1.63	0.64
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.30	0.63
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.31	0.63
1:2A:1226:A:OP1	17:2V:84:LYS:NZ	2.21	0.63
1:2A:2624:G:N7	61:2A:6351:HOH:O	2.30	0.63
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.80	0.63
20:2Y:86:ARG:HD2	20:2Y:100:ALA:HA	1.80	0.63
1:1A:822:U:OP2	61:1A:6645:HOH:O	2.15	0.63
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.79	0.63
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.31	0.63
1:2A:1025:G:O2'	61:2A:5647:HOH:O	2.15	0.63
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.79	0.63
1:2A:1007:C:O2	1:2A:1022:G:N1	17.99	0.63
29:17:8:ASN:HB3	29:17:11:LYS:HB3	1.79	0.63
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.81	0.63
1:1A:1309:G:H4'	29:17:7:PRO:HB2	1.81	0.63
1:1A:1840:G:N7	61:1A:5163:HOH:O	2.31	0.63
6:1G:18:GLU:OE2	6:1G:21:ARG:NH1	2.32	0.63
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.81	0.63
1:2A:2287:A:H62	1:2A:2344:U:H3	1.46	0.63
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.34	0.63
1:1A:2727:G:O2'	10:1O:70:LYS:NZ	2.30	0.63
1:1A:1048:A:OP2	1:1A:1109:C:N4	2.23	0.62
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.80	0.62
1:1A:2140:C:N3	1:1A:2151:G:O6	2.32	0.62
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.16	0.62
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.80	0.62
1:2A:652(B):A:H61	1:2A:655:A:H1'	1.64	0.62
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.32	0.62
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.80	0.62
1:2A:1378:A:O2'	1:2A:1380:G:N7	2.28	0.62
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1509(A):A:H3'	1:1A:1509(B):A:H8	1.65	0.62
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.81	0.62
24:22:39:ALA:HB2	24:22:44:LEU:HD23	1.81	0.62
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.34	0.62
6:1G:142:PRO:HB2	26:14:31:ILE:HD13	1.81	0.62
1:2A:531:C:OP1	1:2A:561:G:N1	2.31	0.62
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.81	0.62
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.33	0.62
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.82	0.62
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.80	0.62
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.33	0.62
1:2A:2317:C:N4	1:2A:2318:G:O6	2.33	0.62
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.33	0.62
1:2A:2136:C:H42	1:2A:2155:G:H1	1.45	0.61
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.00	0.61
10:2O:63:VAL:HG11	10:2O:85:VAL:HG23	1.82	0.61
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.35	0.61
1:1A:833:U:O2	11:1P:55:ARG:NH2	2.33	0.61
1:2A:2134:A:OP2	1:2A:2135:A:N6	2.32	0.61
1:2A:889:C:O2'	1:2A:890:A:O4'	2.17	0.61
1:2A:2657:A:O3'	7:2H:160:LYS:NZ	2.26	0.61
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.63	0.61
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.33	0.61
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.83	0.61
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.20	0.61
12:2Q:16:ARG:HE	12:2Q:18:LYS:HD3	1.65	0.61
1:1A:2142:C:N3	1:1A:2149:G:O6	2.32	0.61
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	1.83	0.61
12:1Q:35:VAL:HG13	12:1Q:130:LYS:HB3	1.82	0.61
1:2A:132:G:O6	61:2A:5539:HOH:O	2.15	0.61
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	1.82	0.61
1:2A:1434:A:H61	1:2A:1558:A:H62	1.48	0.61
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.35	0.61
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.00	0.61
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.33	0.61
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.82	0.61
1:2A:2336:A:H61	22:20:43:THR:HG22	1.66	0.61
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.18	0.61
1:1A:1176:G:N2	1:1A:1178:C:OP1	2.34	0.61
1:1A:859:G:O2'	1:1A:916:G:O6	2.17	0.61
1:2A:2035:G:O6	61:2A:4288:HOH:O	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:276:A:H5'	1:2A:277:C:H5'	1.83	0.61
1:2A:18:C:O2'	1:2A:554:U:OP1	2.19	0.61
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.81	0.61
5:2F:156:LEU:HD21	5:2F:163:VAL:HG12	1.82	0.61
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.33	0.61
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.83	0.61
18:1W:11:ARG:NH1	18:1W:99:ARG:O	2.33	0.61
1:2A:2127:G:C5	1:2A:2161:C:N4	2.68	0.61
29:27:2:LYS:NZ	61:27:201:HOH:O	2.34	0.60
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.34	0.60
1:1A:674:G:OP2	61:1A:7223:HOH:O	2.17	0.60
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.82	0.60
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.83	0.60
2:2B:110:G:H2'	2:2B:111:G:H5'	1.82	0.60
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.35	0.60
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.01	0.60
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.36	0.60
7:2H:149:ARG:NH1	7:2H:167:GLU:OE2	2.34	0.60
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.34	0.60
1:1A:586:A:H5'	5:1F:89:VAL:HG21	1.84	0.60
18:1W:82:LEU:HB2	18:1W:98:LYS:HB2	1.83	0.60
1:2A:568:U:H5'	1:2A:945:A:N1	2.16	0.60
1:2A:2882:A:OP1	13:2R:96:ARG:NH1	2.33	0.60
3:1D:242:ARG:HD2	3:1D:246:PRO:HG3	1.82	0.60
1:2A:223:A:O2'	1:2A:420:C:O2	2.18	0.60
1:2A:532:A:N6	1:2A:1206:G:O2'	62.37	0.60
1:1A:1754:C:OP1	15:1T:96:ARG:NH1	2.35	0.60
8:1I:5:LEU:HD11	8:1I:19:VAL:HG22	1.82	0.60
1:1A:2728:U:H5'	10:1O:70:LYS:HZ3	1.65	0.60
25:23:7:LYS:HB2	25:23:34:GLU:HG3	1.82	0.60
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.19	0.60
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.83	0.60
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.36	0.60
1:1A:2596:U:OP1	61:1A:4205:HOH:O	2.17	0.60
1:1A:581:C:OP1	16:1U:33:ARG:HG3	2.02	0.60
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.83	0.60
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.82	0.60
4:2E:48:GLN:NE2	4:2E:78:LEU:HD23	2.17	0.60
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.84	0.60
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.37	0.59
1:2A:2126:A:H61	1:2A:2162:G:HO2'	1.49	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.34	0.59
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.37	0.59
1:1A:1226:A:OP1	17:1V:84:LYS:NZ	2.26	0.59
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.84	0.59
1:1A:272(F):C:H42	1:1A:363(D):G:H1	1.51	0.59
1:1A:566:U:H5''	11:1P:29:LYS:HE3	1.85	0.59
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.37	0.59
1:2A:927:G:O6	1:2A:928:G:N2	2.36	0.59
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.37	0.59
1:1A:1452:A:OP2	61:1A:4749:HOH:O	2.17	0.59
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.02	0.59
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.84	0.59
1:1A:2627:G:O2'	1:1A:2781:A:N1	2.30	0.59
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.85	0.59
14:1S:11:LYS:HE2	14:1S:15:ARG:HH12	1.67	0.59
21:1Z:151:HIS:HA	21:1Z:170:THR:HA	1.84	0.59
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.21	0.59
1:1A:1002:G:H3'	1:1A:1003:G:H4'	5.35	0.59
1:2A:1169:G:H1	1:2A:1180:C:H42	1.51	0.59
1:2A:860:U:H1'	1:2A:2268:A:H5'	1.83	0.59
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	99.81	0.59
1:1A:1153:C:OP2	61:1A:5679:HOH:O	2.17	0.59
1:2A:1865:G:OP1	61:2A:3902:HOH:O	2.17	0.59
1:2A:882:G:H1	1:2A:894:C:H42	1.50	0.59
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	1.84	0.59
1:1A:2822:G:OP2	61:1A:6915:HOH:O	2.16	0.59
1:2A:668:G:H5'	1:2A:669:G:OP2	2.03	0.59
20:2Y:64:GLU:OE1	20:2Y:64:GLU:N	2.29	0.59
25:13:6:VAL:HG12	25:13:28:LEU:HD11	1.84	0.59
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.38	0.59
61:2A:6385:HOH:O	4:2E:127:ASP:OD2	2.17	0.59
1:1A:1094:U:H1'	1:1A:1097:U:H5	1.68	0.58
1:1A:624:C:O2'	1:1A:657:U:OP1	2.19	0.58
8:1I:12:LEU:HD22	8:1I:19:VAL:HG21	1.85	0.58
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.35	0.58
11:2P:121:LYS:HG2	11:2P:123:LEU:HG	1.85	0.58
1:1A:764:A:H5''	3:1D:210:GLY:HA2	1.83	0.58
4:1E:128:SER:OG	4:1E:129:HIS:N	2.34	0.58
4:1E:48:GLN:HE21	4:1E:78:LEU:HG	1.68	0.58
1:2A:2144:U:H1'	1:2A:2148:G:N2	2.17	0.58
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:452:G:OP2	61:1A:7439:HOH:O	2.17	0.58
1:1A:878:A:N6	1:1A:899:A:O2'	2.34	0.58
4:1E:8:LYS:HG2	4:1E:192:ASN:HA	1.85	0.58
15:2T:50:ILE:HG22	15:2T:102:ILE:HD11	1.83	0.58
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.36	0.58
1:2A:481:G:N7	61:2A:3913:HOH:O	2.32	0.58
1:2A:90:U:H1'	1:2A:92:A:C8	2.37	0.58
21:2Z:91:LEU:HD11	21:2Z:96:VAL:HG11	1.83	0.58
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.33	0.58
1:1A:744:G:OP1	61:1A:5723:HOH:O	2.16	0.58
2:2B:22:U:H3	2:2B:61:G:H1	1.51	0.58
61:2A:5566:HOH:O	19:2X:44:GLU:OE2	2.17	0.58
1:1A:1702:G:N7	61:1A:6157:HOH:O	2.32	0.58
1:1A:946:G:OP1	61:1A:5865:HOH:O	2.17	0.58
28:26:35:GLU:OE2	28:26:50:ARG:NH1	2.36	0.58
1:2A:1309:G:H4'	29:27:7:PRO:HB2	1.85	0.58
1:2A:1568:G:N7	61:2A:5809:HOH:O	2.32	0.58
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.26	0.58
21:2Z:151:HIS:HA	21:2Z:170:THR:HA	1.84	0.58
21:1Z:21:ALA:O	21:1Z:23:LYS:NZ	2.35	0.58
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.38	0.58
1:2A:111:A:O2'	24:22:65:ASN:ND2	2.37	0.58
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.39	0.58
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.86	0.58
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HB	1.84	0.58
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.85	0.58
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.86	0.57
1:1A:2336:A:H61	22:10:43:THR:CG2	2.17	0.57
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.36	0.57
1:1A:2038:G:O6	61:1A:5710:HOH:O	2.16	0.57
1:1A:2706:G:N7	61:1A:5748:HOH:O	2.32	0.57
61:2A:4994:HOH:O	11:2P:54:GLY:O	2.17	0.57
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.40	0.57
1:1A:532:A:N6	1:1A:1206:G:O2'	61.83	0.57
1:2A:140:G:H1'	1:2A:141:A:H2	1.68	0.57
1:2A:873:G:H1	1:2A:904:C:H42	1.50	0.57
16:2U:92:ARG:HA	16:2U:95:LEU:HB2	1.86	0.57
1:1A:1913:A:H4'	1:1A:1914:C:H5''	1.86	0.57
1:1A:570:G:O6	61:1A:6393:HOH:O	2.17	0.57
1:1A:588:U:H2'	1:1A:589:C:C6	2.39	0.57
1:1A:897:C:N3	1:1A:898:C:N4	2.52	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1119:C:H2'	1:2A:1120:G:H8	2.42	0.57
1:2A:458:G:O2'	1:2A:469:G:O6	2.19	0.57
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	1.85	0.57
1:1A:662:G:H5'	11:1P:16:ARG:HG2	1.85	0.57
1:1A:883:G:H22	1:1A:893:C:H42	1.51	0.57
1:2A:1021:A:H62	1:2A:1141:U:H3	1.52	0.57
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.40	0.57
1:1A:1199:U:OP1	61:1A:5824:HOH:O	2.17	0.57
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.19	0.57
4:1E:11:MET:HG2	4:1E:24:THR:HB	1.87	0.57
9:1N:70:LYS:HD3	9:1N:87:LEU:HD12	1.87	0.57
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.20	0.57
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.85	0.57
5:2F:195:ASP:HB3	5:2F:198:ALA:H	1.69	0.57
1:1A:441:U:O2	5:1F:46:ARG:NH2	2.34	0.57
5:1F:11:VAL:HB	5:1F:18:ARG:HG3	1.85	0.57
7:1H:17:VAL:HG22	7:1H:26:VAL:HG22	1.86	0.57
1:2A:1383:C:O2	61:2A:6037:HOH:O	2.17	0.57
1:2A:247:G:H4'	1:2A:386:G:C5	2.39	0.57
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.86	0.57
2:1B:1:U:O2'	2:1B:2:C:OP1	2.20	0.57
1:2A:686:G:N2	1:2A:788:A:H61	2.02	0.57
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.38	0.57
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.87	0.57
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.20	0.57
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.40	0.57
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.38	0.57
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.18	0.57
1:1A:560:C:H5'	16:1U:52:ARG:HH21	1.69	0.56
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.04	0.56
8:2I:123:LEU:HD22	8:2I:144:VAL:HB	1.87	0.56
6:1G:7:LEU:HD11	6:1G:107:LEU:HD12	1.87	0.56
1:1A:642:G:N2	1:1A:645:C:OP2	2.36	0.56
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.39	0.56
22:10:11:ARG:O	22:10:14:ARG:NH2	2.37	0.56
30:18:15:LYS:NZ	61:18:211:HOH:O	2.37	0.56
1:1A:2136:C:N4	1:1A:2155:G:N1	2.29	0.56
1:1A:910:A:N3	1:1A:2264:C:O2'	2.35	0.56
7:1H:3:ARG:HE	7:1H:54:ARG:HH12	1.53	0.56
1:1A:1007:C:N3	1:1A:1022:G:O6	16.44	0.56
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.77	0.56
1:2A:1645:G:H5''	1:2A:1646:C:H5'	1.87	0.56
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.65	0.56
11:2P:36:LYS:O	61:2P:305:HOH:O	2.17	0.56
1:1A:919:G:N2	1:1A:2269:A:OP2	2.39	0.56
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.06	0.56
1:1A:2853:C:H2'	1:1A:2854:G:C8	2.41	0.56
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.88	0.56
1:2A:122:G:N3	61:2A:3915:HOH:O	2.33	0.56
2:2B:117:G:N7	61:2B:301:HOH:O	2.33	0.56
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.69	0.56
12:2Q:125:LEU:HD12	12:2Q:129:THR:HG21	1.88	0.56
1:1A:668:G:H5'	1:1A:669:G:OP2	2.06	0.56
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	1.88	0.56
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.40	0.56
1:1A:2478:A:OP2	31:19:2:LYS:NZ	2.24	0.56
4:1E:111:ARG:HG3	4:1E:160:TYR:CD2	2.41	0.56
12:1Q:16:ARG:HG3	12:1Q:18:LYS:HG3	1.88	0.56
12:1Q:10:ARG:NH1	12:1Q:90:VAL:H	2.04	0.56
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.40	0.56
1:1A:1862:G:H2'	1:1A:1863:G:H8	1.71	0.56
5:1F:178:PRO:HB2	5:1F:201:VAL:HG21	1.88	0.56
1:1A:616:G:H5'	5:1F:205:ARG:HD3	1.88	0.56
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.71	0.56
1:2A:581:C:H2'	1:2A:582:G:C8	2.41	0.56
6:2G:44:GLY:N	6:2G:88:ILE:O	2.39	0.56
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.41	0.56
1:2A:631:A:OP1	11:2P:65:ARG:NE	2.26	0.56
2:2B:14:U:O3'	2:2B:108:U:O2'	2.23	0.56
6:2G:122:PRO:HB3	6:2G:170:ARG:HH12	1.71	0.56
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.87	0.56
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	1.87	0.55
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.40	0.55
1:1A:740:U:OP2	61:1A:5734:HOH:O	2.18	0.55
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.88	0.55
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.41	0.55
15:1T:49:VAL:HG12	15:1T:63:VAL:HG22	1.88	0.55
1:1A:2390:U:P	30:18:35:GLN:HE22	2.29	0.55
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.89	0.55
26:24:24:THR:OG1	26:24:25:TYR:N	2.33	0.55
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:68:ILE:HG22	12:2Q:101:ARG:HE	1.71	0.55
20:2Y:97:ARG:NH1	20:2Y:107:ASP:O	2.40	0.55
18:1W:77:ASP:OD1	61:1W:301:HOH:O	2.18	0.55
1:2A:236:C:H2'	1:2A:237:C:C6	2.42	0.55
1:1A:579:G:OP1	61:1A:7016:HOH:O	2.18	0.55
1:1A:2467:C:H4'	12:1Q:123:HIS:CD2	2.41	0.55
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.71	0.55
1:1A:1507:A:O2'	1:1A:1509(A):A:N6	2.40	0.55
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.21	0.55
1:1A:2128:C:H42	1:1A:2160:G:H1	1.55	0.55
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.89	0.55
1:2A:1406:U:O2	1:2A:1517:G:N2	33.03	0.55
1:2A:2104:G:H1	1:2A:2185:C:H42	1.54	0.55
1:2A:819:A:OP2	1:2A:1187:G:N2	2.30	0.55
2:2B:41:U:H5	6:2G:70:VAL:H	1.55	0.55
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.70	0.55
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.88	0.55
1:1A:1057:A:H61	1:1A:1081:U:H3	1.54	0.55
1:1A:1537:G:OP1	61:1A:4207:HOH:O	2.18	0.55
1:1A:793:A:OP2	1:1A:2071:A:O2'	2.23	0.55
3:1D:274:ARG:NH1	61:1D:401:HOH:O	2.40	0.55
4:1E:181:LEU:HD11	15:1T:6:LEU:HD23	1.88	0.55
28:26:9:LEU:HD22	28:26:25:LYS:HD2	1.89	0.55
31:19:17:ILE:HD13	31:19:26:ILE:HD13	1.89	0.55
1:1A:1779:U:H2'	61:1A:6221:HOH:O	2.06	0.55
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.42	0.55
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.88	0.55
1:2A:1311:G:H2'	29:27:47:ARG:HH22	1.70	0.55
1:2A:800:A:OP1	1:2A:800:A:H8	1.90	0.55
2:2B:113:G:N2	14:2S:45:GLY:O	2.26	0.55
25:13:18:ASP:OD1	25:13:18:ASP:N	2.40	0.55
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.42	0.55
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.42	0.55
21:2Z:98:MET:O	21:2Z:126:VAL:N	2.39	0.55
16:1U:52:ARG:HH11	16:1U:55:ARG:HH21	1.55	0.55
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.40	0.55
24:12:32:LEU:HD22	24:12:36:ARG:HH11	1.72	0.54
25:13:37:LEU:HB3	25:13:43:ILE:HD13	1.89	0.54
25:13:6:VAL:HG13	25:13:54:VAL:HG11	1.89	0.54
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.22	0.54
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:73:ASP:OD2	15:2T:32:TYR:OH	2.20	0.54
1:1A:2125:G:N1	1:1A:2172:U:OP1	2.29	0.54
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.89	0.54
1:2A:2144:U:H1'	1:2A:2148:G:H22	1.73	0.54
1:2A:740:U:H2'	1:2A:741:G:C8	2.43	0.54
1:1A:857:C:H4'	22:10:23:VAL:HG21	1.88	0.54
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.42	0.54
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.41	0.54
10:1O:35:VAL:HG21	10:1O:69:ILE:HD13	1.89	0.54
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.88	0.54
1:2A:136:G:H1	1:2A:143(A):C:H42	1.53	0.54
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.55	0.54
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.07	0.54
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.19	0.54
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.43	0.54
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.41	0.54
1:2A:1007:C:N3	1:2A:1022:G:C6	16.85	0.54
1:2A:2499:C:OP1	61:2A:6007:HOH:O	2.17	0.54
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.89	0.54
7:2H:28:GLY:HA3	7:2H:79:VAL:HB	1.88	0.54
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.36	0.54
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.88	0.54
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.89	0.54
1:2A:1159:U:H2'	1:2A:1160:G:H8	1.71	0.54
1:2A:441:U:O2	5:2F:46:ARG:NH2	2.36	0.54
1:1A:1094:U:H1'	1:1A:1097:U:C5	2.43	0.54
1:1A:1668:A:O2'	1:1A:1674:G:N7	2.38	0.54
6:1G:43:LEU:HD11	6:1G:153:ARG:HD2	1.90	0.54
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	1.89	0.54
21:1Z:150:LEU:HB3	21:1Z:171:ILE:HD11	1.89	0.54
5:1F:167:ALA:HB1	5:1F:173:VAL:HG11	1.89	0.54
1:2A:630:G:N2	1:2A:633:A:OP2	2.36	0.54
1:2A:900:A:O2'	1:2A:901:A:OP1	2.20	0.54
3:2D:3:VAL:HG13	3:2D:17:THR:HB	1.89	0.54
6:1G:67:LYS:HD3	26:14:5:ILE:HD12	1.90	0.54
1:1A:1069:A:H2'	1:1A:1073:A:N7	2.23	0.54
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.08	0.54
1:1A:2815:C:H5'	27:15:29:THR:HG21	1.89	0.54
8:1I:65:ALA:HB1	8:1I:136:VAL:HG11	1.89	0.54
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.19	0.54
1:2A:2127:G:N1	1:2A:2161:C:C5	2.75	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.90	0.54
7:2H:9:ILE:HB	7:2H:50:VAL:HB	1.90	0.54
1:1A:2001:A:OP1	13:1R:9:LYS:NZ	2.38	0.54
1:1A:576:U:H2'	1:1A:577:G:C8	2.42	0.54
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.40	0.54
1:2A:2619:C:OP1	4:2E:152:LYS:NZ	2.28	0.54
1:2A:789:A:N1	61:2A:4447:HOH:O	2.33	0.54
1:2A:882:G:H2'	1:2A:883:G:H8	1.73	0.54
1:1A:2130:U:H2'	1:1A:2158:A:N1	2.23	0.53
1:1A:721:C:H2'	1:1A:722:A:C8	2.43	0.53
1:2A:1826:G:H4'	3:2D:242:ARG:NH1	2.23	0.53
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.42	0.53
15:2T:127:ALA:C	15:2T:129:ARG:H	2.12	0.53
1:2A:2117:A:O2'	1:2A:2118:U:H5''	2.07	0.53
1:2A:2126:A:N6	1:2A:2162:G:HO2'	2.05	0.53
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.08	0.53
1:2A:2751:G:O2'	1:2A:2752:C:O4'	2.26	0.53
1:2A:686:G:H21	1:2A:788:A:H61	1.55	0.53
1:1A:84:A:H5''	20:1Y:8:LYS:HG2	1.90	0.53
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.90	0.53
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.91	0.53
1:1A:2305:A:H5''	6:1G:134:GLY:HA3	1.89	0.53
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.43	0.53
1:2A:845:G:N2	1:2A:845:G:OP2	2.36	0.53
5:2F:95:ARG:NH1	5:2F:97:TYR:OH	2.42	0.53
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.41	0.53
12:2Q:81:VAL:HG12	22:20:5:LYS:HD2	1.90	0.53
13:2R:33:ARG:NH1	13:2R:115:GLU:OE1	2.35	0.53
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.29	0.53
1:1A:1619:G:N7	61:1A:6580:HOH:O	2.34	0.53
1:1A:271(M):G:O2'	1:1A:271(N):U:H5''	2.08	0.53
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.89	0.53
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.91	0.53
15:1T:127:ALA:C	15:1T:129:ARG:H	2.12	0.53
26:24:48:ARG:HE	26:24:52:THR:HA	1.74	0.53
1:2A:1204:A:H5'	1:2A:1206:G:H1'	1.90	0.53
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.25	0.53
1:2A:2168:G:H8	1:2A:2170:A:N7	2.07	0.53
1:2A:400:G:N7	61:2A:5225:HOH:O	2.33	0.53
4:2E:26:ILE:HD11	4:2E:188:VAL:HG21	1.91	0.53
10:2O:68:GLU:HB3	10:2O:78:ARG:HG3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:16:8:LYS:HD3	30:18:34:TRP:CD2	2.44	0.53
1:1A:1426:G:O2'	1:1A:1572:A:N6	2.42	0.53
1:1A:1675:C:O2	4:1E:128:SER:OG	2.27	0.53
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.89	0.53
61:1A:6915:HOH:O	13:1R:3:HIS:NE2	2.34	0.53
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.15	0.53
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.44	0.53
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	1.90	0.53
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.91	0.53
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.90	0.53
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.89	0.53
1:2A:212:G:H2'	1:2A:213:A:O4'	2.09	0.53
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.42	0.53
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.91	0.53
1:2A:979:G:H5''	1:2A:980:A:H5''	1.90	0.53
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.42	0.53
20:2Y:28:LYS:HB3	20:2Y:38:ILE:HG22	1.91	0.53
26:14:57:GLU:HG2	26:14:58:ARG:HH11	1.73	0.53
26:14:58:ARG:O	26:14:61:ARG:N	2.28	0.53
1:1A:278:A:H2'	1:1A:279:C:C6	2.43	0.53
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.89	0.53
12:1Q:20:ALA:HB2	21:1Z:79:ARG:HG3	1.90	0.53
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.27	0.53
7:2H:80:SER:OG	7:2H:81:GLU:OE1	2.26	0.53
1:1A:2522:U:O2'	1:1A:2647:U:OP1	2.16	0.53
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	1.90	0.53
1:1A:2590:A:H2'	1:1A:2591:C:C6	2.42	0.53
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.44	0.53
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.90	0.53
1:1A:336:C:HO2'	20:1Y:35:TYR:HH	1.52	0.53
13:2R:33:ARG:NH2	27:25:57:VAL:O	2.26	0.53
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.91	0.53
1:1A:1419:A:O2'	1:1A:1421:G:N7	2.33	0.52
1:1A:2386:C:O2'	61:1A:4208:HOH:O	2.19	0.52
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.25	0.52
1:2A:817:C:O2'	1:2A:839:U:H5''	2.09	0.52
2:2B:110:G:C2'	2:2B:111:G:H5'	2.39	0.52
3:2D:26:LYS:HB3	3:2D:83:GLU:HG2	1.90	0.52
1:1A:1420:U:O2'	1:1A:1421:G:O5'	2.21	0.52
1:1A:800:A:OP1	1:1A:800:A:H8	1.92	0.52
5:1F:140:LEU:HD11	5:1F:170:LEU:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2114:A:N6	1:2A:2115:G:H21	2.07	0.52
1:2A:2773:C:OP1	4:2E:166:THR:OG1	2.21	0.52
1:2A:642:G:H21	1:2A:646:A:H2	1.57	0.52
1:2A:856:C:H2'	1:2A:857:C:C6	2.44	0.52
1:1A:72:U:H5'	24:12:61:LEU:HD12	1.91	0.52
1:2A:796:C:H2'	1:2A:797:C:C6	2.44	0.52
5:2F:12:LEU:HB2	5:2F:124:LEU:HD11	1.92	0.52
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.90	0.52
1:1A:1286:A:H2'	1:1A:1287:A:H4'	6.71	0.52
1:1A:1453:U:OP1	13:1R:77:ARG:NH1	2.32	0.52
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.10	0.52
12:1Q:10:ARG:NH1	12:1Q:11:LYS:HE2	2.24	0.52
1:2A:112:U:H5'	24:22:65:ASN:ND2	2.24	0.52
1:2A:2134:A:N3	1:2A:2134:A:H2'	2.24	0.52
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.10	0.52
1:2A:492:A:H2'	1:2A:493:G:O4'	2.08	0.52
1:2A:538:G:H5'	9:2N:5:VAL:HG11	1.92	0.52
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.10	0.52
1:1A:2121:G:H1	1:1A:2177:C:N4	2.07	0.52
1:1A:534:U:H2'	1:1A:535:C:C6	2.44	0.52
1:1A:637:A:OP1	11:1P:133:SER:OG	2.26	0.52
1:1A:971:C:O2'	1:1A:983:A:N3	2.36	0.52
1:2A:2524:G:N7	61:2A:6346:HOH:O	2.34	0.52
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.91	0.52
1:2A:1693:U:H1'	3:2D:14:ARG:NH2	2.25	0.52
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.10	0.52
1:1A:2171:A:O2'	1:1A:2172:U:H5''	2.09	0.52
1:1A:272(J):C:H2'	1:1A:274:G:C8	2.39	0.52
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.42	0.52
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.91	0.52
25:23:7:LYS:NZ	25:23:32:GLN:O	2.42	0.52
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	1.90	0.52
26:14:64:GLY:O	26:14:66:SER:N	2.42	0.52
1:1A:1045:A:H5'	1:1A:1046:A:H5'	1.91	0.52
1:1A:1358:G:O2'	1:1A:1373:A:N6	2.41	0.52
1:1A:2129:C:N4	1:1A:2159:G:H1	2.04	0.52
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.45	0.52
1:2A:1865:G:N2	1:2A:1877:A:OP2	2.38	0.52
1:2A:2061:G:N2	1:2A:2062:A:N1	2.57	0.52
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.91	0.52
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:16:CYS:SG	26:24:17:GLY:N	2.83	0.52
1:2A:861:A:N3	2:2B:79:C:O2'	2.37	0.52
10:2O:64:ARG:HB2	10:2O:79:PHE:CG	2.45	0.52
20:2Y:43:ASN:HD22	20:2Y:67:LEU:HD23	1.75	0.52
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.25	0.52
1:1A:1653:G:H3'	13:1R:2:ARG:HD3	1.91	0.52
1:1A:1826:G:H4'	3:1D:242:ARG:CZ	2.39	0.52
6:1G:108:ASN:HD22	26:14:22:ILE:HG21	1.75	0.52
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.28	0.52
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.10	0.52
1:2A:2392:A:OP2	30:28:31:HIS:NE2	2.42	0.52
1:2A:860:U:OP2	61:2A:6253:HOH:O	2.19	0.52
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.10	0.52
26:14:64:GLY:C	26:14:66:SER:H	2.13	0.52
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.10	0.52
1:1A:922:U:H2'	1:1A:923:C:C6	2.45	0.52
1:2A:2285:C:OP2	28:26:6:ARG:HD3	2.10	0.52
1:2A:973:A:H8	1:2A:973:A:OP1	1.93	0.52
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.74	0.51
3:1D:21:PHE:HB3	3:1D:24:ILE:HD12	1.91	0.51
11:1P:65:ARG:HD2	30:18:25:MET:SD	2.50	0.51
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.10	0.51
26:24:64:GLY:C	26:24:66:SER:H	2.13	0.51
1:2A:1658:C:OP1	4:2E:135:HIS:NE2	2.37	0.51
1:2A:2552:2MU:OP2	61:2A:5426:HOH:O	2.19	0.51
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.09	0.51
8:1I:38:LEU:HD13	8:1I:40:THR:HG23	1.92	0.51
12:1Q:42:ILE:HD11	12:1Q:127:ILE:HD13	1.92	0.51
1:1A:1754:C:H5	15:1T:96:ARG:HH21	1.58	0.51
1:2A:2121:G:N1	1:2A:2177:C:N4	2.42	0.51
6:2G:120:LEU:N	6:2G:179:PRO:O	2.32	0.51
9:2N:54:VAL:HB	9:2N:122:VAL:HG22	1.93	0.51
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.92	0.51
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.09	0.51
1:1A:674:G:H2'	1:1A:675:A:H8	4.76	0.51
5:1F:117:ARG:NH2	5:1F:189:THR:O	2.41	0.51
6:1G:4:ASP:OD1	6:1G:9:ARG:NH1	2.41	0.51
9:1N:73:THR:HG23	9:1N:82:LEU:HD11	1.93	0.51
1:2A:1128:A:N7	1:2A:2489:G:O2'	2.43	0.51
1:2A:586:A:H5'	5:2F:89:VAL:HG21	1.93	0.51
1:1A:1002:G:H3'	1:1A:1003:G:C4'	4.90	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1466:G:HO2'	1:1A:1546:C:HO2'	1.55	0.51
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.10	0.51
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.45	0.51
1:2A:2615:U:C2	27:25:7:PRO:HA	2.45	0.51
1:2A:700:G:O2'	1:2A:1632:A:N3	2.31	0.51
1:2A:790:C:OP2	61:2A:4442:HOH:O	2.19	0.51
1:1A:1066:U:N3	1:1A:1069:A:OP2	2.43	0.51
1:1A:1256:G:H1'	5:1F:82:ILE:HD11	1.93	0.51
1:1A:2238:G:H2'	1:1A:2238:G:N3	2.25	0.51
1:1A:2497:A:O2'	61:1A:5717:HOH:O	2.16	0.51
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.24	0.51
1:2A:340:A:H2'	1:2A:341:G:O4'	2.10	0.51
1:2A:144:C:H5'	19:2X:2:LYS:HZ2	1.75	0.51
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.24	0.51
1:1A:2276:G:N7	61:1A:7102:HOH:O	2.33	0.51
2:1B:91:C:OP2	12:1Q:16:ARG:NH1	2.43	0.51
1:2A:1006:C:H2'	1:2A:1007:C:C6	3.10	0.51
1:2A:99:U:O4	20:2Y:8:LYS:NZ	2.40	0.51
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.46	0.51
1:1A:1054:A:H3'	1:1A:1055:G:C8	2.46	0.51
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.45	0.51
1:1A:2150:U:H2'	1:1A:2151:G:C8	2.46	0.51
1:1A:2168:G:O6	1:1A:2171:A:H5''	2.10	0.51
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.93	0.51
17:1V:60:GLU:HB2	17:1V:97:LYS:HE2	1.92	0.51
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.46	0.51
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.75	0.51
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.11	0.51
7:1H:51:ARG:NH2	7:1H:53:GLU:OE2	2.43	0.51
1:2A:2379:G:O2'	14:2S:17:ARG:NH2	2.44	0.51
1:1A:1190:G:OP1	11:1P:30:THR:OG1	2.28	0.51
1:1A:1301:A:O2'	1:1A:1302:A:H3'	2.10	0.51
1:1A:1442:G:H2'	1:1A:1442:G:N3	2.84	0.51
1:2A:1604:C:OP2	61:2A:5432:HOH:O	2.20	0.51
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.18	0.51
1:2A:661:C:H2'	1:2A:662:G:C8	2.45	0.51
1:2A:821:A:N1	61:2A:4694:HOH:O	2.33	0.51
1:2A:839:U:H3'	1:2A:840:C:C6	3.93	0.51
1:1A:278:A:H4'	1:1A:279:C:OP1	2.11	0.51
1:1A:2848:G:C8	15:1T:97:ALA:HB2	2.45	0.51
9:1N:62:VAL:HG11	9:1N:66:LYS:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:8:ARG:HG3	13:1R:43:GLU:OE2	2.11	0.51
18:1W:65:LEU:HD12	18:1W:68:ARG:HE	1.76	0.51
1:2A:1203:G:OP2	1:2A:1204:A:O2'	2.20	0.51
1:2A:1906:G:OP2	1:2A:1929:G:O2'	2.29	0.51
1:2A:1920:4OC:HM22	1:2A:1921:G:H5'	1.93	0.51
6:2G:126:ASP:OD2	6:2G:130:ASN:ND2	2.44	0.51
21:2Z:54:HIS:CD2	21:2Z:101:PRO:HG3	2.46	0.51
31:19:32:HIS:O	31:19:34:GLN:HG3	2.11	0.50
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.93	0.50
1:2A:2142:C:H2'	1:2A:2143:C:O4'	2.11	0.50
7:2H:35:VAL:HG13	7:2H:71:LEU:HD23	1.93	0.50
8:2I:43:ASN:ND2	23:21:75:GLU:OE1	2.44	0.50
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.93	0.50
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.11	0.50
1:1A:1517:G:N3	1:1A:1919:A:O2'	105.17	0.50
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.11	0.50
1:1A:365:C:OP2	61:1A:6825:HOH:O	2.20	0.50
5:1F:39:TRP:CZ2	5:1F:43:LYS:HE3	2.46	0.50
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	1.93	0.50
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.40	0.50
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.44	0.50
1:2A:652(B):A:N6	1:2A:655:A:H1'	2.26	0.50
1:1A:1498:C:OP1	61:1A:7295:HOH:O	2.19	0.50
20:1Y:98:VAL:HG12	20:1Y:105:ALA:HA	1.93	0.50
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.46	0.50
1:2A:2198:A:OP1	8:2I:33:ARG:NH2	2.44	0.50
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.92	0.50
31:19:16:VAL:HG22	31:19:25:VAL:HG22	1.93	0.50
1:1A:1210:A:H5''	1:1A:1212:G:O4'	2.11	0.50
21:1Z:125:LEU:HB3	21:1Z:165:VAL:HG13	1.94	0.50
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.44	0.50
1:2A:659:C:H2'	1:2A:660:G:H8	1.75	0.50
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.94	0.50
10:2O:86:ILE:HG22	10:2O:94:ARG:HD3	1.93	0.50
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.42	0.50
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.26	0.50
1:1A:184:C:H2'	1:1A:185:U:C6	2.46	0.50
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.46	0.50
1:1A:880:G:H2'	1:1A:881:G:C8	2.38	0.50
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.47	0.50
1:2A:1415:U:O2'	1:2A:1417:C:OP1	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.26	0.50
1:2A:818:G:OP2	61:2A:4377:HOH:O	2.19	0.50
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.12	0.50
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.46	0.50
29:17:5:TRP:NE1	29:17:7:PRO:HG3	2.26	0.50
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.11	0.50
1:1A:831:G:N2	11:1P:53:GLY:O	2.44	0.50
4:1E:1:MET:HE3	4:1E:199:ARG:HB3	1.94	0.50
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.12	0.50
14:1S:8:GLU:HA	14:1S:11:LYS:HB2	1.92	0.50
1:2A:407:G:H2'	1:2A:408:G:H8	1.77	0.50
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	1.91	0.50
10:2O:87:ILE:HD12	10:2O:91:LEU:HA	1.92	0.50
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.93	0.50
1:1A:1053:C:N4	1:1A:1106:G:H1	2.07	0.50
1:1A:2128:C:H2'	1:1A:2129:C:O4'	2.11	0.50
28:26:6:ARG:HH11	28:26:26:ASN:HB2	1.75	0.50
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.92	0.50
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.93	0.50
1:2A:2504:U:OP2	61:2A:4814:HOH:O	2.20	0.50
1:2A:854:G:H2'	1:2A:855:G:C8	2.43	0.50
10:2O:21:CYS:HB2	10:2O:39:ILE:HD12	1.94	0.50
1:1A:1066:U:H2'	1:1A:1068:G:OP2	2.12	0.50
1:1A:1174:A:H1'	1:1A:1175:U:O5'	2.12	0.50
1:1A:1439:A:OP1	61:1A:6792:HOH:O	2.19	0.50
4:1E:56:PRO:HG3	4:1E:74:PRO:HG2	1.93	0.50
5:1F:123:LEU:HD13	5:1F:192:LEU:HB3	1.94	0.50
17:1V:43:GLU:N	17:1V:43:GLU:OE1	2.43	0.50
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.47	0.50
25:23:6:VAL:HG22	25:23:56:VAL:HG22	1.94	0.50
27:25:41:PRO:O	27:25:44:THR:OG1	2.23	0.50
1:2A:27:G:N2	1:2A:512:G:H1'	2.27	0.50
8:2I:116:LEU:HD11	8:2I:120:ILE:HG13	1.93	0.50
11:2P:99:LEU:HD23	11:2P:102:ARG:HH21	1.76	0.50
1:1A:2110:G:OP1	1:1A:2118:U:N3	2.38	0.50
1:1A:249:C:O2'	11:1P:64:LYS:NZ	2.31	0.50
1:1A:785:G:N2	1:1A:797:C:O2	28.27	0.50
2:1B:91:C:H5'	12:1Q:18:LYS:HA	1.92	0.50
1:2A:2870:C:H5''	13:2R:65:LEU:HD21	1.94	0.50
1:2A:288:C:H2'	1:2A:289:A:H8	1.76	0.50
1:2A:743:G:OP1	4:2E:130:GLY:HA2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:77:ILE:HG12	4:2E:195:LEU:HD12	1.93	0.50
10:2O:36:GLY:HA2	10:2O:106:LEU:HD23	1.94	0.50
15:2T:51:ARG:HB2	15:2T:98:LYS:HD2	1.93	0.50
1:1A:2336:A:H61	22:10:43:THR:HG21	1.77	0.49
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.11	0.49
1:1A:191:A:H2'	1:1A:192:C:C6	2.47	0.49
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.12	0.49
1:1A:2185:C:H2'	1:1A:2186:G:H8	1.77	0.49
1:1A:2552:2MU:O5'	1:1A:2552:2MU:H6	2.12	0.49
1:1A:524:U:H2'	1:1A:525:U:C6	2.47	0.49
1:1A:769:G:N7	61:1A:7107:HOH:O	2.34	0.49
1:1A:862:G:H2'	1:1A:863:A:O4'	2.12	0.49
5:1F:110:LEU:HD11	5:1F:181:LEU:HG	1.94	0.49
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.47	0.49
18:1W:80:PRO:O	18:1W:100:THR:OG1	2.29	0.49
1:2A:1899:G:O2'	1:2A:1900:A:OP2	2.28	0.49
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.47	0.49
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.47	0.49
1:2A:2218:U:N3	23:21:55:GLY:O	2.45	0.49
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.12	0.49
1:2A:2473:U:H2'	1:2A:2473:U:O2	2.12	0.49
1:2A:2564:A:OP1	1:2A:2648:C:H4'	2.11	0.49
1:2A:657:U:H2'	1:2A:658:C:C6	2.46	0.49
1:2A:879:G:H5'	1:2A:880:G:OP2	2.12	0.49
4:2E:48:GLN:HA	4:2E:80:GLU:HA	1.93	0.49
1:1A:1047:G:O2'	1:1A:1048:A:H8	1.95	0.49
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.47	0.49
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.47	0.49
1:2A:2498:C:OP1	61:2A:4156:HOH:O	2.20	0.49
4:2E:167:VAL:HG22	4:2E:170:LEU:HD11	1.94	0.49
6:2G:97:ASP:OD1	6:2G:97:ASP:N	2.43	0.49
7:2H:3:ARG:HH11	7:2H:4:ILE:H	1.58	0.49
1:2A:2641:G:H5''	9:2N:76:SER:HB3	1.93	0.49
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	1.94	0.49
1:1A:1082:U:C4	1:1A:1086:A:N1	2.75	0.49
1:1A:765:G:N1	1:1A:812:C:O2'	83.92	0.49
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.29	0.49
1:2A:184:C:H2'	1:2A:185:U:C6	2.47	0.49
1:2A:236:C:H2'	1:2A:237:C:H6	1.77	0.49
1:2A:34:C:H2'	1:2A:35:G:H8	4.19	0.49
1:2A:484:C:H2'	1:2A:485:C:C6	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:105:A:H5'	2:2B:106:G:OP2	2.12	0.49
2:2B:40:U:O2'	2:2B:43:C:OP2	2.24	0.49
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.27	0.49
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.12	0.49
1:1A:438:G:H2'	1:1A:440:G:C8	2.47	0.49
1:1A:657:U:H2'	1:1A:658:C:C6	2.47	0.49
1:1A:2310:A:N1	6:1G:79:ASN:ND2	2.60	0.49
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.78	0.49
11:1P:106:LEU:HD22	11:1P:112:LEU:HD13	1.94	0.49
13:1R:36:THR:HG22	13:1R:37:THR:H	1.77	0.49
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	1.94	0.49
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.60	0.49
1:2A:890:A:H2'	1:2A:892:G:H8	1.77	0.49
2:2B:50:G:OP1	14:2S:63:THR:N	2.40	0.49
6:2G:11:TYR:OH	6:2G:16:ARG:NH1	2.46	0.49
19:2X:26:TYR:HB3	19:2X:92:LEU:HD22	1.94	0.49
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.48	0.49
1:1A:2350:C:OP2	61:1A:6676:HOH:O	2.18	0.49
1:1A:740:U:H2'	1:1A:741:G:C8	2.47	0.49
1:1A:848:G:H2'	1:1A:849:A:C8	2.48	0.49
1:2A:2127:G:H2'	1:2A:2128:C:C6	2.47	0.49
1:2A:65:C:O2'	1:2A:456:C:N3	2.36	0.49
1:1A:1418:G:OP2	61:1A:5574:HOH:O	2.20	0.49
1:1A:1508:A:O2'	1:1A:1509:C:H5''	2.12	0.49
1:1A:286:C:H2'	1:1A:287:C:C6	2.48	0.49
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.12	0.49
1:2A:852:G:H2'	1:2A:853:G:C8	2.47	0.49
2:2B:51:G:N7	14:2S:62:LYS:NZ	2.52	0.49
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.94	0.49
2:1B:13:A:N1	2:1B:69:G:O2'	2.36	0.49
4:1E:24:THR:HG23	4:1E:184:VAL:HG12	1.94	0.49
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.47	0.49
21:1Z:153:SER:HA	21:1Z:167:PRO:HB3	1.95	0.49
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.94	0.49
1:2A:1670:C:OP1	61:2A:6087:HOH:O	2.19	0.49
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.48	0.49
1:2A:2781:A:H5''	1:2A:2782:G:H5'	1.95	0.49
1:2A:524:U:H2'	1:2A:525:U:C6	2.48	0.49
1:2A:833:U:H2'	1:2A:834:C:C6	2.74	0.49
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.19	0.49
9:2N:103:VAL:HG11	9:2N:120:LEU:HD22	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:34:HIS:O	14:2S:97:ARG:NH2	2.45	0.49
1:1A:2127:G:H1	1:1A:2161:C:H42	1.60	0.49
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.46	0.49
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.60	0.49
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.47	0.49
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.48	0.49
6:2G:122:PRO:HB3	6:2G:170:ARG:NH1	2.28	0.49
15:2T:74:ARG:HG2	15:2T:76:PHE:CZ	2.48	0.49
1:1A:1364:G:N7	23:11:3:LYS:HD2	2.27	0.49
1:1A:1756:G:H4'	1:1A:1758:G:O4'	2.12	0.49
1:1A:2705:A:N3	61:1R:301:HOH:O	2.35	0.49
1:1A:639:U:H2'	1:1A:640:C:C6	2.47	0.49
2:1B:21:G:N7	61:1B:302:HOH:O	2.35	0.49
10:1O:64:ARG:HD3	10:1O:79:PHE:CD1	2.48	0.49
25:23:12:PRO:HB2	25:23:20:LYS:HG2	1.94	0.49
1:2A:2343:C:O3'	1:2A:2373:G:H4'	2.12	0.49
1:2A:2590:A:H5''	3:2D:239:ARG:HG3	1.94	0.49
1:2A:93:G:H2'	1:2A:94:C:H6	1.78	0.49
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.48	0.49
1:1A:414:C:H2'	1:1A:415:A:C8	2.47	0.49
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	1.95	0.49
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.42	0.49
1:2A:275:G:H2'	1:2A:276:A:O4'	2.13	0.49
1:2A:1751:C:O2'	1:2A:2861:G:O2'	2.28	0.49
1:2A:848:G:N3	1:2A:933:A:H1'	2.28	0.49
6:2G:173:LEU:HB3	6:2G:178:PHE:CD2	2.48	0.49
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.94	0.48
61:1A:6898:HOH:O	16:1U:16:LYS:HD3	2.13	0.48
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	1.95	0.48
19:1X:43:VAL:HG21	19:1X:81:VAL:HG11	1.96	0.48
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.94	0.48
1:2A:1023:U:O2'	1:2A:1122:G:H5'	2.14	0.48
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.95	0.48
1:2A:249:C:O2	30:28:12:LYS:NZ	2.38	0.48
1:2A:2526:G:O3'	31:29:33:LYS:NZ	2.46	0.48
1:2A:531:C:H4'	1:2A:532:A:H5''	1.95	0.48
3:2D:242:ARG:HH11	3:2D:242:ARG:HG3	1.79	0.48
4:2E:5:LEU:HD21	4:2E:79:ARG:HB2	1.94	0.48
5:2F:179:GLU:OE1	5:2F:179:GLU:N	2.45	0.48
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.77	0.48
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:74:VAL:HG22	21:2Z:86:VAL:HG12	1.95	0.48
1:1A:1230:C:H2'	1:1A:1231:G:C8	2.49	0.48
1:1A:2096:U:H3	1:1A:2193:G:H1	1.61	0.48
1:1A:2804:C:H2'	1:1A:2805:G:O4'	2.12	0.48
12:1Q:31:ASP:OD1	12:1Q:134:ARG:NH1	2.43	0.48
2:2B:40:U:H2'	26:24:2:LYS:HE3	1.95	0.48
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.27	0.48
30:28:30:ARG:HB3	30:28:31:HIS:HD2	1.78	0.48
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.48	0.48
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.44	0.48
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.47	0.48
1:2A:661:C:H2'	1:2A:662:G:H8	1.78	0.48
2:2B:14:U:OP2	2:2B:70:C:O2'	2.25	0.48
1:1A:18:C:O2'	1:1A:554:U:OP1	2.29	0.48
2:1B:2:C:H2'	2:1B:3:C:C6	2.48	0.48
21:1Z:130:PRO:HA	21:1Z:133:ILE:HG13	1.96	0.48
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.95	0.48
2:1B:12:C:H2'	22:10:73:GLY:HA3	1.96	0.48
1:1A:1085:A:O2'	1:1A:1104:C:O2'	2.19	0.48
1:1A:1670:C:O2	4:1E:129:HIS:NE2	2.39	0.48
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.48	0.48
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.14	0.48
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.48	0.48
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.77	0.48
1:2A:1016:G:O6	1:2A:1147:C:N4	2.46	0.48
1:2A:1023:U:OP2	61:2A:5647:HOH:O	2.20	0.48
1:2A:140:G:N2	1:2A:1596:A:H4'	2.28	0.48
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.12	0.48
1:2A:251:A:C5	1:2A:252:G:H1'	2.48	0.48
1:2A:887:A:H4'	1:2A:888:C:C5	2.49	0.48
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.79	0.48
11:1P:98:GLU:O	11:1P:101:VAL:HG12	2.14	0.48
16:1U:49:HIS:HA	16:1U:52:ARG:HB3	1.94	0.48
18:1W:12:ILE:HD13	18:1W:17:VAL:HG13	1.95	0.48
19:1X:26:TYR:HB3	19:1X:92:LEU:HD22	1.95	0.48
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.14	0.48
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.44	0.48
11:2P:120:ALA:HB2	11:2P:137:LYS:HB3	1.94	0.48
1:1A:528:A:O2'	1:1A:529:A:H5'	2.14	0.48
1:1A:796:C:H2'	1:1A:797:C:C6	2.48	0.48
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.48	0.48
1:2A:172:C:H2'	1:2A:173:G:H8	1.78	0.48
1:2A:834:C:O2	1:2A:852:G:N2	38.24	0.48
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.31	0.48
1:1A:2790:A:H5'	1:1A:2893:G:H21	1.78	0.48
1:1A:883:G:H22	1:1A:893:C:N4	2.12	0.48
2:1B:66:A:H61	2:1B:109:C:H5'	1.77	0.48
1:2A:118:A:N3	1:2A:178:G:H1'	2.28	0.48
1:2A:208:C:H2'	1:2A:209:C:C6	2.48	0.48
1:2A:582:G:H2'	1:2A:583:G:C8	2.49	0.48
1:2A:839:U:H3'	1:2A:840:C:H6	3.23	0.48
1:2A:878:A:N6	1:2A:899:A:O2'	2.46	0.48
2:2B:90:A:C5	2:2B:91:C:H1'	2.48	0.48
3:2D:206:LEU:HA	3:2D:211:ARG:HE	1.79	0.48
7:2H:4:ILE:O	7:2H:69:ARG:HD2	2.14	0.48
30:28:31:HIS:ND1	30:28:32:LEU:HD13	2.28	0.48
1:2A:1442:G:N3	1:2A:1442:G:H2'	2.84	0.48
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.49	0.48
1:2A:645:C:H5''	1:2A:646:A:OP2	2.14	0.48
1:2A:832:G:H5'	11:2P:45:LEU:HD21	1.95	0.48
23:11:82:LEU:HD13	23:11:90:ILE:HG23	1.94	0.48
1:1A:2478:A:H5'	31:19:31:LYS:HD3	1.96	0.48
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.14	0.48
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.37	0.48
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.95	0.48
1:1A:1766:U:H2'	1:1A:1767:C:H6	1.79	0.48
1:1A:218:A:C2	1:1A:235:U:H4'	2.49	0.48
1:1A:297:C:OP1	20:1Y:87:LYS:NZ	2.42	0.48
1:1A:881:G:H3'	1:1A:882:G:H8	1.78	0.48
30:28:26:LYS:HB2	30:28:44:LYS:O	2.14	0.48
1:2A:1747:G:H2'	1:2A:1747(A):G:H8	1.79	0.48
1:2A:857:C:H1'	22:20:26:TYR:CE1	2.49	0.48
4:2E:181:LEU:HD11	15:2T:6:LEU:HD23	1.95	0.48
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	1.96	0.48
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.87	0.48
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.51	0.48
20:2Y:38:ILE:HD11	20:2Y:66:PRO:HG3	1.96	0.48
1:1A:839:U:H2'	1:1A:840:C:C6	2.49	0.48
7:1H:56:SER:HB3	7:1H:61:HIS:ND1	2.28	0.48
26:24:40:HIS:CD2	26:24:41:PRO:HD2	2.49	0.48
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.14	0.48
1:2A:902:C:H2'	1:2A:903:C:C6	2.49	0.48
5:2F:187:VAL:HG12	11:2P:3:LEU:HD12	1.95	0.48
61:2A:5563:HOH:O	19:2X:40:LYS:NZ	2.47	0.48
1:1A:1717:G:H2'	1:1A:1718:G:H8	1.79	0.47
1:1A:2137:C:H2'	1:1A:2138:C:C6	2.49	0.47
1:1A:2409:G:O2'	61:1A:6964:HOH:O	2.20	0.47
1:1A:324:A:N6	1:1A:338:G:O2'	2.47	0.47
1:1A:540:C:H2'	1:1A:541:C:C6	2.49	0.47
22:20:27:GLU:HG3	22:20:68:GLU:HA	1.96	0.47
28:26:9:LEU:HD13	28:26:51:GLU:HB2	1.95	0.47
1:2A:1973:G:OP2	61:2A:4871:HOH:O	2.19	0.47
1:2A:2062:A:H2'	1:2A:2062:A:N3	2.29	0.47
1:2A:2127:G:N3	1:2A:2161:C:N3	2.61	0.47
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.14	0.47
1:2A:2345:G:H1'	1:2A:2382:G:H5'	1.96	0.47
1:2A:336:C:H2'	1:2A:337:C:C6	2.80	0.47
1:2A:434:U:H2'	1:2A:435:C:C6	6.26	0.47
1:2A:947:G:H2'	1:2A:948:G:C8	2.49	0.47
1:1A:1057:A:N6	1:1A:1087:G:OP2	2.47	0.47
1:1A:1420:U:O2'	1:1A:1421:G:H8	1.97	0.47
1:1A:2228:G:OP1	3:1D:263:ARG:NH2	2.42	0.47
1:1A:2595:G:N2	1:1A:2598:A:OP2	2.45	0.47
1:1A:741:G:H2'	1:1A:742:G:O4'	2.51	0.47
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.79	0.47
1:2A:1237:A:OP2	61:2A:5390:HOH:O	2.20	0.47
1:2A:196:A:N3	1:2A:196:A:H2'	2.29	0.47
1:2A:893:C:H2'	1:2A:894:C:C5	2.49	0.47
5:2F:28:ILE:HG12	5:2F:112:MET:HG2	1.95	0.47
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.96	0.47
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.49	0.47
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.29	0.47
1:1A:1062:G:P	1:1A:1070:A:H1'	2.54	0.47
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.14	0.47
1:1A:2532:G:O2'	1:1A:2657:A:N1	2.45	0.47
1:1A:747:U:H1'	18:1W:92:ARG:HH12	1.79	0.47
12:2Q:81:VAL:HB	22:20:7:LEU:HD21	1.96	0.47
28:26:9:LEU:HA	28:26:54:ILE:HB	1.95	0.47
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.96	0.47
1:2A:1509(B):A:H2'	1:2A:1510:G:H8	1.79	0.47
1:2A:383:U:H2'	1:2A:385:C:H5	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:629:G:H1'	1:2A:639:U:O2'	2.14	0.47
1:2A:93:G:H2'	1:2A:94:C:C6	2.49	0.47
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.31	0.47
22:10:26:TYR:H	22:10:29:GLN:NE2	2.11	0.47
1:1A:2250:G:O2'	1:1A:2496:C:OP1	2.29	0.47
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.15	0.47
1:2A:218:A:C2	1:2A:235:U:H4'	2.49	0.47
1:2A:479:A:N3	1:2A:481:G:H5''	2.29	0.47
2:2B:95:C:H2'	2:2B:96:U:C6	2.49	0.47
1:2A:778:G:H5''	3:2D:48:ARG:HD2	1.96	0.47
1:2A:2680:C:H5'	4:2E:189:PRO:HA	1.96	0.47
1:1A:2134:A:H4'	1:1A:2135:A:OP1	2.15	0.47
13:1R:59:ASP:N	13:1R:59:ASP:OD1	2.47	0.47
1:2A:2498:C:H3'	61:2A:5660:HOH:O	2.14	0.47
1:2A:866:A:H2	1:2A:867:C:C4	2.31	0.47
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.50	0.47
8:2I:65:ALA:O	8:2I:69:LYS:N	2.45	0.47
9:2N:67:LEU:HA	9:2N:87:LEU:HD22	1.95	0.47
26:14:24:THR:OG1	26:14:25:TYR:N	2.48	0.47
1:1A:1014:U:OP2	61:1A:6533:HOH:O	2.20	0.47
1:2A:1161:C:H2'	1:2A:1162:G:H8	1.78	0.47
1:2A:526:A:N3	1:2A:2044:C:H1'	2.30	0.47
2:2B:24:G:N3	2:2B:26:A:N6	2.62	0.47
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.14	0.47
21:2Z:48:PHE:CE1	21:2Z:52:SER:HA	2.49	0.47
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.14	0.47
1:1A:2127:G:H1	1:1A:2161:C:N4	2.11	0.47
1:1A:247:G:H4'	1:1A:386:G:C5	2.49	0.47
1:1A:2533:A:H2'	1:1A:2534:A:O4'	2.15	0.47
1:1A:2803:C:H2'	1:1A:2804:C:C6	2.49	0.47
1:1A:853:G:C2'	1:1A:854:G:H5'	2.44	0.47
1:2A:2127:G:N2	1:2A:2161:C:N1	2.63	0.47
1:2A:848:G:H2'	1:2A:849:A:C8	2.49	0.47
2:2B:91:C:OP1	12:2Q:16:ARG:HG3	2.14	0.47
7:2H:127:GLU:OE1	7:2H:130:ARG:NE	2.46	0.47
19:2X:94:GLY:N	19:2X:95:LEU:HA	2.30	0.47
20:2Y:35:TYR:CE2	20:2Y:69:ALA:HB3	2.50	0.47
1:1A:1075:C:H42	1:1A:1077:A:H62	1.62	0.47
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.15	0.47
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.15	0.47
1:1A:2126:A:N3	1:1A:2127:G:H1'	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:34:C:H5''	1:1A:35:G:OP2	2.15	0.47
1:1A:34:C:H2'	1:1A:35:G:C8	6.34	0.47
1:1A:643:A:N1	1:1A:2369:A:O2'	2.43	0.47
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.50	0.47
1:2A:484:C:H2'	1:2A:485:C:H6	1.80	0.47
1:2A:76:C:H42	1:2A:93:G:H1	26.83	0.47
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.97	0.47
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.49	0.47
9:2N:121:LYS:HD3	9:2N:130:HIS:CE1	2.50	0.47
13:2R:44:LEU:HD23	13:2R:44:LEU:HA	1.81	0.47
1:1A:1364:G:P	23:11:3:LYS:HG3	2.55	0.47
1:1A:1936:A:OP1	1:1A:1937:A:H5'	2.15	0.47
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.50	0.47
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.40	0.47
1:1A:56:A:H2'	1:1A:57:C:O4'	2.15	0.47
1:1A:684:G:OP1	29:17:16:HIS:ND1	2.45	0.47
3:1D:211:ARG:HG3	3:1D:214:TRP:CE3	2.50	0.47
5:1F:156:LEU:HD21	5:1F:163:VAL:HG12	1.97	0.47
1:1A:614(C):A:C4	5:1F:180:GLY:HA2	2.50	0.47
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.15	0.47
1:2A:629:G:H2'	1:2A:630:G:O4'	2.68	0.47
1:2A:888:C:H2'	1:2A:889:C:C4	2.50	0.47
6:2G:124:SER:HB2	6:2G:131:TYR:CE1	2.50	0.47
1:2A:2658:C:P	7:2H:160:LYS:HZ1	2.36	0.47
10:2O:68:GLU:OE1	10:2O:78:ARG:NH1	2.47	0.47
14:2S:7:TYR:CZ	14:2S:91:PRO:HG3	2.50	0.47
24:12:32:LEU:HD11	24:12:54:LYS:HG2	1.97	0.47
25:13:10:LYS:HB3	25:13:53:LEU:HA	1.97	0.47
1:1A:579:G:H2'	1:1A:580:C:C6	2.50	0.47
1:1A:1252:G:O4'	16:1U:33:ARG:HD2	2.15	0.47
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG22	1.96	0.47
1:2A:2723:C:OP1	13:2R:3:HIS:ND1	2.38	0.47
1:2A:2751:G:H5'	7:2H:2:SER:HA	1.96	0.47
1:2A:839:U:H2'	1:2A:840:C:C6	2.50	0.47
1:2A:903:C:H2'	1:2A:904:C:C6	2.49	0.47
2:2B:24:G:N7	2:2B:56:G:H2'	2.29	0.47
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.47	0.47
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.95	0.47
22:10:38:VAL:HB	22:10:59:LEU:HB2	1.96	0.47
1:1A:1091:G:C6	1:1A:1101:U:C2	3.03	0.47
1:1A:1432:C:H2'	1:1A:1433:U:O4'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.50	0.47
1:1A:625:G:O6	11:1P:107:LYS:NZ	2.44	0.47
1:1A:918:A:H5''	2:1B:98:G:O2'	2.15	0.47
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.15	0.47
1:2A:1246:A:OP1	5:2F:38:ARG:NH2	2.39	0.47
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.50	0.47
1:2A:2483:C:N3	12:2Q:124:LYS:HE3	2.30	0.47
1:2A:2705:A:O2'	1:2A:2852:G:OP1	2.20	0.47
1:2A:658:C:H2'	1:2A:659:C:C6	2.50	0.47
1:2A:70:G:H1	1:2A:99:U:H3	37.10	0.47
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.97	0.47
7:2H:64:LEU:O	7:2H:68:THR:OG1	2.24	0.47
17:2V:62:LEU:HD21	17:2V:95:LEU:HB2	1.97	0.47
1:1A:1047:G:HO2'	1:1A:1048:A:P	2.38	0.46
1:1A:1092:C:H2'	1:1A:1093:G:O4'	2.15	0.46
1:1A:264:C:O2'	1:1A:265:A:H2'	2.15	0.46
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.50	0.46
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.96	0.46
21:1Z:98:MET:O	21:1Z:125:LEU:HD12	2.15	0.46
22:20:53:MET:HG2	22:20:57:PHE:HA	1.95	0.46
29:27:34:ARG:NH2	29:27:39:ARG:HG2	2.30	0.46
1:2A:1011:G:N2	1:2A:1018:C:C2	21.59	0.46
1:2A:597:U:H2'	1:2A:598:G:C8	2.51	0.46
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.46	0.46
1:2A:968:G:H2'	1:2A:969:U:C6	2.49	0.46
1:2A:979:G:H5''	1:2A:980:A:C5'	2.46	0.46
6:2G:122:PRO:HG3	6:2G:182:LYS:H	1.80	0.46
7:2H:156:ALA:O	7:2H:172:LYS:HG2	2.15	0.46
1:1A:1118:C:H2'	1:1A:1119:C:C6	2.85	0.46
1:1A:2066:C:H5''	61:1A:5237:HOH:O	2.15	0.46
1:1A:2252:G:N7	22:10:4:LYS:NZ	2.63	0.46
16:1U:55:ARG:O	16:1U:59:ARG:HG3	2.15	0.46
1:2A:1351:C:O3'	1:2A:1571:A:O2'	2.33	0.46
1:2A:1711:C:H2'	1:2A:1712:C:H6	1.80	0.46
28:16:19:ARG:HD3	61:16:201:HOH:O	2.14	0.46
1:1A:1052:C:H2'	1:1A:1053:C:C6	2.50	0.46
1:1A:1792:G:O2'	1:1A:1830:C:OP1	2.32	0.46
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.35	0.46
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.16	0.46
1:1A:2785:C:OP1	4:1E:41:LYS:NZ	2.46	0.46
1:1A:784:A:O4'	3:1D:227:ASN:ND2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:18:GLU:HG3	6:1G:22:ARG:HD2	1.96	0.46
1:2A:1358:G:O2'	1:2A:1373:A:N6	2.45	0.46
1:2A:1578:U:C2'	1:2A:1579:A:H5'	2.46	0.46
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.50	0.46
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.45	0.46
1:2A:921:G:H4'	1:2A:2269:A:C5	2.49	0.46
4:2E:76:ARG:HB2	4:2E:77:ILE:HD12	1.97	0.46
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.97	0.46
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.80	0.46
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.96	0.46
26:14:58:ARG:N	26:14:58:ARG:HD2	2.29	0.46
3:1D:69:ARG:HE	3:1D:130:ALA:HB2	1.81	0.46
6:1G:101:ILE:O	6:1G:105:LYS:NZ	2.49	0.46
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.15	0.46
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.16	0.46
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.31	0.46
1:2A:2238:G:N3	1:2A:2238:G:H2'	2.29	0.46
1:2A:2398:U:H2'	1:2A:2399:G:H8	1.80	0.46
1:2A:289:A:H2'	1:2A:290:G:O4'	2.16	0.46
1:2A:2061:G:O6	57:2A:3888:CLM:H3	2.14	0.46
1:2A:900:A:HO2'	1:2A:901:A:P	2.37	0.46
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.13	0.46
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.47	0.46
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	1.98	0.46
14:2S:35:ILE:HG23	14:2S:69:VAL:HG11	1.97	0.46
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.96	0.46
1:1A:2090:G:N2	23:11:45:ASN:OD1	2.32	0.46
1:1A:1818:U:H2'	3:1D:157:ARG:HG3	1.98	0.46
1:1A:747:U:O2	1:1A:2014:A:H1'	2.16	0.46
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.50	0.46
1:1A:2689:U:OP2	1:1A:2719:G:N2	2.33	0.46
1:1A:841:A:H2'	1:1A:842:G:C8	2.50	0.46
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.97	0.46
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.98	0.46
1:2A:34:C:H2'	1:2A:35:G:C8	5.00	0.46
2:2B:25:A:H2'	2:2B:26:A:C8	2.51	0.46
2:2B:32:C:H42	2:2B:50:G:H1	1.61	0.46
3:2D:18:VAL:HG12	3:2D:211:ARG:HH12	1.80	0.46
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.42	0.46
4:2E:48:GLN:HE21	4:2E:78:LEU:HD23	1.78	0.46
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:28:ARG:NH1	16:2U:38:THR:OG1	2.45	0.46
1:2A:1156:A:O4'	16:2U:51:LYS:NZ	2.49	0.46
1:1A:97:C:OP1	24:12:2:LYS:HE2	2.16	0.46
1:1A:1035:U:H2'	1:1A:1036:G:C8	2.51	0.46
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.50	0.46
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.97	0.46
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.98	0.46
16:1U:17:ILE:HG23	16:1U:39:LEU:HD12	1.98	0.46
20:1Y:13:VAL:HG12	20:1Y:74:PRO:HA	1.97	0.46
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.51	0.46
1:2A:191:A:H2'	1:2A:192:C:C6	2.50	0.46
1:2A:2137:C:O2'	1:2A:2138:C:OP2	2.31	0.46
1:2A:884:C:H3'	1:2A:885:C:C6	2.50	0.46
3:2D:134:ARG:HD2	3:2D:135:PHE:CZ	2.50	0.46
1:2A:1818:U:H2'	3:2D:157:ARG:HG3	1.97	0.46
4:2E:1:MET:O	4:2E:84:PHE:HB2	2.15	0.46
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.56	0.46
28:16:9:LEU:HD13	28:16:51:GLU:HB2	1.98	0.46
1:1A:119:A:H4'	1:1A:120:U:OP1	2.15	0.46
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.50	0.46
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.51	0.46
1:1A:286:C:H2'	1:1A:287:C:H6	1.81	0.46
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.31	0.46
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.97	0.46
5:1F:178:PRO:HB2	5:1F:201:VAL:CG2	2.46	0.46
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.51	0.46
1:2A:2393:A:HO2'	30:28:13:ARG:HH12	1.63	0.46
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.81	0.46
1:2A:585:G:O6	1:2A:756:C:N4	56.82	0.46
1:2A:774:A:N3	1:2A:774:A:H2'	2.31	0.46
1:2A:765:G:N1	1:2A:812:C:O2'	83.32	0.46
1:2A:848:G:C2	1:2A:933:A:H1'	2.50	0.46
7:2H:3:ARG:HH21	7:2H:54:ARG:NH1	2.14	0.46
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.47	0.46
1:1A:1930:G:O2'	1:1A:1968:G:O6	2.28	0.46
1:1A:2142:C:O2	1:1A:2149:G:N1	2.40	0.46
1:1A:458:G:O2'	1:1A:469:G:O6	2.30	0.46
5:1F:13:SER:OG	5:1F:16:GLY:O	2.30	0.46
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.16	0.46
21:1Z:6:LYS:HE3	21:1Z:8:TYR:OH	2.15	0.46
28:26:40:CYS:O	28:26:44:ARG:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2394:C:P	30:28:30:ARG:HH21	2.39	0.46
1:2A:1481:U:H2'	1:2A:1482:G:C8	6.68	0.46
1:2A:248:G:C2	1:2A:2431:U:H4'	2.50	0.46
1:2A:320:A:H4'	1:2A:322:A:C8	2.51	0.46
1:2A:350:U:H2'	1:2A:351:G:O4'	2.16	0.46
2:2B:107:G:H2'	2:2B:108:U:H5''	1.98	0.46
2:2B:28:C:H2'	2:2B:29:A:O4'	2.15	0.46
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.97	0.46
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.16	0.46
21:2Z:101:PRO:HA	21:2Z:123:ASP:HA	1.97	0.46
1:1A:335:C:H4'	20:1Y:73:ARG:HD2	1.98	0.46
1:2A:2432:A:C8	23:21:33:LYS:HD2	2.51	0.46
1:2A:1195:G:N7	11:2P:15:ARG:NH2	2.61	0.46
1:2A:1592:C:H2'	1:2A:1593:G:C8	2.50	0.46
1:2A:1517:G:H1'	1:2A:1919:A:O3'	102.63	0.46
1:2A:359:A:H3'	1:2A:360:G:H8	1.80	0.46
1:1A:330:A:H8	1:1A:1210:A:C4	2.34	0.46
1:1A:2319:G:H22	14:1S:3:ARG:NH1	2.14	0.46
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	1.97	0.46
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.73	0.46
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.16	0.46
21:1Z:123:ASP:N	21:1Z:123:ASP:OD1	2.47	0.46
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.53	0.46
21:1Z:24:LEU:HB2	21:1Z:41:LEU:HD12	1.98	0.46
1:2A:380:U:H2'	1:2A:381:G:H8	1.81	0.46
1:2A:646:A:H2'	1:2A:647:G:O4'	2.16	0.46
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.97	0.46
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.17	0.45
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.31	0.45
5:1F:89:VAL:HG12	5:1F:90:PHE:CD2	2.51	0.45
8:1I:79:ILE:HG22	8:1I:81:VAL:HG13	1.98	0.45
12:1Q:54:MET:HG2	12:1Q:117:ALA:HB1	1.98	0.45
18:1W:92:ARG:NH1	61:1W:302:HOH:O	2.38	0.45
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.51	0.45
1:2A:1390:U:H2'	1:2A:1391:U:C6	3.33	0.45
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.51	0.45
1:2A:1456:G:N7	61:2A:5365:HOH:O	2.36	0.45
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.15	0.45
1:2A:185:U:H4'	1:2A:218:A:H4'	1.97	0.45
1:2A:1910:G:H22	1:2A:1920:4OC:C2	2.28	0.45
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1853:A:N1	1:2A:2087:G:H1'	2.31	0.45
1:2A:2110:G:OP2	1:2A:2149:G:O2'	2.27	0.45
1:2A:299:A:H5''	20:2Y:86:ARG:NH2	2.30	0.45
1:2A:458:G:O2'	29:27:39:ARG:HD2	2.16	0.45
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	1.98	0.45
1:2A:2744:G:N2	7:2H:143:GLN:OE1	2.48	0.45
16:2U:76:TYR:OH	16:2U:92:ARG:NE	2.39	0.45
29:17:12:ARG:HH21	29:17:44:PRO:HB3	1.81	0.45
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.51	0.45
1:1A:27:G:N2	1:1A:512:G:H1'	2.31	0.45
5:1F:25:PRO:HD2	5:1F:115:ALA:HB2	1.97	0.45
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.80	0.45
1:2A:1814:G:OP1	3:2D:40:THR:OG1	2.33	0.45
1:2A:2059:A:C8	1:2A:2503:2MA:HM23	2.51	0.45
1:2A:2307:G:OP1	1:2A:2307:G:H8	1.99	0.45
1:2A:2786:U:H2'	1:2A:2787:C:C6	2.51	0.45
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.98	0.45
9:2N:15:LEU:HD23	9:2N:137:LYS:HG3	1.99	0.45
1:1A:323:G:H1'	1:1A:1205:U:O2	2.16	0.45
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	1.98	0.45
5:1F:135:LYS:HB2	5:1F:138:GLU:CD	2.37	0.45
1:1A:825:C:O2'	11:1P:55:ARG:HD3	2.16	0.45
1:2A:1288:U:O2'	1:2A:1647:G:N2	2.50	0.45
1:2A:971:C:H2'	1:2A:972:G:O4'	2.16	0.45
7:2H:107:VAL:HG11	7:2H:162:ILE:HD11	1.98	0.45
13:2R:87:TYR:HD1	13:2R:90:ARG:HD2	1.82	0.45
16:2U:66:ASN:HD21	16:2U:70:ARG:HH21	1.64	0.45
21:2Z:75:ASN:O	21:2Z:84:GLU:N	2.37	0.45
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.16	0.45
1:1A:570:G:H2'	1:1A:2030:A:N7	2.32	0.45
1:1A:2155:G:H3'	1:1A:2156:G:C8	2.50	0.45
1:1A:435:C:H2'	1:1A:436:C:H6	3.74	0.45
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.45	0.45
5:1F:161:GLU:HG2	5:1F:164:ARG:NH2	2.30	0.45
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.52	0.45
18:1W:73:ALA:HB3	18:1W:106:ILE:HB	1.98	0.45
21:1Z:91:LEU:HD12	21:1Z:91:LEU:HA	1.75	0.45
26:24:62:ARG:HA	26:24:62:ARG:HD3	1.72	0.45
30:28:14:VAL:HG22	30:28:24:ALA:HB2	1.98	0.45
1:2A:839:U:H1'	1:2A:1191:G:H1'	1.98	0.45
1:2A:2702:U:H4'	1:2A:2703:C:OP1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2705:A:H2'	1:2A:2706:G:O4'	2.17	0.45
1:2A:879:G:H3'	1:2A:880:G:C8	2.52	0.45
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.16	0.45
1:2A:2495:G:H5''	12:2Q:82:ARG:HG2	1.98	0.45
13:2R:57:ARG:HH22	13:2R:61:HIS:CD2	2.35	0.45
13:2R:63:ARG:O	13:2R:67:LEU:HB2	2.17	0.45
14:2S:87:PHE:CZ	14:2S:102:ALA:HB2	2.51	0.45
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.52	0.45
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.81	0.45
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.51	0.45
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.81	0.45
13:1R:22:ARG:HG2	13:1R:69:ASP:HB3	1.97	0.45
31:29:7:VAL:HG12	31:29:34:GLN:HB3	1.99	0.45
1:2A:892:G:H3'	1:2A:893:C:H5''	1.99	0.45
3:2D:142:VAL:HG23	3:2D:193:VAL:HA	1.98	0.45
1:2A:2638:G:P	4:2E:82:ARG:HH12	2.39	0.45
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.16	0.45
1:1A:1667:G:O2'	1:1A:1991:U:O4	2.32	0.45
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.17	0.45
1:1A:222:A:H5''	1:1A:421:U:OP1	2.15	0.45
4:1E:12:THR:HG21	15:1T:11:GLU:HG2	1.98	0.45
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.98	0.45
13:1R:2:ARG:NH1	13:1R:5:LYS:O	2.50	0.45
16:1U:52:ARG:NH1	16:1U:55:ARG:HH21	2.14	0.45
61:2A:3999:HOH:O	23:21:3:LYS:HE2	2.17	0.45
24:22:1:MET:SD	24:22:56:GLN:NE2	2.89	0.45
1:2A:943:U:N3	1:2A:1341:U:O2	98.72	0.45
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.17	0.45
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.30	0.45
1:2A:2717:G:H2'	1:2A:2718:G:O4'	2.17	0.45
1:2A:274:G:H2'	1:2A:275:G:C8	2.52	0.45
15:2T:16:ARG:NH2	15:2T:18:ASP:OD2	2.37	0.45
1:2A:2014:A:H4'	18:2W:92:ARG:HH11	1.81	0.45
1:1A:1826:G:H4'	3:1D:242:ARG:NH1	2.32	0.45
1:1A:2855:C:H2'	1:1A:2856:C:C6	2.52	0.45
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.16	0.45
6:1G:53:LEU:HD11	6:1G:87:PRO:HB2	1.98	0.45
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.16	0.45
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.50	0.45
1:2A:721:C:H2'	1:2A:722:A:C8	2.52	0.45
5:2F:32:LEU:HD22	5:2F:112:MET:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.99	0.45
21:2Z:93:ASP:HB3	21:2Z:131:ARG:HH22	1.81	0.45
27:15:42:PRO:HB2	27:15:43:HIS:ND1	2.30	0.45
1:1A:2183:C:O2'	1:1A:2184:G:OP1	2.33	0.45
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.99	0.45
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.51	0.45
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.52	0.45
3:1D:142:VAL:HG23	3:1D:193:VAL:HA	1.98	0.45
7:1H:127:GLU:HG3	7:1H:127:GLU:H	1.60	0.45
1:1A:2319:G:H22	14:1S:3:ARG:HA	1.82	0.45
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.35	0.45
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.17	0.45
1:2A:30:G:O2'	1:2A:1214:A:N3	2.46	0.45
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.52	0.45
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.82	0.45
1:2A:335:C:H4'	20:2Y:73:ARG:HD2	1.97	0.45
1:2A:1903:G:OP1	3:2D:241:PRO:HB2	2.17	0.45
4:2E:52:LEU:HB3	4:2E:76:ARG:HD3	1.98	0.45
9:2N:73:THR:HG23	9:2N:82:LEU:HD11	1.98	0.45
18:2W:33:ARG:NH2	18:2W:52:GLU:OE1	2.40	0.45
1:1A:2126:A:N6	1:1A:2162:G:O2'	2.50	0.45
1:1A:839:U:H3'	1:1A:840:C:H5'	4.11	0.45
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.46	0.45
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.65	0.45
10:1O:64:ARG:NH2	10:1O:99:PHE:O	2.50	0.45
29:27:47:ARG:HA	29:27:47:ARG:HD3	1.61	0.45
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.24	0.45
1:2A:1821:A:H2'	1:2A:1822:G:C8	2.52	0.45
1:2A:1913:A:H4'	1:2A:1914:C:C5'	2.47	0.45
1:2A:2884:U:OP2	61:2A:4777:HOH:O	2.21	0.45
4:2E:7:VAL:HG12	4:2E:27:LEU:HB3	1.99	0.45
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.98	0.45
1:2A:614(B):G:N3	5:2F:44:ARG:HG2	2.32	0.45
11:2P:52:GLU:HB3	11:2P:55:ARG:CZ	2.46	0.45
20:2Y:28:LYS:N	20:2Y:38:ILE:O	2.50	0.45
23:11:59:THR:O	23:11:91:LYS:NZ	2.50	0.45
28:16:13:CYS:SG	28:16:47:THR:HG21	2.57	0.45
1:1A:1310:G:H1'	1:1A:1611:C:H5'	1.99	0.45
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.52	0.45
1:1A:515:A:H1'	1:1A:581:C:H1'	1.99	0.45
1:2A:1002:G:H5'	1:2A:1003:G:OP2	5.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1037:G:H1	1:2A:1118:C:H42	1.63	0.45
1:2A:1248:G:C5	16:2U:3:ARG:HB2	2.52	0.45
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.17	0.45
1:2A:1607:C:H5''	1:2A:1608:A:H5'	1.99	0.45
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.52	0.45
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.80	0.45
1:2A:747:U:O2	1:2A:2014:A:H1'	2.17	0.45
1:2A:813:U:H2'	1:2A:814:C:C6	2.53	0.45
3:2D:75:ILE:HG21	3:2D:99:ASP:HB2	1.99	0.45
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.99	0.45
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.98	0.45
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.17	0.45
16:2U:49:HIS:HA	16:2U:52:ARG:HB3	1.98	0.45
1:1A:1032:A:H2	1:1A:1122:G:H22	1.65	0.44
1:1A:1052:C:H2'	1:1A:1053:C:H6	1.82	0.44
1:1A:1218:C:H42	1:1A:1231:G:H1	1.66	0.44
1:1A:1935:G:H1'	1:1A:1964:G:N2	2.32	0.44
1:1A:1972:A:H2'	1:1A:1973:G:H8	1.81	0.44
1:1A:2155:G:H3'	1:1A:2156:G:H8	1.82	0.44
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.16	0.44
1:1A:8:A:H2'	1:1A:9:U:C6	2.53	0.44
1:1A:944:G:N7	61:1A:4211:HOH:O	2.36	0.44
21:1Z:99:TYR:HA	21:1Z:124:ILE:O	2.16	0.44
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.52	0.44
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.52	0.44
1:2A:581:C:H2'	1:2A:582:G:H8	1.82	0.44
1:2A:705:A:C2	1:2A:727:A:H1'	2.52	0.44
1:2A:820:A:N3	1:2A:943:U:H4'	2.32	0.44
1:1A:1790:C:H5''	1:1A:1791:A:OP1	2.16	0.44
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.31	0.44
1:1A:2418:A:H2'	1:1A:2419:U:C6	2.52	0.44
1:1A:2712:U:O2'	1:1A:2713:A:H5'	2.17	0.44
1:1A:774:A:N3	1:1A:774:A:H2'	2.32	0.44
3:1D:37:LEU:HB2	3:1D:62:TYR:HB2	1.99	0.44
14:1S:34:HIS:O	14:1S:97:ARG:NH2	2.50	0.44
1:2A:2232:U:P	23:21:40:ARG:HH12	2.40	0.44
1:2A:2845:G:H2'	1:2A:2846:G:C8	2.52	0.44
1:2A:71:A:H5''	1:2A:73:A:C8	2.52	0.44
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.18	0.44
7:2H:74:ASN:O	7:2H:78:GLY:N	2.50	0.44
9:2N:49:GLY:O	9:2N:119:ARG:NH1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.99	0.44
24:12:14:ARG:O	24:12:67:LYS:NZ	2.49	0.44
1:1A:1364:G:C8	23:11:3:LYS:HD2	2.53	0.44
1:1A:2334:G:O6	22:10:74:ARG:NH1	2.44	0.44
1:1A:2557:G:H2'	1:1A:2558:C:C6	2.53	0.44
1:1A:272:G:N7	1:1A:421:U:H2'	2.33	0.44
2:1B:66:A:H61	2:1B:108:U:H2'	1.82	0.44
6:1G:114:ILE:HG12	6:1G:140:ILE:HG12	1.99	0.44
1:2A:2390:U:P	30:28:35:GLN:HE22	2.39	0.44
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.52	0.44
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.52	0.44
1:2A:1952:A:N3	1:2A:2560:C:O2'	2.43	0.44
1:2A:2062:A:OP1	61:2A:4300:HOH:O	2.21	0.44
1:2A:2152:G:C2	1:2A:2153:G:H1'	2.52	0.44
2:2B:42:C:C4	2:2B:43:C:C4	3.06	0.44
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.98	0.44
5:2F:36:VAL:O	5:2F:40:GLN:HG3	2.17	0.44
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.15	0.44
12:2Q:2:LEU:HD12	12:2Q:69:PHE:HE1	1.82	0.44
15:2T:65:LYS:HE2	15:2T:65:LYS:HB3	1.78	0.44
28:16:14:THR:HG21	28:16:48:VAL:HG13	1.99	0.44
2:1B:88:C:H2'	2:1B:89:G:O4'	2.18	0.44
4:1E:181:LEU:HA	4:1E:181:LEU:HD12	1.72	0.44
6:1G:170:ARG:NH2	6:1G:182:LYS:O	2.48	0.44
7:1H:113:VAL:HG11	7:1H:151:ILE:HG21	1.98	0.44
1:1A:24:G:O2'	18:1W:78:GLU:O	2.26	0.44
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.53	0.44
1:2A:2033:A:O2'	1:2A:2035:G:OP2	2.25	0.44
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.98	0.44
1:2A:521:G:H2'	1:2A:522:G:H8	1.83	0.44
1:2A:882:G:H1	1:2A:894:C:N4	2.14	0.44
1:2A:927:G:H2'	1:2A:928:G:O4'	2.16	0.44
1:2A:94(A):G:H2'	1:2A:95:G:O4'	2.17	0.44
3:2D:18:VAL:HG12	3:2D:211:ARG:NH1	2.32	0.44
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.18	0.44
9:2N:138:LEU:HD23	9:2N:138:LEU:HA	1.85	0.44
26:14:49:PHE:HB3	26:14:50:VAL:H	1.51	0.44
1:1A:1401:G:H2'	1:1A:1402:C:O4'	2.17	0.44
1:1A:1406:U:H2'	1:1A:1407:C:H6	1.79	0.44
1:1A:2102:U:H3	1:1A:2187:G:H1	1.65	0.44
1:1A:2336:A:H61	22:10:43:THR:HG22	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:101:GLU:OE2	3:1D:103:ARG:NE	2.42	0.44
1:1A:1823:G:P	3:1D:54:ARG:HH21	2.40	0.44
6:1G:43:LEU:HD12	6:1G:43:LEU:HA	1.81	0.44
12:1Q:134:ARG:NH1	21:1Z:122:ARG:HH21	2.15	0.44
1:2A:250:G:OP1	30:28:13:ARG:NH2	2.50	0.44
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.99	0.44
1:2A:1231:G:H2'	1:2A:1232:G:H8	1.82	0.44
1:2A:2875:C:H2'	1:2A:2876:G:O4'	2.18	0.44
1:2A:1007:C:P	9:2N:37:LYS:HZ2	2.40	0.44
9:2N:67:LEU:O	9:2N:88:GLU:HG3	2.17	0.44
17:2V:58:VAL:HB	17:2V:98:GLU:HG3	2.00	0.44
1:2A:571:A:O2'	17:2V:78:LYS:HE2	2.18	0.44
1:1A:11:G:O2'	1:1A:506:G:N2	53.36	0.44
1:1A:2121:G:H2'	1:1A:2122:U:C6	2.53	0.44
1:1A:2181:G:HO2'	1:1A:2182:G:P	2.39	0.44
1:1A:614(B):G:N2	5:1F:44:ARG:O	2.46	0.44
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.54	0.44
21:1Z:99:TYR:HB3	21:1Z:123:ASP:OD2	2.18	0.44
1:2A:1637:A:H5'	1:2A:1760:A:O2'	2.18	0.44
1:2A:2516:G:C6	1:2A:2517:C:C4	3.06	0.44
1:2A:2689:U:P	1:2A:2719:G:H22	2.41	0.44
2:2B:34:U:O4	2:2B:44:G:O2'	2.33	0.44
12:2Q:50:ALA:HB1	12:2Q:121:ALA:HB1	1.99	0.44
1:2A:1155:A:H5''	16:2U:55:ARG:NE	2.32	0.44
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.52	0.44
1:1A:1566:A:OP1	3:1D:211:ARG:NH1	2.49	0.44
1:1A:234:C:H2'	1:1A:235:U:H6	1.82	0.44
1:1A:2590:A:H2'	1:1A:2591:C:H6	1.82	0.44
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.52	0.44
19:1X:35:THR:HG22	19:1X:37:THR:H	1.83	0.44
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.23	0.44
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.41	0.44
3:2D:3:VAL:HG21	3:2D:203:ASN:HB2	2.00	0.44
3:2D:77:ALA:HA	3:2D:97:TYR:HA	2.00	0.44
17:2V:48:GLY:HA2	17:2V:52:VAL:HG13	1.99	0.44
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.53	0.44
1:1A:1069:A:H2	1:1A:1095:A:O2'	2.01	0.44
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.53	0.44
1:1A:1275:A:H4'	61:1A:7623:HOH:O	2.17	0.44
1:1A:2179:C:H2'	1:1A:2180:U:C6	2.53	0.44
1:1A:407:G:H2'	1:1A:408:G:H8	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:438:G:H2'	1:1A:440:G:H8	1.83	0.44
1:1A:586:A:N1	1:1A:809:G:O2'	2.44	0.44
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.82	0.44
9:1N:36:GLY:HA2	9:1N:38:HIS:CE1	2.53	0.44
10:1O:64:ARG:HB2	10:1O:79:PHE:CD2	2.53	0.44
13:1R:54:LEU:HA	13:1R:54:LEU:HD12	1.83	0.44
16:1U:104:GLN:NE2	16:1U:105:VAL:HG23	2.33	0.44
12:1Q:134:ARG:CZ	21:1Z:122:ARG:HH21	2.31	0.44
1:2A:1017:G:N7	61:2A:5060:HOH:O	2.46	0.44
1:2A:551:G:O2'	1:2A:1220:A:N3	2.37	0.44
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.47	0.44
1:2A:271(R):G:OP1	23:21:76:ARG:NH1	2.51	0.44
1:2A:35:G:H2'	1:2A:36:G:O4'	2.17	0.44
1:2A:407:G:H2'	1:2A:408:G:C8	2.52	0.44
1:2A:489:G:H2'	1:2A:491:G:O4'	2.18	0.44
7:2H:80:SER:OG	7:2H:81:GLU:N	2.51	0.44
21:2Z:91:LEU:HD12	21:2Z:91:LEU:HA	1.85	0.44
1:1A:1047:G:O2'	1:1A:1048:A:O5'	2.33	0.44
1:1A:1065:U:N3	1:1A:1070:A:OP1	2.42	0.44
1:1A:1420:U:H6	1:1A:1420:U:H2'	1.62	0.44
1:1A:1637:A:OP2	61:1A:7206:HOH:O	2.21	0.44
1:1A:185:U:H2'	1:1A:186:G:H8	1.83	0.44
1:1A:2330:G:H2'	1:1A:2331:G:O4'	2.18	0.44
1:1A:674:G:H2'	1:1A:675:A:C8	5.03	0.44
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.18	0.44
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.18	0.44
1:2A:1270:C:HO2'	1:2A:1313:U:HO2'	22.24	0.44
1:2A:2562:U:H4'	10:2O:25:LEU:HD21	2.00	0.44
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.53	0.44
1:2A:2820:A:OP1	13:2R:2:ARG:NH2	2.47	0.44
1:2A:322:A:H5'	1:2A:340:A:H1'	1.99	0.44
1:2A:752:A:P	29:27:3:ARG:HH22	2.41	0.44
1:2A:892:G:H3'	1:2A:893:C:C5'	2.48	0.44
2:2B:41:U:H5	6:2G:70:VAL:N	2.16	0.44
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.99	0.44
1:2A:1012:U:O4	9:2N:28:THR:HG21	2.18	0.44
1:1A:1068:G:OP2	1:1A:1068:G:H8	2.61	0.43
1:1A:1355:G:H2'	1:1A:1356:G:C8	2.98	0.43
1:1A:1754:C:N3	1:1A:2716:U:O2'	2.44	0.43
1:1A:242:G:C8	30:18:5:LYS:HG2	2.53	0.43
1:1A:2441:C:OP2	1:1A:2586:C:O2'	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:266:G:H2'	1:1A:266:G:N3	3.31	0.43
1:1A:271(K):U:H4'	1:1A:271(L):U:OP2	2.16	0.43
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.18	0.43
11:1P:124:LYS:HA	11:1P:144:GLU:HB3	1.98	0.43
11:1P:3:LEU:HD12	11:1P:3:LEU:HA	1.90	0.43
12:1Q:25:ASP:N	12:1Q:25:ASP:OD1	2.50	0.43
11:2P:52:GLU:HG3	30:28:57:ARG:HH22	1.82	0.43
1:2A:1028:A:H61	1:2A:1125:G:H2'	1.81	0.43
1:2A:1427:A:H4'	1:2A:1428:C:O5'	2.18	0.43
1:2A:2127:G:H2'	1:2A:2128:C:H6	1.82	0.43
1:2A:2547:U:H2'	1:2A:2548:G:C8	2.53	0.43
1:2A:2853:C:H2'	1:2A:2854:G:H8	1.82	0.43
2:2B:55:U:H1'	6:2G:29:TRP:CD1	2.53	0.43
5:2F:57:VAL:HG13	5:2F:59:TYR:H	1.83	0.43
8:2I:125:GLU:OE1	8:2I:143:SER:HB3	2.18	0.43
13:2R:13:HIS:CE1	13:2R:16:HIS:HB2	2.53	0.43
1:1A:118:A:C8	1:1A:119:A:C8	3.05	0.43
1:1A:1448:G:H5''	1:1A:1542:A:OP2	2.19	0.43
1:1A:1504:C:H2'	1:1A:1505:C:C6	2.54	0.43
1:1A:324:A:H2'	1:1A:325:G:O4'	2.18	0.43
2:1B:74:U:H2'	2:1B:75:G:O4'	2.18	0.43
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.29	0.43
5:1F:106:ARG:HG2	5:1F:106:ARG:H	1.56	0.43
5:1F:32:LEU:HB3	5:1F:112:MET:HE1	2.00	0.43
7:1H:89:ILE:O	7:1H:129:THR:OG1	2.34	0.43
11:1P:3:LEU:HD12	11:1P:6:LEU:HD12	2.00	0.43
1:1A:1754:C:H5	15:1T:96:ARG:NH2	2.16	0.43
1:2A:1576:U:H2'	1:2A:1577:C:C6	2.53	0.43
1:2A:1754:C:N3	1:2A:2716:U:O2'	2.47	0.43
1:2A:2065:C:H4'	1:2A:2251:OMG:HM22	2.00	0.43
1:2A:2251:OMG:OP2	1:2A:2251:OMG:H8	2.01	0.43
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.53	0.43
1:2A:362:U:O2'	1:2A:363:G:H5'	2.18	0.43
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.46	0.43
1:2A:660:G:H5'	5:2F:99:TYR:CE1	2.53	0.43
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.53	0.43
11:2P:70:GLN:O	11:2P:73:GLY:N	2.36	0.43
21:2Z:53:ILE:HG22	21:2Z:71:VAL:O	2.18	0.43
26:14:63:TYR:CD1	26:14:63:TYR:N	2.85	0.43
1:1A:1155:A:OP1	16:1U:55:ARG:HD2	2.19	0.43
1:1A:121:G:H4'	1:1A:149:A:H5'	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1692:U:O2'	1:1A:1693:U:H2'	2.18	0.43
1:1A:2120:G:C2'	1:1A:2121:G:H5'	2.48	0.43
1:1A:2788:C:O2'	1:1A:2809:A:N3	2.41	0.43
1:1A:602:G:O2'	1:1A:655:A:N6	2.51	0.43
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	2.00	0.43
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.65	0.43
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	1.99	0.43
11:1P:50:ARG:HD3	30:18:7:HIS:HD2	1.79	0.43
28:26:8:LYS:HD3	30:28:34:TRP:CD2	2.54	0.43
1:2A:1364:G:P	23:21:3:LYS:HG3	2.58	0.43
1:2A:1598:C:H2'	1:2A:1599:C:C6	2.53	0.43
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.53	0.43
1:2A:208:C:H2'	1:2A:209:C:H6	1.83	0.43
1:2A:2108:C:H42	1:2A:2181:G:H1	1.64	0.43
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.18	0.43
2:2B:24:G:H4'	2:2B:25:A:C8	2.54	0.43
3:2D:183:ARG:HG3	3:2D:270:ILE:HG12	2.01	0.43
3:2D:9:TYR:CD1	3:2D:10:THR:HG23	2.53	0.43
6:2G:49:ASP:OD1	6:2G:49:ASP:N	2.48	0.43
8:2I:79:ILE:O	8:2I:144:VAL:HA	2.18	0.43
12:2Q:38:GLU:OE2	12:2Q:128:LYS:N	2.40	0.43
20:2Y:6:HIS:ND1	20:2Y:7:VAL:HG23	2.33	0.43
30:18:63:PRO:HG2	30:18:64:TYR:CE2	2.53	0.43
1:1A:768:G:O2'	1:1A:1379:A:N1	2.41	0.43
1:1A:1652:A:OP1	13:1R:8:ARG:NH1	2.51	0.43
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.83	0.43
1:1A:182:A:N3	1:1A:433:C:O2'	2.44	0.43
1:1A:2206:G:H4'	1:1A:2206:G:OP2	2.17	0.43
1:1A:2691:C:O3'	1:1A:2871:C:H4'	2.18	0.43
3:1D:218:ARG:HB3	3:1D:219:PRO:HD2	1.99	0.43
5:1F:129:PHE:HB3	5:1F:132:VAL:HG13	2.00	0.43
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.18	0.43
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.51	0.43
24:22:10:LEU:HD21	24:22:59:ARG:HG2	1.98	0.43
30:28:23:VAL:HG11	30:28:47:LYS:HD3	2.00	0.43
1:2A:1660:C:H2'	1:2A:1661:G:H8	1.83	0.43
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.83	0.43
1:2A:2287:A:H2	1:2A:2346:A:H62	1.64	0.43
1:2A:284:U:H2'	1:2A:285:C:C6	2.54	0.43
1:2A:822:U:OP2	61:2A:5949:HOH:O	2.21	0.43
61:2A:4490:HOH:O	3:2D:237:GLU:OE2	2.20	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:36:LYS:HD3	6:2G:95:ARG:NH1	2.33	0.43
8:2I:62:LYS:O	8:2I:66:GLU:HG2	2.18	0.43
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.99	0.43
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	2.00	0.43
1:1A:125:G:H1'	29:17:48:LYS:HD3	2.01	0.43
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.51	0.43
1:1A:26:G:H1'	1:1A:515:A:H61	1.84	0.43
7:1H:90:LYS:HD2	7:1H:159:GLU:HG2	1.99	0.43
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	2.00	0.43
1:1A:747:U:H1'	18:1W:92:ARG:NH1	2.32	0.43
28:26:13:CYS:SG	28:26:47:THR:HG21	2.58	0.43
1:2A:1537:G:H2'	1:2A:1538:G:C8	2.49	0.43
1:2A:1814:G:H2'	1:2A:1815:A:C8	2.54	0.43
1:2A:210:C:H2'	1:2A:211:A:C8	2.53	0.43
1:2A:2322:A:H2'	1:2A:2323:G:O4'	2.18	0.43
1:2A:565:C:H2'	1:2A:566:U:O4'	2.19	0.43
1:2A:589:C:H2'	1:2A:590:A:C8	2.53	0.43
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	2.00	0.43
6:2G:135:LEU:O	6:2G:155:MET:N	2.40	0.43
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.54	0.43
13:2R:66:VAL:HG12	13:2R:70:LEU:HD12	1.99	0.43
15:2T:33:LYS:HB3	15:2T:82:LEU:HD22	2.00	0.43
15:2T:88:ILE:HG21	15:2T:91:ARG:NE	2.32	0.43
1:1A:1111:A:H4'	1:1A:1112:G:OP1	2.19	0.43
1:1A:1441:G:O6	61:1A:6075:HOH:O	2.21	0.43
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.34	0.43
1:1A:2049:G:N7	61:1A:6385:HOH:O	2.37	0.43
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.19	0.43
1:1A:53:A:H2'	1:1A:54:G:O4'	2.19	0.43
1:1A:2639:A:O2'	9:1N:97:ARG:NH2	2.52	0.43
1:2A:1422:G:O3'	10:2O:49:ARG:NH1	99.52	0.43
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.53	0.43
1:2A:2563:U:H4'	10:2O:28:SER:HA	2.00	0.43
1:2A:752:A:H4'	1:2A:753:C:H5'	1.99	0.43
1:2A:884:C:H3'	1:2A:885:C:H6	1.84	0.43
10:2O:29:ASN:OD1	10:2O:29:ASN:N	2.51	0.43
13:2R:72:ASP:HB3	13:2R:75:LEU:HB3	2.00	0.43
16:2U:6:THR:HG21	16:2U:10:ARG:HH21	1.84	0.43
28:16:12:GLU:HA	28:16:19:ARG:HA	2.01	0.43
1:1A:1470:G:N2	1:1A:1520:G:OP2	2.34	0.43
1:1A:185:U:H2'	1:1A:186:G:C8	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1952:A:C6	1:1A:1953:A:N1	2.86	0.43
1:1A:2168:G:C6	1:1A:2171:A:C8	3.07	0.43
1:1A:2188:C:H2'	1:1A:2189:U:O4'	2.18	0.43
1:1A:666:G:N1	1:1A:740:U:O2	75.04	0.43
3:1D:155:LEU:HD23	3:1D:155:LEU:HA	4.48	0.43
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	2.01	0.43
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.51	0.43
1:2A:1022:G:N2	1:2A:1023:U:O4	2.45	0.43
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.84	0.43
1:2A:1423:G:H2'	1:2A:1424:G:H8	1.83	0.43
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.19	0.43
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.18	0.43
1:2A:469:G:N7	29:27:37:LYS:NZ	2.63	0.43
1:2A:684:G:N7	61:2A:3918:HOH:O	2.37	0.43
1:2A:855:G:H2'	1:2A:856:C:C6	2.53	0.43
1:2A:863:A:H2'	1:2A:864:G:C8	2.54	0.43
1:1A:1118:C:H2'	1:1A:1119:C:H6	2.19	0.43
1:1A:1638:C:H5''	1:1A:2710:C:O2'	2.18	0.43
1:1A:35:G:H2'	1:1A:36:G:O4'	2.19	0.43
5:1F:116:ASP:OD2	11:1P:1:MET:N	2.42	0.43
9:1N:4:TYR:CE2	16:1U:100:VAL:HG11	2.53	0.43
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.18	0.43
23:21:89:GLU:O	23:21:93:GLU:HG2	2.18	0.43
1:2A:458:G:C8	29:27:37:LYS:HG2	2.54	0.43
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.18	0.43
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.18	0.43
1:2A:2841:C:H2'	1:2A:2842:G:C8	2.53	0.43
1:2A:741:G:H2'	1:2A:742:G:O4'	2.64	0.43
1:2A:848:G:O6	1:2A:928:G:H2'	2.18	0.43
2:2B:68:C:H2'	2:2B:69:G:H8	1.82	0.43
14:2S:64:GLU:CD	14:2S:64:GLU:H	3.82	0.43
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.19	0.43
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.53	0.43
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.54	0.43
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.54	0.43
1:1A:2135:A:H2	1:1A:2136:C:C2	2.37	0.43
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.54	0.43
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.54	0.43
1:1A:1783:A:C5'	1:1A:2608:G:H4'	2.49	0.43
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.83	0.43
11:1P:59:LEU:HD21	30:18:10:ALA:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2011:U:OP1	18:1W:42:ARG:NH1	2.51	0.43
2:1B:92:C:H5''	21:1Z:79:ARG:NH1	2.33	0.43
1:2A:1504:C:H2'	1:2A:1505:C:H6	1.83	0.43
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.19	0.43
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.54	0.43
1:2A:2840:C:H2'	1:2A:2841:C:C6	2.54	0.43
1:2A:729:G:C8	3:2D:208:LYS:HD2	2.54	0.43
1:2A:744:G:H2'	1:2A:745:G:O4'	2.18	0.43
2:2B:66:A:H61	2:2B:108:U:H2'	1.84	0.43
2:2B:11:C:H3'	2:2B:12:C:C6	2.53	0.43
6:2G:3:LEU:HD12	6:2G:8:LYS:NZ	2.34	0.43
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.52	0.43
21:2Z:50:GLN:N	21:2Z:50:GLN:OE1	2.51	0.43
1:1A:1010:A:N3	1:1A:1153:C:H1'	2.33	0.43
1:1A:1054:A:N6	1:1A:1105:U:N3	2.49	0.43
1:1A:1058:G:N1	1:1A:1080:C:N4	2.34	0.43
1:1A:1409:C:H2'	1:1A:1410:G:C8	2.54	0.43
1:1A:1418:G:O5'	1:1A:1418:G:H8	2.02	0.43
1:1A:1665:A:H2'	1:1A:1666:G:O4'	2.19	0.43
1:1A:234:C:H2'	1:1A:235:U:C6	2.54	0.43
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	2.00	0.43
1:2A:1568:G:H5''	3:2D:61:LEU:HD13	2.00	0.43
1:2A:2474:C:H5''	1:2A:2475:C:OP2	2.19	0.43
1:2A:2658:C:H5'	7:2H:160:LYS:HZ2	1.83	0.43
1:2A:2689:U:H4'	1:2A:2690:C:O5'	2.19	0.43
1:2A:613:G:O2'	1:2A:614(C):A:N1	2.43	0.43
1:2A:898:C:H2'	1:2A:899:A:H5'	2.01	0.43
7:2H:122:THR:O	7:2H:134:SER:OG	2.33	0.43
10:2O:64:ARG:HG2	10:2O:83:ALA:HB3	2.01	0.43
30:18:62:LEU:HB3	30:18:65:GLU:HG2	2.01	0.42
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.53	0.42
1:1A:143:G:H4'	19:1X:35:THR:HG21	2.00	0.42
1:1A:2611:U:H6	1:1A:2611:U:H5'	1.84	0.42
1:1A:2801(A):A:H5''	1:1A:2802:G:C8	2.54	0.42
1:1A:957:A:H4'	12:1Q:74:TYR:OH	2.19	0.42
1:2A:1263:U:C4	1:2A:1264:G:C6	3.06	0.42
1:2A:1354:A:O3'	3:2D:38:LYS:HE3	2.19	0.42
1:2A:139:G:H2'	1:2A:140:G:N7	2.34	0.42
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.18	0.42
1:2A:877:U:O2'	1:2A:900:A:N6	2.52	0.42
1:2A:923:C:H2'	1:2A:924:C:H6	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:19:G:H2'	2:2B:20:C:O4'	2.19	0.42
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.19	0.42
3:2D:70:TRP:CE2	3:2D:150:LYS:HG3	2.54	0.42
7:2H:43:VAL:HG13	7:2H:52:VAL:HG22	2.00	0.42
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.17	0.42
19:2X:5:TYR:CZ	24:22:30:ARG:HB2	2.53	0.42
28:16:11:LEU:HD23	28:16:11:LEU:HA	1.91	0.42
1:1A:570:G:H2'	1:1A:2030:A:C5	2.54	0.42
1:1A:2314:C:H2'	1:1A:2315:G:C8	2.54	0.42
1:1A:2478:A:O2'	1:1A:2536:G:N2	2.52	0.42
1:1A:751:A:H5'	18:1W:90:ARG:HA	2.01	0.42
1:1A:2484:G:H1'	12:1Q:124:LYS:HD2	2.00	0.42
13:1R:72:ASP:HB3	13:1R:75:LEU:HB3	2.01	0.42
1:2A:2389:G:H5"	1:2A:2390:U:O4'	2.19	0.42
1:2A:588:U:H2'	1:2A:589:C:C6	2.54	0.42
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.51	0.42
12:2Q:57:HIS:NE2	12:2Q:116:GLU:HB3	2.34	0.42
10:2O:101:PRO:HD3	15:2T:68:TYR:HB2	2.00	0.42
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.83	0.42
12:2Q:20:ALA:HB2	21:2Z:79:ARG:HG2	2.00	0.42
1:1A:2232:U:P	23:11:40:ARG:HH12	2.43	0.42
24:12:53:LEU:HA	24:12:53:LEU:HD23	1.81	0.42
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.55	0.42
1:1A:472:A:H2'	1:1A:473:G:O4'	4.76	0.42
7:1H:56:SER:OG	7:1H:57:ASP:N	2.52	0.42
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	2.00	0.42
15:1T:94:ALA:HB1	15:1T:99:LEU:HD21	2.00	0.42
16:1U:27:LEU:HB3	16:1U:31:SER:HB3	1.99	0.42
1:2A:1364:G:C8	23:21:3:LYS:HD2	2.54	0.42
24:22:49:LYS:HE2	24:22:49:LYS:HB3	1.75	0.42
1:2A:1580:A:H3'	1:2A:1581:G:C8	2.51	0.42
1:2A:598:G:H2'	1:2A:599:G:O4'	2.19	0.42
3:2D:242:ARG:HD2	3:2D:246:PRO:HG3	2.00	0.42
3:2D:69:ARG:HH11	3:2D:105:ILE:HG21	1.85	0.42
5:2F:184:TYR:CZ	5:2F:188:ARG:HD2	2.54	0.42
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.19	0.42
17:2V:85:LYS:HB2	17:2V:85:LYS:HE3	1.70	0.42
21:2Z:126:VAL:CG1	21:2Z:161:VAL:HG23	2.49	0.42
23:11:64:ALA:HA	23:11:67:ILE:HG13	2.00	0.42
1:1A:1178:C:O5'	1:1A:1178:C:H6	2.01	0.42
1:1A:1431:U:H2'	1:1A:1432:C:C6	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.47	0.42
1:1A:478:A:N1	1:1A:500:G:H4'	2.33	0.42
13:1R:98:LEU:HB2	13:1R:113:LEU:HD11	2.02	0.42
14:1S:10:ARG:HG3	14:1S:13:ARG:NH2	2.33	0.42
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	2.03	0.42
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.52	0.42
1:2A:807:U:O2'	1:2A:2060:A:N1	2.50	0.42
1:2A:2586:C:OP2	1:2A:2608:G:N1	2.42	0.42
1:2A:2792:G:N3	1:2A:2792:G:H2'	2.35	0.42
1:2A:648:G:H2'	1:2A:649:G:C8	2.54	0.42
1:2A:751:A:H2	1:2A:789:A:HO2'	1.66	0.42
4:2E:11:MET:HG2	4:2E:24:THR:HB	2.00	0.42
10:2O:1:MET:HG3	10:2O:67:LYS:HG2	2.00	0.42
10:2O:64:ARG:HB2	10:2O:79:PHE:CD2	2.54	0.42
11:2P:101:VAL:HA	11:2P:106:LEU:O	2.19	0.42
13:2R:26:LYS:HE2	13:2R:70:LEU:O	2.19	0.42
21:2Z:54:HIS:HB3	21:2Z:101:PRO:HD3	2.02	0.42
26:14:55:ARG:H	26:14:56:VAL:HA	1.85	0.42
1:1A:1055:G:N2	1:1A:1104:C:N3	2.58	0.42
1:1A:1027:A:C2	1:1A:2488:A:H5'	2.54	0.42
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.19	0.42
1:1A:27:G:C2	1:1A:512:G:N3	2.87	0.42
2:1B:42:C:O2'	6:1G:66:GLN:HG2	2.19	0.42
3:1D:208:LYS:HG3	3:1D:210:GLY:H	1.84	0.42
4:1E:9:VAL:HB	15:1T:3:ARG:HG2	2.02	0.42
1:1A:2378:A:H2'	14:1S:21:THR:HG21	2.02	0.42
15:1T:95:ARG:HB2	15:1T:96:ARG:HH12	1.84	0.42
17:1V:40:LEU:HB2	17:1V:46:VAL:HG22	2.01	0.42
25:23:6:VAL:HG13	25:23:54:VAL:HG11	2.01	0.42
1:2A:459:U:OP2	29:27:39:ARG:NH1	2.52	0.42
1:2A:817:C:N4	1:2A:1529:G:O6	111.69	0.42
1:2A:1847:A:H3'	1:2A:1848:A:H5'	2.01	0.42
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.54	0.42
1:2A:2494:G:OP1	22:20:3:HIS:N	2.43	0.42
1:2A:250:G:C6	1:2A:251:A:C6	3.08	0.42
1:2A:2612:C:OP2	27:25:2:ALA:N	2.52	0.42
1:2A:2748:A:H2	7:2H:63:SER:HB3	1.84	0.42
1:2A:320:A:H4'	1:2A:322:A:N7	2.34	0.42
1:2A:476:G:H2'	1:2A:477:A:H8	3.55	0.42
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.54	0.42
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.19	0.42
8:2I:26:ALA:O	8:2I:31:LEU:HB2	2.20	0.42
11:2P:83:VAL:HG22	11:2P:112:LEU:HD11	2.01	0.42
14:2S:62:LYS:O	14:2S:66:ALA:N	2.51	0.42
25:13:23:LEU:HD13	25:13:50:VAL:HG11	2.01	0.42
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	2.01	0.42
26:14:53:GLU:O	26:14:56:VAL:HG13	2.19	0.42
1:1A:1057:A:N6	1:1A:1081:U:H3	2.15	0.42
1:1A:1645:G:H5''	1:1A:1646:C:O4'	2.20	0.42
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.55	0.42
1:1A:1821:A:H2'	1:1A:1822:G:C8	2.55	0.42
1:1A:573:G:O2'	1:1A:574:C:H3'	2.20	0.42
1:1A:817:C:H4'	1:1A:932:G:C5	2.55	0.42
1:1A:744:G:OP1	4:1E:132:HIS:ND1	2.50	0.42
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.54	0.42
6:1G:49:ASP:N	6:1G:49:ASP:OD1	2.53	0.42
9:1N:66:LYS:HB3	9:1N:70:LYS:HB2	2.00	0.42
11:1P:62:LEU:O	30:18:13:ARG:HD3	2.20	0.42
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.54	0.42
19:1X:28:PHE:CE1	19:1X:92:LEU:HD11	2.55	0.42
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.54	0.42
1:2A:1262:A:H2	27:25:10:LYS:HD2	1.83	0.42
1:2A:115:C:O2'	1:2A:127:A:O2'	2.36	0.42
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.54	0.42
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.53	0.42
1:2A:1540:U:H2'	1:2A:1541:G:O4'	2.20	0.42
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.43	0.42
1:2A:2305:A:H5''	6:2G:134:GLY:HA3	2.00	0.42
1:2A:2617:C:H2'	1:2A:2618:G:O4'	2.20	0.42
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.54	0.42
1:2A:797:C:H2'	1:2A:798:G:O4'	2.20	0.42
7:2H:56:SER:OG	7:2H:57:ASP:N	2.53	0.42
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	2.01	0.42
11:2P:138:LEU:HG	11:2P:143:GLY:HA3	2.00	0.42
13:2R:87:TYR:CD1	13:2R:90:ARG:HD2	2.55	0.42
20:2Y:14:LEU:HG	20:2Y:15:VAL:N	2.34	0.42
20:2Y:19:LYS:HE2	20:2Y:19:LYS:HB3	1.84	0.42
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.73	0.42
25:13:39:ASP:OD1	25:13:44:ARG:NH1	2.52	0.42
1:1A:1064:C:H2'	1:1A:1065:U:H5'	2.01	0.42
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1190:G:H5''	11:1P:32:THR:O	2.20	0.42
1:1A:762:U:OP1	61:1A:6670:HOH:O	2.22	0.42
2:1B:83:G:OP1	25:13:19:GLN:NE2	2.49	0.42
19:1X:40:LYS:O	19:1X:44:GLU:HG3	2.19	0.42
25:23:6:VAL:HG13	25:23:54:VAL:CG1	2.49	0.42
1:2A:2116:G:N2	1:2A:2162:G:OP1	2.52	0.42
1:2A:2398:U:H2'	1:2A:2399:G:C8	2.55	0.42
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.19	0.42
1:2A:259:G:H2'	1:2A:260:G:O4'	2.84	0.42
1:2A:746:A:H2'	1:2A:2612:C:H5''	2.00	0.42
5:2F:33:LEU:HD11	5:2F:112:MET:HB3	2.01	0.42
12:2Q:36:ALA:HA	12:2Q:129:THR:HG22	2.02	0.42
15:2T:51:ARG:HG2	15:2T:62:THR:HB	2.02	0.42
1:1A:1069:A:H1'	1:1A:1096:A:H4'	2.02	0.42
1:1A:1274:A:N3	1:1A:1297:C:H1'	2.35	0.42
1:1A:1489:U:HO2'	1:1A:1490:A:H8	1.68	0.42
1:1A:27:G:O2'	1:1A:28:A:OP2	2.35	0.42
1:1A:629:G:H2'	1:1A:630:G:O4'	2.65	0.42
1:1A:686:G:N2	1:1A:788:A:H61	2.18	0.42
2:1B:28:C:H2'	2:1B:29:A:O4'	2.20	0.42
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.42	0.42
14:1S:10:ARG:HG3	14:1S:13:ARG:HH22	1.85	0.42
16:1U:47:TYR:HA	16:1U:50:ARG:NH2	2.34	0.42
18:1W:65:LEU:HB2	18:1W:68:ARG:HD2	2.01	0.42
20:1Y:106:LEU:O	20:1Y:107:ASP:HB2	2.19	0.42
20:1Y:28:LYS:HD2	20:1Y:40:GLU:OE1	2.20	0.42
27:25:40:LYS:NZ	27:25:44:THR:O	2.44	0.42
1:2A:1022:G:OP2	9:2N:69:GLN:NE2	2.46	0.42
1:2A:1832:C:H2'	1:2A:1833:U:O4'	2.20	0.42
1:2A:2133:G:C6	1:2A:2157:G:C6	3.08	0.42
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.55	0.42
1:2A:297:C:H2'	1:2A:298:G:O4'	2.20	0.42
1:2A:729:G:O5'	3:2D:208:LYS:NZ	2.53	0.42
2:2B:15:A:OP2	2:2B:69:G:N2	2.53	0.42
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.50	0.42
4:2E:181:LEU:HA	4:2E:181:LEU:HD12	1.74	0.42
10:2O:7:TYR:CZ	10:2O:44:LYS:HG3	2.55	0.42
15:2T:19:LEU:HD13	15:2T:86:ILE:HD12	2.02	0.42
16:2U:88:ILE:HG22	16:2U:90:VAL:HG23	2.01	0.42
21:2Z:149:SER:HG	21:2Z:170:THR:HG1	1.64	0.42
25:13:19:GLN:OE1	25:13:52:HIS:NE2	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:13:3:ARG:HB2	25:13:59:VAL:HG23	2.01	0.42
1:1A:1653:G:O3'	13:1R:2:ARG:HB2	2.19	0.42
1:1A:196:A:N3	1:1A:196:A:H2'	2.35	0.42
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.55	0.42
1:1A:284:U:H2'	1:1A:285:C:C6	2.55	0.42
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	2.02	0.42
5:1F:125:LEU:HD21	5:1F:199:TRP:CD2	2.55	0.42
61:1A:5688:HOH:O	11:1P:43:GLY:HA3	2.20	0.42
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.54	0.42
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.20	0.42
1:2A:631:A:H1'	11:2P:66:GLY:HA2	2.02	0.42
6:2G:27:ASN:HB3	6:2G:30:GLU:HB2	2.01	0.42
7:2H:152:ARG:HD3	7:2H:152:ARG:HA	1.86	0.42
14:2S:20:ARG:HD2	14:2S:20:ARG:HA	1.94	0.42
21:2Z:158:PRO:HA	21:2Z:159:PRO:HD3	1.97	0.42
21:2Z:128:VAL:HG23	21:2Z:160:GLY:O	2.20	0.42
30:18:30:ARG:O	61:18:207:HOH:O	2.22	0.42
1:1A:106:C:HO2'	1:1A:294:A:HO2'	1.66	0.42
1:1A:1156:A:OP1	16:1U:55:ARG:NH1	2.45	0.42
1:1A:1216:G:O6	61:1A:4803:HOH:O	2.21	0.42
1:1A:129:C:H2'	1:1A:130:C:H6	1.85	0.42
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.20	0.42
1:1A:2141:G:C6	1:1A:2142:C:C2	3.07	0.42
1:1A:251:A:C5	1:1A:252:G:H1'	2.54	0.42
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.20	0.42
1:1A:479:A:N3	1:1A:481:G:H5''	2.35	0.42
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.20	0.42
6:1G:62:LEU:HA	26:14:27:THR:HG21	2.02	0.42
8:1I:26:ALA:O	8:1I:31:LEU:HB2	2.20	0.42
9:1N:62:VAL:CG1	9:1N:66:LYS:HB2	2.50	0.42
18:1W:36:LEU:HD13	18:1W:48:ALA:HA	2.02	0.42
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.20	0.42
26:24:18:CYS:SG	26:24:20:ASN:HB2	2.60	0.42
1:2A:1639:U:H4'	1:2A:2699:C:H4'	2.02	0.42
1:2A:1713:U:H2'	1:2A:1714:G:H8	1.84	0.42
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.35	0.42
1:2A:1902:C:H5'	3:2D:246:PRO:HD3	2.02	0.42
1:2A:2313:C:H2'	1:2A:2314:C:C6	2.55	0.42
1:2A:266:G:H2'	1:2A:266:G:N3	3.19	0.42
1:2A:359:A:H2'	1:2A:360:G:O4'	2.20	0.42
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:51:ARG:HD3	24:12:55:ARG:NH1	2.35	0.41
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.92	0.41
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.53	0.41
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.84	0.41
1:1A:2032:G:OP2	1:1A:2454:G:O2'	2.29	0.41
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.53	0.41
1:1A:629:G:H3'	1:1A:630:G:H5''	4.63	0.41
1:1A:669:G:N2	61:1A:4261:HOH:O	2.44	0.41
8:1I:50:ARG:HB3	8:1I:50:ARG:CZ	2.50	0.41
15:1T:33:LYS:HD3	15:1T:82:LEU:HD22	2.02	0.41
15:1T:95:ARG:HB2	15:1T:96:ARG:NH1	2.35	0.41
1:1A:1156:A:C8	16:1U:51:LYS:HD2	2.54	0.41
21:1Z:44:PHE:CZ	21:1Z:86:VAL:HG11	2.55	0.41
1:2A:2011:U:H2'	1:2A:2012:G:O4'	2.20	0.41
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.20	0.41
1:2A:2166:G:N7	1:2A:2168:G:N2	2.68	0.41
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.34	0.41
1:2A:784:A:OP1	1:2A:2588:G:H5''	2.19	0.41
1:2A:2755:C:HO2'	1:2A:2756:U:H6	1.65	0.41
1:2A:948:G:H21	1:2A:985:C:P	2.43	0.41
2:2B:30:C:H2'	2:2B:31:C:H5'	2.02	0.41
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	2.02	0.41
6:2G:141:PHE:HE2	6:2G:155:MET:HE1	1.85	0.41
13:2R:29:LEU:HA	13:2R:29:LEU:HD12	1.85	0.41
2:2B:50:G:P	14:2S:62:LYS:HB2	2.60	0.41
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	2.01	0.41
1:1A:2432:A:N9	23:11:33:LYS:HD3	2.35	0.41
1:1A:271(H):G:H4'	23:11:81:LYS:HG2	2.02	0.41
26:14:49:PHE:HD1	26:14:49:PHE:HA	1.73	0.41
1:1A:271(V):G:O6	61:1A:5975:HOH:O	2.22	0.41
1:1A:596:G:H2'	1:1A:597:U:O4'	2.20	0.41
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.55	0.41
6:1G:28:VAL:O	6:1G:31:VAL:HG12	2.20	0.41
8:1I:60:GLU:HG3	8:1I:61:ARG:NH1	2.35	0.41
11:1P:128:HIS:NE2	11:1P:148:LEU:HD11	2.35	0.41
1:1A:996:A:O3'	16:1U:91:ASP:HB2	2.20	0.41
26:24:40:HIS:O	26:24:44:THR:HG22	2.20	0.41
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.36	0.41
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.56	0.41
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.20	0.41
1:2A:2643:G:H2'	1:2A:2644:G:O4'	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2697:G:H2'	1:2A:2698:U:O4'	2.21	0.41
1:2A:434:U:H2'	1:2A:435:C:H6	5.74	0.41
1:2A:56:A:H2'	1:2A:57:C:O4'	2.21	0.41
7:2H:56:SER:HB3	7:2H:61:HIS:HD1	1.83	0.41
13:2R:44:LEU:HD11	13:2R:79:LEU:HD13	10.81	0.41
15:2T:73:GLU:OE2	15:2T:103:ARG:NE	2.53	0.41
2:2B:75:G:H1	21:2Z:73:GLN:NE2	2.19	0.41
1:1A:1119:C:N4	61:1A:6713:HOH:O	2.53	0.41
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.20	0.41
1:1A:2206:G:H5''	1:1A:2207:G:N7	2.35	0.41
1:1A:2376:A:H2'	1:1A:2377:A:O4'	2.20	0.41
1:1A:2715:C:H2'	1:1A:2716:U:C6	2.56	0.41
1:2A:1619:G:N2	29:27:1:MET:O	2.47	0.41
1:2A:1235:G:C6	1:2A:1236:G:N1	2.87	0.41
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.36	0.41
1:2A:1510:G:H2'	1:2A:1511:C:O4'	2.20	0.41
1:2A:1770:G:H4'	1:2A:1938:A:OP1	2.20	0.41
1:2A:2185:C:H2'	1:2A:2186:G:O4'	2.21	0.41
1:2A:2419:U:H2'	1:2A:2420:C:H6	1.85	0.41
1:2A:288:C:H2'	1:2A:289:A:C8	2.54	0.41
1:2A:307:G:N2	1:2A:330:A:H62	2.16	0.41
1:2A:597:U:H2'	1:2A:598:G:H8	1.86	0.41
2:2B:43:C:O4'	6:2G:66:GLN:NE2	2.53	0.41
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.20	0.41
6:2G:5:VAL:HG22	6:2G:8:LYS:HE2	2.02	0.41
9:2N:99:LEU:HA	9:2N:99:LEU:HD23	1.84	0.41
26:14:16:CYS:SG	26:14:17:GLY:N	2.93	0.41
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.55	0.41
1:1A:129:C:H2'	1:1A:130:C:C6	2.55	0.41
1:1A:1853:A:H2'	1:1A:1854:A:C8	2.55	0.41
1:1A:2223:G:OP1	3:1D:172:TYR:OH	2.25	0.41
1:1A:238:C:H2'	1:1A:239:U:O4'	2.21	0.41
2:1B:1:U:HO2'	2:1B:2:C:P	2.42	0.41
4:1E:52:LEU:HA	4:1E:53:PRO:HD3	1.91	0.41
13:1R:28:LEU:HD22	13:1R:44:LEU:HD13	2.03	0.41
1:2A:116:C:H2'	1:2A:117:G:O4'	2.21	0.41
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.19	0.41
1:2A:2351:G:HO2'	1:2A:2352:A:H8	1.67	0.41
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.56	0.41
1:2A:2712:U:O2'	1:2A:2713:A:H5'	2.21	0.41
1:2A:579:G:H2'	1:2A:580:C:C6	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:42:C:O2	6:2G:93:THR:N	2.33	0.41
1:2A:2679:A:H4'	4:2E:165:VAL:HG11	2.01	0.41
6:2G:3:LEU:HD12	6:2G:8:LYS:HZ3	1.85	0.41
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.85	0.41
9:2N:67:LEU:HD12	9:2N:87:LEU:HD22	2.02	0.41
14:2S:53:SER:O	14:2S:57:LYS:N	2.47	0.41
22:10:10:THR:HA	61:10:205:HOH:O	2.20	0.41
1:1A:1766:U:H2'	1:1A:1767:C:C6	2.55	0.41
1:1A:582:G:H2'	1:1A:583:G:C8	2.55	0.41
1:1A:83:G:N7	61:1A:7268:HOH:O	2.37	0.41
1:1A:1997:G:H5''	4:1E:117:MET:CE	2.51	0.41
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	2.02	0.41
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	2.03	0.41
9:1N:14:VAL:HG11	9:1N:138:LEU:HD12	2.01	0.41
1:2A:2046:G:O5'	27:25:19:ARG:HA	2.19	0.41
1:2A:1278:A:H2'	1:2A:1279:G:C8	2.56	0.41
1:2A:1471:A:OP2	1:2A:1519:G:N2	2.41	0.41
1:2A:265:A:C8	1:2A:266:G:H1'	2.55	0.41
1:2A:2690:C:N4	1:2A:2713:A:H1'	2.35	0.41
1:2A:493:G:H2'	1:2A:494:G:O4'	2.21	0.41
1:2A:569:U:H1'	1:2A:947:G:O4'	2.21	0.41
1:2A:852:G:H2'	1:2A:853:G:H8	1.84	0.41
13:2R:62:ALA:O	13:2R:66:VAL:HG23	2.21	0.41
16:2U:29:SER:OG	16:2U:30:LYS:NZ	2.44	0.41
20:2Y:20:TYR:CE2	20:2Y:43:ASN:HA	2.56	0.41
24:12:2:LYS:O	24:12:6:VAL:HG23	2.21	0.41
24:12:51:ARG:O	24:12:55:ARG:HG2	2.20	0.41
1:1A:1862:G:H2'	1:1A:1863:G:C8	2.53	0.41
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.20	0.41
1:1A:38:A:H2'	1:1A:39:C:C6	2.55	0.41
1:1A:548:A:H61	17:1V:18:LEU:HA	1.86	0.41
3:1D:80:ALA:HB3	3:1D:94:LEU:HD13	2.03	0.41
14:1S:43:GLU:OE2	22:10:49:LYS:HE3	2.20	0.41
1:2A:940:G:N3	1:2A:1191:G:H4'	2.36	0.41
1:2A:1368:G:OP1	29:27:28:ARG:NH2	2.53	0.41
1:2A:570:G:H2'	1:2A:2030:A:C5	2.55	0.41
1:2A:2165:G:H2'	1:2A:2166:G:O4'	2.20	0.41
1:2A:2313:C:H2'	1:2A:2314:C:H6	1.85	0.41
1:2A:253:C:H2'	1:2A:254:G:O4'	2.21	0.41
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.03	0.41
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2812:G:H2'	1:2A:2813:A:C8	2.55	0.41
3:2D:260:ARG:NH1	3:2D:267:SER:OG	2.54	0.41
9:2N:103:VAL:O	9:2N:107:LEU:HG	2.20	0.41
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	2.01	0.41
28:16:25:LYS:HE3	28:16:27:LYS:HA	2.03	0.41
1:1A:944:G:O6	1:1A:1337:G:H8	83.18	0.41
1:1A:2695:C:H2'	1:1A:2696:U:C6	2.56	0.41
1:1A:620:G:H5'	1:1A:620:G:N3	2.36	0.41
1:1A:764:A:O4'	3:1D:213:ARG:HG3	2.21	0.41
13:1R:24:GLN:HB3	13:1R:44:LEU:HD11	2.01	0.41
10:1O:76:ALA:HB3	15:1T:75:ILE:HD12	2.02	0.41
21:1Z:54:HIS:CG	21:1Z:101:PRO:HG3	2.56	0.41
1:2A:199:A:OP1	61:2A:5372:HOH:O	2.22	0.41
1:2A:2584:U:H2'	1:2A:2585:U:H2'	2.03	0.41
1:2A:262:A:H2'	1:2A:263:C:O4'	2.20	0.41
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.55	0.41
1:2A:2822:G:OP2	61:2A:6428:HOH:O	2.21	0.41
1:2A:2836:U:H2'	1:2A:2837:G:H8	1.82	0.41
1:2A:921:G:C6	1:2A:922:U:C4	3.09	0.41
1:2A:925:C:H2'	1:2A:926:A:H8	1.85	0.41
2:2B:67:G:H2'	2:2B:68:C:C6	2.55	0.41
15:2T:39:ARG:HH12	15:2T:41:ARG:HB3	1.86	0.41
19:2X:44:GLU:O	19:2X:48:LYS:N	2.50	0.41
61:1A:6401:HOH:O	25:13:13:ILE:O	2.22	0.41
1:1A:1310:G:OP2	29:17:9:ARG:NH2	2.54	0.41
30:18:23:VAL:HG13	30:18:47:LYS:HB3	2.02	0.41
1:1A:1086:A:H3'	1:1A:1086:A:N3	2.35	0.41
1:1A:1093:G:H3'	1:1A:1094:U:H5''	2.02	0.41
1:1A:1957:C:H2'	1:1A:1958:C:C6	2.56	0.41
1:1A:2379:G:O2'	14:1S:17:ARG:NH2	2.54	0.41
1:1A:629:G:H1'	1:1A:639:U:H1'	2.03	0.41
1:1A:644:A:H4'	1:1A:645:C:H5	1.85	0.41
1:1A:646:A:H2'	1:1A:647:G:O4'	2.20	0.41
1:1A:755:C:H2'	1:1A:756:C:C6	2.55	0.41
1:1A:783:A:O2'	1:1A:785:G:OP1	2.30	0.41
1:1A:1288:U:O4	13:1R:106:GLY:HA3	2.21	0.41
15:1T:26:ASP:O	15:1T:49:VAL:HG22	2.21	0.41
15:1T:27:THR:HB	15:1T:90:GLN:HB3	2.03	0.41
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	2.02	0.41
23:21:64:ALA:HA	23:21:67:ILE:HG13	2.03	0.41
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1031:G:H21	31:29:36:GLN:HE22	1.67	0.41
1:2A:1856:G:H1	1:2A:1886:C:H42	1.68	0.41
1:2A:2135:A:H5'	1:2A:2159:G:H1'	2.03	0.41
1:2A:2334:G:O6	22:20:74:ARG:NH1	2.46	0.41
1:2A:26:G:C6	1:2A:27:G:N1	2.89	0.41
1:2A:1999:C:H5''	1:2A:2723:C:O2'	2.21	0.41
1:2A:2745:C:C4	1:2A:2746:U:C4	3.09	0.41
1:2A:473:G:H2'	1:2A:474:G:H8	2.63	0.41
1:2A:747:U:O2'	18:2W:92:ARG:NH2	2.44	0.41
1:2A:984:A:H5''	1:2A:985:C:H5	1.86	0.41
4:2E:170:LEU:HB3	4:2E:184:VAL:CG2	2.51	0.41
6:2G:100:TRP:O	6:2G:104:GLU:HB2	2.20	0.41
6:2G:63:ILE:HD13	6:2G:141:PHE:CD2	2.55	0.41
61:2A:6160:HOH:O	19:2X:57:LEU:HA	2.20	0.41
1:1A:1183:G:O2'	25:13:29:ARG:NH1	2.54	0.41
1:1A:1889:A:H2'	1:1A:1890:A:C8	2.56	0.41
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.21	0.41
1:1A:2352:A:N6	1:1A:2365:G:O2'	2.53	0.41
1:1A:124:G:N2	1:1A:237:C:O2	57.46	0.41
1:1A:589:C:H2'	1:1A:590:A:C8	2.56	0.41
1:1A:662:G:H5'	11:1P:14:LYS:O	2.21	0.41
11:1P:135:LEU:HA	11:1P:135:LEU:HD23	1.85	0.41
13:1R:2:ARG:HG2	13:1R:5:LYS:HB2	2.03	0.41
1:1A:996:A:H4'	16:1U:91:ASP:OD2	2.21	0.41
24:22:1:MET:N	24:22:52:ASP:OD1	2.51	0.41
28:26:8:LYS:HG2	30:28:34:TRP:CD1	2.56	0.41
1:2A:1031:G:N2	31:29:36:GLN:HE22	2.18	0.41
1:2A:2218:U:H1'	23:21:52:ARG:HH12	1.86	0.41
1:2A:2784:C:H2'	1:2A:2785:C:C6	2.55	0.41
1:2A:355:G:H2'	1:2A:356:G:O4'	2.21	0.41
1:2A:723:G:H2'	1:2A:724:U:O4'	2.21	0.41
3:2D:211:ARG:HG3	3:2D:214:TRP:CE3	2.55	0.41
4:2E:12:THR:HG21	15:2T:11:GLU:HG2	2.03	0.41
6:2G:51:ARG:HD3	6:2G:52:ILE:H	1.85	0.41
10:2O:70:LYS:HB3	10:2O:70:LYS:HE2	1.92	0.41
15:2T:102:ILE:HB	15:2T:110:ILE:HG12	2.03	0.41
17:2V:3:ALA:HB3	17:2V:14:VAL:HG23	2.03	0.41
30:18:26:LYS:HB2	30:18:44:LYS:O	2.21	0.41
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.36	0.41
1:1A:1213:A:N3	1:1A:1238:G:O2'	2.51	0.41
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.83	0.41
1:1A:2140:C:H2'	1:1A:2141:G:C8	2.55	0.41
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.56	0.41
1:1A:536:A:H2'	1:1A:537:C:C6	2.56	0.41
1:1A:735:A:N7	1:1A:761:A:H2	2.19	0.41
61:1A:5688:HOH:O	11:1P:42:SER:O	2.21	0.41
16:1U:8:VAL:HG23	16:1U:11:ARG:HH21	1.86	0.41
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.20	0.41
23:21:83:GLU:N	23:21:83:GLU:OE1	2.54	0.41
1:2A:1599:C:H2'	1:2A:1600:C:C6	2.56	0.41
1:2A:2295:C:H41	14:2S:13:ARG:NH1	2.18	0.41
1:2A:2300:G:C6	1:2A:2301:C:C4	3.09	0.41
1:2A:2579:C:OP1	61:2A:3903:HOH:O	2.22	0.41
1:2A:656:G:H2'	1:2A:657:U:O4'	2.20	0.41
2:2B:59:A:H2'	2:2B:60:C:O4'	2.21	0.41
17:2V:62:LEU:HD23	17:2V:93:GLU:HG2	2.03	0.41
61:1A:4208:HOH:O	22:10:41:ARG:HA	2.21	0.41
1:1A:1063:G:C5	1:1A:1064:C:N4	2.89	0.41
1:1A:1286:A:C6	1:1A:1329:U:C2	3.09	0.41
1:1A:2134:A:O2'	1:1A:2135:A:O5'	2.31	0.41
1:1A:2364:C:OP1	22:10:55:ARG:NH1	2.54	0.41
1:1A:2448:A:OP1	61:1A:6393:HOH:O	2.22	0.41
1:1A:969:U:H2'	1:1A:970:C:C6	2.56	0.41
3:1D:168:ARG:HA	3:1D:173:VAL:HA	2.03	0.41
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.55	0.41
11:1P:88:LEU:HD11	11:1P:114:ILE:HD12	2.03	0.41
12:1Q:38:GLU:HG3	12:1Q:127:ILE:HB	2.02	0.41
14:1S:87:PHE:CZ	14:1S:102:ALA:HB2	2.55	0.41
1:2A:1409:C:O2	1:2A:1491:G:N2	42.71	0.41
1:2A:2356:C:H2'	1:2A:2357:U:O4'	2.21	0.41
1:2A:2400:G:H2'	1:2A:2401:U:H6	1.86	0.41
1:2A:380:U:H2'	1:2A:381:G:C8	2.55	0.41
4:2E:12:THR:HG22	4:2E:13:ARG:H	1.86	0.41
6:2G:41:GLN:HG2	6:2G:154:GLY:O	2.21	0.41
1:1A:1336:A:H2'	1:1A:1337:G:C8	2.56	0.40
1:1A:1655:A:H3'	1:1A:1656:C:C6	2.56	0.40
1:1A:1920:4OC:O5'	1:1A:1920:4OC:H6	2.21	0.40
1:1A:228:A:H3'	1:1A:229:A:C5'	2.49	0.40
1:1A:2408:U:H2'	1:1A:2409:G:C8	2.56	0.40
1:1A:942:G:OP2	11:1P:39:LYS:HE2	2.21	0.40
1:1A:993:G:H2'	1:1A:995:C:H41	14.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1789:A:H5''	3:1D:220:HIS:O	2.21	0.40
4:1E:9:VAL:HG13	4:1E:25:VAL:O	2.21	0.40
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.37	0.40
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.21	0.40
10:1O:86:ILE:HG22	10:1O:94:ARG:HD3	2.03	0.40
14:1S:5:THR:OG1	14:1S:8:GLU:HG2	2.21	0.40
18:1W:18:ARG:HG2	18:1W:76:VAL:HB	2.02	0.40
1:2A:136:G:H2'	1:2A:137:C:C6	2.56	0.40
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.19	0.40
1:2A:2053:G:OP2	61:2A:4832:HOH:O	2.22	0.40
1:2A:271(Z):C:OP2	61:2A:6005:HOH:O	2.22	0.40
3:2D:68:LYS:C	3:2D:70:TRP:H	2.24	0.40
12:2Q:2:LEU:HD12	12:2Q:69:PHE:CE1	2.57	0.40
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	2.03	0.40
15:2T:64:ARG:HB2	15:2T:73:GLU:HG2	2.02	0.40
1:2A:1252:G:N2	16:2U:37:GLU:OE2	2.48	0.40
1:1A:1106:G:H2'	1:1A:1107:G:O4'	2.21	0.40
1:1A:1139:G:H4'	1:1A:1140:C:H5'	4.54	0.40
1:1A:1156:A:OP2	61:1A:6455:HOH:O	2.21	0.40
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.56	0.40
1:1A:1862:G:C2	1:1A:1881:C:C2	3.09	0.40
1:1A:2142:C:H2'	1:1A:2143:C:C6	2.56	0.40
1:1A:2443:C:OP1	5:1F:68:LYS:HD3	2.21	0.40
1:1A:30:G:H2'	1:1A:31:C:C6	2.56	0.40
1:1A:330:A:N7	1:1A:1210:A:O2'	2.35	0.40
1:1A:857:C:N4	1:1A:858:U:O4	2.55	0.40
5:1F:135:LYS:HB3	5:1F:135:LYS:HE3	1.90	0.40
9:1N:61:ARG:HA	9:1N:61:ARG:HD3	1.87	0.40
20:1Y:19:LYS:HE2	20:1Y:19:LYS:HB3	1.78	0.40
22:20:11:ARG:O	22:20:14:ARG:NH2	2.54	0.40
24:22:51:ARG:O	24:22:55:ARG:HG2	2.21	0.40
24:22:64:LEU:HD11	24:22:68:ARG:NH2	2.35	0.40
25:23:11:SER:HA	25:23:31:LEU:HD21	2.02	0.40
1:2A:1353:A:H2'	1:2A:1354:A:C8	2.56	0.40
1:2A:1448:G:H2'	1:2A:1449:A:C8	2.57	0.40
1:2A:2119:A:H2	1:2A:2171:A:H5'	1.86	0.40
1:2A:271:A:N6	1:2A:271(X):G:H1'	2.37	0.40
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.56	0.40
1:2A:113:G:O2'	1:2A:354:G:H5'	48.30	0.40
5:2F:140:LEU:HD11	5:2F:170:LEU:HD11	2.03	0.40
9:2N:104:LYS:HA	9:2N:107:LEU:HD12	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:4:PRO:HD3	10:2O:24:VAL:HG23	2.02	0.40
1:1A:1038:C:H42	1:1A:1117:G:H1	1.67	0.40
1:1A:1608:A:H1'	1:1A:1610:A:OP2	2.22	0.40
1:1A:858:U:O2	1:1A:2268:A:H2'	2.21	0.40
1:1A:34:C:H2'	1:1A:35:G:H8	5.53	0.40
1:1A:580:C:H2'	1:1A:581:C:C6	2.56	0.40
1:1A:695:G:OP1	1:1A:1380:G:O2'	2.35	0.40
1:1A:781:A:OP1	3:1D:218:ARG:NH2	2.55	0.40
5:1F:197:ASP:O	5:1F:201:VAL:HG13	2.21	0.40
1:2A:857:C:H4'	22:20:23:VAL:HG21	2.03	0.40
1:2A:109:G:H2'	1:2A:110:G:O4'	2.22	0.40
1:2A:1027:A:N6	1:2A:1126:A:C4	2.90	0.40
1:2A:1147:C:H2'	1:2A:1148:A:C8	2.56	0.40
1:2A:1270:C:H5''	1:2A:1271:G:O5'	2.22	0.40
1:2A:1614:A:P	1:2A:1614:A:H8	2.44	0.40
1:2A:2324:C:H2'	1:2A:2385:C:H5	1.87	0.40
1:2A:2652:C:H42	1:2A:2668:G:H1	1.69	0.40
1:2A:527:C:H4'	1:2A:528:A:O5'	2.21	0.40
1:2A:847:U:H5'	1:2A:848:G:OP2	2.21	0.40
1:2A:902:C:H2'	1:2A:903:C:H6	1.86	0.40
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.54	0.40
7:2H:25:LYS:HE2	7:2H:27:LYS:NZ	2.36	0.40
16:2U:65:ILE:HD13	16:2U:95:LEU:HD23	2.04	0.40
20:2Y:82:PRO:O	20:2Y:101:LYS:NZ	2.41	0.40
1:2A:297:C:OP1	20:2Y:87:LYS:HG3	2.20	0.40
21:2Z:80:ARG:HB3	21:2Z:82:ARG:HD3	2.04	0.40
25:13:6:VAL:HG13	25:13:54:VAL:CG1	2.50	0.40
28:16:9:LEU:HD11	28:16:34:LEU:HD12	2.04	0.40
1:1A:86:C:H4'	1:1A:104:U:H1'	2.03	0.40
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.57	0.40
1:1A:1923:U:H2'	1:1A:1924:C:C6	2.55	0.40
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.56	0.40
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.57	0.40
1:1A:336:C:O2'	20:1Y:35:TYR:OH	2.28	0.40
1:1A:612:C:N3	1:1A:628:G:N1	45.84	0.40
1:1A:625:G:H2'	1:1A:626:U:C6	3.02	0.40
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.20	0.40
24:22:12:GLU:O	24:22:16:LEU:HG	2.22	0.40
27:25:16:ARG:HG3	27:25:17:ASP:N	2.37	0.40
1:2A:1541:G:H3'	1:2A:1542:A:H8	1.86	0.40
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2843:G:H1	1:2A:2874:C:H42	1.69	0.40
1:2A:384:U:H2'	1:2A:385:C:H6	1.86	0.40
4:2E:169:ASN:HB2	4:2E:203:LYS:HG3	2.03	0.40
1:2A:863:A:P	12:2Q:22:LYS:HG3	2.61	0.40
15:2T:11:GLU:OE1	15:2T:57:PHE:HB3	2.21	0.40
15:2T:82:LEU:HD23	15:2T:82:LEU:HA	1.82	0.40
1:1A:214:G:O2'	1:1A:216:A:O2'	2.31	0.40
11:1P:111:ARG:HB3	11:1P:128:HIS:CG	2.56	0.40
11:1P:120:ALA:HB2	11:1P:137:LYS:HB3	2.03	0.40
1:2A:1372:U:H2'	1:2A:1373:A:O4'	2.21	0.40
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.21	0.40
1:2A:1987:G:H2'	1:2A:1988:C:C6	2.56	0.40
1:2A:2050:C:N4	1:2A:2051:A:N1	2.70	0.40
1:2A:918:A:C5	1:2A:919:G:H1'	2.57	0.40
19:2X:5:TYR:CZ	24:22:30:ARG:HD2	2.57	0.40
21:2Z:71:VAL:HG22	21:2Z:88:PHE:CE1	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%)	11 (4%)	1 (0%)	34	57
3	2D	273/276 (99%)	261 (96%)	11 (4%)	1 (0%)	34	57
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	52
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	52
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	29	52
5	2F	201/210 (96%)	197 (98%)	1 (0%)	3 (2%)	10	21
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	2G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	14	30
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	25	47
7	2H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	13	27
8	1I	144/148 (97%)	137 (95%)	7 (5%)	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%)	116 (97%)	4 (3%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
12	1Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	124 (96%)	5 (4%)	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%)	93 (94%)	5 (5%)	1 (1%)	15	32
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	32
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	1Z	148/206 (72%)	140 (95%)	8 (5%)	0	100	100
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	30
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	57 (85%)	7 (10%)	3 (4%)	2	3
26	24	67/71 (94%)	54 (81%)	11 (16%)	2 (3%)	4	7
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	4	6
33	2b	229/256 (90%)	203 (89%)	20 (9%)	6 (3%)	5	9
34	1c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	15	32
34	2c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	15	32
35	1d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	52
35	2d	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	15	32
36	1e	146/162 (90%)	140 (96%)	5 (3%)	1 (1%)	22	43
36	2e	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	12	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	2g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	12	24
39	1h	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
40	2i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
41	1j	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	3	3
41	2j	94/105 (90%)	81 (86%)	6 (6%)	7 (7%)	1	1
42	1k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8	16
42	2k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8	16
43	1l	119/132 (90%)	112 (94%)	6 (5%)	1 (1%)	19	39
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	111 (92%)	9 (8%)	0	100	100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
47	2p	80/88 (91%)	77 (96%)	3 (4%)	0	100	100
48	1q	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	15	32
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	15	32
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	13	27
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4	6
51	2t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	4	6
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10749 (94%)	549 (5%)	72 (1%)	25	47

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
23	11	3	LYS
26	14	58	ARG
33	1b	10	LEU
33	1b	22	LYS
7	2H	126	PRO
26	24	55	ARG
26	24	65	ASP
33	2b	10	LEU
41	2j	75	ILE
51	2t	10	LEU
33	1b	9	GLU
41	1j	55	LYS
41	1j	75	ILE
35	2d	181	MET
38	2g	7	ALA
41	2j	33	GLN
42	2k	49	GLY
3	1D	3	VAL
6	1G	43	LEU
26	14	65	ASP
35	1d	5	ILE
48	1q	33	GLY
51	1t	10	LEU
51	1t	97	ALA
34	2c	156	ARG
41	2j	29	ARG
41	2j	78	ASN
41	2j	79	ARG
4	1E	52	LEU
33	1b	20	GLU
33	1b	125	PRO
34	1c	107	GLN
38	1g	114	ARG
41	1j	33	GLN
41	1j	78	ASN
4	2E	52	LEU
5	2F	130	ALA
7	2H	47	GLU
17	2V	79	VAL
33	2b	16	HIS
33	2b	20	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	85	ARG
51	2t	97	ALA
17	1V	79	VAL
33	1b	17	PHE
33	1b	37	ASN
38	1g	80	VAL
43	1l	91	LYS
3	2D	3	VAL
5	2F	26	ALA
6	2G	49	ASP
6	2G	52	ILE
33	2b	17	PHE
35	2d	5	ILE
38	2g	80	VAL
48	2q	68	ARG
51	2t	47	GLY
34	1c	66	VAL
51	1t	47	GLY
5	2F	89	VAL
33	2b	9	GLU
50	2s	9	VAL
26	14	64	GLY
42	1k	105	VAL
33	2b	127	ILE
42	2k	105	VAL
36	1e	69	VAL
41	2j	24	VAL
41	2j	39	PRO
42	1k	49	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	200 (93%)	15 (7%)	15	30
3	2D	215/218 (99%)	201 (94%)	14 (6%)	17	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	1E	164/166 (99%)	151 (92%)	13 (8%)	12	24
4	2E	164/166 (99%)	156 (95%)	8 (5%)	25	48
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	23
5	2F	159/166 (96%)	147 (92%)	12 (8%)	13	27
6	1G	143/156 (92%)	136 (95%)	7 (5%)	25	48
6	2G	143/156 (92%)	129 (90%)	14 (10%)	8	15
7	1H	144/148 (97%)	137 (95%)	7 (5%)	25	48
7	2H	144/148 (97%)	140 (97%)	4 (3%)	43	69
8	1I	113/124 (91%)	108 (96%)	5 (4%)	28	53
8	2I	105/124 (85%)	96 (91%)	9 (9%)	10	20
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19	39
9	2N	118/119 (99%)	114 (97%)	4 (3%)	37	63
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	67
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	67
11	1P	115/116 (99%)	110 (96%)	5 (4%)	29	54
11	2P	115/116 (99%)	111 (96%)	4 (4%)	36	62
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	27	52
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	44	71
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	11
13	2R	101/101 (100%)	90 (89%)	11 (11%)	6	11
14	1S	86/88 (98%)	82 (95%)	4 (5%)	26	50
14	2S	85/88 (97%)	84 (99%)	1 (1%)	71	87
15	1T	115/127 (91%)	111 (96%)	4 (4%)	36	62
15	2T	113/127 (89%)	111 (98%)	2 (2%)	59	80
16	1U	93/94 (99%)	89 (96%)	4 (4%)	29	54
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39	65
17	1V	80/82 (98%)	69 (86%)	11 (14%)	3	6
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6	10
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21	42
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28	53
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	72
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	14	29
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	19	39
21	1Z	135/179 (75%)	127 (94%)	8 (6%)	19	39
21	2Z	137/179 (76%)	135 (98%)	2 (2%)	65	83
22	10	65/67 (97%)	62 (95%)	3 (5%)	27	51
22	20	65/67 (97%)	64 (98%)	1 (2%)	65	83
23	11	80/83 (96%)	76 (95%)	4 (5%)	24	47
23	21	80/83 (96%)	76 (95%)	4 (5%)	24	47
24	12	65/67 (97%)	63 (97%)	2 (3%)	40	66
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	39
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	57
26	14	59/63 (94%)	52 (88%)	7 (12%)	5	9
26	24	53/63 (84%)	51 (96%)	2 (4%)	33	59
27	15	50/52 (96%)	47 (94%)	3 (6%)	19	39
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	57
28	16	51/52 (98%)	49 (96%)	2 (4%)	32	58
28	26	50/52 (96%)	48 (96%)	2 (4%)	31	57
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	9
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	9
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	28
30	28	54/55 (98%)	52 (96%)	2 (4%)	34	60
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	68
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	39
33	1b	192/220 (87%)	186 (97%)	6 (3%)	40	66
33	2b	187/220 (85%)	180 (96%)	7 (4%)	34	60
34	1c	142/188 (76%)	138 (97%)	4 (3%)	43	69
34	2c	140/188 (74%)	134 (96%)	6 (4%)	29	54
35	1d	169/181 (93%)	156 (92%)	13 (8%)	13	25
35	2d	173/181 (96%)	163 (94%)	10 (6%)	20	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	1e	113/123 (92%)	108 (96%)	5 (4%)	28	53
36	2e	114/123 (93%)	111 (97%)	3 (3%)	46	72
37	1f	84/90 (93%)	79 (94%)	5 (6%)	19	39
37	2f	85/90 (94%)	82 (96%)	3 (4%)	36	62
38	1g	119/127 (94%)	114 (96%)	5 (4%)	30	55
38	2g	120/127 (94%)	117 (98%)	3 (2%)	47	73
39	1h	114/119 (96%)	108 (95%)	6 (5%)	22	45
39	2h	114/119 (96%)	108 (95%)	6 (5%)	22	45
40	1i	90/99 (91%)	87 (97%)	3 (3%)	38	64
40	2i	89/99 (90%)	84 (94%)	5 (6%)	21	42
41	1j	66/92 (72%)	63 (96%)	3 (4%)	27	52
41	2j	69/92 (75%)	66 (96%)	3 (4%)	29	54
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49	74
42	2k	83/99 (84%)	82 (99%)	1 (1%)	71	87
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	55
43	2l	96/108 (89%)	92 (96%)	4 (4%)	30	55
44	1m	93/101 (92%)	91 (98%)	2 (2%)	52	76
44	2m	92/101 (91%)	86 (94%)	6 (6%)	17	34
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7	14
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	14
46	1o	78/80 (98%)	77 (99%)	1 (1%)	69	86
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	86
47	1p	69/74 (93%)	66 (96%)	3 (4%)	29	54
47	2p	68/74 (92%)	64 (94%)	4 (6%)	19	39
48	1q	94/97 (97%)	90 (96%)	4 (4%)	29	54
48	2q	94/97 (97%)	93 (99%)	1 (1%)	73	88
49	1r	59/77 (77%)	56 (95%)	3 (5%)	24	46
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	32
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67	85
50	2s	67/80 (84%)	62 (92%)	5 (8%)	13	27
51	1t	70/82 (85%)	66 (94%)	4 (6%)	20	41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	42
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8841 (95%)	462 (5%)	24	47

All (462) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	14	ARG
3	1D	22	SER
3	1D	32	SER
3	1D	37	LEU
3	1D	94	LEU
3	1D	99	ASP
3	1D	142	VAL
3	1D	155	LEU
3	1D	157	ARG
3	1D	162	SER
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
4	1E	19	ARG
4	1E	21	VAL
4	1E	24	THR
4	1E	47	VAL
4	1E	75	VAL
4	1E	78	LEU
4	1E	111	ARG
4	1E	113	PHE
4	1E	116	VAL
4	1E	170	LEU
4	1E	175	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	33	LEU
5	1F	43	LYS
5	1F	44	ARG
5	1F	53	THR
5	1F	57	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	162	LEU
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	21	ARG
6	1G	43	LEU
6	1G	49	ASP
6	1G	82	LEU
6	1G	140	ILE
6	1G	159	VAL
7	1H	15	VAL
7	1H	23	ARG
7	1H	51	ARG
7	1H	71	LEU
7	1H	84	SER
7	1H	122	THR
7	1H	124	GLU
8	1I	9	LEU
8	1I	38	LEU
8	1I	92	VAL
8	1I	116	LEU
8	1I	129	THR
9	1N	28	THR
9	1N	32	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	99	LEU
9	1N	121	LYS
10	1O	10	VAL
10	1O	35	VAL
10	1O	98	VAL
11	1P	3	LEU
11	1P	95	VAL
11	1P	101	VAL
11	1P	125	VAL
11	1P	147	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	35	VAL
12	1Q	75	THR
12	1Q	101	ARG
13	1R	15	SER
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	96	ARG
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	17	ARG
14	1S	69	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	89	VAL
15	1T	96	ARG
15	1T	128	GLU
16	1U	59	ARG
16	1U	74	LEU
16	1U	83	LEU
16	1U	95	LEU
17	1V	1	MET
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	56	SER
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	82	ARG
18	1W	11	ARG
18	1W	17	VAL
18	1W	90	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	1W	100	THR
18	1W	107	LEU
19	1X	38	GLU
19	1X	72	LYS
20	1Y	7	VAL
20	1Y	31	LEU
20	1Y	63	LYS
20	1Y	72	VAL
20	1Y	97	ARG
20	1Y	99	CYS
21	1Z	41	LEU
21	1Z	42	VAL
21	1Z	53	ILE
21	1Z	61	LEU
21	1Z	91	LEU
21	1Z	136	PHE
21	1Z	154	ASP
21	1Z	170	THR
22	10	39	ARG
22	10	55	ARG
22	10	74	ARG
23	11	11	ARG
23	11	30	VAL
23	11	80	LEU
23	11	95	LEU
24	12	3	LEU
24	12	30	ARG
25	13	23	LEU
25	13	34	GLU
25	13	60	GLU
26	14	13	ARG
26	14	31	ILE
26	14	49	PHE
26	14	53	GLU
26	14	56	VAL
26	14	58	ARG
26	14	63	TYR
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
28	16	9	LEU
28	16	48	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	17	9	ARG
29	17	29	LYS
29	17	39	ARG
29	17	43	THR
29	17	46	VAL
30	18	29	LYS
30	18	30	ARG
30	18	31	HIS
30	18	32	LEU
31	19	4	ARG
33	1b	83	MET
33	1b	93	VAL
33	1b	115	LEU
33	1b	121	LEU
33	1b	142	LEU
33	1b	160	ASP
34	1c	3	ASN
34	1c	89	GLU
34	1c	112	SER
34	1c	196	LEU
35	1d	5	ILE
35	1d	8	VAL
35	1d	10	ARG
35	1d	49	ARG
35	1d	52	SER
35	1d	53	ASP
35	1d	135	LEU
35	1d	140	VAL
35	1d	144	ASP
35	1d	175	SER
35	1d	182	LYS
35	1d	190	ASP
35	1d	194	LEU
36	1e	20	GLN
36	1e	41	VAL
36	1e	81	GLU
36	1e	91	LEU
36	1e	120	THR
37	1f	17	SER
37	1f	19	LEU
37	1f	25	ILE
37	1f	55	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	1f	72	VAL
38	1g	6	ARG
38	1g	9	VAL
38	1g	24	THR
38	1g	79	ARG
38	1g	98	SER
39	1h	25	ASP
39	1h	52	ASP
39	1h	82	HIS
39	1h	104	ARG
39	1h	112	LEU
39	1h	137	VAL
40	1i	86	VAL
40	1i	108	VAL
40	1i	128	ARG
41	1j	19	SER
41	1j	81	THR
41	1j	92	THR
42	1k	48	ILE
42	1k	120	ARG
43	1l	27	LEU
43	1l	33	ARG
43	1l	54	LYS
43	1l	83	VAL
44	1m	43	THR
44	1m	70	LEU
45	1n	13	THR
45	1n	18	VAL
45	1n	22	THR
45	1n	31	ARG
45	1n	33	VAL
46	1o	66	LEU
47	1p	20	VAL
47	1p	21	VAL
47	1p	62	VAL
48	1q	6	LEU
48	1q	9	VAL
48	1q	35	VAL
48	1q	63	ARG
49	1r	35	ARG
49	1r	47	THR
49	1r	76	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1s	12	ASP
51	1t	8	ARG
51	1t	13	LEU
51	1t	31	SER
51	1t	84	LEU
52	1u	17	THR
3	2D	14	ARG
3	2D	54	ARG
3	2D	94	LEU
3	2D	99	ASP
3	2D	116	GLN
3	2D	134	ARG
3	2D	138	VAL
3	2D	141	VAL
3	2D	142	VAL
3	2D	157	ARG
3	2D	169	GLU
3	2D	211	ARG
3	2D	221	VAL
3	2D	260	ARG
4	2E	7	VAL
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	38	THR
4	2E	116	VAL
4	2E	175	VAL
4	2E	181	LEU
5	2F	12	LEU
5	2F	46	ARG
5	2F	57	VAL
5	2F	70	THR
5	2F	88	VAL
5	2F	106	ARG
5	2F	132	VAL
5	2F	170	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	195	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	9	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	28	VAL
6	2G	31	VAL
6	2G	43	LEU
6	2G	49	ASP
6	2G	70	VAL
6	2G	79	ASN
6	2G	97	ASP
6	2G	109	VAL
6	2G	130	ASN
6	2G	140	ILE
6	2G	145	THR
6	2G	159	VAL
7	2H	15	VAL
7	2H	70	THR
7	2H	134	SER
7	2H	139	GLN
8	2I	3	VAL
8	2I	38	LEU
8	2I	47	LEU
8	2I	77	LEU
8	2I	92	VAL
8	2I	123	LEU
8	2I	127	VAL
8	2I	142	VAL
8	2I	144	VAL
9	2N	33	LEU
9	2N	34	LEU
9	2N	67	LEU
9	2N	99	LEU
10	2O	63	VAL
10	2O	69	ILE
10	2O	98	VAL
11	2P	95	VAL
11	2P	105	LEU
11	2P	131	SER
11	2P	133	SER
12	2Q	1	MET
12	2Q	38	GLU
12	2Q	75	THR
13	2R	24	GLN
13	2R	29	LEU
13	2R	33	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	2R	36	THR
13	2R	44	LEU
13	2R	54	LEU
13	2R	65	LEU
13	2R	86	ARG
13	2R	91	GLN
13	2R	96	ARG
13	2R	111	LEU
14	2S	25	ARG
15	2T	57	PHE
15	2T	96	ARG
16	2U	8	VAL
16	2U	55	ARG
16	2U	95	LEU
17	2V	14	VAL
17	2V	52	VAL
17	2V	61	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
17	2V	95	LEU
17	2V	98	GLU
18	2W	11	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	107	LEU
19	2X	62	LYS
19	2X	81	VAL
20	2Y	21	LYS
20	2Y	55	TYR
20	2Y	88	LYS
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	96	VAL
21	2Z	154	ASP
22	20	14	ARG
23	21	11	ARG
23	21	21	ARG
23	21	35	THR
23	21	38	SER
25	23	30	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	23	57	GLU
26	24	50	VAL
26	24	67	TYR
27	25	29	THR
27	25	33	CYS
28	26	25	LYS
28	26	48	VAL
29	27	39	ARG
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
29	27	48	LYS
30	28	11	LYS
30	28	30	ARG
31	29	4	ARG
31	29	7	VAL
33	2b	35	GLU
33	2b	93	VAL
33	2b	124	SER
33	2b	154	LEU
33	2b	189	ASP
33	2b	195	ASP
33	2b	213	LEU
34	2c	3	ASN
34	2c	18	TRP
34	2c	59	ARG
34	2c	103	VAL
34	2c	154	SER
34	2c	196	LEU
35	2d	8	VAL
35	2d	10	ARG
35	2d	19	LEU
35	2d	31	CYS
35	2d	34	GLU
35	2d	83	SER
35	2d	108	LEU
35	2d	135	LEU
35	2d	170	VAL
35	2d	194	LEU
36	2e	20	GLN
36	2e	41	VAL
36	2e	83	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	2f	61	LEU
37	2f	72	VAL
37	2f	75	LEU
38	2g	52	GLU
38	2g	79	ARG
38	2g	113	GLU
39	2h	2	LEU
39	2h	8	ASP
39	2h	25	ASP
39	2h	51	VAL
39	2h	69	ARG
39	2h	114	THR
40	2i	23	ASN
40	2i	102	LEU
40	2i	107	ARG
40	2i	108	VAL
40	2i	128	ARG
41	2j	16	LEU
41	2j	72	VAL
41	2j	81	THR
42	2k	48	ILE
43	2l	18	VAL
43	2l	27	LEU
43	2l	113	ARG
43	2l	117	ARG
44	2m	3	ARG
44	2m	15	VAL
44	2m	64	TRP
44	2m	73	GLU
44	2m	103	THR
44	2m	114	ARG
45	2n	3	ARG
45	2n	6	LEU
45	2n	18	VAL
45	2n	22	THR
45	2n	33	VAL
46	2o	39	LEU
47	2p	20	VAL
47	2p	21	VAL
47	2p	44	THR
47	2p	67	THR
48	2q	68	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	2r	21	LYS
49	2r	47	THR
49	2r	76	LEU
49	2r	85	LEU
50	2s	5	LEU
50	2s	33	THR
50	2s	47	HIS
50	2s	77	THR
50	2s	83	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
4	1E	48	GLN
4	1E	121	ASN
5	1F	69	HIS
6	1G	26	GLN
6	1G	108	ASN
8	1I	11	ASN
10	1O	3	GLN
12	1Q	123	HIS
15	1T	58	ASN
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	54	HIS
22	10	29	GLN
27	15	4	HIS
34	1c	6	HIS
34	1c	162	GLN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	1i	58	HIS
40	1i	73	GLN
40	1i	89	ASN
40	1i	124	GLN
41	1j	21	GLN
41	1j	56	HIS
43	1l	99	HIS
46	1o	46	HIS
47	1p	65	GLN
50	1s	57	HIS
50	1s	69	HIS
3	2D	116	GLN
3	2D	126	GLN
5	2F	69	HIS
5	2F	204	ASN
11	2P	35	HIS
12	2Q	89	ASN
12	2Q	123	HIS
13	2R	13	HIS
15	2T	58	ASN
17	2V	80	GLN
19	2X	31	HIS
20	2Y	43	ASN
21	2Z	73	GLN
22	20	29	GLN
22	20	35	ASN
24	22	65	ASN
26	24	46	GLN
33	2b	40	HIS
33	2b	78	GLN
33	2b	94	ASN
34	2c	176	HIS
35	2d	74	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	125	HIS
36	2e	78	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	37	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	2g	86	GLN
38	2g	109	ASN
39	2h	15	ASN
39	2h	78	GLN
40	2i	3	GLN
40	2i	58	HIS
41	2j	56	HIS
42	2k	117	ASN
43	2l	99	HIS
46	2o	62	GLN
47	2p	16	HIS
49	2r	63	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	42	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	431 (15%)	29 (1%)
1	2A	2788/2915 (95%)	482 (17%)	24 (0%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	33 (27%)	0
32	1a	1494/1521 (98%)	238 (15%)	0
32	2a	1498/1521 (98%)	284 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	71/76 (93%)	23 (32%)	0
54	1y	71/76 (93%)	19 (26%)	0
54	2w	68/76 (89%)	22 (32%)	0
54	2y	69/76 (90%)	21 (30%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	13 (17%)	0
All	All	9332/9620 (97%)	1593 (17%)	54 (0%)

All (1593) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	9	U
1	1A	12	U
1	1A	13	A
1	1A	27	G
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	51	G
1	1A	55	G
1	1A	58	G
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	102	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	136	G
1	1A	139(A)	G
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	200	U
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	232	G
1	1A	248	G
1	1A	269	U
1	1A	271(E)	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	271(S)	G
1	1A	271(U)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	510	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	587	C
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	615	G
1	1A	621	A
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	740	U
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	854	G
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	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	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1063	G
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1082	U
1	1A	1083	U
1	1A	1084	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1101	U
1	1A	1102	C
1	1A	1103	A
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1211	U
1	1A	1220	A
1	1A	1244	G
1	1A	1247	A
1	1A	1250	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1275	A
1	1A	1276	A
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1313	U
1	1A	1352	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1386	C
1	1A	1416	G
1	1A	1417	C
1	1A	1421	G
1	1A	1428	C
1	1A	1439	A
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1478	G
1	1A	1482	G
1	1A	1490	A
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1558	A
1	1A	1559	G
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1669	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1722	A
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1786	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1847	A
1	1A	1858	G
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1915	5MU
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2110	G
1	1A	2111	C
1	1A	2113	U
1	1A	2118	U
1	1A	2119	A
1	1A	2121	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2140	C
1	1A	2141	G
1	1A	2142	C
1	1A	2144	U
1	1A	2147	G
1	1A	2150	U
1	1A	2151	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2192	G
1	1A	2198	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2309	A
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2361	A
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2400	G
1	1A	2406	U
1	1A	2408	U
1	1A	2410	G
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2449	U
1	1A	2474	C
1	1A	2476	A
1	1A	2484	G
1	1A	2491	U
1	1A	2498	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	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	2761	G
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2818	G
1	1A	2820	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2821	A
1	1A	2834	G
1	1A	2835	A
1	1A	2858	C
1	1A	2872	G
1	1A	2873	A
1	1A	2876	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	12	C
2	1B	21	G
2	1B	25	A
2	1B	35	U
2	1B	50	G
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	109	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	33	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	65	U
32	1a	91	C
32	1a	98	G
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	180	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	183	G
32	1a	189(D)	C
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	219	C
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	452	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	453	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
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	528	C
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	629	G
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	686	U
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	859	A
32	1a	870	U
32	1a	872	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	932	C
32	1a	934	C
32	1a	955	U
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1039	C
32	1a	1045	C
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1087	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1104	G
32	1a	1108	G
32	1a	1121	U
32	1a	1125	U
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1156	G
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1166	G
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1212	U
32	1a	1213	A
32	1a	1222	G
32	1a	1226	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1246	C
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1276	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1368	G
32	1a	1370	G
32	1a	1378	C
32	1a	1394	A
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	23	A
54	1w	24	G
54	1w	25	C
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	63	G
54	1w	68	C
54	1w	70	G
54	1w	71	G
54	1w	73	A
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	14	A
55	1x	19	G
55	1x	21	A
55	1x	22	G
55	1x	47	U
55	1x	63	G
55	1x	64	G
55	1x	76	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1y	6	G
54	1y	8	4SU
54	1y	9	A
54	1y	11	C
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	22	G
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	57	G
54	1y	59	U
54	1y	61	C
54	1y	70	G
1	2A	10	G
1	2A	11	G
1	2A	15	G
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	83	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	96	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	266	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	304	G
1	2A	311	A
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	386	G
1	2A	389	G
1	2A	396	G
1	2A	411	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	412	A
1	2A	422	A
1	2A	435	C
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	586	A
1	2A	592	G
1	2A	595	C
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	653	A
1	2A	661	C
1	2A	669	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	686	G
1	2A	701	G
1	2A	712	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	778	G
1	2A	782	A
1	2A	783	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	806	C
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	847	U
1	2A	854	G
1	2A	856	C
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	873	G
1	2A	874	G
1	2A	875	G
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	890	A
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	936	C
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	979	G
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	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1130	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1166	C
1	2A	1167	U
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1229	G
1	2A	1237	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1309	G
1	2A	1314	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1376	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1444	G
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1537	G
1	2A	1543	C
1	2A	1544	A
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1579	A
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1648	C
1	2A	1654	A
1	2A	1663	C
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
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	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2027	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2050	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	2093	G
1	2A	2096	U
1	2A	2103	C
1	2A	2111	C
1	2A	2113	U
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2148	G
1	2A	2150	U
1	2A	2153	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2180	U
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2239	G
1	2A	2273	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2294	C
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2352	A
1	2A	2353	G
1	2A	2361	A
1	2A	2376	A
1	2A	2377	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2468	G
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2478	A
1	2A	2480	C
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2586	C
1	2A	2602	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2609	U
1	2A	2610	C
1	2A	2611	U
1	2A	2612	C
1	2A	2623	G
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2662	A
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2759	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2779	U
1	2A	2780	G
1	2A	2789	C
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2850	A
1	2A	2872	G
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	4	C
2	2B	5	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	8	U
2	2B	13	A
2	2B	19	G
2	2B	20	C
2	2B	25	A
2	2B	30	C
2	2B	34	U
2	2B	42	C
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	64	C
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	72	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	94	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	114	C
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	6	G
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	73	G
32	2a	79	G
32	2a	88	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	89	C
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	117	G
32	2a	121	C
32	2a	124	G
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	146	G
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	180	U
32	2a	182	U
32	2a	184	G
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	269	C
32	2a	281	G
32	2a	289	G
32	2a	318	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	415	A
32	2a	421	U
32	2a	423	G
32	2a	429	U
32	2a	430	A
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
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	517	G
32	2a	518	C
32	2a	528	C
32	2a	531	U
32	2a	532	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	574	A
32	2a	576	G
32	2a	577	G
32	2a	596	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	598	U
32	2a	618	C
32	2a	630	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	694	A
32	2a	695	A
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	874	G
32	2a	880	C
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	959	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	983	A
32	2a	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1013	G
32	2a	1017	G
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(D)	A
32	2a	1031	G
32	2a	1033	G
32	2a	1035	A
32	2a	1038	C
32	2a	1039	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1040	U
32	2a	1044	A
32	2a	1045	C
32	2a	1046	A
32	2a	1051	C
32	2a	1053	G
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1103	C
32	2a	1113	C
32	2a	1115	C
32	2a	1116	C
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	1145	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1171	G
32	2a	1172	C
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1189	C
32	2a	1196	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1197	G
32	2a	1202	G
32	2a	1209	C
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1228	C
32	2a	1233	G
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1248	A
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1264	C
32	2a	1270	C
32	2a	1273	G
32	2a	1275	A
32	2a	1276	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1319	A
32	2a	1320	C
32	2a	1347	G
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1397	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1496	C
32	2a	1497	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	18	G
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	29	G
54	2w	36	A
54	2w	38	A
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	56	C
54	2w	59	U
54	2w	62	C
54	2w	63	G
54	2w	65	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2w	68	C
54	2w	69	G
54	2w	72	C
54	2w	74	C
55	2x	9	G
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	46	G
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	56	C
55	2x	63	G
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	5	G
54	2y	6	G
54	2y	8	4SU
54	2y	11	C
54	2y	12	U
54	2y	13	C
54	2y	19	G
54	2y	35	A
54	2y	41	C
54	2y	44	G
54	2y	45	U
54	2y	46	7MG
54	2y	48	C
54	2y	52	G
54	2y	53	G
54	2y	57	G
54	2y	59	U
54	2y	61	C
54	2y	65	G
54	2y	70	G
54	2y	73	A

All (54) RNA pucker outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
-----	-------	-----	------

Mol	Chain	Res	Type
1	1A	90	U
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	895	U
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1210	A
1	1A	1275	A
1	1A	1379	A
1	1A	1420	U
1	1A	1442	G
1	1A	1508	A
1	1A	1653	G
1	1A	2134	A
1	1A	2170	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2430	A
1	1A	2689	U
1	1A	2756	U
2	1B	1	U
1	2A	34	C
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1493	C
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2351	G
1	2A	2689	U

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

84 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	PSU	1A	1911	1	17,21,22	1.58	2 (11%)	20,30,33	3.08	6 (30%)
1	5MU	2A	1939	1,56	15,22,23	1.09	2 (13%)	16,32,35	1.74	2 (12%)
32	5MC	2a	967	32	15,22,23	1.34	1 (6%)	19,32,35	1.35	3 (15%)
1	PSU	2A	2605	1	17,21,22	1.55	3 (17%)	20,30,33	3.09	6 (30%)
1	5MU	1A	1939	1,56	15,22,23	1.05	2 (13%)	16,32,35	1.84	2 (12%)
32	PSU	2a	516	32	17,21,22	1.52	2 (11%)	20,30,33	3.17	5 (25%)
32	5MC	2a	1404	32	15,22,23	1.36	1 (6%)	19,32,35	1.37	3 (15%)
32	MA6	2a	1518	32	19,26,27	0.97	1 (5%)	18,38,41	1.67	4 (22%)
32	M2G	1a	966	32	20,27,28	1.38	3 (15%)	22,40,43	2.17	5 (22%)
54	5MU	2y	54	54	15,22,23	1.07	2 (13%)	16,32,35	2.19	1 (6%)
54	7MG	2w	46	54	22,26,27	1.75	4 (18%)	28,39,42	2.72	9 (32%)
32	MA6	2a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.58	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	0TD	2l	92	43	4,9,10	3.09	1 (25%)	3,11,13	3.67	1 (33%)
54	PSU	2w	55	54	17,21,22	1.47	2 (11%)	20,30,33	3.27	6 (30%)
54	MIA	2y	37	54	18,24,32	1.11	2 (11%)	18,35,47	1.26	2 (11%)
1	2MU	1A	2552	1,56	14,22,24	0.87	0	14,31,36	0.72	0
32	2MG	1a	1207	32	19,26,27	1.24	2 (10%)	21,38,41	2.23	7 (33%)
1	4OC	1A	1920	1	15,22,24	0.67	0	17,31,35	1.48	2 (11%)
32	UR3	2a	1498	32	14,22,23	0.82	1 (7%)	15,32,35	0.80	1 (6%)
1	5MC	2A	1962	1,56	15,22,23	1.33	1 (6%)	19,32,35	1.32	3 (15%)
32	7MG	2a	527	32,56	22,26,27	1.77	4 (18%)	28,39,42	2.78	9 (32%)
32	4OC	2a	1402	32,56	16,23,24	0.61	0	17,32,35	1.38	1 (5%)
32	2MG	2a	1207	32	19,26,27	1.31	2 (10%)	21,38,41	2.34	8 (38%)
54	4SU	1w	8	54	14,21,22	1.27	2 (14%)	15,30,33	1.63	2 (13%)
55	PSU	2x	55	55	17,21,22	1.58	2 (11%)	20,30,33	3.12	6 (30%)
54	5MU	1w	54	54	15,22,23	1.10	1 (6%)	16,32,35	1.71	2 (12%)
54	PSU	2w	39	54	17,21,22	1.46	2 (11%)	20,30,33	3.27	6 (30%)
1	PSU	2A	1917	1	17,21,22	1.51	2 (11%)	20,30,33	3.11	6 (30%)
32	5MC	2a	1407	32	15,22,23	1.28	1 (6%)	19,32,35	1.37	2 (10%)
1	5MU	1A	1915	1	15,22,23	1.06	1 (6%)	16,32,35	1.84	2 (12%)
55	5MU	2x	54	55	15,22,23	1.10	1 (6%)	16,32,35	1.92	2 (12%)
32	5MC	2a	1400	32	15,22,23	1.31	1 (6%)	19,32,35	1.34	3 (15%)
54	4SU	1y	8	54	14,21,22	1.28	1 (7%)	15,30,33	1.50	2 (13%)
54	PSU	2y	32	54	17,21,22	1.50	3 (17%)	20,30,33	3.07	6 (30%)
54	PSU	2w	32	54	17,21,22	1.53	2 (11%)	20,30,33	3.13	6 (30%)
54	PSU	1y	55	54	17,21,22	1.53	3 (17%)	20,30,33	3.11	6 (30%)
54	PSU	2y	55	54	17,21,22	1.57	2 (11%)	20,30,33	3.23	6 (30%)
54	PSU	1w	39	54	17,21,22	1.57	2 (11%)	20,30,33	3.13	6 (30%)
32	M2G	2a	966	32	20,27,28	1.44	3 (15%)	22,40,43	2.14	5 (22%)
1	PSU	1A	2605	1,56	17,21,22	1.53	2 (11%)	20,30,33	3.23	6 (30%)
54	4SU	2y	8	54	14,21,22	1.36	2 (14%)	15,30,33	1.52	2 (13%)
1	5MC	1A	1942	1	15,22,23	1.28	1 (6%)	19,32,35	1.37	3 (15%)
1	5MC	2A	1942	1	15,22,23	1.30	1 (6%)	19,32,35	1.40	3 (15%)
1	PSU	2A	1911	1	17,21,22	1.54	2 (11%)	20,30,33	3.11	6 (30%)
54	7MG	2y	46	54	22,26,27	1.83	3 (13%)	28,39,42	3.00	9 (32%)
1	2MA	2A	2503	1,56	17,25,26	1.37	2 (11%)	19,37,40	2.03	3 (15%)
32	UR3	1a	1498	32	14,22,23	0.79	1 (7%)	15,32,35	0.75	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	1w	32	54	17,21,22	1.54	2 (11%)	20,30,33	3.17	6 (30%)
32	7MG	1a	527	32,56	22,26,27	1.77	4 (18%)	28,39,42	2.71	9 (32%)
54	7MG	1y	46	54	22,26,27	1.79	3 (13%)	28,39,42	2.84	9 (32%)
32	4OC	1a	1402	32	16,23,24	0.66	0	17,32,35	1.36	1 (5%)
1	2MU	2A	2552	1,56	14,22,24	0.88	0	14,31,36	0.87	0
1	PSU	1A	1917	1	17,21,22	1.57	2 (11%)	20,30,33	3.12	6 (30%)
1	5MC	1A	1962	1,56	15,22,23	1.32	1 (6%)	19,32,35	1.29	3 (15%)
32	MA6	1a	1519	32	19,26,27	1.01	1 (5%)	18,38,41	1.63	4 (22%)
32	5MC	1a	1407	32	15,22,23	1.35	1 (6%)	19,32,35	1.30	3 (15%)
32	PSU	1a	516	32	17,21,22	1.55	3 (17%)	20,30,33	3.15	6 (30%)
32	5MC	1a	1400	32	15,22,23	1.33	1 (6%)	19,32,35	1.34	3 (15%)
55	4SU	2x	8	55,56	14,21,22	1.36	2 (14%)	15,30,33	1.99	2 (13%)
54	MIA	2w	37	54	20,27,32	1.75	3 (15%)	22,39,47	1.80	7 (31%)
54	PSU	1y	32	54	17,21,22	1.47	2 (11%)	20,30,33	3.07	5 (25%)
54	MIA	1y	37	54	18,24,32	1.11	2 (11%)	18,35,47	1.28	2 (11%)
54	PSU	1w	55	54	17,21,22	1.47	2 (11%)	20,30,33	3.35	6 (30%)
55	5MU	1x	54	55,56	15,22,23	1.08	1 (6%)	16,32,35	1.92	2 (12%)
55	4SU	1x	8	55	14,21,22	1.41	2 (14%)	15,30,33	2.36	2 (13%)
1	OMG	1A	2251	1,55,56	18,26,27	1.21	2 (11%)	20,38,41	2.22	6 (30%)
1	2MA	1A	2503	1,56	17,25,26	1.36	2 (11%)	19,37,40	2.08	3 (15%)
1	4OC	2A	1920	1	15,22,24	0.65	0	17,31,35	1.45	2 (11%)
32	5MC	1a	967	32	15,22,23	1.28	1 (6%)	19,32,35	1.31	3 (15%)
55	5MC	2x	32	55	15,22,23	1.31	1 (6%)	19,32,35	1.35	3 (15%)
55	5MC	1x	32	55	15,22,23	1.35	1 (6%)	19,32,35	1.43	3 (15%)
54	7MG	1w	46	54	22,26,27	1.78	4 (18%)	28,39,42	2.82	8 (28%)
54	PSU	2y	39	54	17,21,22	1.59	2 (11%)	20,30,33	3.21	6 (30%)
54	4SU	2w	8	54	14,21,22	1.29	1 (7%)	15,30,33	1.15	2 (13%)
1	5MU	2A	1915	1	15,22,23	1.08	1 (6%)	16,32,35	1.84	2 (12%)
54	MIA	1w	37	54	24,31,32	2.21	4 (16%)	26,44,47	2.59	10 (38%)
55	PSU	1x	55	55,56	17,21,22	1.64	2 (11%)	20,30,33	3.18	6 (30%)
32	5MC	1a	1404	32	15,22,23	1.36	1 (6%)	19,32,35	1.28	3 (15%)
54	5MU	1y	54	54	15,22,23	1.05	1 (6%)	16,32,35	1.77	2 (12%)
54	5MU	2w	54	54	15,22,23	1.06	1 (6%)	16,32,35	2.08	1 (6%)
32	MA6	1a	1518	32	19,26,27	0.96	1 (5%)	18,38,41	1.69	5 (27%)
1	OMG	2A	2251	1,55,56	18,26,27	1.18	2 (11%)	20,38,41	2.09	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	1y	39	54	17,21,22	1.50	2 (11%)	20,30,33	3.04	6 (30%)
43	0TD	1l	92	43	4,9,10	3.12	1 (25%)	3,11,13	5.72	1 (33%)

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	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/5/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,56	-	0/5/25/26	0/2/2/2
32	PSU	2a	516	32	-	1/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	5MU	2y	54	54	-	0/5/25/26	0/2/2/2
54	7MG	2w	46	54	-	3/7/37/38	0/3/3/3
32	MA6	2a	1519	32	-	6/7/29/30	0/3/3/3
43	0TD	2l	92	43	-	2/3/12/14	-
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/3/25/34	0/3/3/3
1	2MU	1A	2552	1,56	-	0/7/27/28	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	4OC	1A	1920	1	-	1/7/27/30	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	1/7/37/38	0/3/3/3
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/5/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/5/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4SU	1y	8	54	-	3/5/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	2/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	4/7/37/38	0/3/3/3
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
54	PSU	1w	32	54	-	1/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
54	7MG	1y	46	54	-	4/7/37/38	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
1	2MU	2A	2552	1,56	-	0/7/27/28	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	2/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	1/5/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/5/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
1	OMG	1A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	1A	2503	1,56	-	2/3/25/26	0/3/3/3
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
32	5MC	1a	967	32	-	1/5/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	1/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
54	5MU	1y	54	54	-	1/5/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
1	OMG	2A	2251	1,55,56	-	1/5/27/28	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.14	1.52	1.32
54	1w	37	MIA	C2-S10	-6.54	1.70	1.75
54	2w	37	MIA	C2-S10	-6.28	1.70	1.75
43	1l	92	0TD	CB-SB	-5.98	1.69	1.84
43	2l	92	0TD	CB-SB	-5.92	1.69	1.84
32	2a	527	7MG	C6-C5	4.96	1.48	1.41
54	2y	46	7MG	C6-C5	4.93	1.48	1.41
32	2a	1404	5MC	C5-C4	4.87	1.48	1.41
54	1y	46	7MG	C6-C5	4.85	1.48	1.41
32	1a	527	7MG	C6-C5	4.85	1.48	1.41
32	2a	967	5MC	C5-C4	4.84	1.48	1.41
55	1x	32	5MC	C5-C4	4.84	1.48	1.41
32	1a	1404	5MC	C5-C4	4.83	1.48	1.41
55	2x	32	5MC	C5-C4	4.76	1.48	1.41
54	2y	46	7MG	C5-C4	4.74	1.48	1.39
32	1a	1400	5MC	C5-C4	4.74	1.48	1.41
32	1a	1407	5MC	C5-C4	4.73	1.48	1.41
1	1A	1962	5MC	C5-C4	4.73	1.48	1.41
1	2A	1962	5MC	C5-C4	4.73	1.48	1.41
55	1x	55	PSU	C5-C1'	-4.71	1.48	1.52
54	2w	46	7MG	C6-C5	4.69	1.47	1.41
1	2A	1942	5MC	C5-C4	4.68	1.48	1.41
32	2a	1400	5MC	C5-C4	4.68	1.48	1.41
1	1A	2503	2MA	C6-C5	4.63	1.48	1.41
54	1y	46	7MG	C5-C4	4.62	1.48	1.39
32	1a	967	5MC	C5-C4	4.61	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2503	2MA	C6-C5	4.59	1.48	1.41
54	2y	55	PSU	C5-C1'	-4.58	1.48	1.52
1	1A	1942	5MC	C5-C4	4.57	1.48	1.41
54	1w	46	7MG	C5-C4	4.55	1.48	1.39
32	2a	1407	5MC	C5-C4	4.49	1.48	1.41
32	2a	1207	2MG	C6-C5	4.49	1.49	1.41
32	2a	527	7MG	C5-C4	4.48	1.47	1.39
32	1a	527	7MG	C5-C4	4.46	1.47	1.39
54	2y	39	PSU	C5-C1'	-4.45	1.48	1.52
54	2w	46	7MG	C5-C4	4.44	1.47	1.39
54	1w	46	7MG	C6-C5	4.36	1.47	1.41
54	1w	39	PSU	C5-C1'	-4.35	1.48	1.52
55	2x	55	PSU	C5-C1'	-4.33	1.48	1.52
1	1A	1917	PSU	C5-C1'	-4.33	1.48	1.52
32	2a	966	M2G	C6-C5	4.31	1.48	1.41
54	1y	55	PSU	C5-C1'	-4.22	1.48	1.52
1	2A	2605	PSU	C5-C1'	-4.20	1.48	1.52
32	1a	1207	2MG	C6-C5	4.20	1.48	1.41
54	2w	8	4SU	C4-S4	-4.18	1.59	1.67
32	1a	966	M2G	C6-C5	4.18	1.48	1.41
1	1A	1911	PSU	C5-C1'	-4.16	1.48	1.52
54	2y	8	4SU	C4-S4	-4.15	1.59	1.67
1	1A	2605	PSU	C5-C1'	-4.14	1.48	1.52
1	2A	1911	PSU	C5-C1'	-4.13	1.48	1.52
55	2x	8	4SU	C4-S4	-4.13	1.59	1.67
32	1a	516	PSU	C5-C1'	-4.05	1.48	1.52
1	1A	2251	OMG	C6-C5	4.03	1.48	1.41
55	1x	8	4SU	C4-S4	-4.00	1.60	1.67
1	2A	2251	OMG	C6-C5	3.95	1.48	1.41
54	1y	39	PSU	C5-C1'	-3.94	1.48	1.52
54	2w	32	PSU	C5-C1'	-3.94	1.48	1.52
54	1w	32	PSU	C5-C1'	-3.92	1.48	1.52
54	1w	8	4SU	C4-S4	-3.91	1.60	1.67
54	1y	8	4SU	C4-S4	-3.91	1.60	1.67
1	2A	1917	PSU	C5-C1'	-3.90	1.48	1.52
54	2w	39	PSU	C5-C1'	-3.85	1.49	1.52
54	2y	32	PSU	C5-C1'	-3.78	1.49	1.52
32	2a	516	PSU	C5-C1'	-3.71	1.49	1.52
54	1w	55	PSU	C5-C1'	-3.70	1.49	1.52
32	2a	516	PSU	C4-C5	3.67	1.49	1.41
54	1y	32	PSU	C4-C5	3.63	1.49	1.41
54	2w	55	PSU	C5-C1'	-3.59	1.49	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	32	PSU	C4-C5	3.59	1.49	1.41
54	1w	46	7MG	C5-N7	-3.56	1.33	1.39
54	2w	55	PSU	C4-C5	3.54	1.49	1.41
54	2y	46	7MG	C5-N7	-3.53	1.33	1.39
54	2w	32	PSU	C4-C5	3.52	1.49	1.41
55	2x	55	PSU	C4-C5	3.52	1.49	1.41
54	1y	32	PSU	C5-C1'	-3.52	1.49	1.52
1	2A	1915	5MU	C4-C5	3.51	1.49	1.41
32	2a	966	M2G	C2-N2	3.50	1.40	1.34
54	1w	54	5MU	C4-C5	3.46	1.48	1.41
1	1A	1911	PSU	C4-C5	3.46	1.48	1.41
54	1y	46	7MG	C5-N7	-3.44	1.33	1.39
54	2y	39	PSU	C4-C5	3.43	1.48	1.41
54	2y	32	PSU	C4-C5	3.43	1.48	1.41
32	2a	527	7MG	C5-N7	-3.42	1.34	1.39
55	2x	54	5MU	C4-C5	3.40	1.48	1.41
1	2A	1911	PSU	C4-C5	3.39	1.48	1.41
54	1y	39	PSU	C4-C5	3.39	1.48	1.41
1	2A	1917	PSU	C4-C5	3.39	1.48	1.41
32	1a	527	7MG	C5-N7	-3.39	1.34	1.39
32	1a	966	M2G	C2-N2	3.38	1.40	1.34
54	1y	54	5MU	C4-C5	3.38	1.48	1.41
55	1x	54	5MU	C4-C5	3.37	1.48	1.41
32	1a	516	PSU	C4-C5	3.36	1.48	1.41
54	2w	46	7MG	C5-N7	-3.35	1.34	1.39
1	2A	1939	5MU	C4-C5	3.35	1.48	1.41
1	2A	2605	PSU	C4-C5	3.31	1.48	1.41
54	2w	54	5MU	C4-C5	3.31	1.48	1.41
1	1A	1915	5MU	C4-C5	3.30	1.48	1.41
55	1x	55	PSU	C4-C5	3.30	1.48	1.41
54	2y	54	5MU	C4-C5	3.30	1.48	1.41
1	1A	1917	PSU	C4-C5	3.29	1.48	1.41
54	1w	39	PSU	C4-C5	3.29	1.48	1.41
54	1w	55	PSU	C4-C5	3.27	1.48	1.41
54	2y	55	PSU	C4-C5	3.24	1.48	1.41
1	1A	1939	5MU	C4-C5	3.20	1.48	1.41
54	2w	39	PSU	C4-C5	3.18	1.48	1.41
54	1y	55	PSU	C4-C5	3.16	1.48	1.41
1	1A	2605	PSU	C4-C5	3.10	1.48	1.41
55	1x	8	4SU	C2-N3	-3.04	1.32	1.38
32	2a	1519	MA6	C5-C4	2.68	1.48	1.40
54	2w	37	MIA	C5-C4	2.67	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	37	MIA	C2-N3	2.64	1.36	1.32
54	2y	37	MIA	C5-C4	2.63	1.47	1.40
54	1y	37	MIA	C5-C4	2.61	1.47	1.40
32	2a	1518	MA6	C5-C4	2.61	1.47	1.40
54	1w	37	MIA	C5-C4	2.61	1.47	1.40
54	1y	37	MIA	C2-N3	2.58	1.36	1.32
55	2x	8	4SU	C2-N3	-2.55	1.33	1.38
54	1w	46	7MG	C4-N9	-2.52	1.33	1.38
32	1a	1519	MA6	C5-C4	2.49	1.47	1.40
32	2a	1207	2MG	C5-C4	2.49	1.47	1.40
32	1a	1518	MA6	C5-C4	2.48	1.47	1.40
32	2a	966	M2G	C5-C4	2.46	1.47	1.40
1	2A	2251	OMG	C5-C4	2.46	1.47	1.40
54	2w	46	7MG	C4-N9	-2.45	1.33	1.38
32	1a	1207	2MG	C5-C4	2.40	1.47	1.40
1	1A	2503	2MA	C5-C4	2.40	1.47	1.40
32	1a	966	M2G	C5-C4	2.39	1.47	1.40
1	1A	2251	OMG	C5-C4	2.38	1.47	1.40
32	1a	527	7MG	C4-N9	-2.36	1.33	1.38
1	2A	2503	2MA	C5-C4	2.36	1.47	1.40
32	1a	1498	UR3	C4-N3	2.18	1.41	1.38
54	2w	37	MIA	C6-N1	2.14	1.35	1.32
54	2y	54	5MU	C2-N3	-2.13	1.33	1.38
32	2a	1498	UR3	C4-N3	2.11	1.41	1.38
54	1w	8	4SU	C2-N3	-2.10	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.10	1.34	1.38
54	1y	55	PSU	O4'-C1'	-2.10	1.41	1.44
54	2y	8	4SU	C2-N3	-2.09	1.34	1.38
32	1a	516	PSU	O4'-C1'	-2.08	1.41	1.44
1	1A	1939	5MU	C2-N3	-2.04	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.02	1.34	1.38
54	1w	37	MIA	C6-N1	2.01	1.35	1.32
32	2a	527	7MG	C4-N9	-2.01	1.34	1.38
54	2y	32	PSU	O4'-C1'	-2.00	1.41	1.44

All (344) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	46	7MG	N3-C4-N9	10.07	139.84	126.91
43	1l	92	0TD	CSB-SB-CB	-9.80	82.57	101.85
54	1y	46	7MG	N3-C4-N9	9.36	138.94	126.91
32	2a	527	7MG	N3-C4-N9	9.24	138.78	126.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	39	PSU	N1-C2-N3	-9.07	121.22	128.43
32	1a	527	7MG	N3-C4-N9	9.02	138.49	126.91
54	1w	46	7MG	N3-C4-N9	8.89	138.33	126.91
32	2a	516	PSU	N1-C2-N3	-8.70	121.52	128.43
1	1A	2605	PSU	N1-C2-N3	-8.69	121.52	128.43
32	1a	516	PSU	N1-C2-N3	-8.66	121.55	128.43
54	2w	46	7MG	N3-C4-N9	8.61	137.97	126.91
54	1w	32	PSU	N1-C2-N3	-8.56	121.62	128.43
54	1y	32	PSU	N1-C2-N3	-8.46	121.70	128.43
54	2w	55	PSU	N1-C2-N3	-8.46	121.71	128.43
54	1w	37	MIA	C12-C13-C14	-8.42	110.76	127.14
1	1A	1917	PSU	N1-C2-N3	-8.41	121.75	128.43
54	2y	39	PSU	N1-C2-N3	-8.40	121.75	128.43
54	1y	55	PSU	N1-C2-N3	-8.38	121.77	128.43
1	2A	1911	PSU	N1-C2-N3	-8.38	121.77	128.43
54	2w	32	PSU	N1-C2-N3	-8.37	121.77	128.43
55	1x	55	PSU	N1-C2-N3	-8.37	121.78	128.43
54	2y	32	PSU	N1-C2-N3	-8.33	121.81	128.43
1	2A	2605	PSU	N1-C2-N3	-8.29	121.84	128.43
54	1w	39	PSU	N1-C2-N3	-8.28	121.84	128.43
54	2y	55	PSU	N1-C2-N3	-8.28	121.85	128.43
54	2y	54	5MU	C4-N3-C2	8.25	122.11	115.14
54	1y	39	PSU	N1-C2-N3	-8.23	121.88	128.43
1	2A	1917	PSU	N1-C2-N3	-8.21	121.91	128.43
1	1A	1911	PSU	N1-C2-N3	-8.21	121.91	128.43
54	1w	55	PSU	N1-C2-N3	-8.18	121.93	128.43
55	2x	55	PSU	N1-C2-N3	-8.16	121.94	128.43
55	1x	8	4SU	C2-N3-C4	8.01	126.76	115.15
54	2w	54	5MU	C4-N3-C2	7.84	121.76	115.14
54	2w	39	PSU	C4-N3-C2	7.34	121.34	115.14
32	2a	516	PSU	C4-N3-C2	7.31	121.31	115.14
54	1w	32	PSU	C4-N3-C2	7.17	121.20	115.14
55	1x	54	5MU	C4-N3-C2	7.13	121.16	115.14
32	1a	516	PSU	C4-N3-C2	7.05	121.10	115.14
1	1A	2605	PSU	C4-N3-C2	7.01	121.06	115.14
54	2w	55	PSU	C4-N3-C2	6.98	121.04	115.14
54	2w	32	PSU	C4-N3-C2	6.93	120.99	115.14
54	1w	55	PSU	C4-N3-C2	6.89	120.96	115.14
55	2x	54	5MU	C4-N3-C2	6.87	120.94	115.14
54	1y	32	PSU	C4-N3-C2	6.87	120.94	115.14
54	2y	32	PSU	C4-N3-C2	6.83	120.91	115.14
54	1w	39	PSU	C4-N3-C2	6.79	120.87	115.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	55	PSU	C4-N3-C2	6.77	120.85	115.14
1	2A	1911	PSU	C4-N3-C2	6.72	120.81	115.14
55	1x	55	PSU	C4-N3-C2	6.71	120.81	115.14
1	1A	1915	5MU	C4-N3-C2	6.68	120.78	115.14
54	1y	55	PSU	C4-N3-C2	6.68	120.78	115.14
54	2y	39	PSU	C4-N3-C2	6.67	120.77	115.14
1	2A	1915	5MU	C4-N3-C2	6.66	120.77	115.14
1	1A	1917	PSU	C4-N3-C2	6.63	120.74	115.14
55	2x	8	4SU	C2-N3-C4	6.58	124.69	115.15
1	1A	1911	PSU	C4-N3-C2	6.57	120.69	115.14
54	2y	55	PSU	C4-N3-C2	6.56	120.68	115.14
1	2A	1917	PSU	C4-N3-C2	6.55	120.67	115.14
1	1A	2503	2MA	C2-N3-C4	6.51	120.81	115.52
1	2A	2605	PSU	C4-N3-C2	6.46	120.60	115.14
1	2A	2503	2MA	C2-N3-C4	6.41	120.73	115.52
54	1y	39	PSU	C4-N3-C2	6.36	120.51	115.14
54	1y	54	5MU	C4-N3-C2	6.34	120.49	115.14
43	2l	92	0TD	CSB-SB-CB	-6.24	89.59	101.85
54	1w	54	5MU	C4-N3-C2	6.23	120.41	115.14
54	1w	55	PSU	C5-C1'-C2'	-6.22	104.22	115.32
1	1A	1939	5MU	C4-N3-C2	6.20	120.38	115.14
54	2y	46	7MG	C5-C4-N3	-5.82	116.99	126.49
1	2A	1939	5MU	C4-N3-C2	5.77	120.02	115.14
54	1w	46	7MG	C6-N1-C2	5.71	125.00	115.93
32	2a	516	PSU	C5-C4-N3	-5.65	118.08	125.36
54	1w	32	PSU	C5-C4-N3	-5.63	118.10	125.36
55	2x	55	PSU	C5-C4-N3	-5.61	118.13	125.36
54	2w	32	PSU	C5-C4-N3	-5.58	118.17	125.36
54	1w	39	PSU	C5-C4-N3	-5.55	118.20	125.36
32	1a	516	PSU	C5-C4-N3	-5.52	118.25	125.36
54	2y	32	PSU	C5-C4-N3	-5.51	118.27	125.36
55	1x	55	PSU	C5-C4-N3	-5.50	118.27	125.36
54	2w	55	PSU	C5-C4-N3	-5.45	118.34	125.36
54	1y	55	PSU	C5-C4-N3	-5.45	118.34	125.36
54	1w	55	PSU	C5-C4-N3	-5.45	118.34	125.36
32	2a	527	7MG	C5-C4-N3	-5.42	117.64	126.49
54	2y	39	PSU	C5-C4-N3	-5.40	118.40	125.36
54	2w	39	PSU	C5-C4-N3	-5.37	118.45	125.36
54	1y	46	7MG	C5-C4-N3	-5.36	117.74	126.49
32	1a	966	M2G	C6-N1-C2	5.35	122.55	116.18
1	1A	1911	PSU	C5-C4-N3	-5.35	118.47	125.36
1	2A	1911	PSU	C5-C4-N3	-5.35	118.47	125.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	55	PSU	C5-C4-N3	-5.34	118.48	125.36
1	2A	1917	PSU	C5-C4-N3	-5.33	118.49	125.36
54	2w	46	7MG	N7-C8-N9	-5.33	95.75	103.38
54	1y	32	PSU	C5-C4-N3	-5.29	118.54	125.36
1	1A	1917	PSU	C5-C4-N3	-5.27	118.57	125.36
54	1y	39	PSU	C5-C4-N3	-5.26	118.58	125.36
54	1w	46	7MG	N7-C8-N9	-5.23	95.89	103.38
1	1A	2605	PSU	C5-C4-N3	-5.23	118.62	125.36
32	2a	966	M2G	C6-N1-C2	5.22	122.39	116.18
32	1a	527	7MG	N7-C8-N9	-5.20	95.94	103.38
32	1a	527	7MG	C5-C4-N3	-5.07	118.20	126.49
32	2a	527	7MG	N7-C8-N9	-5.06	96.14	103.38
1	2A	2605	PSU	C5-C4-N3	-5.06	118.84	125.36
54	2w	46	7MG	C6-N1-C2	5.03	123.93	115.93
54	1w	8	4SU	C2-N3-C4	5.01	122.42	115.15
1	1A	2251	OMG	C2-N3-C4	4.99	121.06	115.36
54	1y	46	7MG	N7-C8-N9	-4.91	96.36	103.38
32	2a	966	M2G	C2-N3-C4	4.91	120.85	115.28
32	2a	1207	2MG	C2-N3-C4	4.90	120.84	115.28
54	2y	46	7MG	N7-C8-N9	-4.86	96.42	103.38
32	1a	966	M2G	C2-N3-C4	4.85	120.79	115.28
54	1y	46	7MG	C6-N1-C2	4.84	123.62	115.93
54	2w	55	PSU	C5-C1'-C2'	-4.80	106.75	115.32
54	2y	46	7MG	C6-N1-C2	4.78	123.52	115.93
32	1a	1207	2MG	C2-N3-C4	4.77	120.70	115.28
54	2y	46	7MG	C6-C5-C4	4.75	120.30	115.20
1	2A	2251	OMG	C2-N3-C4	4.75	120.78	115.36
1	2A	2503	2MA	C5-C6-N1	-4.74	118.09	123.06
54	2w	46	7MG	C5-C4-N3	-4.71	118.80	126.49
32	2a	1402	4OC	CM4-N4-C4	-4.68	118.95	122.97
1	1A	2503	2MA	C5-C6-N1	-4.68	118.15	123.06
54	2y	8	4SU	C2-N3-C4	4.60	121.82	115.15
1	1A	1920	4OC	C2-N3-C4	4.56	120.96	116.34
32	1a	1402	4OC	CM4-N4-C4	-4.55	119.06	122.97
1	2A	1920	4OC	C2-N3-C4	4.54	120.94	116.34
54	2y	55	PSU	C5-C1'-C2'	-4.51	107.27	115.32
54	1w	46	7MG	C5-C4-N3	-4.48	119.17	126.49
54	2w	37	MIA	C2-N3-C4	4.47	121.48	115.32
54	1y	8	4SU	C2-N3-C4	4.46	121.61	115.15
32	2a	527	7MG	C6-C5-C4	4.46	119.98	115.20
54	2y	55	PSU	C5-C6-N1	-4.45	118.97	124.44
54	1y	46	7MG	C6-C5-C4	4.40	119.92	115.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	39	PSU	C5-C6-N1	-4.37	119.07	124.44
32	2a	1207	2MG	C5-C6-N1	-4.37	117.46	123.43
1	2A	2605	PSU	C5-C6-N1	-4.34	119.10	124.44
32	1a	527	7MG	C6-N1-C2	4.33	122.81	115.93
1	1A	1911	PSU	C5-C6-N1	-4.31	119.15	124.44
54	1w	37	MIA	C2-N3-C4	4.30	121.26	115.32
55	1x	55	PSU	C5-C6-N1	-4.28	119.18	124.44
32	2a	1207	2MG	C6-N1-C2	4.25	122.79	115.18
54	1w	39	PSU	C5-C6-N1	-4.23	119.24	124.44
32	2a	527	7MG	C6-N1-C2	4.22	122.63	115.93
1	2A	1917	PSU	C5-C6-N1	-4.20	119.28	124.44
54	1y	39	PSU	C5-C6-N1	-4.20	119.28	124.44
32	1a	1207	2MG	C5-C6-N1	-4.19	117.70	123.43
54	2y	39	PSU	C6-N1-C2	4.18	122.26	115.36
1	2A	2605	PSU	C6-N1-C2	4.18	122.25	115.36
1	1A	1917	PSU	C5-C6-N1	-4.17	119.31	124.44
55	2x	55	PSU	C5-C6-N1	-4.17	119.32	124.44
1	1A	1911	PSU	C6-N1-C2	4.17	122.23	115.36
1	1A	2251	OMG	C6-N1-C2	4.14	122.52	115.93
54	1y	39	PSU	C6-N1-C2	4.13	122.17	115.36
32	2a	966	M2G	C5-C6-N1	-4.12	117.79	123.43
32	1a	1207	2MG	C6-N1-C2	4.11	122.54	115.18
54	2w	39	PSU	C6-N1-C2	4.11	122.14	115.36
1	1A	1917	PSU	C6-N1-C2	4.10	122.13	115.36
54	1w	37	MIA	C15-C14-C13	-4.10	110.79	122.65
54	2w	39	PSU	C5-C6-N1	-4.10	119.40	124.44
32	1a	966	M2G	C6-C5-C4	-4.09	116.89	120.80
32	1a	516	PSU	C6-N1-C2	4.09	122.11	115.36
54	2y	55	PSU	C6-N1-C2	4.08	122.09	115.36
54	1w	46	7MG	C5-C6-N1	-4.07	114.77	123.14
1	2A	1911	PSU	C5-C6-N1	-4.07	119.43	124.44
54	2y	32	PSU	C5-C6-N1	-4.07	119.44	124.44
55	1x	55	PSU	C6-N1-C2	4.07	122.07	115.36
1	2A	1917	PSU	C6-N1-C2	4.06	122.05	115.36
1	2A	1911	PSU	C6-N1-C2	4.05	122.05	115.36
54	1y	55	PSU	C5-C6-N1	-4.05	119.46	124.44
1	2A	2251	OMG	C5-C6-N1	-4.05	117.89	123.43
1	2A	2251	OMG	C6-N1-C2	4.04	122.35	115.93
1	1A	2605	PSU	C5-C6-N1	-4.04	119.47	124.44
54	1w	39	PSU	C6-N1-C2	4.03	122.01	115.36
54	2y	32	PSU	C6-N1-C2	4.02	121.99	115.36
54	1w	32	PSU	C6-N1-C2	4.02	121.99	115.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	516	PSU	C6-N1-C2	4.02	121.99	115.36
54	1y	32	PSU	C6-N1-C2	4.01	121.98	115.36
32	1a	966	M2G	C5-C6-N1	-4.01	117.95	123.43
55	2x	55	PSU	C6-N1-C2	4.01	121.97	115.36
1	1A	2605	PSU	C6-N1-C2	4.01	121.97	115.36
32	1a	527	7MG	C6-C5-C4	4.01	119.50	115.20
32	2a	1207	2MG	C6-C5-C4	-4.00	116.98	120.80
54	2w	32	PSU	C6-N1-C2	4.00	121.96	115.36
54	1y	55	PSU	C6-N1-C2	3.99	121.95	115.36
54	2w	55	PSU	C6-N1-C2	3.99	121.95	115.36
54	2w	32	PSU	C5-C6-N1	-3.99	119.54	124.44
54	2y	39	PSU	C5-C1'-C2'	-3.97	108.23	115.32
1	1A	2251	OMG	C5-C6-N1	-3.95	118.03	123.43
32	1a	516	PSU	C5-C6-N1	-3.94	119.59	124.44
32	2a	1407	5MC	C2-N3-C4	3.89	120.72	116.02
54	1w	37	MIA	C16-C14-C13	-3.89	111.40	122.65
1	1A	2251	OMG	C6-C5-C4	-3.88	117.09	120.80
55	1x	8	4SU	C5-C4-N3	-3.87	118.65	123.83
54	1w	46	7MG	C6-C5-C4	3.87	119.36	115.20
32	2a	1518	MA6	C9-N6-C6	-3.87	107.80	119.51
54	1y	32	PSU	C5-C6-N1	-3.85	119.71	124.44
55	2x	32	5MC	C2-N3-C4	3.84	120.65	116.02
54	1w	55	PSU	C6-N1-C2	3.82	121.67	115.36
32	1a	1400	5MC	C2-N3-C4	3.81	120.62	116.02
54	2w	55	PSU	C5-C6-N1	-3.80	119.77	124.44
54	2w	46	7MG	C5-C6-N1	-3.80	115.34	123.14
54	1w	32	PSU	C5-C6-N1	-3.79	119.78	124.44
32	1a	1207	2MG	C6-C5-C4	-3.79	117.18	120.80
54	1y	46	7MG	C5-C6-N1	-3.78	115.37	123.14
1	1A	2605	PSU	C5-C1'-C2'	-3.76	108.60	115.32
55	1x	55	PSU	C5-C1'-C2'	-3.73	108.66	115.32
32	2a	967	5MC	C2-N3-C4	3.72	120.50	116.02
54	2y	46	7MG	C5-C6-N1	-3.70	115.54	123.14
32	2a	1400	5MC	C2-N3-C4	3.70	120.48	116.02
32	2a	1518	MA6	C4-C5-N7	-3.70	105.55	109.40
54	2w	46	7MG	C6-C5-C4	3.68	119.15	115.20
1	1A	1962	5MC	C2-N3-C4	3.67	120.45	116.02
32	2a	516	PSU	C5-C6-N1	-3.66	119.94	124.44
1	2A	1942	5MC	C2-N3-C4	3.65	120.42	116.02
54	1w	55	PSU	C5-C6-N1	-3.63	119.98	124.44
32	2a	527	7MG	C5-C6-N1	-3.62	115.70	123.14
32	1a	1407	5MC	C2-N3-C4	3.60	120.36	116.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2251	OMG	N3-C2-N1	-3.58	122.44	127.22
55	1x	32	5MC	C2-N3-C4	3.55	120.30	116.02
54	1y	37	MIA	N3-C2-N1	-3.54	123.14	128.68
32	1a	967	5MC	C2-N3-C4	3.54	120.29	116.02
32	1a	527	7MG	C5-C6-N1	-3.54	115.87	123.14
32	2a	966	M2G	C6-C5-C4	-3.54	117.42	120.80
32	2a	1404	5MC	C2-N3-C4	3.53	120.28	116.02
54	2w	37	MIA	C5-C6-N1	-3.53	117.88	120.81
32	1a	1404	5MC	C2-N3-C4	3.51	120.25	116.02
54	1w	37	MIA	C5-C6-N1	-3.49	117.91	120.81
32	1a	1519	MA6	C4-C5-N7	-3.48	105.78	109.40
55	2x	8	4SU	C5-C4-N3	-3.46	119.20	123.83
54	2y	37	MIA	N3-C2-N1	-3.45	123.28	128.68
32	1a	1518	MA6	N3-C2-N1	-3.43	123.32	128.68
32	1a	1518	MA6	C9-N6-C6	-3.40	109.21	119.51
1	2A	2251	OMG	C6-C5-C4	-3.39	117.56	120.80
32	2a	1519	MA6	C4-C5-N7	-3.39	105.86	109.40
1	1A	1942	5MC	C2-N3-C4	3.38	120.10	116.02
1	2A	1962	5MC	C2-N3-C4	3.38	120.09	116.02
32	2a	1518	MA6	N3-C2-N1	-3.37	123.41	128.68
32	1a	1518	MA6	C4-C5-N7	-3.33	105.92	109.40
32	1a	1519	MA6	C9-N6-C6	-3.32	109.47	119.51
32	2a	1207	2MG	C4-C5-N7	-3.31	105.95	109.40
1	1A	1917	PSU	C5-C1'-C2'	-3.27	109.48	115.32
1	2A	1917	PSU	C5-C1'-C2'	-3.26	109.50	115.32
1	2A	2605	PSU	C5-C1'-C2'	-3.25	109.51	115.32
32	2a	1519	MA6	C9-N6-C6	-3.23	109.73	119.51
32	2a	1519	MA6	N3-C2-N1	-3.21	123.65	128.68
54	1w	8	4SU	C5-C4-N3	-3.20	119.54	123.83
1	2A	2251	OMG	N3-C2-N1	-3.19	122.97	127.22
54	1y	8	4SU	C5-C4-N3	-3.16	119.59	123.83
32	1a	1207	2MG	CM2-N2-C2	-3.11	119.84	123.59
55	2x	55	PSU	C5-C1'-C2'	-3.09	109.81	115.32
54	1w	37	MIA	C12-N6-C6	-3.06	118.02	122.55
54	2w	8	4SU	C2-N3-C4	3.04	119.56	115.15
32	1a	1519	MA6	N3-C2-N1	-3.03	123.94	128.68
1	2A	1939	5MU	C5-C6-N1	-3.03	118.93	122.19
1	2A	1911	PSU	C5-C1'-C2'	-2.98	110.00	115.32
54	1w	39	PSU	C5-C1'-C2'	-2.93	110.08	115.32
54	2w	37	MIA	C12-N6-C6	-2.93	120.35	122.87
32	1a	1207	2MG	C4-C5-N7	-2.92	106.35	109.40
54	2y	8	4SU	C5-C4-N3	-2.92	119.92	123.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	5MU	C5-C6-N1	-2.89	119.08	122.19
54	1w	37	MIA	C2-N1-C6	2.88	122.34	117.19
32	2a	1207	2MG	CM2-N2-C2	-2.87	120.13	123.59
1	2A	1942	5MC	N4-C4-N3	2.87	121.09	117.03
32	2a	1407	5MC	N4-C4-N3	2.82	121.02	117.03
54	1w	46	7MG	C5-C4-N9	-2.82	102.50	106.44
54	1y	55	PSU	C5-C1'-C2'	-2.80	110.32	115.32
32	2a	966	M2G	C4-C5-N7	-2.75	106.53	109.40
55	1x	32	5MC	C5-C6-N1	-2.75	119.23	122.19
54	2w	37	MIA	C2-N1-C6	2.74	122.09	117.19
32	2a	1400	5MC	N4-C4-N3	2.72	120.88	117.03
54	1y	37	MIA	C4-C5-N7	-2.71	106.57	109.40
1	1A	1911	PSU	C5-C1'-C2'	-2.70	110.50	115.32
54	2y	37	MIA	C4-C5-N7	-2.70	106.59	109.40
54	2y	46	7MG	C8-N7-C5	2.69	115.95	108.94
32	2a	527	7MG	C8-N7-C5	2.69	115.94	108.94
1	2A	1962	5MC	C5-C6-N1	-2.68	119.30	122.19
1	1A	1942	5MC	N4-C4-N3	2.65	120.78	117.03
32	1a	527	7MG	C8-N7-C5	2.63	115.79	108.94
32	1a	967	5MC	N4-C4-N3	2.60	120.70	117.03
54	2w	46	7MG	C8-N7-C5	2.59	115.68	108.94
54	1y	46	7MG	C8-N7-C5	2.58	115.66	108.94
1	2A	1962	5MC	N4-C4-N3	2.58	120.67	117.03
1	1A	1942	5MC	C5-C6-N1	-2.58	119.42	122.19
54	1y	39	PSU	C5-C1'-C2'	-2.57	110.73	115.32
1	1A	2503	2MA	C4-C5-N7	-2.57	106.72	109.40
1	1A	2251	OMG	C4-C5-N7	-2.55	106.75	109.40
1	2A	2503	2MA	C4-C5-N7	-2.53	106.76	109.40
54	1w	37	MIA	C4-C5-N7	-2.52	106.77	109.40
54	2w	8	4SU	C5-C4-N3	-2.51	120.47	123.83
55	2x	32	5MC	N4-C4-N3	2.50	120.57	117.03
32	1a	1400	5MC	N4-C4-N3	2.50	120.56	117.03
54	1w	37	MIA	N3-C2-N1	-2.50	122.39	126.98
32	2a	1207	2MG	N2-C2-N1	2.48	119.34	116.96
54	2w	32	PSU	C5-C1'-C2'	-2.47	110.91	115.32
54	1y	54	5MU	C5-C6-N1	-2.46	119.54	122.19
32	2a	1404	5MC	N4-C4-N3	2.46	120.51	117.03
54	2w	37	MIA	C4-C5-N7	-2.46	106.83	109.40
32	1a	1404	5MC	C5-C6-N1	-2.45	119.55	122.19
54	2w	37	MIA	N3-C2-N1	-2.45	122.48	126.98
54	1w	46	7MG	C8-N7-C5	2.45	115.30	108.94
32	1a	966	M2G	C4-C5-N7	-2.44	106.86	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1404	5MC	C5-C6-N1	-2.42	119.59	122.19
1	2A	1915	5MU	C5-C6-N1	-2.42	119.59	122.19
32	1a	1407	5MC	N4-C4-N3	2.41	120.44	117.03
55	2x	54	5MU	C5-C6-N1	-2.37	119.64	122.19
1	1A	1962	5MC	N4-C4-N3	2.36	120.37	117.03
54	2y	46	7MG	C5-C4-N9	-2.35	103.15	106.44
1	1A	1920	4OC	N4-C4-N3	2.35	120.20	116.49
1	2A	2251	OMG	C4-C5-N7	-2.34	106.96	109.40
32	1a	1518	MA6	C10-N6-C9	-2.34	108.58	116.12
32	2a	967	5MC	N4-C4-N3	2.32	120.31	117.03
55	1x	32	5MC	N4-C4-N3	2.31	120.31	117.03
54	2y	46	7MG	C2-N3-C4	2.31	120.28	113.89
54	2w	46	7MG	C5-C4-N9	-2.30	103.22	106.44
32	2a	1518	MA6	C10-N6-C9	-2.30	108.71	116.12
54	1w	37	MIA	C11-S10-C2	-2.30	100.55	102.27
1	2A	1942	5MC	C5-C6-N1	-2.30	119.72	122.19
32	2a	967	5MC	C5-C6-N1	-2.28	119.73	122.19
54	2w	37	MIA	N6-C6-N1	2.27	121.34	118.50
54	2w	39	PSU	C5-C1'-C2'	-2.26	111.29	115.32
32	1a	527	7MG	C5-C4-N9	-2.26	103.28	106.44
32	2a	1498	UR3	C3U-N3-C4	2.24	121.09	118.12
54	1y	46	7MG	C5-C4-N9	-2.23	103.31	106.44
32	1a	1519	MA6	N1-C6-N6	2.23	119.40	117.06
32	1a	1498	UR3	C3U-N3-C4	2.21	121.05	118.12
32	1a	967	5MC	C5-C6-N1	-2.21	119.81	122.19
54	1y	46	7MG	C2-N3-C4	2.20	119.97	113.89
32	2a	1207	2MG	N3-C2-N1	-2.20	122.75	126.23
32	1a	1518	MA6	C10-N6-C6	-2.18	112.93	119.51
1	1A	1962	5MC	C5-C6-N1	-2.17	119.86	122.19
32	2a	527	7MG	C2-N3-C4	2.17	119.88	113.89
54	1w	54	5MU	C5-C6-N1	-2.16	119.86	122.19
32	1a	1404	5MC	N4-C4-N3	2.16	120.09	117.03
1	2A	1920	4OC	N4-C4-N3	2.14	119.87	116.49
32	1a	1400	5MC	C5-C6-N1	-2.12	119.91	122.19
32	1a	527	7MG	C2-N3-C4	2.12	119.74	113.89
55	1x	54	5MU	C5-C6-N1	-2.11	119.92	122.19
1	1A	1915	5MU	C5-C6-N1	-2.11	119.92	122.19
32	1a	1207	2MG	N3-C2-N1	-2.09	122.92	126.23
54	2w	46	7MG	C2-N3-C4	2.08	119.63	113.89
32	2a	1400	5MC	C5-C6-N1	-2.07	119.96	122.19
32	2a	527	7MG	C5-C4-N9	-2.05	103.57	106.44
54	2y	32	PSU	O4'-C1'-C2'	2.03	107.94	104.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	32	PSU	C5-C1'-C2'	-2.02	111.72	115.32
55	2x	32	5MC	C5-C6-N1	-2.01	120.03	122.19
32	1a	516	PSU	O4'-C1'-C2'	2.01	107.91	104.66
32	1a	1407	5MC	C5-C6-N1	-2.00	120.04	122.19

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
1	1A	1920	4OC	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	1a	1518	MA6	C5-C6-N6-C10
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	2y	8	4SU	O4'-C4'-C5'-O5'
54	2y	46	7MG	C4'-C5'-O5'-P
54	1y	46	7MG	C4'-C5'-O5'-P
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB
55	2x	8	4SU	C2'-C1'-N1-C6
54	2w	8	4SU	O4'-C1'-N1-C6
54	1w	37	MIA	C12-C13-C14-C16
1	1A	1915	5MU	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	2y	8	4SU	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
1	1A	1915	5MU	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	8	4SU	O4'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1519	MA6	N1-C6-N6-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1400	5MC	O4'-C4'-C5'-O5'
54	2w	46	7MG	C2'-C1'-N9-C8
54	2y	46	7MG	C2'-C1'-N9-C8
54	1y	46	7MG	C2'-C1'-N9-C8
54	1w	46	7MG	C2'-C1'-N9-C8
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
54	2w	46	7MG	C2'-C1'-N9-C4
32	2a	527	7MG	C4'-C5'-O5'-P
54	2y	46	7MG	C2'-C1'-N9-C4
54	1y	46	7MG	C2'-C1'-N9-C4
54	2w	46	7MG	O4'-C1'-N9-C8
54	2y	46	7MG	O4'-C1'-N9-C8
54	1y	54	5MU	O4'-C4'-C5'-O5'
54	1w	46	7MG	O4'-C1'-N9-C8
32	2a	516	PSU	C2'-C1'-C5-C6
54	1w	32	PSU	C2'-C1'-C5-C6
54	1y	46	7MG	O4'-C1'-N9-C8
32	1a	967	5MC	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	2251	OMG	C4'-C5'-O5'-P
54	1y	8	4SU	C4'-C5'-O5'-P
32	1a	527	7MG	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	1	0
1	1A	1939	5MU	1	0
1	1A	2552	2MU	1	0
1	1A	1920	4OC	1	0
1	2A	1917	PSU	1	0
1	2A	2503	2MA	2	0
1	2A	2552	2MU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1920	4OC	2	0
1	2A	1915	5MU	1	0
1	2A	2251	OMG	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2840 ligands modelled in this entry, 2836 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	CLM	2A	3888	-	19,20,20	0.94	2 (10%)	23,27,27	1.01	1 (4%)
60	SF4	2d	302	35	0,12,12	0.00	-	-		
60	SF4	1d	302	35	0,12,12	0.00	-	-		
57	CLM	1A	4102	-	19,20,20	0.92	1 (5%)	23,27,27	0.75	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
57	CLM	2A	3888	-	-	6/20/22/22	0/1/1/1
60	SF4	2d	302	35	-	-	0/6/5/5
60	SF4	1d	302	35	-	-	0/6/5/5
57	CLM	1A	4102	-	-	7/20/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3888	CLM	C6-C5	-2.42	1.48	1.51
57	1A	4102	CLM	C6-C5	-2.10	1.48	1.51
57	2A	3888	CLM	C9-N9	-2.09	1.40	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3888	CLM	C6-C5-C3	-2.83	106.66	111.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	2A	3888	CLM	C1-C2-N2-C3
57	2A	3888	CLM	O2-C2-N2-C3
57	2A	3888	CLM	C4-C3-N2-C2
57	2A	3888	CLM	N2-C3-C4-O4
57	2A	3888	CLM	C5-C3-C4-O4
57	1A	4102	CLM	O2-C2-N2-C3
57	1A	4102	CLM	C1-C2-N2-C3
57	1A	4102	CLM	C5-C3-C4-O4
57	1A	4102	CLM	N2-C3-C4-O4
57	1A	4102	CLM	C5-C3-N2-C2
57	1A	4102	CLM	C4-C3-N2-C2
57	1A	4102	CLM	C4-C3-C5-O5
57	2A	3888	CLM	C4-C3-C5-O5

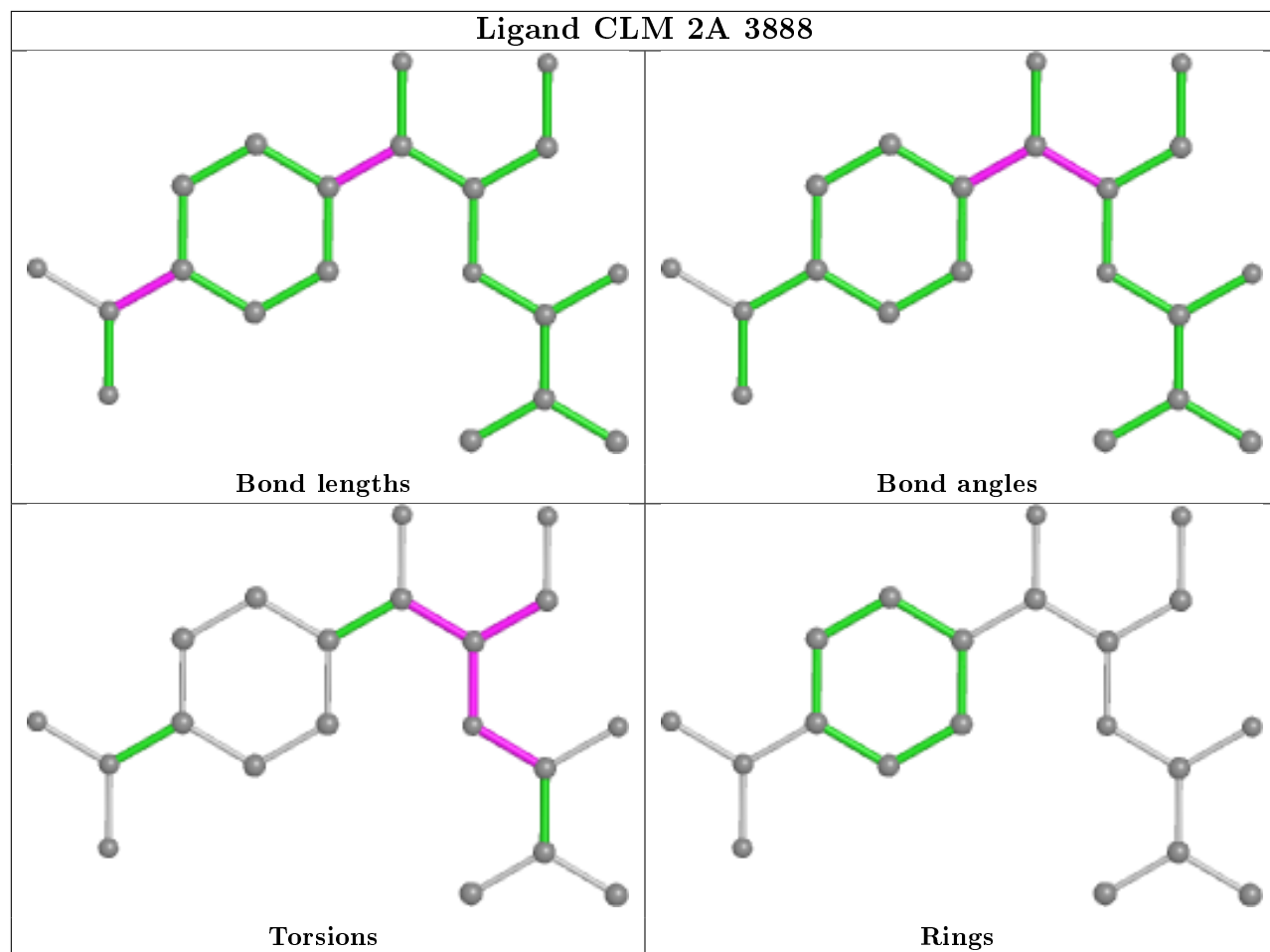
There are no ring outliers.

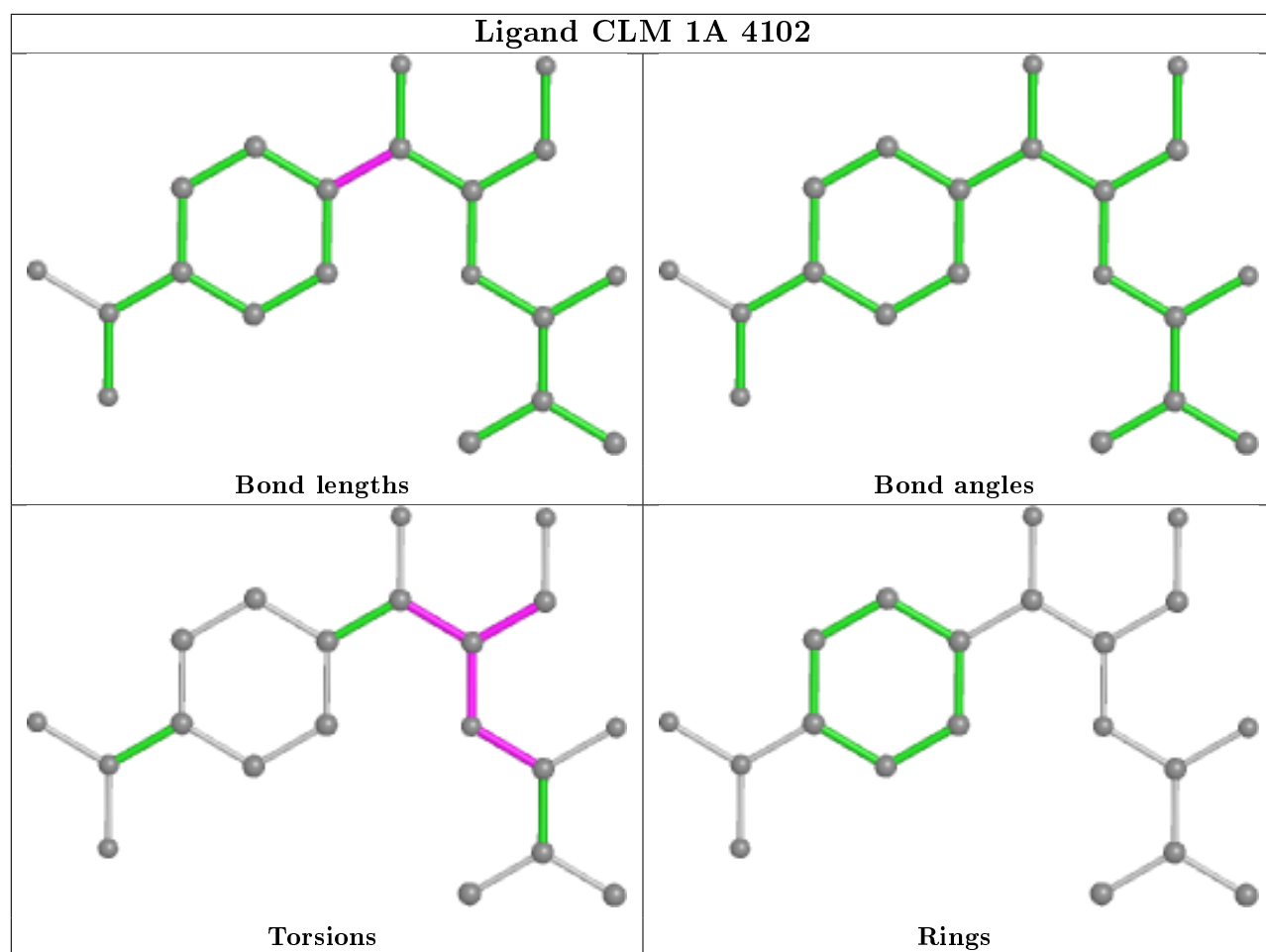
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	2A	3888	CLM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.40	45 (1%) 72 68	17, 34, 87, 101	0
1	2A	2789/2915 (95%)	0.16	58 (2%) 63 58	34, 57, 87, 102	0
2	1B	120/121 (99%)	0.09	0 100 100	27, 48, 58, 79	0
2	2B	120/121 (99%)	-0.34	0 100 100	58, 78, 85, 87	0
3	1D	275/276 (99%)	0.48	5 (1%) 68 64	20, 35, 50, 73	0
3	2D	275/276 (99%)	0.70	12 (4%) 34 27	33, 51, 62, 73	0
4	1E	204/206 (99%)	0.53	2 (0%) 82 80	18, 40, 57, 73	0
4	2E	204/206 (99%)	0.45	7 (3%) 45 38	35, 58, 69, 79	0
5	1F	203/210 (96%)	0.36	0 100 100	16, 41, 63, 80	0
5	2F	203/210 (96%)	0.57	7 (3%) 45 38	37, 64, 77, 83	0
6	1G	181/182 (99%)	0.15	1 (0%) 89 88	39, 56, 69, 78	0
6	2G	181/182 (99%)	0.73	23 (12%) 3 2	68, 77, 85, 93	0
7	1H	174/180 (96%)	0.12	0 100 100	37, 50, 62, 71	0
7	2H	174/180 (96%)	1.38	47 (27%) 0 0	67, 78, 84, 91	0
8	1I	146/148 (98%)	0.05	2 (1%) 75 71	45, 70, 77, 81	0
8	2I	146/148 (98%)	0.33	11 (7%) 14 10	53, 70, 80, 85	0
9	1N	140/140 (100%)	0.37	1 (0%) 87 86	26, 38, 54, 72	0
9	2N	140/140 (100%)	1.15	29 (20%) 1 0	46, 64, 75, 80	0
10	1O	122/122 (100%)	0.46	0 100 100	26, 40, 55, 61	0
10	2O	122/122 (100%)	0.59	5 (4%) 37 30	44, 57, 68, 73	0
11	1P	149/150 (99%)	0.72	5 (3%) 45 38	17, 44, 64, 72	0
11	2P	149/150 (99%)	1.50	45 (30%) 0 0	38, 64, 77, 83	0
12	1Q	141/141 (100%)	0.38	1 (0%) 87 86	27, 41, 54, 74	0
12	2Q	141/141 (100%)	0.79	15 (10%) 6 4	52, 65, 74, 80	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%)	0.41	0 100 100	22, 34, 47, 55	0
13	2R	118/118 (100%)	0.36	0 100 100	38, 51, 59, 67	0
14	1S	110/112 (98%)	0.16	0 100 100	37, 49, 61, 65	0
14	2S	110/112 (98%)	0.55	10 (9%) 9 6	63, 73, 80, 84	0
15	1T	131/146 (89%)	0.47	0 100 100	33, 43, 64, 70	0
15	2T	131/146 (89%)	0.35	4 (3%) 49 42	49, 59, 74, 79	0
16	1U	116/118 (98%)	0.48	1 (0%) 84 82	20, 29, 47, 60	0
16	2U	116/118 (98%)	1.01	17 (14%) 2 1	47, 61, 74, 80	0
17	1V	101/101 (100%)	0.35	0 100 100	20, 39, 56, 69	0
17	2V	101/101 (100%)	0.95	14 (13%) 2 1	42, 68, 76, 82	0
18	1W	112/113 (99%)	0.40	0 100 100	21, 30, 46, 75	0
18	2W	112/113 (99%)	0.56	2 (1%) 68 64	38, 50, 66, 88	0
19	1X	95/96 (98%)	0.30	0 100 100	24, 36, 55, 72	0
19	2X	95/96 (98%)	0.31	3 (3%) 47 40	44, 58, 70, 81	0
20	1Y	107/110 (97%)	0.28	0 100 100	33, 48, 66, 74	0
20	2Y	107/110 (97%)	1.02	17 (15%) 1 1	59, 68, 75, 84	0
21	1Z	154/206 (74%)	0.13	1 (0%) 89 88	41, 60, 77, 85	0
21	2Z	160/206 (77%)	0.44	4 (2%) 57 51	66, 78, 86, 88	0
22	10	83/85 (97%)	0.80	7 (8%) 11 7	27, 37, 60, 72	0
22	20	83/85 (97%)	1.50	19 (22%) 0 0	53, 64, 74, 83	0
23	11	97/98 (98%)	0.51	2 (2%) 63 58	24, 43, 63, 68	0
23	21	97/98 (98%)	1.11	16 (16%) 1 1	40, 56, 71, 73	0
24	12	70/72 (97%)	0.20	1 (1%) 75 71	32, 46, 57, 65	0
24	22	70/72 (97%)	0.43	1 (1%) 75 71	54, 68, 73, 76	0
25	13	59/60 (98%)	0.40	1 (1%) 70 66	25, 36, 58, 78	0
25	23	59/60 (98%)	2.02	27 (45%) 0 0	53, 64, 77, 79	0
26	14	69/71 (97%)	-0.07	0 100 100	49, 71, 81, 85	0
26	24	69/71 (97%)	0.26	7 (10%) 7 4	76, 82, 88, 91	0
27	15	59/60 (98%)	0.44	1 (1%) 70 66	18, 29, 45, 63	0
27	25	59/60 (98%)	0.33	2 (3%) 45 38	38, 50, 63, 67	0
28	16	53/54 (98%)	0.58	0 100 100	30, 41, 55, 61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	1.21	10 (18%) 1 0	49, 61, 68, 75	0
29	17	48/49 (97%)	0.70	3 (6%) 20 15	18, 24, 52, 58	0
29	27	48/49 (97%)	1.07	7 (14%) 2 1	32, 41, 60, 68	0
30	18	64/65 (98%)	0.76	2 (3%) 49 42	26, 31, 38, 54	0
30	28	64/65 (98%)	1.55	17 (26%) 0 0	45, 54, 60, 71	0
31	19	37/37 (100%)	0.27	0 100 100	27, 38, 54, 57	0
31	29	37/37 (100%)	1.47	11 (29%) 0 0	59, 66, 73, 76	0
32	1a	1488/1521 (97%)	-0.02	24 (1%) 72 68	33, 65, 87, 100	0
32	2a	1491/1521 (98%)	0.10	50 (3%) 45 38	50, 75, 91, 99	0
33	1b	231/256 (90%)	0.21	7 (3%) 50 43	63, 74, 82, 87	0
33	2b	231/256 (90%)	1.42	63 (27%) 0 0	71, 83, 88, 92	0
34	1c	206/239 (86%)	0.94	35 (16%) 1 1	59, 70, 78, 83	0
34	2c	206/239 (86%)	1.89	90 (43%) 0 0	72, 82, 87, 91	0
35	1d	208/209 (99%)	0.51	12 (5%) 23 17	56, 69, 80, 84	0
35	2d	208/209 (99%)	0.27	3 (1%) 75 71	57, 67, 75, 82	0
36	1e	148/162 (91%)	0.40	3 (2%) 65 60	49, 63, 70, 76	0
36	2e	148/162 (91%)	0.76	19 (12%) 3 2	67, 76, 81, 88	0
37	1f	100/101 (99%)	0.21	0 100 100	50, 64, 70, 73	0
37	2f	100/101 (99%)	0.16	2 (2%) 65 60	60, 70, 77, 81	0
38	1g	155/156 (99%)	0.97	19 (12%) 4 2	50, 67, 76, 87	0
38	2g	155/156 (99%)	1.36	33 (21%) 0 0	66, 75, 82, 88	0
39	1h	137/138 (99%)	0.55	5 (3%) 42 35	56, 64, 71, 75	0
39	2h	137/138 (99%)	0.69	11 (8%) 12 9	67, 75, 80, 86	0
40	1i	127/128 (99%)	0.67	10 (7%) 12 9	52, 72, 77, 79	0
40	2i	127/128 (99%)	2.01	56 (44%) 0 0	68, 80, 86, 89	0
41	1j	97/105 (92%)	1.06	15 (15%) 2 1	58, 76, 83, 89	0
41	2j	96/105 (91%)	2.13	48 (50%) 0 0	71, 82, 88, 96	0
42	1k	114/129 (88%)	1.15	17 (14%) 2 1	38, 61, 70, 74	0
42	2k	114/129 (88%)	1.20	22 (19%) 1 0	56, 72, 77, 82	0
43	1l	121/132 (91%)	0.34	3 (2%) 57 51	42, 56, 66, 69	0
43	2l	121/132 (91%)	0.72	12 (9%) 7 5	58, 69, 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	123/126 (97%)	0.06	5 (4%) 37 30	55, 67, 75, 81	0
44	2m	122/126 (96%)	1.72	43 (35%) 0 0	71, 79, 85, 88	0
45	1n	60/61 (98%)	1.16	12 (20%) 1 0	60, 68, 73, 76	0
45	2n	60/61 (98%)	3.35	44 (73%) 0 0	74, 82, 86, 90	0
46	1o	88/89 (98%)	0.34	2 (2%) 60 54	48, 60, 70, 74	0
46	2o	88/89 (98%)	0.54	4 (4%) 33 26	60, 70, 78, 82	0
47	1p	82/88 (93%)	0.85	5 (6%) 21 16	56, 70, 76, 79	0
47	2p	82/88 (93%)	0.22	0 100 100	58, 65, 74, 80	0
48	1q	99/105 (94%)	0.52	2 (2%) 65 60	50, 63, 71, 73	0
48	2q	99/105 (94%)	1.01	17 (17%) 1 0	62, 69, 77, 81	0
49	1r	68/88 (77%)	0.75	6 (8%) 10 7	55, 64, 73, 75	0
49	2r	68/88 (77%)	0.57	6 (8%) 10 7	62, 71, 78, 82	0
50	1s	83/93 (89%)	0.00	0 100 100	60, 70, 77, 80	0
50	2s	83/93 (89%)	1.58	27 (32%) 0 0	75, 82, 87, 91	0
51	1t	96/106 (90%)	0.41	6 (6%) 20 15	58, 68, 76, 81	0
51	2t	96/106 (90%)	0.68	11 (11%) 4 3	57, 69, 76, 79	0
52	1u	23/27 (85%)	0.85	3 (13%) 3 2	59, 64, 69, 71	0
52	2u	23/27 (85%)	2.05	11 (47%) 0 0	74, 77, 81, 85	0
53	1v	13/24 (54%)	1.28	5 (38%) 0 0	47, 66, 80, 86	0
53	2v	13/24 (54%)	1.67	5 (38%) 0 0	69, 82, 92, 92	0
54	1w	67/76 (88%)	1.66	19 (28%) 0 0	59, 87, 94, 98	0
54	1y	67/76 (88%)	1.36	18 (26%) 0 0	38, 86, 93, 96	0
54	2w	65/76 (85%)	2.95	39 (60%) 0 0	74, 91, 96, 101	0
54	2y	66/76 (86%)	1.92	33 (50%) 0 0	57, 92, 96, 99	0
55	1x	72/77 (93%)	0.22	1 (1%) 75 71	37, 62, 77, 85	0
55	2x	72/77 (93%)	0.15	1 (1%) 75 71	55, 78, 86, 89	0
All	All	20875/21748 (95%)	0.50	1412 (6%) 17 12	16, 62, 85, 102	0

All (1412) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	11.9
38	2g	80	VAL	11.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	1w	71	G	10.9
38	1g	80	VAL	10.4
44	2m	6	GLY	9.0
45	2n	25	VAL	8.9
54	1w	72	C	8.5
38	2g	81	GLY	8.4
54	1w	70	G	8.3
22	20	2	ALA	8.1
50	2s	79	THR	8.0
54	2w	76	A	7.9
44	2m	120	LYS	7.9
38	1g	82	GLY	7.8
54	2w	71	G	7.8
3	2D	2	ALA	7.6
45	2n	44	LEU	7.6
32	2a	1030(B)	C	7.6
44	2m	123	ALA	7.6
44	2m	102	ARG	7.5
54	2w	4	C	7.3
54	2w	72	C	7.2
34	1c	39	ILE	7.2
41	2j	47	PHE	7.2
54	2w	31	A	7.2
54	2w	70	G	7.2
22	20	5	LYS	7.1
40	2i	115	GLY	7.1
25	23	26	LEU	6.9
22	10	7	LEU	6.7
23	21	2	SER	6.7
1	2A	2146	C	6.7
38	2g	82	GLY	6.7
54	1w	73	A	6.6
54	2w	3	C	6.6
54	2w	73	A	6.5
54	2w	75	C	6.5
40	2i	123	PRO	6.4
38	1g	79	ARG	6.3
32	2a	1034	G	6.3
45	2n	38	GLY	6.3
45	2n	34	TYR	6.3
45	2n	39	LEU	6.3
40	2i	7	THR	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	1y	20	U	6.2
45	1n	2	ALA	6.2
22	10	5	LYS	6.1
1	2A	229	A	6.1
38	1g	85	TYR	6.1
45	2n	36	PHE	6.0
33	2b	165	VAL	6.0
40	2i	36	TYR	6.0
38	2g	78	ARG	5.9
22	10	6	GLY	5.9
20	2Y	5	MET	5.8
33	2b	187	LEU	5.7
32	2a	1030(A)	G	5.7
54	2y	36	A	5.7
44	1m	124	PRO	5.7
31	29	37	GLY	5.7
38	2g	154	TYR	5.7
34	2c	64	VAL	5.7
22	10	4	LYS	5.7
40	2i	124	GLN	5.6
32	2a	1033	G	5.6
34	2c	53	ALA	5.6
34	2c	65	ALA	5.6
50	2s	80	TYR	5.5
44	2m	5	ALA	5.5
45	2n	35	ARG	5.5
38	2g	156	TRP	5.5
32	1a	1036	G	5.5
54	2w	74	C	5.5
44	2m	121	LYS	5.4
45	2n	12	ARG	5.4
22	20	7	LEU	5.4
41	2j	85	LEU	5.4
45	2n	42	ILE	5.3
12	2Q	104	PHE	5.3
38	2g	84	ASN	5.3
52	2u	14	TRP	5.3
34	2c	8	ILE	5.2
32	2a	1036	G	5.2
34	2c	182	ILE	5.2
50	2s	82	GLY	5.2
41	2j	65	LEU	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	47	LEU	5.2
1	1A	2145	C	5.1
34	2c	4	LYS	5.1
38	1g	154	TYR	5.0
40	2i	127	LYS	5.0
45	2n	22	THR	5.0
40	2i	114	TYR	5.0
32	2a	1001(A)	G	5.0
40	2i	106	ALA	4.9
54	1w	76	A	4.9
33	2b	37	ASN	4.9
36	2e	109	ILE	4.9
40	2i	52	ALA	4.9
25	23	59	VAL	4.9
1	2A	2145	C	4.8
41	2j	55	LYS	4.8
1	2A	652(B)	A	4.8
7	2H	107	VAL	4.8
34	2c	59	ARG	4.8
22	20	76	GLY	4.8
54	2w	5	G	4.8
54	2w	28	G	4.8
33	2b	215	LEU	4.8
34	2c	33	LEU	4.8
40	2i	81	ILE	4.7
54	1w	3	C	4.7
32	2a	1035	A	4.7
54	1y	35	A	4.7
34	2c	80	GLY	4.7
45	2n	11	LYS	4.7
44	2m	66	LEU	4.7
45	2n	53	LEU	4.6
54	1w	2	C	4.6
54	2w	69	G	4.6
34	2c	202	ILE	4.6
1	1A	2146	C	4.6
38	1g	156	TRP	4.6
44	2m	90	LEU	4.6
7	2H	35	VAL	4.6
34	2c	190	ARG	4.6
38	2g	85	TYR	4.6
34	2c	198	VAL	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	2l	18	VAL	4.6
1	1A	2159	G	4.5
22	10	3	HIS	4.5
33	2b	201	ILE	4.5
45	2n	10	ALA	4.5
41	2j	50	ILE	4.5
1	1A	2112	G	4.5
50	2s	53	ASN	4.5
25	23	29	ARG	4.5
45	2n	29	ARG	4.5
34	2c	81	GLY	4.5
41	2j	48	THR	4.5
45	2n	37	PHE	4.5
33	2b	214	ILE	4.5
33	2b	216	SER	4.5
53	1v	12	A	4.5
45	2n	31	ARG	4.5
38	1g	83	ALA	4.5
33	2b	152	PHE	4.4
40	2i	109	VAL	4.4
8	2l	12	LEU	4.4
32	2a	1001	A	4.4
33	2b	118	LEU	4.4
45	2n	56	VAL	4.4
40	2i	53	VAL	4.4
50	2s	14	HIS	4.4
41	2j	93	GLY	4.4
1	1A	2129	C	4.4
35	1d	180	GLY	4.4
45	2n	58	LYS	4.4
42	2k	50	TYR	4.4
34	2c	91	LEU	4.3
34	2c	134	ILE	4.3
3	1D	276	LYS	4.3
40	2i	14	VAL	4.3
33	2b	131	PRO	4.3
44	2m	60	VAL	4.3
34	2c	200	ALA	4.3
40	2i	82	ALA	4.3
33	2b	185	ILE	4.3
1	2A	2144	U	4.3
22	10	8	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	78	ILE	4.3
38	2g	79	ARG	4.3
50	2s	52	TYR	4.3
41	1j	98	ILE	4.3
40	2i	79	LEU	4.3
41	2j	41	PRO	4.3
32	1a	1532	U	4.3
42	2k	25	TYR	4.3
6	2G	157	ILE	4.3
34	2c	57	ILE	4.3
41	2j	98	ILE	4.3
38	2g	16	LEU	4.2
44	2m	119	GLY	4.2
20	2Y	106	LEU	4.2
7	2H	123	PHE	4.2
1	1A	1509	C	4.2
38	2g	4	ARG	4.2
40	2i	125	TYR	4.2
45	2n	7	ILE	4.2
52	2u	5	ASP	4.2
41	2j	66	ARG	4.2
54	2w	2	C	4.2
34	2c	186	PHE	4.2
53	2v	12	A	4.2
44	2m	122	LYS	4.2
41	2j	96	ILE	4.2
1	1A	2141	G	4.1
34	2c	87	LEU	4.1
33	2b	163	PHE	4.1
38	2g	147	ALA	4.1
34	2c	5	ILE	4.1
29	27	23	ARG	4.1
22	20	4	LYS	4.1
41	1j	97	GLU	4.1
34	2c	124	ILE	4.1
34	2c	52	LEU	4.1
33	2b	71	VAL	4.1
33	2b	101	MET	4.1
41	2j	62	HIS	4.1
1	1A	2158	A	4.1
11	2P	79	ARG	4.1
7	2H	24	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2140	C	4.1
41	2j	63	PHE	4.1
6	2G	152	LEU	4.0
7	2H	103	LEU	4.0
7	2H	72	ILE	4.0
7	2H	101	ARG	4.0
54	1y	36	A	4.0
33	2b	203	GLY	4.0
54	1w	4	C	4.0
44	2m	92	HIS	4.0
1	2A	2112	G	4.0
7	2H	115	VAL	4.0
32	1a	1030(B)	C	4.0
21	2Z	149	SER	4.0
44	2m	88	ARG	4.0
45	2n	24	CYS	4.0
34	2c	178	LEU	4.0
45	2n	59	ALA	4.0
44	2m	87	TYR	3.9
32	1a	1531	A	3.9
33	2b	93	VAL	3.9
42	2k	109	VAL	3.9
45	1n	59	ALA	3.9
54	2w	56	C	3.9
42	1k	25	TYR	3.9
34	2c	179	ARG	3.9
41	2j	10	GLY	3.9
34	2c	188	LEU	3.9
34	2c	184	TYR	3.9
41	2j	67	THR	3.9
33	2b	81	VAL	3.9
45	2n	6	LEU	3.9
16	2U	90	VAL	3.9
26	24	50	VAL	3.9
44	2m	95	GLY	3.9
34	2c	206	GLU	3.8
1	2A	2154	G	3.8
52	2u	11	GLY	3.8
9	2N	69	GLN	3.8
44	2m	94	ARG	3.8
17	2V	73	SER	3.8
41	2j	72	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	645	C	3.8
54	2w	23	A	3.8
54	2y	23	A	3.8
14	2S	20	ARG	3.8
1	1A	2113	U	3.8
40	2i	19	LEU	3.8
54	1w	44	G	3.8
33	2b	186	ALA	3.8
40	2i	128	ARG	3.8
45	2n	13	THR	3.8
52	2u	6	ARG	3.8
40	2i	41	VAL	3.8
28	26	54	ILE	3.8
54	2w	13	C	3.8
25	23	47	VAL	3.8
41	2j	59	SER	3.8
34	2c	113	ALA	3.7
40	2i	108	VAL	3.7
33	2b	228	GLY	3.7
50	2s	31	ILE	3.7
31	29	25	VAL	3.7
54	1w	74	C	3.7
25	23	60	GLU	3.7
38	2g	32	ARG	3.7
43	2l	13	LYS	3.7
51	2t	24	LEU	3.7
38	2g	83	ALA	3.7
1	1A	2109	U	3.7
50	2s	32	LYS	3.7
54	2y	35	A	3.7
9	2N	5	VAL	3.7
9	2N	10	GLU	3.7
20	2Y	45	VAL	3.7
23	21	28	GLY	3.7
11	2P	45	LEU	3.7
45	2n	16	PHE	3.7
41	1j	46	ARG	3.7
54	1w	1	G	3.7
11	2P	91	PHE	3.7
38	2g	152	ALA	3.7
40	2i	122	ALA	3.7
42	1k	92	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	2V	71	LEU	3.6
41	2j	27	ALA	3.6
32	2a	1026	G	3.6
42	2k	60	ALA	3.6
11	2P	109	GLY	3.6
32	2a	1257	U	3.6
25	23	28	LEU	3.6
48	2q	22	LEU	3.6
25	23	21	ALA	3.6
54	2w	6	G	3.6
7	2H	106	THR	3.6
31	29	12	ASP	3.6
54	2w	14	A	3.6
32	2a	1030	C	3.6
33	2b	207	ALA	3.6
34	2c	177	THR	3.6
8	2I	1	MET	3.6
35	1d	135	LEU	3.6
39	2h	2	LEU	3.6
38	1g	81	GLY	3.6
40	1i	117	HIS	3.6
22	10	2	ALA	3.6
44	1m	123	ALA	3.6
6	2G	39	ILE	3.6
36	2e	12	LEU	3.6
11	2P	31	ALA	3.6
19	2X	92	LEU	3.6
1	1A	2131	G	3.6
54	2y	53	G	3.6
48	2q	30	PRO	3.6
6	2G	139	LEU	3.6
38	1g	78	ARG	3.5
54	1y	47	U	3.5
52	2u	17	THR	3.5
32	1a	1001(A)	G	3.5
34	1c	12	LEU	3.5
1	1A	2132	U	3.5
54	2w	45	U	3.5
25	23	6	VAL	3.5
45	2n	41	ARG	3.5
30	28	29	LYS	3.5
38	2g	155	ARG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2128	C	3.5
50	2s	84	GLY	3.5
41	2j	46	ARG	3.5
41	2j	44	VAL	3.5
32	2a	1032	G	3.5
54	1w	69	G	3.5
54	2y	65	G	3.5
32	2a	1321	C	3.5
3	2D	38	LYS	3.5
34	2c	174	PRO	3.5
41	2j	89	ASP	3.5
1	1A	2138	C	3.5
32	1a	1257	U	3.5
7	2H	94	TYR	3.5
40	2i	105	ASP	3.5
36	2e	81	GLU	3.4
1	1A	2111	C	3.4
11	2P	110	TYR	3.4
33	2b	31	TYR	3.4
34	2c	149	ALA	3.4
42	2k	23	ALA	3.4
53	2v	23	A	3.4
35	1d	170	VAL	3.4
33	2b	90	MET	3.4
54	2w	41	C	3.4
45	2n	57	ARG	3.4
34	1c	15	THR	3.4
54	2w	19	G	3.4
23	2l	29	GLY	3.4
31	29	16	VAL	3.4
11	2P	118	GLY	3.4
33	2b	161	ALA	3.4
6	2G	51	ARG	3.4
40	2i	9	ARG	3.4
20	2Y	1	MET	3.4
30	28	25	MET	3.4
32	1a	1002	G	3.4
32	2a	1003	G	3.4
42	1k	97	ALA	3.4
50	2s	13	ASP	3.4
40	2i	90	PRO	3.4
6	1G	139	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	23	23	LEU	3.4
34	1c	64	VAL	3.4
41	2j	71	LEU	3.4
9	2N	116	LEU	3.4
34	2c	205	GLY	3.4
45	2n	8	GLU	3.4
50	2s	30	LEU	3.4
1	2A	883	G	3.3
21	2Z	144	LEU	3.3
33	2b	164	VAL	3.3
53	2v	24	A	3.3
54	2w	38	A	3.3
32	2a	1030(C)	G	3.3
36	2e	31	LEU	3.3
45	2n	50	LYS	3.3
29	17	46	VAL	3.3
26	24	51	ASP	3.3
43	2l	56	ALA	3.3
1	2A	2155	G	3.3
54	2y	34	G	3.3
8	2I	3	VAL	3.3
22	20	3	HIS	3.3
33	2b	211	ILE	3.3
7	2H	102	ALA	3.3
33	2b	83	MET	3.3
4	2E	195	LEU	3.3
12	2Q	37	LEU	3.3
34	2c	204	LEU	3.3
49	1r	78	LEU	3.3
53	2v	13	A	3.3
20	2Y	44	ILE	3.3
6	2G	2	PRO	3.3
11	2P	92	GLU	3.3
40	2i	86	VAL	3.3
45	1n	7	ILE	3.3
7	2H	96	ALA	3.3
32	2a	1002	G	3.3
34	2c	19	GLU	3.3
6	2G	49	ASP	3.3
1	2A	2169	A	3.3
33	2b	77	ALA	3.3
40	2i	116	LYS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2151	G	3.3
34	2c	12	LEU	3.3
54	2y	52	G	3.3
28	26	52	VAL	3.2
23	21	69	LYS	3.2
40	1i	106	ALA	3.2
41	1j	18	ALA	3.2
1	2A	1847	A	3.2
40	2i	121	ARG	3.2
44	2m	70	LEU	3.2
44	2m	106	ASN	3.2
43	2l	39	VAL	3.2
36	2e	86	ALA	3.2
6	2G	29	TRP	3.2
42	1k	123	LYS	3.2
54	1y	21	A	3.2
7	2H	76	VAL	3.2
40	2i	28	VAL	3.2
52	2u	16	GLY	3.2
7	2H	148	ILE	3.2
12	2Q	6	ARG	3.2
41	2j	16	LEU	3.2
45	2n	61	TRP	3.2
34	2c	120	VAL	3.2
48	2q	23	VAL	3.2
33	2b	92	TYR	3.2
45	2n	23	ARG	3.2
1	1A	2190	G	3.2
38	1g	84	ASN	3.2
22	20	6	GLY	3.2
34	2c	37	GLN	3.2
36	1e	89	ILE	3.2
34	1c	180	ALA	3.2
6	2G	133	LEU	3.2
1	2A	2133	G	3.2
34	2c	6	HIS	3.2
40	2i	117	HIS	3.2
45	2n	45	ARG	3.2
34	2c	10	PHE	3.2
42	1k	15	ALA	3.2
41	2j	88	LEU	3.2
44	2m	99	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1037	C	3.2
26	24	49	PHE	3.2
36	2e	16	THR	3.2
42	2k	125	PHE	3.2
32	1a	1030(A)	G	3.2
32	2a	1202	G	3.2
54	2y	15	G	3.2
7	2H	128	PRO	3.2
34	1c	87	LEU	3.2
41	2j	56	HIS	3.1
28	26	5	VAL	3.1
1	2A	2174	C	3.1
1	2A	2149	G	3.1
42	2k	126	ARG	3.1
52	2u	23	PRO	3.1
17	2V	72	VAL	3.1
34	2c	153	VAL	3.1
26	24	68	ARG	3.1
44	2m	4	ILE	3.1
50	2s	81	ARG	3.1
14	2S	58	LEU	3.1
35	1d	21	LEU	3.1
54	2y	24	G	3.1
22	20	37	LEU	3.1
44	2m	23	TYR	3.1
41	2j	54	PHE	3.1
10	2O	99	PHE	3.1
9	2N	23	LEU	3.1
23	11	2	SER	3.1
34	1c	34	LEU	3.1
34	2c	189	ALA	3.1
34	2c	7	PRO	3.1
30	28	46	ARG	3.1
1	1A	1847	A	3.1
1	1A	2161	C	3.1
45	2n	4	LYS	3.1
35	1d	105	VAL	3.1
33	2b	232	PRO	3.1
1	2A	2118	U	3.1
25	23	35	ARG	3.1
34	2c	69	HIS	3.1
45	2n	49	HIS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	166	GLY	3.1
33	2b	122	PHE	3.1
34	2c	21	ARG	3.1
34	2c	152	ILE	3.1
48	2q	91	ARG	3.1
26	24	63	TYR	3.0
36	2e	133	TYR	3.0
9	2N	9	VAL	3.0
11	2P	101	VAL	3.0
54	2w	22	G	3.0
53	1v	13	A	3.0
34	2c	23	TYR	3.0
40	2i	102	LEU	3.0
25	23	12	PRO	3.0
30	28	16	ILE	3.0
33	2b	208	ILE	3.0
34	2c	55	VAL	3.0
12	2Q	33	GLY	3.0
41	2j	6	ILE	3.0
45	2n	55	GLY	3.0
54	1y	56	C	3.0
9	2N	48	MET	3.0
9	2N	73	THR	3.0
54	2y	33	U	3.0
7	2H	36	PRO	3.0
16	2U	62	ILE	3.0
44	2m	7	VAL	3.0
54	2w	30	G	3.0
49	1r	40	LEU	3.0
1	2A	2109	U	3.0
12	2Q	66	ILE	3.0
20	2Y	61	ILE	3.0
29	27	47	ARG	3.0
48	2q	42	TYR	3.0
11	1P	108	LYS	3.0
5	2F	37	VAL	3.0
25	23	53	LEU	3.0
32	2a	1114	C	3.0
36	2e	21	ALA	3.0
54	2w	29	G	3.0
48	2q	100	LYS	3.0
38	2g	151	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	103	THR	3.0
11	2P	148	LEU	3.0
41	2j	49	VAL	3.0
44	2m	100	GLY	3.0
7	2H	89	ILE	2.9
1	1A	2160	G	2.9
1	2A	2159	G	2.9
5	2F	89	VAL	2.9
7	2H	45	VAL	2.9
12	1Q	81	VAL	2.9
3	1D	2	ALA	2.9
45	2n	2	ALA	2.9
39	1h	13	ILE	2.9
32	2a	1040	U	2.9
32	2a	973	G	2.9
4	2E	52	LEU	2.9
40	1i	47	LEU	2.9
36	2e	90	VAL	2.9
49	2r	86	VAL	2.9
9	2N	102	ALA	2.9
33	2b	97	TRP	2.9
34	2c	17	ASP	2.9
34	2c	176	HIS	2.9
1	2A	2111	C	2.9
51	1t	69	GLY	2.9
24	22	60	LEU	2.9
30	28	60	LEU	2.9
39	2h	112	LEU	2.9
1	1A	2162	G	2.9
32	2a	1220	G	2.9
43	2l	68	ALA	2.9
54	2y	63	G	2.9
30	28	65	GLU	2.9
34	2c	157	ILE	2.9
44	2m	25	ILE	2.9
34	1c	72	LYS	2.9
41	2j	60	ARG	2.9
49	1r	31	LEU	2.9
4	1E	1	MET	2.9
30	28	23	VAL	2.9
32	1a	1030	C	2.9
32	2a	1027	C	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	2P	78	PRO	2.9
38	1g	153	HIS	2.9
41	1j	5	ARG	2.9
34	2c	145	GLY	2.9
35	1d	101	LEU	2.9
40	2i	110	GLU	2.9
48	2q	9	VAL	2.9
29	27	48	LYS	2.9
38	2g	88	PRO	2.9
54	1y	13	C	2.9
44	2m	84	ILE	2.9
32	2a	1224	G	2.9
54	2w	15	G	2.9
54	2y	1	G	2.9
6	2G	149	VAL	2.9
7	2H	113	VAL	2.9
7	2H	114	VAL	2.9
9	2N	1	MET	2.9
34	1c	193	TYR	2.9
46	2o	27	VAL	2.9
1	1A	271(K)	U	2.9
7	2H	21	PRO	2.9
34	2c	71	ALA	2.9
51	2t	9	ASN	2.9
52	1u	14	TRP	2.9
1	1A	2108	C	2.9
54	2w	40	C	2.9
1	2A	2127	G	2.9
44	2m	104	ARG	2.9
11	2P	97	PRO	2.9
40	2i	4	TYR	2.9
14	2S	35	ILE	2.8
33	2b	132	LYS	2.8
50	2s	38	SER	2.8
38	1g	99	LEU	2.8
9	2N	46	VAL	2.8
50	2s	50	ALA	2.8
54	2y	45	U	2.8
1	2A	2142	C	2.8
32	1a	1027	C	2.8
7	2H	34	GLU	2.8
41	2j	64	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2119	A	2.8
29	17	48	LYS	2.8
40	2i	27	THR	2.8
29	27	1	MET	2.8
32	1a	1028	C	2.8
42	2k	89	ALA	2.8
44	1m	2	ALA	2.8
3	1D	275	LYS	2.8
30	28	41	ILE	2.8
36	2e	89	ILE	2.8
11	2P	85	LEU	2.8
23	21	98	LEU	2.8
1	2A	1026	U	2.8
29	27	46	VAL	2.8
32	2a	1222	G	2.8
34	2c	185	GLY	2.8
50	2s	40	ILE	2.8
41	1j	100	THR	2.8
54	2y	47	U	2.8
6	2G	160	VAL	2.8
17	2V	1	MET	2.8
36	2e	82	VAL	2.8
45	2n	18	VAL	2.8
9	2N	104	LYS	2.8
38	2g	149	ARG	2.8
1	1A	2119	A	2.8
1	2A	2110	G	2.8
11	2P	74	GLU	2.8
34	2c	39	ILE	2.8
39	2h	83	ILE	2.8
41	2j	11	PHE	2.8
54	2y	48	C	2.8
34	2c	41	GLY	2.8
34	1c	66	VAL	2.8
8	2I	85	GLU	2.8
40	2i	126	SER	2.8
1	2A	2116	G	2.8
1	2A	2153	G	2.8
1	2A	2166	G	2.8
7	2H	105	LEU	2.8
34	1c	196	LEU	2.8
54	2y	18	G	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2174	C	2.8
16	2U	43	GLY	2.8
51	2t	26	ASN	2.8
38	2g	40	ALA	2.7
34	1c	201	TYR	2.7
17	2V	101	GLY	2.7
33	1b	196	LEU	2.7
44	2m	19	LEU	2.7
3	2D	271	ILE	2.7
1	2A	2128	C	2.7
1	2A	2147	G	2.7
32	1a	1030(C)	G	2.7
32	2a	998	G	2.7
33	1b	136	VAL	2.7
35	2d	32	ALA	2.7
38	2g	89	MET	2.7
33	2b	96	ARG	2.7
41	1j	47	PHE	2.7
34	1c	152	ILE	2.7
40	1i	65	VAL	2.7
44	2m	118	ALA	2.7
1	2A	2170	A	2.7
53	1v	14	A	2.7
1	1A	2100	G	2.7
32	2a	1061	G	2.7
54	1w	5	G	2.7
11	2P	59	LEU	2.7
29	17	47	ARG	2.7
34	1c	43	LEU	2.7
47	1p	59	TRP	2.7
48	2q	32	TYR	2.7
54	2y	66	U	2.7
11	2P	75	ILE	2.7
25	23	43	ILE	2.7
12	2Q	22	LYS	2.7
33	2b	112	VAL	2.7
33	2b	130	ARG	2.7
45	1n	57	ARG	2.7
32	2a	1225	A	2.7
1	2A	2125	G	2.7
1	2A	2802	G	2.7
34	2c	201	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2y	6	G	2.7
34	1c	14	ILE	2.7
7	2H	29	PRO	2.7
20	2Y	65	ALA	2.7
44	2m	97	PRO	2.7
8	2I	19	VAL	2.7
33	2b	48	MET	2.7
40	2i	67	GLY	2.7
38	2g	86	GLN	2.7
33	2b	33	TYR	2.7
40	2i	88	TYR	2.7
54	2y	56	C	2.7
32	2a	1532	U	2.7
41	2j	74	ILE	2.7
1	2A	2160	G	2.7
38	2g	77	SER	2.7
11	2P	90	ARG	2.7
11	2P	68	GLN	2.7
33	2b	95	GLN	2.7
7	2H	88	LEU	2.7
32	1a	345	C	2.7
1	2A	2132	U	2.7
54	1w	20	U	2.7
54	2w	12	U	2.7
34	2c	187	ALA	2.7
54	2y	22	G	2.7
21	1Z	1	MET	2.7
11	2P	105	LEU	2.7
9	2N	75	TYR	2.7
33	2b	58	ILE	2.7
33	2b	109	SER	2.7
16	2U	117	GLN	2.6
4	2E	167	VAL	2.6
23	2I	14	VAL	2.6
33	2b	98	LEU	2.6
54	2w	44	G	2.6
23	2I	26	ARG	2.6
40	2i	83	ARG	2.6
44	2m	93	ARG	2.6
11	2P	116	GLY	2.6
34	1c	185	GLY	2.6
7	2H	19	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	23	54	VAL	2.6
54	1w	75	C	2.6
5	2F	131	GLY	2.6
30	28	38	GLY	2.6
5	2F	81	PRO	2.6
34	2c	60	ALA	2.6
21	2Z	139	VAL	2.6
45	1n	33	VAL	2.6
1	1A	2130	U	2.6
9	2N	107	LEU	2.6
11	2P	147	LEU	2.6
36	2e	25	ARG	2.6
34	2c	56	ASP	2.6
54	2y	2	C	2.6
33	2b	32	ILE	2.6
48	2q	36	ILE	2.6
23	21	68	PRO	2.6
28	26	35	GLU	2.6
1	1A	2115	G	2.6
1	1A	2116	G	2.6
11	1P	15	ARG	2.6
42	1k	126	ARG	2.6
41	2j	40	LEU	2.6
1	2A	2113	U	2.6
22	20	45	PHE	2.6
30	28	15	LYS	2.6
54	2y	3	C	2.6
40	2i	5	TYR	2.6
43	2l	64	TYR	2.6
6	2G	136	ARG	2.6
11	2P	65	ARG	2.6
28	26	20	ASN	2.6
54	2y	73	A	2.6
7	2H	13	LYS	2.6
9	2N	113	GLY	2.6
33	2b	133	LYS	2.6
49	2r	43	PHE	2.6
42	2k	43	SER	2.6
44	2m	68	GLY	2.6
33	2b	223	ILE	2.6
39	2h	92	ARG	2.6
40	2i	103	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	120	ALA	2.6
54	1y	23	A	2.6
40	2i	33	PHE	2.6
28	26	28	ARG	2.6
34	2c	172	ARG	2.6
54	1w	29	G	2.6
27	25	29	THR	2.6
41	1j	96	ILE	2.6
7	2H	73	ALA	2.6
14	2S	34	HIS	2.6
25	23	51	ALA	2.6
1	1A	2164	C	2.6
40	1i	112	LYS	2.6
6	2G	28	VAL	2.6
16	2U	8	VAL	2.6
20	2Y	13	VAL	2.6
46	2o	60	VAL	2.6
48	2q	11	VAL	2.6
54	2w	42	C	2.6
23	21	46	LEU	2.6
34	1c	206	GLU	2.6
11	2P	28	GLY	2.6
34	1c	41	GLY	2.6
51	1t	8	ARG	2.6
53	2v	14	A	2.6
9	2N	84	LYS	2.5
51	2t	63	ILE	2.5
16	2U	35	ALA	2.5
1	2A	2100	G	2.5
1	2A	2182	G	2.5
11	2P	125	VAL	2.5
34	1c	101	LEU	2.5
41	1j	8	LEU	2.5
45	1n	56	VAL	2.5
50	2s	41	VAL	2.5
1	2A	2139	C	2.5
46	2o	68	ARG	2.5
9	2N	47	ALA	2.5
42	2k	31	THR	2.5
42	2k	68	ALA	2.5
54	2w	7	A	2.5
32	1a	841	U	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	100	GLY	2.5
17	2V	5	VAL	2.5
23	21	62	VAL	2.5
3	2D	217	ARG	2.5
51	2t	8	ARG	2.5
54	1y	15	G	2.5
55	2x	70	G	2.5
1	1A	2142	C	2.5
28	26	2	ALA	2.5
42	2k	29	ILE	2.5
50	2s	12	ASP	2.5
50	2s	49	ILE	2.5
11	2P	76	LYS	2.5
25	23	15	TYR	2.5
34	1c	33	LEU	2.5
34	2c	101	LEU	2.5
40	2i	120	ARG	2.5
17	2V	75	PHE	2.5
54	1y	24	G	2.5
54	2w	24	G	2.5
54	2y	62	C	2.5
6	2G	114	ILE	2.5
8	2I	35	LEU	2.5
27	25	58	LEU	2.5
34	1c	207	VAL	2.5
34	2c	66	VAL	2.5
54	1y	14	A	2.5
16	2U	2	PRO	2.5
16	2U	113	ALA	2.5
35	2d	49	ARG	2.5
38	2g	7	ALA	2.5
42	1k	89	ALA	2.5
43	2l	15	ARG	2.5
47	1p	7	ALA	2.5
51	2t	25	ARG	2.5
54	2y	71	G	2.5
41	1j	65	LEU	2.5
25	23	24	LYS	2.5
38	1g	32	ARG	2.5
40	2i	107	ARG	2.5
52	2u	15	ARG	2.5
22	20	42	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	15	THR	2.5
7	2H	37	VAL	2.5
32	2a	1066	C	2.5
38	1g	87	VAL	2.5
39	2h	137	VAL	2.5
40	2i	17	VAL	2.5
49	1r	22	VAL	2.5
17	2V	81	TYR	2.5
34	2c	203	PHE	2.5
51	1t	9	ASN	2.5
41	2j	17	ASP	2.5
16	2U	89	GLU	2.5
41	2j	91	PRO	2.5
20	2Y	48	ALA	2.5
41	2j	68	HIS	2.5
12	2Q	79	LEU	2.5
51	1t	13	LEU	2.5
45	2n	27	CYS	2.5
11	2P	18	ARG	2.5
33	2b	111	ARG	2.5
40	2i	66	ARG	2.5
51	2t	22	ARG	2.5
1	1A	2152	G	2.5
1	2A	2157	G	2.5
32	1a	1034	G	2.5
41	2j	15	THR	2.4
42	1k	57	THR	2.4
1	1A	2117	A	2.4
9	2N	103	VAL	2.4
11	2P	83	VAL	2.4
31	29	19	ARG	2.4
33	2b	144	ARG	2.4
20	2Y	29	GLU	2.4
44	2m	82	MET	2.4
36	2e	85	GLY	2.4
54	2y	61	C	2.4
11	2P	122	PRO	2.4
32	2a	204	U	2.4
40	2i	61	ALA	2.4
42	2k	87	THR	2.4
50	2s	75	ALA	2.4
6	2G	19	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	2N	87	LEU	2.4
15	2T	102	ILE	2.4
23	21	37	ILE	2.4
39	1h	133	LEU	2.4
49	1r	76	LEU	2.4
49	2r	85	LEU	2.4
28	26	42	TRP	2.4
41	2j	61	GLU	2.4
14	2S	57	LYS	2.4
39	2h	90	GLY	2.4
11	2P	30	THR	2.4
16	2U	46	ALA	2.4
32	2a	1219	U	2.4
35	1d	158	ILE	2.4
47	1p	6	LEU	2.4
48	2q	65	ILE	2.4
3	2D	18	VAL	2.4
8	2I	37	VAL	2.4
35	1d	110	PHE	2.4
41	2j	52	GLY	2.4
53	1v	23	A	2.4
54	2y	64	A	2.4
42	1k	98	LEU	2.4
50	2s	71	LEU	2.4
1	2A	885	C	2.4
16	2U	17	ILE	2.4
9	2N	51	PHE	2.4
26	24	42	PHE	2.4
40	2i	8	GLY	2.4
1	1A	1176	G	2.4
30	28	64	TYR	2.4
32	2a	80	G	2.4
54	1w	15	G	2.4
7	2H	175	LYS	2.4
11	1P	107	LYS	2.4
41	2j	83	GLU	2.4
15	2T	48	ILE	2.4
23	21	13	ILE	2.4
37	2f	52	ILE	2.4
54	2w	58	A	2.4
1	1A	1026	U	2.4
34	2c	167	TRP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	171	GLY	2.4
42	1k	88	GLY	2.4
25	23	48	GLU	2.4
38	2g	112	PRO	2.4
3	1D	37	LEU	2.4
11	2P	32	THR	2.4
11	2P	115	LEU	2.4
22	20	62	LEU	2.4
33	1b	188	ALA	2.4
34	2c	196	LEU	2.4
54	1y	19	G	2.4
11	2P	95	VAL	2.4
37	2f	6	VAL	2.4
40	2i	37	PHE	2.4
47	1p	21	VAL	2.4
48	1q	27	PHE	2.4
1	2A	2117	A	2.4
32	2a	965	A	2.4
40	1i	121	ARG	2.4
53	1v	24	A	2.4
1	1A	2178	C	2.4
1	2A	2143	C	2.4
25	13	60	GLU	2.4
54	1y	48	C	2.4
14	2S	7	TYR	2.4
45	2n	21	TYR	2.4
4	1E	195	LEU	2.4
18	2W	13	SER	2.4
25	23	8	LEU	2.4
17	2V	42	GLY	2.4
12	2Q	18	LYS	2.4
31	29	15	LYS	2.4
33	2b	162	ILE	2.4
6	2G	48	GLU	2.4
9	1N	140	VAL	2.4
11	2P	15	ARG	2.4
50	2s	36	ARG	2.4
1	1A	1175	U	2.3
1	1A	2144	U	2.3
1	2A	2189	U	2.3
12	2Q	1	MET	2.3
50	2s	83	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	2I	44	LEU	2.3
14	2S	32	LEU	2.3
33	2b	51	LEU	2.3
33	2b	123	ALA	2.3
45	2n	60	SER	2.3
33	2b	129	GLU	2.3
34	1c	8	ILE	2.3
34	2c	143	GLU	2.3
38	2g	6	ARG	2.3
46	1o	88	ARG	2.3
48	2q	90	ILE	2.3
52	1u	15	ARG	2.3
7	2H	52	VAL	2.3
32	1a	1026	G	2.3
16	2U	47	TYR	2.3
25	23	10	LYS	2.3
32	2a	961	U	2.3
1	2A	2138	C	2.3
6	2G	78	SER	2.3
20	2Y	31	LEU	2.3
35	1d	120	LEU	2.3
50	2s	15	LEU	2.3
7	2H	48	GLY	2.3
9	2N	43	THR	2.3
26	24	52	THR	2.3
38	2g	24	THR	2.3
22	20	44	ARG	2.3
23	11	26	ARG	2.3
34	1c	57	ILE	2.3
40	2i	77	ILE	2.3
48	1q	36	ILE	2.3
3	2D	229	VAL	2.3
22	20	79	VAL	2.3
33	2b	17	PHE	2.3
38	1g	86	GLN	2.3
45	1n	61	TRP	2.3
3	2D	276	LYS	2.3
33	1b	133	LYS	2.3
6	2G	146	TYR	2.3
7	2H	47	GLU	2.3
35	1d	167	GLY	2.3
51	1t	12	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	29	26	ILE	2.3
54	1w	11	C	2.3
54	2w	35	A	2.3
3	2D	275	LYS	2.3
7	2H	125	VAL	2.3
27	15	60	VAL	2.3
36	2e	105	VAL	2.3
7	2H	116	GLU	2.3
22	20	71	ASP	2.3
16	2U	20	LEU	2.3
44	2m	71	ARG	2.3
49	2r	66	LEU	2.3
32	2a	1308	U	2.3
54	2y	57	G	2.3
4	2E	134	ILE	2.3
6	2G	140	ILE	2.3
34	1c	202	ILE	2.3
32	2a	1030(D)	A	2.3
41	2j	70	ARG	2.3
6	2G	11	TYR	2.3
4	2E	116	VAL	2.3
33	1b	129	GLU	2.3
38	2g	8	GLU	2.3
50	2s	51	VAL	2.3
54	1y	44	G	2.3
1	2A	884	C	2.3
36	2e	22	GLY	2.3
40	1i	113	LYS	2.3
47	1p	27	LYS	2.3
34	2c	111	LEU	2.3
12	2Q	121	ALA	2.3
30	28	10	ALA	2.3
31	29	24	TYR	2.3
34	2c	146	ALA	2.3
42	2k	97	ALA	2.3
44	2m	109	THR	2.3
22	20	68	GLU	2.3
44	2m	67	GLU	2.3
44	2m	73	GLU	2.3
1	1A	1963	U	2.3
33	2b	39	ILE	2.3
34	2c	54	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	2r	26	LEU	2.3
1	2A	2108	C	2.3
32	2a	1226	C	2.3
7	2H	32	GLU	2.3
20	2Y	50	ARG	2.3
23	21	21	ARG	2.3
33	2b	209	ARG	2.3
10	2O	19	ILE	2.3
45	2n	9	LYS	2.3
41	1j	10	GLY	2.2
11	2P	1	MET	2.2
28	26	11	LEU	2.2
45	2n	54	PRO	2.2
34	2c	168	ALA	2.2
49	1r	73	ALA	2.2
48	2q	38	ARG	2.2
34	2c	197	GLY	2.2
43	2l	65	GLU	2.2
3	2D	182	LEU	2.2
9	2N	18	ALA	2.2
40	1i	78	LYS	2.2
11	2P	102	ARG	2.2
20	2Y	83	THR	2.2
42	1k	96	ARG	2.2
34	1c	184	TYR	2.2
1	1A	2143	C	2.2
54	1y	1	G	2.2
54	2w	18	G	2.2
7	2H	18	GLU	2.2
11	2P	100	LEU	2.2
30	28	63	PRO	2.2
32	1a	1030(D)	A	2.2
32	2a	1016	A	2.2
40	2i	78	LYS	2.2
51	2t	29	LYS	2.2
39	2h	84	ARG	2.2
40	2i	42	ARG	2.2
52	2u	22	ARG	2.2
36	1e	134	ALA	2.2
33	2b	220	ASP	2.2
12	2Q	86	GLY	2.2
33	2b	55	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	105	GLU	2.2
12	2Q	94	VAL	2.2
38	2g	27	ILE	2.2
34	2c	181	ASN	2.2
48	2q	99	SER	2.2
54	2w	68	C	2.2
1	2A	2148	G	2.2
11	1P	105	LEU	2.2
16	2U	39	LEU	2.2
40	1i	120	ARG	2.2
54	2w	34	G	2.2
29	27	45	ALA	2.2
34	2c	67	THR	2.2
54	1y	38	A	2.2
16	1U	117	GLN	2.2
46	1o	89	GLY	2.2
14	2S	11	LYS	2.2
16	2U	32	PHE	2.2
17	2V	47	VAL	2.2
25	23	9	VAL	2.2
36	2e	13	ILE	2.2
40	2i	65	VAL	2.2
31	29	22	ARG	2.2
35	1d	3	ARG	2.2
34	1c	91	LEU	2.2
54	2w	67	C	2.2
42	2k	42	TRP	2.2
33	1b	207	ALA	2.2
1	2A	614(A)	U	2.2
3	2D	110	GLY	2.2
39	2h	120	THR	2.2
43	2l	16	GLU	2.2
44	1m	105	THR	2.2
54	2y	51	U	2.2
1	2A	2173	A	2.2
33	1b	163	PHE	2.2
43	2l	32	PHE	2.2
3	2D	51	VAL	2.2
9	2N	140	VAL	2.2
34	2c	20	SER	2.2
41	2j	38	ILE	2.2
11	2P	88	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	18	60	LEU	2.2
34	1c	47	LEU	2.2
40	2i	49	PRO	2.2
1	2A	888	C	2.2
1	2A	2140	C	2.2
54	2y	25	C	2.2
23	21	60	PHE	2.2
38	1g	6	ARG	2.2
21	2Z	57	ILE	2.2
42	2k	108	ILE	2.2
32	2a	1041	A	2.2
7	2H	98	LEU	2.2
11	2P	149	GLU	2.2
17	2V	35	LEU	2.2
33	2b	8	LYS	2.2
25	23	25	ALA	2.2
34	1c	100	ALA	2.2
34	2c	158	GLY	2.2
44	2m	72	ALA	2.2
16	2U	106	PHE	2.2
32	2a	91	C	2.2
54	2y	72	C	2.2
10	2O	7	TYR	2.1
14	2S	92	TYR	2.1
20	2Y	35	TYR	2.1
20	2Y	47	LYS	2.1
44	1m	87	TYR	2.1
6	2G	35	GLU	2.1
6	2G	38	VAL	2.1
14	2S	18	ILE	2.1
20	2Y	75	ILE	2.1
34	2c	28	GLN	2.1
7	2H	117	PRO	2.1
48	2q	53	LEU	2.1
32	2a	1031	G	2.1
54	2y	19	G	2.1
1	1A	229	A	2.1
7	2H	97	ARG	2.1
10	2O	65	THR	2.1
39	2h	24	THR	2.1
17	2V	76	LYS	2.1
30	28	21	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	45	LYS	2.1
4	2E	51	PHE	2.1
1	2A	2896	C	2.1
15	2T	52	ILE	2.1
38	2g	75	VAL	2.1
40	2i	74	ILE	2.1
8	2I	47	LEU	2.1
22	20	75	LEU	2.1
33	2b	102	LEU	2.1
45	1n	49	HIS	2.1
25	23	30	ARG	2.1
34	1c	126	ARG	2.1
34	1c	190	ARG	2.1
41	2j	29	ARG	2.1
11	2P	39	LYS	2.1
29	27	22	MET	2.1
31	29	13	LYS	2.1
34	2c	150	LYS	2.1
38	2g	73	MET	2.1
7	2H	159	GLU	2.1
32	1a	162	A	2.1
32	1a	1035	A	2.1
42	2k	57	THR	2.1
9	2N	8	GLN	2.1
8	1I	3	VAL	2.1
35	2d	198	VAL	2.1
39	2h	35	ILE	2.1
41	2j	75	ILE	2.1
34	1c	56	ASP	2.1
24	12	69	ARG	2.1
32	1a	204	U	2.1
32	2a	1000	U	2.1
32	2a	1214	C	2.1
33	2b	40	HIS	2.1
42	1k	63	LEU	2.1
42	1k	81	ASP	2.1
50	2s	69	HIS	2.1
1	2A	958	U	2.1
51	2t	30	LYS	2.1
36	2e	138	ALA	2.1
34	2c	22	TRP	2.1
22	20	12	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2135	A	2.1
1	2A	614(B)	G	2.1
7	2H	31	GLY	2.1
11	2P	123	LEU	2.1
18	2W	17	VAL	2.1
25	23	18	ASP	2.1
33	2b	197	VAL	2.1
35	1d	112	VAL	2.1
39	1h	38	ILE	2.1
52	2u	21	TYR	2.1
17	2V	50	PRO	2.1
45	2n	14	PRO	2.1
32	2a	962	C	2.1
34	1c	19	GLU	2.1
43	2l	26	ALA	2.1
9	2N	13	TRP	2.1
10	2O	1	MET	2.1
5	2F	83	PHE	2.1
22	20	69	PHE	2.1
42	1k	125	PHE	2.1
7	2H	25	LYS	2.1
43	2l	28	LYS	2.1
6	2G	134	GLY	2.1
8	1I	19	VAL	2.1
8	2I	38	LEU	2.1
34	2c	47	LEU	2.1
39	1h	2	LEU	2.1
41	1j	85	LEU	2.1
48	2q	33	GLY	2.1
50	2s	45	VAL	2.1
1	2A	6	A	2.1
1	2A	2141	G	2.1
23	2l	71	TYR	2.1
32	2a	1236	A	2.1
5	2F	80	ALA	2.1
42	2k	13	GLN	2.1
32	2a	723	U	2.1
32	2a	979	C	2.1
9	2N	114	ARG	2.1
12	2Q	5	ARG	2.1
19	2X	60	ARG	2.1
36	2e	84	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	4	SER	2.1
9	2N	80	GLY	2.1
11	2P	20	GLY	2.1
40	2i	54	ASP	2.1
12	2Q	17	LEU	2.1
17	2V	79	VAL	2.1
30	28	7	HIS	2.1
33	2b	200	ILE	2.1
34	1c	198	VAL	2.1
34	2c	207	VAL	2.1
38	2g	22	LEU	2.1
39	1h	112	LEU	2.1
1	1A	2181	G	2.1
1	2A	2131	G	2.1
9	2N	118	LYS	2.1
45	1n	11	LYS	2.1
38	1g	155	ARG	2.1
41	2j	92	THR	2.1
8	2I	20	ASP	2.1
22	20	57	PHE	2.1
45	1n	37	PHE	2.1
48	2q	27	PHE	2.1
25	23	27	GLY	2.1
32	2a	1028	C	2.1
34	2c	148	GLY	2.1
45	2n	51	GLY	2.1
54	1w	13	C	2.1
11	2P	112	LEU	2.1
40	2i	99	LEU	2.1
34	2c	48	TYR	2.1
38	1g	151	TYR	2.1
42	2k	70	LYS	2.1
42	2k	117	ASN	2.1
44	2m	91	ARG	2.1
51	2t	80	ARG	2.1
41	1j	48	THR	2.1
32	1a	1003	G	2.0
54	1y	59	U	2.0
55	1x	70	G	2.0
20	2Y	63	LYS	2.0
30	28	61	LEU	2.0
32	2a	1019	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	16	LEU	2.0
9	2N	108	PRO	2.0
39	2h	65	TYR	2.0
19	2X	68	ARG	2.0
25	23	3	ARG	2.0
36	1e	48	ALA	2.0
41	1j	45	ARG	2.0
42	2k	96	ARG	2.0
45	1n	20	ALA	2.0
52	1u	6	ARG	2.0
11	2P	144	GLU	2.0
38	2g	113	GLU	2.0
4	2E	6	GLY	2.0
41	2j	19	SER	2.0
28	26	8	LYS	2.0
30	28	47	LYS	2.0
44	2m	64	TRP	2.0
32	2a	1020	U	2.0
41	2j	21	GLN	2.0
46	2o	62	GLN	2.0
32	1a	160	A	2.0
7	2H	151	ILE	2.0
32	1a	1033	G	2.0
34	2c	138	VAL	2.0
34	1c	182	ILE	2.0
42	1k	95	ILE	2.0
43	1l	7	ILE	2.0
51	2t	23	ARG	2.0
52	2u	13	ILE	2.0
1	1A	2136	C	2.0
5	2F	56	GLU	2.0
30	18	65	GLU	2.0
42	2k	59	TYR	2.0
54	2y	13	C	2.0
34	2c	180	ALA	2.0
33	2b	67	THR	2.0
43	1l	14	GLY	2.0
15	2T	22	PHE	2.0
25	23	2	PRO	2.0
36	2e	33	VAL	2.0
41	1j	66	ARG	2.0
42	1k	29	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	1l	16	GLU	2.0
54	1y	45	U	2.0
3	1D	38	LYS	2.0
1	2A	1170	G	2.0
11	1P	110	TYR	2.0
12	2Q	114	ALA	2.0
40	1i	114	TYR	2.0
23	2l	22	GLY	2.0
40	2i	30	GLY	2.0
34	2c	191	THR	2.0
16	2U	40	PHE	2.0
31	29	1	MET	2.0
3	2D	37	LEU	2.0
7	2H	71	LEU	2.0
11	2P	50	ARG	2.0
11	2P	138	LEU	2.0
34	1c	179	ARG	2.0
34	2c	44	GLU	2.0
41	2j	51	ARG	2.0
44	2m	96	LEU	2.0
49	2r	87	ARG	2.0
42	1k	14	VAL	2.0
45	1n	50	LYS	2.0
51	1t	14	LYS	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
54	PSU	2y	55	20/21	0.69	0.47	90,96,107,107	0
54	PSU	2w	55	20/21	0.74	0.30	81,91,96,98	0
54	4SU	2w	8	20/21	0.74	0.21	83,93,104,117	0
54	7MG	2y	46	24/25	0.76	0.31	86,95,102,123	0
54	PSU	1y	55	20/21	0.76	0.26	80,89,98,103	0
54	7MG	1w	46	24/25	0.79	0.17	77,89,99,107	0
54	7MG	2w	46	24/25	0.79	0.23	80,93,101,121	0
54	5MU	2y	54	21/22	0.80	0.39	84,91,99,112	0
54	5MU	1y	54	21/22	0.82	0.30	79,85,91,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	4SU	1y	8	20/21	0.83	0.21	81,89,98,99	0
54	MIA	2y	37	22/30	0.83	0.26	75,87,99,109	0
54	PSU	2y	32	20/21	0.84	0.25	79,85,93,102	0
54	PSU	2y	39	20/21	0.85	0.26	79,84,92,96	0
54	7MG	1y	46	24/25	0.85	0.32	79,90,98,101	0
54	4SU	1w	8	20/21	0.86	0.17	80,85,93,94	0
54	4SU	2y	8	20/21	0.86	0.21	88,93,99,104	0
55	4SU	2x	8	20/21	0.86	0.17	73,79,87,90	0
54	PSU	1y	32	20/21	0.86	0.29	78,82,87,88	0
54	MIA	2w	37	25/30	0.87	0.27	75,82,88,103	0
54	PSU	2w	39	20/21	0.87	0.42	81,86,88,92	0
32	M2G	2a	966	25/26	0.87	0.24	60,69,84,86	0
54	PSU	2w	32	20/21	0.88	0.43	78,85,93,97	0
32	2MG	2a	1207	24/25	0.89	0.15	63,83,92,95	0
1	5MU	2A	1915	21/22	0.89	0.17	74,78,84,94	0
54	PSU	1w	55	20/21	0.89	0.17	74,83,92,95	0
43	0TD	2l	92	10/11	0.89	0.21	67,71,72,79	0
54	PSU	1w	32	20/21	0.90	0.26	65,76,82,84	0
32	PSU	2a	516	20/21	0.91	0.15	70,77,83,85	0
55	PSU	2x	55	20/21	0.91	0.17	72,80,82,85	0
54	MIA	1y	37	22/30	0.91	0.26	74,78,84,85	0
55	5MU	2x	54	21/22	0.91	0.21	68,77,82,94	0
54	5MU	2w	54	21/22	0.91	0.21	67,82,87,93	0
43	0TD	1l	92	10/11	0.91	0.19	47,55,60,75	0
54	MIA	1w	37	29/30	0.92	0.22	56,65,72,74	0
32	5MC	2a	967	21/22	0.92	0.18	61,70,78,82	0
1	PSU	2A	1911	20/21	0.92	0.17	60,66,73,75	0
1	PSU	2A	1917	20/21	0.92	0.16	62,71,81,87	0
54	PSU	1y	39	20/21	0.93	0.21	74,76,80,80	0
54	PSU	1w	39	20/21	0.93	0.25	67,74,85,85	0
54	5MU	1w	54	21/22	0.94	0.17	64,72,79,82	0
55	5MC	2x	32	21/22	0.94	0.20	60,73,78,82	0
32	5MC	1a	967	21/22	0.94	0.21	52,59,63,64	0
1	5MU	1A	1915	21/22	0.94	0.17	56,61,68,71	0
32	5MC	2a	1404	21/22	0.94	0.19	56,60,65,68	0
1	4OC	2A	1920	21/23	0.94	0.20	61,65,67,71	0
1	PSU	1A	1917	20/21	0.95	0.19	48,57,62,63	0
55	5MU	1x	54	21/22	0.95	0.15	51,64,70,76	0
55	4SU	1x	8	20/21	0.95	0.17	51,59,65,71	0
55	PSU	1x	55	20/21	0.95	0.18	49,63,70,73	0
32	4OC	2a	1402	22/23	0.95	0.16	53,65,69,70	0
32	UR3	2a	1498	21/22	0.95	0.20	55,61,65,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	PSU	1a	516	20/21	0.95	0.12	60,66,71,71	0
32	5MC	2a	1400	21/22	0.95	0.17	60,69,76,83	0
32	2MG	1a	1207	24/25	0.95	0.14	59,67,73,75	0
32	5MC	2a	1407	21/22	0.95	0.17	53,59,63,64	0
32	7MG	2a	527	24/25	0.96	0.15	63,66,72,76	0
1	2MA	2A	2503	23/24	0.96	0.23	32,36,43,45	0
32	MA6	2a	1519	24/25	0.96	0.28	52,63,67,69	0
32	7MG	1a	527	24/25	0.96	0.19	42,49,57,58	0
55	5MC	1x	32	21/22	0.96	0.23	46,54,60,74	0
1	4OC	1A	1920	21/23	0.96	0.22	37,44,48,53	0
32	MA6	2a	1518	24/25	0.96	0.24	55,65,68,71	0
1	5MC	2A	1942	21/22	0.96	0.18	54,60,66,68	0
1	OMG	2A	2251	24/25	0.97	0.24	42,45,51,56	0
1	5MU	2A	1939	21/22	0.97	0.23	36,44,49,51	0
1	PSU	1A	1911	20/21	0.97	0.20	40,49,57,57	0
32	4OC	1a	1402	22/23	0.97	0.21	37,45,51,57	0
1	2MU	2A	2552	21/23	0.97	0.23	35,42,46,62	0
1	5MC	1A	1942	21/22	0.97	0.20	31,40,43,49	0
32	MA6	1a	1519	24/25	0.97	0.21	38,42,47,50	0
32	5MC	1a	1407	21/22	0.97	0.22	36,41,43,45	0
1	5MC	2A	1962	21/22	0.97	0.17	40,52,59,68	0
32	5MC	1a	1400	21/22	0.97	0.20	39,50,54,59	0
32	M2G	1a	966	25/26	0.97	0.19	49,55,59,66	0
1	OMG	1A	2251	24/25	0.98	0.22	19,25,28,29	0
1	2MU	1A	2552	21/23	0.98	0.20	21,29,33,39	0
1	PSU	1A	2605	20/21	0.98	0.21	19,26,35,35	0
32	5MC	1a	1404	21/22	0.98	0.19	35,41,44,44	0
1	5MC	1A	1962	21/22	0.98	0.21	29,36,41,44	0
32	UR3	1a	1498	21/22	0.98	0.21	39,43,46,48	0
32	MA6	1a	1518	24/25	0.98	0.23	34,41,45,49	0
1	5MU	1A	1939	21/22	0.98	0.21	23,29,33,40	0
1	2MA	1A	2503	23/24	0.98	0.22	14,21,24,31	0
1	PSU	2A	2605	20/21	0.98	0.18	34,42,47,47	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	2A	3819	1/1	0.09	0.29	69,69,69,69	0
56	MG	1A	3982	1/1	0.14	0.30	77,77,77,77	0
56	MG	2a	3173	1/1	0.20	0.21	70,70,70,70	0
56	MG	2a	3136	1/1	0.28	0.30	78,78,78,78	0
56	MG	1A	4000	1/1	0.33	0.17	62,62,62,62	0
56	MG	1a	1807	1/1	0.33	0.12	66,66,66,66	0
56	MG	1A	4043	1/1	0.34	0.34	66,66,66,66	0
56	MG	1A	3979	1/1	0.40	0.23	69,69,69,69	0
56	MG	2A	3817	1/1	0.40	0.29	75,75,75,75	0
56	MG	1A	4061	1/1	0.41	0.14	68,68,68,68	0
56	MG	1a	1790	1/1	0.42	0.12	74,74,74,74	0
56	MG	1a	1784	1/1	0.43	0.21	56,56,56,56	0
56	MG	1A	3801	1/1	0.44	0.13	53,53,53,53	0
56	MG	1A	3924	1/1	0.46	0.14	71,71,71,71	0
56	MG	2A	3828	1/1	0.46	0.10	59,59,59,59	0
56	MG	2A	3864	1/1	0.47	0.12	69,69,69,69	0
56	MG	2a	3070	1/1	0.48	0.25	68,68,68,68	0
56	MG	2A	3855	1/1	0.48	0.20	74,74,74,74	0
56	MG	1a	1793	1/1	0.48	0.11	78,78,78,78	0
56	MG	1a	1655	1/1	0.49	0.19	76,76,76,76	0
56	MG	1A	3771	1/1	0.49	0.17	19,19,19,19	0
56	MG	1A	4067	1/1	0.50	0.14	55,55,55,55	0
56	MG	2A	3040	1/1	0.50	0.57	88,88,88,88	0
56	MG	2a	3101	1/1	0.52	0.16	68,68,68,68	0
56	MG	2A	3532	1/1	0.53	0.14	61,61,61,61	0
56	MG	2A	3285	1/1	0.53	0.23	62,62,62,62	0
56	MG	1A	3980	1/1	0.54	0.11	62,62,62,62	0
56	MG	2a	3167	1/1	0.54	0.07	75,75,75,75	0
56	MG	1a	1731	1/1	0.56	0.21	69,69,69,69	0
56	MG	2a	3178	1/1	0.56	0.38	91,91,91,91	0
56	MG	2A	3830	1/1	0.56	0.17	77,77,77,77	0
56	MG	2A	3650	1/1	0.56	0.21	67,67,67,67	0
56	MG	2a	3149	1/1	0.57	0.07	76,76,76,76	0
56	MG	1a	1812	1/1	0.57	0.13	62,62,62,62	0
56	MG	2A	3640	1/1	0.58	0.18	64,64,64,64	0
56	MG	1A	4056	1/1	0.58	0.14	45,45,45,45	0
56	MG	2a	3196	1/1	0.58	0.12	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3188	1/1	0.58	0.14	59,59,59,59	0
56	MG	1A	3985	1/1	0.59	0.17	61,61,61,61	0
56	MG	1A	3332	1/1	0.59	0.20	57,57,57,57	0
56	MG	2a	3199	1/1	0.59	0.12	70,70,70,70	0
56	MG	1A	4083	1/1	0.59	0.17	51,51,51,51	0
56	MG	2a	3176	1/1	0.59	0.12	72,72,72,72	0
56	MG	2a	3182	1/1	0.59	0.07	83,83,83,83	0
56	MG	1a	1714	1/1	0.60	0.22	62,62,62,62	0
56	MG	1A	3998	1/1	0.60	0.25	67,67,67,67	0
56	MG	2a	3142	1/1	0.60	0.08	68,68,68,68	0
56	MG	2a	3031	1/1	0.61	0.60	69,69,69,69	0
56	MG	1a	1766	1/1	0.61	0.13	61,61,61,61	0
56	MG	1A	3784	1/1	0.62	0.09	66,66,66,66	0
56	MG	1A	3996	1/1	0.62	0.16	51,51,51,51	0
56	MG	2D	308	1/1	0.62	0.12	39,39,39,39	0
56	MG	1A	4032	1/1	0.62	0.36	57,57,57,57	0
56	MG	1A	3661	1/1	0.62	0.18	29,29,29,29	0
56	MG	1a	1789	1/1	0.62	0.20	77,77,77,77	0
56	MG	2A	3844	1/1	0.62	0.18	72,72,72,72	0
56	MG	1a	1824	1/1	0.62	0.10	60,60,60,60	0
56	MG	1A	3844	1/1	0.64	0.12	57,57,57,57	0
56	MG	2A	3570	1/1	0.64	0.11	48,48,48,48	0
56	MG	1a	1800	1/1	0.64	0.09	50,50,50,50	0
56	MG	2A	3779	1/1	0.64	0.11	71,71,71,71	0
56	MG	1A	4081	1/1	0.64	0.10	44,44,44,44	0
56	MG	2A	3321	1/1	0.64	0.32	65,65,65,65	0
56	MG	1A	4068	1/1	0.65	0.18	61,61,61,61	0
56	MG	1A	4052	1/1	0.65	0.23	48,48,48,48	0
56	MG	2A	3734	1/1	0.65	0.16	52,52,52,52	0
56	MG	2a	3193	1/1	0.65	0.16	82,82,82,82	0
56	MG	1A	4049	1/1	0.65	0.18	54,54,54,54	0
56	MG	2A	3029	1/1	0.65	0.19	62,62,62,62	0
56	MG	1A	3697	1/1	0.65	0.21	38,38,38,38	0
56	MG	1a	1803	1/1	0.65	0.09	61,61,61,61	0
56	MG	2w	102	1/1	0.66	0.16	72,72,72,72	0
56	MG	2A	3048	1/1	0.66	0.19	65,65,65,65	0
56	MG	2a	3120	1/1	0.66	0.20	66,66,66,66	0
56	MG	2A	3859	1/1	0.66	0.14	60,60,60,60	0
56	MG	2A	3618	1/1	0.66	0.10	49,49,49,49	0
56	MG	2A	3833	1/1	0.67	0.10	53,53,53,53	0
56	MG	2a	3180	1/1	0.67	0.10	71,71,71,71	0
56	MG	2A	3247	1/1	0.68	0.35	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1753	1/1	0.68	0.18	53,53,53,53	0
56	MG	2A	3214	1/1	0.68	0.14	62,62,62,62	0
56	MG	2A	3848	1/1	0.68	0.09	74,74,74,74	0
56	MG	1a	1660	1/1	0.68	0.14	72,72,72,72	0
56	MG	1A	3292	1/1	0.68	0.15	57,57,57,57	0
56	MG	2A	3798	1/1	0.68	0.10	51,51,51,51	0
56	MG	1A	4033	1/1	0.69	0.16	55,55,55,55	0
56	MG	1A	3411	1/1	0.69	0.52	57,57,57,57	0
56	MG	2A	3780	1/1	0.69	0.09	69,69,69,69	0
56	MG	2a	3015	1/1	0.69	0.18	69,69,69,69	0
56	MG	1e	201	1/1	0.69	0.17	73,73,73,73	0
56	MG	1A	3300	1/1	0.69	0.16	44,44,44,44	0
56	MG	2A	3812	1/1	0.69	0.42	76,76,76,76	0
56	MG	2a	3165	1/1	0.69	0.08	78,78,78,78	0
56	MG	2a	3052	1/1	0.69	0.16	56,56,56,56	0
56	MG	2A	3637	1/1	0.69	0.18	47,47,47,47	0
56	MG	1A	3512	1/1	0.69	0.26	60,60,60,60	0
56	MG	1A	3494	1/1	0.70	0.20	56,56,56,56	0
56	MG	1a	1798	1/1	0.70	0.16	76,76,76,76	0
56	MG	1A	3605	1/1	0.70	0.22	37,37,37,37	0
56	MG	1A	3165	1/1	0.70	0.33	39,39,39,39	0
56	MG	1A	3928	1/1	0.70	0.22	69,69,69,69	0
56	MG	1A	3901	1/1	0.70	0.14	53,53,53,53	0
56	MG	2A	3805	1/1	0.70	0.09	67,67,67,67	0
56	MG	1A	3767	1/1	0.70	0.22	30,30,30,30	0
56	MG	1A	3329	1/1	0.70	0.29	51,51,51,51	0
56	MG	1a	1772	1/1	0.71	0.21	60,60,60,60	0
56	MG	2a	3095	1/1	0.71	0.17	79,79,79,79	0
56	MG	1A	3968	1/1	0.71	0.36	43,43,43,43	0
56	MG	2A	3467	1/1	0.71	0.19	74,74,74,74	0
56	MG	1P	206	1/1	0.71	0.32	62,62,62,62	0
56	MG	2A	3869	1/1	0.71	0.12	45,45,45,45	0
56	MG	1a	1806	1/1	0.71	0.12	59,59,59,59	0
56	MG	2a	3225	1/1	0.71	0.23	73,73,73,73	0
56	MG	2A	3793	1/1	0.72	0.23	77,77,77,77	0
56	MG	2a	3201	1/1	0.72	0.16	60,60,60,60	0
56	MG	2A	3291	1/1	0.72	0.34	57,57,57,57	0
56	MG	1a	1746	1/1	0.72	0.12	59,59,59,59	0
56	MG	2A	3474	1/1	0.72	0.20	61,61,61,61	0
56	MG	1a	1609	1/1	0.72	0.11	65,65,65,65	0
56	MG	1A	3360	1/1	0.72	0.16	65,65,65,65	0
56	MG	2A	3762	1/1	0.72	0.15	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3342	1/1	0.72	0.21	60,60,60,60	0
56	MG	2a	3170	1/1	0.72	0.18	73,73,73,73	0
56	MG	2A	3806	1/1	0.72	0.17	50,50,50,50	0
56	MG	2v	101	1/1	0.72	0.12	78,78,78,78	0
56	MG	1A	3987	1/1	0.72	0.09	50,50,50,50	0
56	MG	2A	3543	1/1	0.72	0.13	45,45,45,45	0
56	MG	1A	4059	1/1	0.72	0.20	27,27,27,27	0
56	MG	2A	3838	1/1	0.73	0.17	43,43,43,43	0
56	MG	2A	3334	1/1	0.73	0.17	74,74,74,74	0
56	MG	2A	3714	1/1	0.73	0.18	57,57,57,57	0
56	MG	2A	3711	1/1	0.73	0.18	54,54,54,54	0
56	MG	2A	3735	1/1	0.73	0.08	62,62,62,62	0
56	MG	1A	3561	1/1	0.73	0.34	62,62,62,62	0
56	MG	2a	3049	1/1	0.73	0.16	64,64,64,64	0
56	MG	1A	3742	1/1	0.73	0.24	17,17,17,17	0
56	MG	2A	3207	1/1	0.73	0.15	64,64,64,64	0
56	MG	2A	3554	1/1	0.73	0.11	49,49,49,49	0
56	MG	1A	3247	1/1	0.73	0.18	53,53,53,53	0
56	MG	2A	3875	1/1	0.73	0.14	74,74,74,74	0
56	MG	1A	3392	1/1	0.73	0.27	45,45,45,45	0
56	MG	2A	3169	1/1	0.73	0.31	57,57,57,57	0
56	MG	2A	3596	1/1	0.73	0.14	40,40,40,40	0
56	MG	1a	1818	1/1	0.73	0.16	71,71,71,71	0
56	MG	1a	1721	1/1	0.74	0.27	54,54,54,54	0
56	MG	2A	3804	1/1	0.74	0.17	53,53,53,53	0
56	MG	2a	3153	1/1	0.74	0.09	73,73,73,73	0
56	MG	1A	3689	1/1	0.74	0.22	26,26,26,26	0
56	MG	2A	3568	1/1	0.74	0.15	47,47,47,47	0
56	MG	1a	1780	1/1	0.74	0.15	58,58,58,58	0
56	MG	2A	3002	1/1	0.74	0.21	53,53,53,53	0
56	MG	2a	3041	1/1	0.74	0.21	66,66,66,66	0
56	MG	1A	3869	1/1	0.74	0.18	45,45,45,45	0
56	MG	2A	3820	1/1	0.74	0.12	73,73,73,73	0
56	MG	2a	3145	1/1	0.74	0.24	79,79,79,79	0
59	ZN	24	501	1/1	0.74	0.07	117,117,117,117	0
56	MG	2A	3405	1/1	0.74	0.20	64,64,64,64	0
56	MG	1B	234	1/1	0.74	0.18	56,56,56,56	0
56	MG	2A	3860	1/1	0.74	0.16	73,73,73,73	0
56	MG	2a	3054	1/1	0.74	0.27	71,71,71,71	0
56	MG	1w	109	1/1	0.74	0.20	77,77,77,77	0
56	MG	2A	3382	1/1	0.75	0.52	47,47,47,47	0
56	MG	2A	3353	1/1	0.75	0.16	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3787	1/1	0.75	0.08	72,72,72,72	0
56	MG	1A	3422	1/1	0.75	0.15	58,58,58,58	0
56	MG	2a	3003	1/1	0.75	0.14	63,63,63,63	0
56	MG	1a	1620	1/1	0.75	0.27	55,55,55,55	0
56	MG	1a	1801	1/1	0.75	0.12	64,64,64,64	0
56	MG	2a	3147	1/1	0.75	0.18	80,80,80,80	0
56	MG	2A	3320	1/1	0.75	0.14	54,54,54,54	0
56	MG	1A	3341	1/1	0.75	0.21	50,50,50,50	0
56	MG	2A	3361	1/1	0.75	0.21	61,61,61,61	0
56	MG	1A	3471	1/1	0.75	0.21	51,51,51,51	0
56	MG	1B	228	1/1	0.75	0.18	42,42,42,42	0
56	MG	1A	3402	1/1	0.75	0.36	85,85,85,85	0
56	MG	2a	3082	1/1	0.75	0.11	65,65,65,65	0
56	MG	2A	3063	1/1	0.75	0.21	58,58,58,58	0
56	MG	2A	3337	1/1	0.75	0.25	49,49,49,49	0
56	MG	1a	1787	1/1	0.75	0.15	66,66,66,66	0
56	MG	1A	3489	1/1	0.75	0.71	48,48,48,48	0
56	MG	1A	4089	1/1	0.76	0.21	65,65,65,65	0
56	MG	1A	4012	1/1	0.76	0.09	68,68,68,68	0
56	MG	2A	3116	1/1	0.76	0.13	60,60,60,60	0
56	MG	2A	3230	1/1	0.76	0.30	67,67,67,67	0
56	MG	1A	3923	1/1	0.76	0.17	59,59,59,59	0
56	MG	1A	3297	1/1	0.76	0.15	50,50,50,50	0
56	MG	1A	3404	1/1	0.76	0.33	60,60,60,60	0
56	MG	1A	4006	1/1	0.76	0.19	29,29,29,29	0
56	MG	2A	3308	1/1	0.76	0.12	56,56,56,56	0
56	MG	2A	3476	1/1	0.76	0.15	62,62,62,62	0
56	MG	1A	3224	1/1	0.76	0.15	45,45,45,45	0
56	MG	2A	3352	1/1	0.76	0.23	72,72,72,72	0
56	MG	1O	205	1/1	0.76	0.21	72,72,72,72	0
56	MG	2A	3809	1/1	0.76	0.26	60,60,60,60	0
56	MG	2A	3243	1/1	0.76	0.67	64,64,64,64	0
56	MG	2A	3333	1/1	0.76	0.31	65,65,65,65	0
56	MG	1A	3871	1/1	0.76	0.11	32,32,32,32	0
56	MG	2A	3674	1/1	0.76	0.15	63,63,63,63	0
56	MG	2x	103	1/1	0.76	0.18	60,60,60,60	0
56	MG	2A	3740	1/1	0.76	0.07	67,67,67,67	0
56	MG	1A	3876	1/1	0.76	0.22	34,34,34,34	0
56	MG	1A	3019	1/1	0.76	0.18	41,41,41,41	0
56	MG	2a	3174	1/1	0.77	0.19	75,75,75,75	0
56	MG	2A	3008	1/1	0.77	0.23	60,60,60,60	0
56	MG	2A	3452	1/1	0.77	0.17	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3399	1/1	0.77	0.20	69,69,69,69	0
56	MG	1A	3208	1/1	0.77	0.15	61,61,61,61	0
56	MG	1a	1822	1/1	0.77	0.10	69,69,69,69	0
56	MG	1A	3983	1/1	0.77	0.17	64,64,64,64	0
56	MG	2a	3096	1/1	0.77	0.10	67,67,67,67	0
56	MG	1a	1698	1/1	0.77	0.28	62,62,62,62	0
56	MG	2G	201	1/1	0.77	0.12	65,65,65,65	0
56	MG	2T	202	1/1	0.77	0.13	61,61,61,61	0
56	MG	1A	3800	1/1	0.77	0.22	60,60,60,60	0
56	MG	2A	3255	1/1	0.77	0.32	69,69,69,69	0
56	MG	2A	3802	1/1	0.77	0.12	57,57,57,57	0
56	MG	2A	3217	1/1	0.77	0.38	67,67,67,67	0
56	MG	2A	3493	1/1	0.77	0.25	61,61,61,61	0
56	MG	2j	201	1/1	0.77	0.14	76,76,76,76	0
56	MG	1A	3962	1/1	0.78	0.12	48,48,48,48	0
56	MG	1a	1672	1/1	0.78	0.12	44,44,44,44	0
56	MG	2A	3599	1/1	0.78	0.20	68,68,68,68	0
56	MG	1A	3838	1/1	0.78	0.19	60,60,60,60	0
56	MG	2A	3397	1/1	0.78	0.18	72,72,72,72	0
56	MG	1A	3930	1/1	0.78	0.14	30,30,30,30	0
56	MG	2a	3151	1/1	0.78	0.15	91,91,91,91	0
56	MG	1a	1747	1/1	0.78	0.11	52,52,52,52	0
56	MG	1A	3053	1/1	0.78	0.14	62,62,62,62	0
56	MG	1A	4039	1/1	0.78	0.14	61,61,61,61	0
56	MG	2A	3698	1/1	0.78	0.20	56,56,56,56	0
56	MG	2A	3585	1/1	0.78	0.13	77,77,77,77	0
56	MG	2A	3691	1/1	0.78	0.07	71,71,71,71	0
56	MG	1A	4035	1/1	0.78	0.06	64,64,64,64	0
56	MG	2a	3066	1/1	0.78	0.11	60,60,60,60	0
56	MG	1A	3382	1/1	0.78	0.25	46,46,46,46	0
56	MG	2A	3612	1/1	0.78	0.10	41,41,41,41	0
56	MG	2A	3120	1/1	0.78	0.24	62,62,62,62	0
56	MG	2A	3448	1/1	0.78	0.20	64,64,64,64	0
56	MG	2A	3421	1/1	0.78	0.19	69,69,69,69	0
56	MG	1B	229	1/1	0.79	0.14	38,38,38,38	0
56	MG	1A	3338	1/1	0.79	0.20	48,48,48,48	0
56	MG	1a	1703	1/1	0.79	0.25	60,60,60,60	0
56	MG	1A	3684	1/1	0.79	0.12	36,36,36,36	0
56	MG	2A	3856	1/1	0.79	0.06	58,58,58,58	0
56	MG	1A	3503	1/1	0.79	0.40	57,57,57,57	0
56	MG	2a	3172	1/1	0.79	0.12	62,62,62,62	0
56	MG	1a	1604	1/1	0.79	0.14	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3065	1/1	0.79	0.17	51,51,51,51	0
56	MG	2A	3406	1/1	0.79	0.34	66,66,66,66	0
56	MG	2A	3071	1/1	0.79	0.14	40,40,40,40	0
56	MG	2A	3271	1/1	0.79	0.13	58,58,58,58	0
56	MG	2A	3789	1/1	0.79	0.09	44,44,44,44	0
56	MG	2A	3661	1/1	0.79	0.32	59,59,59,59	0
56	MG	2R	201	1/1	0.79	0.16	65,65,65,65	0
56	MG	2A	3396	1/1	0.79	0.15	63,63,63,63	0
56	MG	2A	3381	1/1	0.79	0.13	57,57,57,57	0
56	MG	1A	4042	1/1	0.79	0.08	40,40,40,40	0
56	MG	1A	3083	1/1	0.79	0.29	37,37,37,37	0
56	MG	1A	3103	1/1	0.79	0.16	60,60,60,60	0
56	MG	1A	3921	1/1	0.79	0.17	41,41,41,41	0
56	MG	2A	3883	1/1	0.79	0.24	68,68,68,68	0
56	MG	1A	3726	1/1	0.79	0.10	53,53,53,53	0
56	MG	2A	3279	1/1	0.79	0.17	62,62,62,62	0
56	MG	1A	4047	1/1	0.80	0.17	47,47,47,47	0
56	MG	2a	3061	1/1	0.80	0.12	53,53,53,53	0
56	MG	1A	3058	1/1	0.80	0.18	32,32,32,32	0
56	MG	1A	3577	1/1	0.80	0.33	47,47,47,47	0
56	MG	2a	3007	1/1	0.80	0.15	63,63,63,63	0
56	MG	2A	3094	1/1	0.80	0.14	62,62,62,62	0
56	MG	2A	3315	1/1	0.80	0.11	62,62,62,62	0
56	MG	2A	3347	1/1	0.80	0.18	66,66,66,66	0
56	MG	1A	3933	1/1	0.80	0.10	49,49,49,49	0
56	MG	2A	3086	1/1	0.80	0.18	66,66,66,66	0
56	MG	1A	4101	1/1	0.80	0.07	53,53,53,53	0
56	MG	1A	3004	1/1	0.80	0.21	22,22,22,22	0
56	MG	1A	3002	1/1	0.80	0.15	51,51,51,51	0
56	MG	1A	3798	1/1	0.80	0.12	39,39,39,39	0
56	MG	2W	203	1/1	0.80	0.26	51,51,51,51	0
56	MG	1A	4016	1/1	0.80	0.20	25,25,25,25	0
56	MG	2A	3551	1/1	0.80	0.12	43,43,43,43	0
56	MG	1a	1711	1/1	0.80	0.19	39,39,39,39	0
56	MG	1A	4034	1/1	0.80	0.07	61,61,61,61	0
56	MG	2A	3176	1/1	0.80	0.30	59,59,59,59	0
56	MG	2A	3800	1/1	0.80	0.04	78,78,78,78	0
56	MG	1A	3639	1/1	0.80	0.18	36,36,36,36	0
56	MG	1a	1813	1/1	0.80	0.10	53,53,53,53	0
56	MG	1a	1656	1/1	0.80	0.11	62,62,62,62	0
56	MG	1A	3478	1/1	0.80	0.28	41,41,41,41	0
56	MG	1A	3148	1/1	0.80	0.31	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3402	1/1	0.80	0.12	65,65,65,65	0
56	MG	1a	1700	1/1	0.80	0.22	68,68,68,68	0
56	MG	2a	3014	1/1	0.80	0.16	63,63,63,63	0
56	MG	1x	109	1/1	0.80	0.12	61,61,61,61	0
56	MG	1A	3317	1/1	0.80	0.18	65,65,65,65	0
56	MG	2A	3264	1/1	0.80	0.14	56,56,56,56	0
56	MG	2A	3414	1/1	0.80	0.13	59,59,59,59	0
56	MG	2A	3486	1/1	0.80	0.17	62,62,62,62	0
56	MG	2A	3107	1/1	0.80	0.16	65,65,65,65	0
56	MG	1A	4060	1/1	0.81	0.46	52,52,52,52	0
56	MG	2y	106	1/1	0.81	0.40	83,83,83,83	0
56	MG	2A	3623	1/1	0.81	0.14	60,60,60,60	0
56	MG	2A	3494	1/1	0.81	0.09	67,67,67,67	0
56	MG	1A	3934	1/1	0.81	0.11	55,55,55,55	0
56	MG	2A	3287	1/1	0.81	0.20	67,67,67,67	0
56	MG	2A	3155	1/1	0.81	0.12	55,55,55,55	0
56	MG	2A	3077	1/1	0.81	0.27	57,57,57,57	0
56	MG	1A	3121	1/1	0.81	0.49	46,46,46,46	0
56	MG	1A	4001	1/1	0.81	0.10	48,48,48,48	0
56	MG	2A	3242	1/1	0.81	0.18	64,64,64,64	0
56	MG	1A	3461	1/1	0.81	0.43	61,61,61,61	0
56	MG	2f	202	1/1	0.81	0.13	65,65,65,65	0
56	MG	1A	3394	1/1	0.81	0.25	50,50,50,50	0
56	MG	1a	1748	1/1	0.81	0.11	36,36,36,36	0
56	MG	2a	3043	1/1	0.81	0.17	66,66,66,66	0
56	MG	2A	3808	1/1	0.81	0.24	63,63,63,63	0
56	MG	1A	3992	1/1	0.81	0.18	25,25,25,25	0
56	MG	2A	3818	1/1	0.81	0.15	64,64,64,64	0
56	MG	2A	3253	1/1	0.81	0.21	64,64,64,64	0
56	MG	1w	110	1/1	0.81	0.23	74,74,74,74	0
56	MG	2a	3006	1/1	0.81	0.11	61,61,61,61	0
56	MG	2A	3824	1/1	0.81	0.23	66,66,66,66	0
56	MG	2A	3684	1/1	0.81	0.12	56,56,56,56	0
56	MG	1A	3922	1/1	0.81	0.10	70,70,70,70	0
56	MG	1G	203	1/1	0.81	0.10	63,63,63,63	0
56	MG	2A	3823	1/1	0.81	0.10	50,50,50,50	0
56	MG	2A	3072	1/1	0.81	0.21	61,61,61,61	0
56	MG	2A	3145	1/1	0.81	0.11	66,66,66,66	0
56	MG	2A	3821	1/1	0.81	0.21	55,55,55,55	0
56	MG	2Q	202	1/1	0.81	0.13	53,53,53,53	0
56	MG	2T	201	1/1	0.81	0.16	54,54,54,54	0
56	MG	2A	3332	1/1	0.81	0.15	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3731	1/1	0.81	0.23	60,60,60,60	0
56	MG	2A	3386	1/1	0.81	0.13	55,55,55,55	0
56	MG	2A	3417	1/1	0.81	0.24	68,68,68,68	0
56	MG	2A	3703	1/1	0.81	0.07	59,59,59,59	0
56	MG	2A	3759	1/1	0.81	0.11	62,62,62,62	0
56	MG	1a	1760	1/1	0.81	0.15	56,56,56,56	0
56	MG	2A	3216	1/1	0.81	0.17	65,65,65,65	0
56	MG	1A	3537	1/1	0.81	0.17	61,61,61,61	0
56	MG	2A	3538	1/1	0.81	0.15	38,38,38,38	0
56	MG	2a	3157	1/1	0.81	0.10	57,57,57,57	0
56	MG	2a	3100	1/1	0.81	0.13	77,77,77,77	0
56	MG	2A	3085	1/1	0.81	0.25	55,55,55,55	0
56	MG	1A	3808	1/1	0.82	0.11	65,65,65,65	0
56	MG	2A	3191	1/1	0.82	0.19	70,70,70,70	0
56	MG	1A	3945	1/1	0.82	0.17	56,56,56,56	0
56	MG	2A	3676	1/1	0.82	0.14	61,61,61,61	0
56	MG	1A	4024	1/1	0.82	0.16	70,70,70,70	0
56	MG	1A	3948	1/1	0.82	0.19	36,36,36,36	0
56	MG	2O	8400	1/1	0.82	0.10	64,64,64,64	0
56	MG	2A	3239	1/1	0.82	0.39	56,56,56,56	0
56	MG	2A	3033	1/1	0.82	0.13	36,36,36,36	0
56	MG	1B	207	1/1	0.82	0.25	70,70,70,70	0
56	MG	2A	3886	1/1	0.82	0.12	71,71,71,71	0
56	MG	2A	3099	1/1	0.82	0.23	68,68,68,68	0
56	MG	2A	3443	1/1	0.82	0.22	59,59,59,59	0
56	MG	1a	1673	1/1	0.82	0.13	63,63,63,63	0
56	MG	2A	3088	1/1	0.82	0.22	78,78,78,78	0
56	MG	1A	4062	1/1	0.82	0.12	32,32,32,32	0
56	MG	2A	3750	1/1	0.82	0.14	55,55,55,55	0
56	MG	2a	3166	1/1	0.82	0.07	67,67,67,67	0
56	MG	2a	3053	1/1	0.82	0.14	70,70,70,70	0
56	MG	2A	3861	1/1	0.82	0.12	62,62,62,62	0
56	MG	1A	3497	1/1	0.82	0.22	50,50,50,50	0
56	MG	1a	1814	1/1	0.82	0.06	67,67,67,67	0
56	MG	2A	3262	1/1	0.82	0.27	60,60,60,60	0
56	MG	2A	3710	1/1	0.82	0.13	42,42,42,42	0
56	MG	2A	3799	1/1	0.82	0.14	75,75,75,75	0
56	MG	2a	3062	1/1	0.82	0.14	71,71,71,71	0
56	MG	1B	215	1/1	0.82	0.07	55,55,55,55	0
56	MG	1A	4074	1/1	0.82	0.12	48,48,48,48	0
56	MG	2A	3622	1/1	0.82	0.10	38,38,38,38	0
56	MG	1A	3340	1/1	0.82	0.15	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3477	1/1	0.82	0.23	53,53,53,53	0
56	MG	1A	3699	1/1	0.82	0.19	37,37,37,37	0
56	MG	2a	3154	1/1	0.82	0.10	69,69,69,69	0
56	MG	1l	104	1/1	0.82	0.12	48,48,48,48	0
56	MG	1a	1693	1/1	0.82	0.15	69,69,69,69	0
56	MG	2a	3209	1/1	0.82	0.24	73,73,73,73	0
56	MG	1a	1611	1/1	0.82	0.13	68,68,68,68	0
56	MG	2a	3197	1/1	0.82	0.09	73,73,73,73	0
56	MG	1A	3753	1/1	0.82	0.20	34,34,34,34	0
56	MG	1A	3336	1/1	0.82	0.16	60,60,60,60	0
56	MG	2a	3086	1/1	0.82	0.15	63,63,63,63	0
56	MG	2B	202	1/1	0.82	0.15	63,63,63,63	0
56	MG	2a	3060	1/1	0.82	0.21	71,71,71,71	0
56	MG	2A	3516	1/1	0.82	0.23	74,74,74,74	0
56	MG	1a	1808	1/1	0.82	0.08	50,50,50,50	0
56	MG	1A	3765	1/1	0.82	0.18	43,43,43,43	0
56	MG	2A	3447	1/1	0.82	0.23	55,55,55,55	0
56	MG	2A	3296	1/1	0.82	0.17	50,50,50,50	0
56	MG	1U	201	1/1	0.82	0.28	51,51,51,51	0
56	MG	1A	3323	1/1	0.82	0.27	50,50,50,50	0
56	MG	1x	117	1/1	0.82	0.20	71,71,71,71	0
56	MG	1A	3703	1/1	0.82	0.18	48,48,48,48	0
56	MG	1A	3665	1/1	0.82	0.12	30,30,30,30	0
56	MG	2A	3250	1/1	0.82	0.73	64,64,64,64	0
56	MG	1a	1706	1/1	0.82	0.20	59,59,59,59	0
56	MG	1A	3564	1/1	0.82	0.17	49,49,49,49	0
56	MG	1A	3777	1/1	0.82	0.12	46,46,46,46	0
56	MG	2A	3614	1/1	0.82	0.15	45,45,45,45	0
56	MG	1A	4004	1/1	0.82	0.11	51,51,51,51	0
56	MG	2A	3546	1/1	0.82	0.17	65,65,65,65	0
56	MG	1A	3418	1/1	0.82	0.23	55,55,55,55	0
56	MG	2A	3522	1/1	0.82	0.09	41,41,41,41	0
56	MG	1A	3480	1/1	0.82	0.14	54,54,54,54	0
56	MG	2A	3123	1/1	0.83	0.11	59,59,59,59	0
56	MG	1s	101	1/1	0.83	0.16	71,71,71,71	0
56	MG	2A	3480	1/1	0.83	0.37	46,46,46,46	0
56	MG	2A	3282	1/1	0.83	0.16	63,63,63,63	0
56	MG	2A	3171	1/1	0.83	0.12	74,74,74,74	0
56	MG	1a	1659	1/1	0.83	0.38	55,55,55,55	0
56	MG	1a	1781	1/1	0.83	0.13	75,75,75,75	0
56	MG	1A	3693	1/1	0.83	0.23	42,42,42,42	0
56	MG	2F	302	1/1	0.83	0.15	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2B	216	1/1	0.83	0.08	65,65,65,65	0
56	MG	1A	3845	1/1	0.83	0.32	57,57,57,57	0
56	MG	2A	3138	1/1	0.83	0.07	70,70,70,70	0
56	MG	2A	3203	1/1	0.83	0.13	48,48,48,48	0
56	MG	2A	3796	1/1	0.83	0.28	77,77,77,77	0
56	MG	1A	3799	1/1	0.83	0.10	38,38,38,38	0
56	MG	1A	3854	1/1	0.83	0.07	60,60,60,60	0
56	MG	2A	3364	1/1	0.83	0.24	66,66,66,66	0
56	MG	2A	3251	1/1	0.83	0.15	62,62,62,62	0
56	MG	2a	3025	1/1	0.83	0.27	59,59,59,59	0
56	MG	2a	3009	1/1	0.83	0.12	72,72,72,72	0
56	MG	1A	3523	1/1	0.83	0.14	53,53,53,53	0
56	MG	2a	3127	1/1	0.83	0.19	63,63,63,63	0
56	MG	1A	3322	1/1	0.83	0.19	43,43,43,43	0
56	MG	1A	3955	1/1	0.83	0.11	65,65,65,65	0
56	MG	1A	4036	1/1	0.83	0.16	41,41,41,41	0
56	MG	2P	203	1/1	0.83	0.10	38,38,38,38	0
56	MG	2a	3175	1/1	0.83	0.16	73,73,73,73	0
56	MG	1D	310	1/1	0.83	0.17	24,24,24,24	0
56	MG	1A	3937	1/1	0.83	0.10	60,60,60,60	0
56	MG	2a	3135	1/1	0.83	0.23	59,59,59,59	0
56	MG	2A	3059	1/1	0.83	0.30	58,58,58,58	0
56	MG	2a	3068	1/1	0.83	0.12	74,74,74,74	0
56	MG	2A	3053	1/1	0.83	0.17	64,64,64,64	0
56	MG	1A	3747	1/1	0.83	0.17	54,54,54,54	0
56	MG	1A	3136	1/1	0.83	0.14	41,41,41,41	0
56	MG	1A	3706	1/1	0.83	0.24	53,53,53,53	0
56	MG	2A	3335	1/1	0.83	0.29	47,47,47,47	0
56	MG	2A	3566	1/1	0.83	0.17	44,44,44,44	0
56	MG	2A	3713	1/1	0.83	0.13	48,48,48,48	0
56	MG	1A	3510	1/1	0.83	0.15	41,41,41,41	0
56	MG	1a	1797	1/1	0.83	0.07	65,65,65,65	0
56	MG	2a	3005	1/1	0.83	0.17	66,66,66,66	0
56	MG	2A	3162	1/1	0.83	0.21	64,64,64,64	0
56	MG	1d	301	1/1	0.83	0.23	48,48,48,48	0
56	MG	2A	3323	1/1	0.83	0.14	57,57,57,57	0
56	MG	1A	3018	1/1	0.83	0.14	30,30,30,30	0
56	MG	1a	1796	1/1	0.83	0.13	59,59,59,59	0
56	MG	1A	3364	1/1	0.83	0.18	37,37,37,37	0
56	MG	2a	3140	1/1	0.83	0.10	57,57,57,57	0
56	MG	1A	3498	1/1	0.83	0.25	59,59,59,59	0
56	MG	2a	3156	1/1	0.83	0.06	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3273	1/1	0.83	0.28	49,49,49,49	0
56	MG	1A	3346	1/1	0.83	0.21	52,52,52,52	0
56	MG	1A	3533	1/1	0.83	0.25	55,55,55,55	0
56	MG	2A	3395	1/1	0.83	0.14	66,66,66,66	0
56	MG	1a	1646	1/1	0.83	0.15	56,56,56,56	0
56	MG	1A	3270	1/1	0.83	0.12	55,55,55,55	0
56	MG	1t	201	1/1	0.84	0.17	59,59,59,59	0
56	MG	2B	213	1/1	0.84	0.22	56,56,56,56	0
56	MG	1A	3039	1/1	0.84	0.21	54,54,54,54	0
56	MG	1A	3367	1/1	0.84	0.26	57,57,57,57	0
56	MG	1Q	206	1/1	0.84	0.16	51,51,51,51	0
56	MG	2A	3508	1/1	0.84	0.15	64,64,64,64	0
56	MG	1B	208	1/1	0.84	0.17	57,57,57,57	0
56	MG	1A	3607	1/1	0.84	0.20	27,27,27,27	0
56	MG	2A	3552	1/1	0.84	0.10	43,43,43,43	0
56	MG	2A	3051	1/1	0.84	0.13	72,72,72,72	0
56	MG	1a	1638	1/1	0.84	0.21	61,61,61,61	0
56	MG	1A	3958	1/1	0.84	0.11	50,50,50,50	0
56	MG	1A	3251	1/1	0.84	0.11	69,69,69,69	0
56	MG	1a	1715	1/1	0.84	0.11	53,53,53,53	0
56	MG	1a	1826	1/1	0.84	0.22	58,58,58,58	0
56	MG	2A	3236	1/1	0.84	0.19	45,45,45,45	0
56	MG	2A	3608	1/1	0.84	0.14	34,34,34,34	0
56	MG	1A	3984	1/1	0.84	0.10	71,71,71,71	0
56	MG	1A	3282	1/1	0.84	0.67	38,38,38,38	0
56	MG	2A	3540	1/1	0.84	0.14	35,35,35,35	0
56	MG	1A	3339	1/1	0.84	0.25	42,42,42,42	0
56	MG	1A	3358	1/1	0.84	0.15	45,45,45,45	0
56	MG	2A	3753	1/1	0.84	0.13	42,42,42,42	0
56	MG	2a	3037	1/1	0.84	0.15	48,48,48,48	0
56	MG	1a	1722	1/1	0.84	0.11	50,50,50,50	0
56	MG	2A	3295	1/1	0.84	0.25	58,58,58,58	0
56	MG	2a	3002	1/1	0.84	0.13	63,63,63,63	0
56	MG	2A	3297	1/1	0.84	0.14	72,72,72,72	0
56	MG	1A	3207	1/1	0.84	0.16	47,47,47,47	0
56	MG	1A	3954	1/1	0.84	0.15	75,75,75,75	0
56	MG	2A	3186	1/1	0.84	0.15	53,53,53,53	0
56	MG	14	101	1/1	0.84	0.10	69,69,69,69	0
56	MG	1A	4092	1/1	0.84	0.23	54,54,54,54	0
56	MG	1A	3074	1/1	0.84	0.30	55,55,55,55	0
56	MG	2a	3138	1/1	0.84	0.12	67,67,67,67	0
56	MG	1a	1606	1/1	0.84	0.25	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3767	1/1	0.84	0.18	51,51,51,51	0
56	MG	1A	3096	1/1	0.84	0.23	57,57,57,57	0
56	MG	2A	3350	1/1	0.84	0.14	68,68,68,68	0
56	MG	2A	3098	1/1	0.84	0.17	61,61,61,61	0
56	MG	2A	3605	1/1	0.84	0.11	51,51,51,51	0
56	MG	1A	3643	1/1	0.84	0.18	56,56,56,56	0
56	MG	1A	4053	1/1	0.84	0.14	34,34,34,34	0
56	MG	2A	3822	1/1	0.84	0.11	61,61,61,61	0
56	MG	2A	3418	1/1	0.84	0.16	66,66,66,66	0
56	MG	1A	3989	1/1	0.84	0.19	31,31,31,31	0
56	MG	2A	3400	1/1	0.84	0.45	59,59,59,59	0
56	MG	2A	3850	1/1	0.84	0.15	55,55,55,55	0
56	MG	2A	3202	1/1	0.84	0.15	47,47,47,47	0
56	MG	1A	3635	1/1	0.84	0.19	33,33,33,33	0
56	MG	1a	1661	1/1	0.84	0.13	58,58,58,58	0
56	MG	1a	1683	1/1	0.84	0.13	43,43,43,43	0
56	MG	2A	3737	1/1	0.84	0.14	70,70,70,70	0
56	MG	1A	3143	1/1	0.84	0.20	37,37,37,37	0
56	MG	2A	3801	1/1	0.84	0.12	80,80,80,80	0
56	MG	1A	3732	1/1	0.84	0.11	61,61,61,61	0
56	MG	1A	3151	1/1	0.84	0.53	42,42,42,42	0
56	MG	1A	3766	1/1	0.84	0.13	26,26,26,26	0
56	MG	1a	1641	1/1	0.84	0.10	57,57,57,57	0
56	MG	2A	3372	1/1	0.84	0.15	50,50,50,50	0
56	MG	2a	3001	1/1	0.84	0.26	57,57,57,57	0
56	MG	2A	3383	1/1	0.84	0.19	66,66,66,66	0
56	MG	2A	3726	1/1	0.84	0.19	50,50,50,50	0
56	MG	2A	3700	1/1	0.84	0.07	58,58,58,58	0
56	MG	1x	104	1/1	0.84	0.25	56,56,56,56	0
56	MG	2w	101	1/1	0.84	0.15	69,69,69,69	0
56	MG	1a	1730	1/1	0.84	0.25	65,65,65,65	0
56	MG	1A	4095	1/1	0.84	0.12	38,38,38,38	0
56	MG	2A	3087	1/1	0.84	0.22	48,48,48,48	0
56	MG	1a	1696	1/1	0.84	0.25	44,44,44,44	0
56	MG	2a	3077	1/1	0.84	0.14	59,59,59,59	0
56	MG	2A	3299	1/1	0.84	0.16	49,49,49,49	0
56	MG	2a	3238	1/1	0.84	0.24	72,72,72,72	0
56	MG	1A	3256	1/1	0.84	0.13	53,53,53,53	0
56	MG	2A	3014	1/1	0.84	0.64	55,55,55,55	0
56	MG	2A	3766	1/1	0.85	0.19	68,68,68,68	0
56	MG	2A	3168	1/1	0.85	0.10	53,53,53,53	0
56	MG	1A	3685	1/1	0.85	0.21	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3885	1/1	0.85	0.19	25,25,25,25	0
56	MG	2g	201	1/1	0.85	0.14	81,81,81,81	0
56	MG	1A	3797	1/1	0.85	0.21	27,27,27,27	0
56	MG	2A	3225	1/1	0.85	0.10	62,62,62,62	0
56	MG	2A	3831	1/1	0.85	0.20	56,56,56,56	0
56	MG	2A	3373	1/1	0.85	0.17	67,67,67,67	0
56	MG	2a	3236	1/1	0.85	0.13	73,73,73,73	0
56	MG	1a	1685	1/1	0.85	0.22	65,65,65,65	0
56	MG	1A	3048	1/1	0.85	0.13	20,20,20,20	0
56	MG	1a	1657	1/1	0.85	0.21	68,68,68,68	0
56	MG	2A	3005	1/1	0.85	0.15	55,55,55,55	0
56	MG	1A	3405	1/1	0.85	0.20	52,52,52,52	0
56	MG	2A	3368	1/1	0.85	0.23	65,65,65,65	0
56	MG	2a	3163	1/1	0.85	0.29	68,68,68,68	0
56	MG	2A	3310	1/1	0.85	0.25	65,65,65,65	0
56	MG	1A	3202	1/1	0.85	0.14	40,40,40,40	0
56	MG	2y	103	1/1	0.85	0.17	76,76,76,76	0
56	MG	2A	3484	1/1	0.85	0.12	58,58,58,58	0
56	MG	1a	1690	1/1	0.85	0.14	56,56,56,56	0
56	MG	1A	3131	1/1	0.85	0.19	63,63,63,63	0
56	MG	1A	3526	1/1	0.85	0.43	42,42,42,42	0
56	MG	2Q	203	1/1	0.85	0.41	56,56,56,56	0
56	MG	2a	3107	1/1	0.85	0.14	74,74,74,74	0
56	MG	2A	3221	1/1	0.85	0.16	57,57,57,57	0
56	MG	1E	301	1/1	0.85	0.39	28,28,28,28	0
56	MG	2A	3657	1/1	0.85	0.29	84,84,84,84	0
56	MG	1A	3468	1/1	0.85	0.41	57,57,57,57	0
56	MG	2A	3193	1/1	0.85	0.10	63,63,63,63	0
56	MG	2A	3205	1/1	0.85	0.39	63,63,63,63	0
56	MG	1A	3960	1/1	0.85	0.11	50,50,50,50	0
56	MG	2A	3129	1/1	0.85	0.43	54,54,54,54	0
56	MG	2A	3263	1/1	0.85	0.20	71,71,71,71	0
56	MG	2A	3419	1/1	0.85	0.16	62,62,62,62	0
56	MG	1A	3412	1/1	0.85	0.20	38,38,38,38	0
56	MG	1A	3378	1/1	0.85	0.19	42,42,42,42	0
56	MG	1B	214	1/1	0.85	0.13	46,46,46,46	0
56	MG	2A	3377	1/1	0.85	0.24	65,65,65,65	0
56	MG	1A	3927	1/1	0.85	0.16	55,55,55,55	0
56	MG	1x	111	1/1	0.85	0.14	71,71,71,71	0
56	MG	2A	3004	1/1	0.85	0.11	58,58,58,58	0
56	MG	2A	3768	1/1	0.85	0.09	42,42,42,42	0
56	MG	2A	3173	1/1	0.85	0.15	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3220	1/1	0.85	0.17	49,49,49,49	0
56	MG	2a	3098	1/1	0.85	0.11	62,62,62,62	0
56	MG	2A	3234	1/1	0.85	0.52	60,60,60,60	0
56	MG	1a	1788	1/1	0.85	0.09	61,61,61,61	0
56	MG	1N	201	1/1	0.85	0.36	51,51,51,51	0
56	MG	1a	1607	1/1	0.85	0.16	55,55,55,55	0
56	MG	2A	3163	1/1	0.85	0.12	57,57,57,57	0
56	MG	1A	3932	1/1	0.85	0.19	48,48,48,48	0
56	MG	1A	3947	1/1	0.85	0.17	27,27,27,27	0
56	MG	1A	4027	1/1	0.85	0.41	65,65,65,65	0
56	MG	1A	4076	1/1	0.85	0.25	36,36,36,36	0
56	MG	2A	3292	1/1	0.85	0.11	57,57,57,57	0
56	MG	2A	3309	1/1	0.85	0.19	55,55,55,55	0
56	MG	1a	1759	1/1	0.85	0.14	61,61,61,61	0
56	MG	2A	3074	1/1	0.85	0.45	41,41,41,41	0
56	MG	2A	3376	1/1	0.85	0.20	53,53,53,53	0
56	MG	2A	3439	1/1	0.85	0.22	55,55,55,55	0
56	MG	1A	3733	1/1	0.85	0.15	45,45,45,45	0
56	MG	2A	3339	1/1	0.85	0.23	64,64,64,64	0
56	MG	2A	3114	1/1	0.85	0.14	64,64,64,64	0
56	MG	2A	3159	1/1	0.85	0.21	66,66,66,66	0
56	MG	2A	3302	1/1	0.86	0.14	61,61,61,61	0
56	MG	1A	3682	1/1	0.86	0.17	61,61,61,61	0
56	MG	1A	4014	1/1	0.86	0.15	46,46,46,46	0
56	MG	1a	1817	1/1	0.86	0.25	58,58,58,58	0
56	MG	1A	3041	1/1	0.86	0.55	34,34,34,34	0
56	MG	2a	3106	1/1	0.86	0.12	65,65,65,65	0
56	MG	1A	3434	1/1	0.86	0.16	40,40,40,40	0
56	MG	2A	3391	1/1	0.86	0.12	68,68,68,68	0
56	MG	1A	3528	1/1	0.86	0.34	47,47,47,47	0
56	MG	2A	3265	1/1	0.86	0.12	57,57,57,57	0
56	MG	1A	3990	1/1	0.86	0.14	33,33,33,33	0
56	MG	1N	203	1/1	0.86	0.16	46,46,46,46	0
56	MG	1A	3626	1/1	0.86	0.12	47,47,47,47	0
56	MG	2A	3479	1/1	0.86	0.24	52,52,52,52	0
56	MG	2a	3137	1/1	0.86	0.13	75,75,75,75	0
56	MG	1A	3147	1/1	0.86	0.26	39,39,39,39	0
56	MG	2A	3495	1/1	0.86	0.16	57,57,57,57	0
56	MG	2q	201	1/1	0.86	0.24	68,68,68,68	0
56	MG	2B	217	1/1	0.86	0.21	84,84,84,84	0
56	MG	1A	3062	1/1	0.86	0.27	51,51,51,51	0
56	MG	2a	3089	1/1	0.86	0.26	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3034	1/1	0.86	0.22	72,72,72,72	0
56	MG	2A	3679	1/1	0.86	0.10	52,52,52,52	0
56	MG	25	104	1/1	0.86	0.25	54,54,54,54	0
56	MG	1a	1679	1/1	0.86	0.11	66,66,66,66	0
56	MG	2A	3490	1/1	0.86	0.15	53,53,53,53	0
56	MG	1A	4031	1/1	0.86	0.10	60,60,60,60	0
56	MG	2D	307	1/1	0.86	0.53	47,47,47,47	0
56	MG	1A	3261	1/1	0.86	0.16	52,52,52,52	0
56	MG	1A	3114	1/1	0.86	0.25	32,32,32,32	0
56	MG	2a	3050	1/1	0.86	0.18	47,47,47,47	0
56	MG	1a	1692	1/1	0.86	0.17	70,70,70,70	0
56	MG	2A	3613	1/1	0.86	0.12	46,46,46,46	0
56	MG	1A	3686	1/1	0.86	0.17	54,54,54,54	0
56	MG	1A	3234	1/1	0.86	0.37	54,54,54,54	0
56	MG	1A	3237	1/1	0.86	0.25	30,30,30,30	0
56	MG	1A	3504	1/1	0.86	0.32	54,54,54,54	0
56	MG	2a	3045	1/1	0.86	0.22	72,72,72,72	0
56	MG	2A	3314	1/1	0.86	0.26	60,60,60,60	0
56	MG	2a	3216	1/1	0.86	0.17	72,72,72,72	0
56	MG	1A	3907	1/1	0.86	0.09	48,48,48,48	0
56	MG	1A	3349	1/1	0.86	0.25	56,56,56,56	0
56	MG	1x	112	1/1	0.86	0.15	58,58,58,58	0
56	MG	2X	101	1/1	0.86	0.12	56,56,56,56	0
56	MG	2A	3497	1/1	0.86	0.17	51,51,51,51	0
56	MG	2A	3457	1/1	0.86	0.14	50,50,50,50	0
56	MG	2a	3227	1/1	0.86	0.21	78,78,78,78	0
56	MG	25	105	1/1	0.86	0.22	49,49,49,49	0
56	MG	2A	3121	1/1	0.86	0.17	48,48,48,48	0
56	MG	1A	3440	1/1	0.86	0.13	36,36,36,36	0
56	MG	1A	3333	1/1	0.86	0.30	56,56,56,56	0
56	MG	2A	3056	1/1	0.86	0.18	59,59,59,59	0
56	MG	2A	3356	1/1	0.86	0.35	62,62,62,62	0
56	MG	2A	3367	1/1	0.86	0.13	54,54,54,54	0
56	MG	1A	3713	1/1	0.86	0.26	63,63,63,63	0
56	MG	2A	3182	1/1	0.86	0.14	49,49,49,49	0
56	MG	2A	3283	1/1	0.86	0.09	57,57,57,57	0
56	MG	2a	3027	1/1	0.86	0.43	70,70,70,70	0
56	MG	1a	1805	1/1	0.86	0.14	55,55,55,55	0
56	MG	1F	308	1/1	0.86	0.20	49,49,49,49	0
56	MG	2a	3084	1/1	0.86	0.15	58,58,58,58	0
56	MG	2a	3117	1/1	0.86	0.13	65,65,65,65	0
56	MG	2A	3416	1/1	0.86	0.20	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3675	1/1	0.86	0.10	24,24,24,24	0
56	MG	2A	3104	1/1	0.86	0.15	51,51,51,51	0
56	MG	1P	209	1/1	0.86	0.14	40,40,40,40	0
56	MG	1A	3400	1/1	0.86	0.54	42,42,42,42	0
56	MG	10	104	1/1	0.86	0.18	59,59,59,59	0
56	MG	1a	1658	1/1	0.86	0.08	63,63,63,63	0
56	MG	1A	3776	1/1	0.87	0.12	31,31,31,31	0
56	MG	1A	3475	1/1	0.87	0.26	48,48,48,48	0
56	MG	2A	3826	1/1	0.87	0.14	55,55,55,55	0
56	MG	1A	3334	1/1	0.87	0.16	43,43,43,43	0
56	MG	1A	3017	1/1	0.87	0.39	50,50,50,50	0
56	MG	2A	3515	1/1	0.87	0.15	36,36,36,36	0
56	MG	2A	3267	1/1	0.87	0.82	67,67,67,67	0
56	MG	1a	1779	1/1	0.87	0.19	88,88,88,88	0
56	MG	1A	3493	1/1	0.87	0.17	48,48,48,48	0
56	MG	1P	207	1/1	0.87	0.08	51,51,51,51	0
56	MG	2A	3463	1/1	0.87	0.12	55,55,55,55	0
56	MG	2A	3611	1/1	0.87	0.13	51,51,51,51	0
56	MG	1A	3585	1/1	0.87	0.31	35,35,35,35	0
56	MG	1B	237	1/1	0.87	0.12	68,68,68,68	0
56	MG	1A	3823	1/1	0.87	0.60	50,50,50,50	0
56	MG	1a	1729	1/1	0.87	0.19	54,54,54,54	0
56	MG	1A	3836	1/1	0.87	0.20	50,50,50,50	0
56	MG	2D	306	1/1	0.87	0.77	47,47,47,47	0
56	MG	2A	3248	1/1	0.87	0.57	65,65,65,65	0
56	MG	2a	3080	1/1	0.87	0.28	62,62,62,62	0
56	MG	1A	3170	1/1	0.87	0.18	47,47,47,47	0
56	MG	1A	3892	1/1	0.87	0.14	30,30,30,30	0
56	MG	2A	3358	1/1	0.87	0.13	56,56,56,56	0
56	MG	2A	3715	1/1	0.87	0.17	68,68,68,68	0
56	MG	1A	3627	1/1	0.87	0.22	18,18,18,18	0
56	MG	2A	3268	1/1	0.87	0.17	57,57,57,57	0
56	MG	2A	3003	1/1	0.87	0.23	44,44,44,44	0
56	MG	1A	3116	1/1	0.87	0.22	36,36,36,36	0
56	MG	2A	3601	1/1	0.87	0.20	58,58,58,58	0
56	MG	12	101	1/1	0.87	0.15	54,54,54,54	0
56	MG	1N	205	1/1	0.87	0.23	57,57,57,57	0
56	MG	2a	3064	1/1	0.87	0.23	64,64,64,64	0
56	MG	2a	3122	1/1	0.87	0.09	73,73,73,73	0
56	MG	1f	202	1/1	0.87	0.13	70,70,70,70	0
56	MG	2A	3043	1/1	0.87	0.19	57,57,57,57	0
56	MG	2a	3183	1/1	0.87	0.14	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3505	1/1	0.87	0.16	39,39,39,39	0
56	MG	1a	1752	1/1	0.87	0.19	74,74,74,74	0
56	MG	2A	3858	1/1	0.87	0.28	64,64,64,64	0
56	MG	1A	4100	1/1	0.87	0.42	85,85,85,85	0
56	MG	1a	1627	1/1	0.87	0.12	55,55,55,55	0
56	MG	2A	3022	1/1	0.87	0.29	56,56,56,56	0
56	MG	2A	3175	1/1	0.87	0.43	50,50,50,50	0
56	MG	1a	1669	1/1	0.87	0.28	75,75,75,75	0
56	MG	2A	3562	1/1	0.87	0.16	35,35,35,35	0
56	MG	1A	3664	1/1	0.87	0.08	40,40,40,40	0
56	MG	2a	3187	1/1	0.87	0.16	70,70,70,70	0
56	MG	2A	3506	1/1	0.87	0.11	36,36,36,36	0
56	MG	2a	3143	1/1	0.87	0.12	75,75,75,75	0
56	MG	1A	4038	1/1	0.87	0.09	52,52,52,52	0
56	MG	1a	1754	1/1	0.87	0.16	57,57,57,57	0
56	MG	2A	3531	1/1	0.87	0.17	55,55,55,55	0
56	MG	2A	3692	1/1	0.87	0.07	66,66,66,66	0
56	MG	2a	3118	1/1	0.87	0.13	62,62,62,62	0
56	MG	1A	3101	1/1	0.87	0.17	56,56,56,56	0
56	MG	1A	3917	1/1	0.87	0.16	34,34,34,34	0
56	MG	1A	3279	1/1	0.87	0.31	39,39,39,39	0
56	MG	2A	3136	1/1	0.87	0.16	38,38,38,38	0
56	MG	2a	3047	1/1	0.87	0.13	55,55,55,55	0
56	MG	1A	3431	1/1	0.87	0.21	54,54,54,54	0
56	MG	1A	3296	1/1	0.87	0.12	32,32,32,32	0
56	MG	1A	3157	1/1	0.87	0.20	40,40,40,40	0
56	MG	2A	3069	1/1	0.87	0.09	54,54,54,54	0
56	MG	2A	3525	1/1	0.87	0.14	60,60,60,60	0
56	MG	2A	3461	1/1	0.87	0.15	44,44,44,44	0
56	MG	1A	4028	1/1	0.87	0.07	61,61,61,61	0
56	MG	1B	212	1/1	0.87	0.14	40,40,40,40	0
56	MG	2t	201	1/1	0.87	0.14	47,47,47,47	0
56	MG	1Y	201	1/1	0.87	0.23	32,32,32,32	0
56	MG	1A	3578	1/1	0.87	0.19	43,43,43,43	0
56	MG	1A	3433	1/1	0.87	0.13	31,31,31,31	0
56	MG	20	101	1/1	0.87	0.11	67,67,67,67	0
56	MG	1x	110	1/1	0.87	0.22	61,61,61,61	0
56	MG	1A	3488	1/1	0.87	0.17	33,33,33,33	0
56	MG	1a	1689	1/1	0.87	0.15	59,59,59,59	0
56	MG	2a	3213	1/1	0.87	0.08	75,75,75,75	0
56	MG	1E	313	1/1	0.87	0.27	54,54,54,54	0
56	MG	1A	3997	1/1	0.87	0.20	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3432	1/1	0.87	0.22	40,40,40,40	0
56	MG	1A	3717	1/1	0.87	0.07	41,41,41,41	0
56	MG	1A	3391	1/1	0.87	0.10	42,42,42,42	0
56	MG	2A	3564	1/1	0.87	0.23	53,53,53,53	0
56	MG	1a	1810	1/1	0.87	0.10	59,59,59,59	0
56	MG	1E	303	1/1	0.87	0.30	38,38,38,38	0
56	MG	2A	3602	1/1	0.87	0.14	55,55,55,55	0
56	MG	1A	3061	1/1	0.87	0.18	67,67,67,67	0
56	MG	1A	3816	1/1	0.87	0.23	54,54,54,54	0
56	MG	2A	3592	1/1	0.87	0.14	46,46,46,46	0
56	MG	1A	3534	1/1	0.87	0.20	63,63,63,63	0
56	MG	2A	3252	1/1	0.87	0.11	48,48,48,48	0
56	MG	2A	3331	1/1	0.87	0.32	72,72,72,72	0
56	MG	2A	3200	1/1	0.87	0.17	48,48,48,48	0
56	MG	1a	1668	1/1	0.87	0.11	66,66,66,66	0
56	MG	2A	3702	1/1	0.87	0.10	31,31,31,31	0
56	MG	1A	3888	1/1	0.87	0.32	44,44,44,44	0
56	MG	2A	3716	1/1	0.87	0.08	51,51,51,51	0
56	MG	2a	3051	1/1	0.87	0.15	62,62,62,62	0
56	MG	2A	3483	1/1	0.87	0.19	68,68,68,68	0
56	MG	2A	3194	1/1	0.88	0.38	60,60,60,60	0
56	MG	1a	1623	1/1	0.88	0.23	55,55,55,55	0
56	MG	1A	3722	1/1	0.88	0.16	59,59,59,59	0
56	MG	1A	3949	1/1	0.88	0.07	54,54,54,54	0
56	MG	1A	3438	1/1	0.88	0.16	50,50,50,50	0
56	MG	2A	3030	1/1	0.88	0.12	46,46,46,46	0
56	MG	2A	3503	1/1	0.88	0.19	39,39,39,39	0
56	MG	1A	3667	1/1	0.88	0.18	28,28,28,28	0
56	MG	1A	4070	1/1	0.88	0.07	52,52,52,52	0
56	MG	1A	4094	1/1	0.88	0.22	47,47,47,47	0
56	MG	2A	3379	1/1	0.88	0.15	56,56,56,56	0
56	MG	1a	1667	1/1	0.88	0.21	58,58,58,58	0
56	MG	1a	1712	1/1	0.88	0.27	53,53,53,53	0
56	MG	1A	3750	1/1	0.88	0.14	34,34,34,34	0
56	MG	1A	3109	1/1	0.88	0.41	31,31,31,31	0
56	MG	1a	1726	1/1	0.88	0.14	61,61,61,61	0
56	MG	1A	4073	1/1	0.88	0.36	59,59,59,59	0
56	MG	2A	3853	1/1	0.88	0.13	49,49,49,49	0
56	MG	1A	3625	1/1	0.88	0.12	53,53,53,53	0
56	MG	2A	3428	1/1	0.88	0.20	50,50,50,50	0
56	MG	1A	4018	1/1	0.88	0.17	35,35,35,35	0
56	MG	1a	1710	1/1	0.88	0.15	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3802	1/1	0.88	0.24	60,60,60,60	0
56	MG	1A	3303	1/1	0.88	0.39	55,55,55,55	0
56	MG	1A	3725	1/1	0.88	0.08	66,66,66,66	0
56	MG	2W	202	1/1	0.88	0.28	45,45,45,45	0
56	MG	2a	3179	1/1	0.88	0.08	69,69,69,69	0
56	MG	2a	3131	1/1	0.88	0.19	60,60,60,60	0
56	MG	1w	102	1/1	0.88	0.20	75,75,75,75	0
56	MG	1A	3276	1/1	0.88	0.12	45,45,45,45	0
56	MG	1A	3617	1/1	0.88	0.13	36,36,36,36	0
56	MG	1A	3506	1/1	0.88	0.27	47,47,47,47	0
56	MG	2A	3375	1/1	0.88	0.18	64,64,64,64	0
56	MG	2A	3343	1/1	0.88	0.08	57,57,57,57	0
56	MG	2A	3370	1/1	0.88	0.12	64,64,64,64	0
56	MG	2A	3270	1/1	0.88	0.20	57,57,57,57	0
56	MG	2A	3011	1/1	0.88	0.09	53,53,53,53	0
56	MG	1A	3889	1/1	0.88	0.18	44,44,44,44	0
56	MG	2A	3470	1/1	0.88	0.62	62,62,62,62	0
56	MG	1A	4046	1/1	0.88	0.15	44,44,44,44	0
56	MG	2A	3509	1/1	0.88	0.15	41,41,41,41	0
56	MG	1A	4051	1/1	0.88	0.32	58,58,58,58	0
56	MG	1A	3470	1/1	0.88	0.24	49,49,49,49	0
56	MG	10	102	1/1	0.88	0.16	41,41,41,41	0
56	MG	1Q	205	1/1	0.88	0.21	55,55,55,55	0
56	MG	1a	1791	1/1	0.88	0.10	64,64,64,64	0
56	MG	16	103	1/1	0.88	0.24	51,51,51,51	0
56	MG	2A	3862	1/1	0.88	0.09	57,57,57,57	0
56	MG	1A	3870	1/1	0.88	0.20	30,30,30,30	0
56	MG	1A	3575	1/1	0.88	0.22	55,55,55,55	0
56	MG	2A	3721	1/1	0.88	0.11	62,62,62,62	0
56	MG	2A	3706	1/1	0.88	0.14	68,68,68,68	0
56	MG	12	102	1/1	0.88	0.21	39,39,39,39	0
56	MG	1A	3690	1/1	0.88	0.20	19,19,19,19	0
56	MG	2A	3847	1/1	0.88	0.11	47,47,47,47	0
56	MG	1A	3335	1/1	0.88	0.17	36,36,36,36	0
56	MG	1A	3519	1/1	0.88	0.11	45,45,45,45	0
56	MG	2A	3150	1/1	0.88	0.35	53,53,53,53	0
56	MG	1G	204	1/1	0.88	0.12	52,52,52,52	0
56	MG	1A	3787	1/1	0.88	0.08	44,44,44,44	0
56	MG	2a	3202	1/1	0.88	0.27	75,75,75,75	0
56	MG	1a	1642	1/1	0.88	0.17	57,57,57,57	0
56	MG	2a	3231	1/1	0.88	0.15	58,58,58,58	0
56	MG	25	103	1/1	0.88	0.22	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3547	1/1	0.88	0.18	42,42,42,42	0
56	MG	1A	3606	1/1	0.88	0.20	36,36,36,36	0
56	MG	2A	3228	1/1	0.88	0.40	72,72,72,72	0
56	MG	1A	3739	1/1	0.88	0.11	51,51,51,51	0
56	MG	1A	3963	1/1	0.88	0.11	33,33,33,33	0
56	MG	1A	3361	1/1	0.88	0.17	56,56,56,56	0
56	MG	2W	201	1/1	0.88	0.26	57,57,57,57	0
56	MG	2a	3023	1/1	0.88	0.16	76,76,76,76	0
56	MG	1B	211	1/1	0.88	0.32	51,51,51,51	0
56	MG	2a	3233	1/1	0.88	0.15	67,67,67,67	0
56	MG	1a	1709	1/1	0.88	0.18	50,50,50,50	0
56	MG	2A	3746	1/1	0.88	0.11	57,57,57,57	0
56	MG	2A	3743	1/1	0.88	0.09	59,59,59,59	0
56	MG	2B	212	1/1	0.88	0.18	57,57,57,57	0
56	MG	1A	3238	1/1	0.88	0.23	56,56,56,56	0
56	MG	2A	3462	1/1	0.88	0.20	60,60,60,60	0
56	MG	2A	3770	1/1	0.88	0.31	54,54,54,54	0
56	MG	2A	3160	1/1	0.88	0.53	57,57,57,57	0
56	MG	1A	3709	1/1	0.88	0.19	41,41,41,41	0
56	MG	1A	3060	1/1	0.88	0.14	39,39,39,39	0
56	MG	1A	3388	1/1	0.88	0.18	44,44,44,44	0
56	MG	2A	3687	1/1	0.88	0.34	71,71,71,71	0
56	MG	1A	3770	1/1	0.88	0.15	32,32,32,32	0
56	MG	2Q	204	1/1	0.88	0.42	62,62,62,62	0
56	MG	2A	3409	1/1	0.88	0.15	66,66,66,66	0
56	MG	2A	3664	1/1	0.88	0.13	57,57,57,57	0
56	MG	1A	3991	1/1	0.88	0.19	22,22,22,22	0
56	MG	2A	3181	1/1	0.88	0.11	44,44,44,44	0
56	MG	2A	3369	1/1	0.88	0.11	64,64,64,64	0
56	MG	2A	3712	1/1	0.88	0.18	70,70,70,70	0
56	MG	1a	1677	1/1	0.88	0.29	57,57,57,57	0
56	MG	2a	3020	1/1	0.88	0.14	71,71,71,71	0
56	MG	1A	3155	1/1	0.88	0.21	43,43,43,43	0
56	MG	1B	233	1/1	0.88	0.09	63,63,63,63	0
56	MG	1F	304	1/1	0.88	0.13	34,34,34,34	0
56	MG	1A	3563	1/1	0.88	0.16	53,53,53,53	0
56	MG	1A	4082	1/1	0.88	0.11	35,35,35,35	0
56	MG	1A	3566	1/1	0.88	0.15	52,52,52,52	0
56	MG	2a	3046	1/1	0.88	0.11	66,66,66,66	0
56	MG	1A	3123	1/1	0.88	0.27	41,41,41,41	0
56	MG	1A	3988	1/1	0.88	0.25	21,21,21,21	0
56	MG	1A	3734	1/1	0.88	0.11	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3792	1/1	0.88	0.41	63,63,63,63	0
56	MG	2a	3148	1/1	0.88	0.14	63,63,63,63	0
56	MG	1a	1666	1/1	0.88	0.14	63,63,63,63	0
56	MG	1a	1762	1/1	0.88	0.19	61,61,61,61	0
56	MG	1A	3458	1/1	0.88	0.14	62,62,62,62	0
56	MG	1a	1691	1/1	0.88	0.14	64,64,64,64	0
56	MG	18	107	1/1	0.88	0.30	56,56,56,56	0
56	MG	1A	3644	1/1	0.88	0.17	58,58,58,58	0
56	MG	2A	3130	1/1	0.88	0.21	54,54,54,54	0
56	MG	1A	4037	1/1	0.88	0.10	68,68,68,68	0
56	MG	2A	3688	1/1	0.88	0.16	57,57,57,57	0
56	MG	2A	3459	1/1	0.88	0.11	41,41,41,41	0
56	MG	1A	3681	1/1	0.88	0.08	47,47,47,47	0
56	MG	1A	3456	1/1	0.88	0.12	49,49,49,49	0
56	MG	2A	3348	1/1	0.88	0.14	65,65,65,65	0
56	MG	1A	3226	1/1	0.89	0.23	43,43,43,43	0
56	MG	1Z	302	1/1	0.89	0.08	60,60,60,60	0
56	MG	1A	3974	1/1	0.89	0.08	54,54,54,54	0
56	MG	1A	3572	1/1	0.89	0.30	39,39,39,39	0
56	MG	1A	3450	1/1	0.89	0.43	50,50,50,50	0
56	MG	1A	3209	1/1	0.89	0.17	38,38,38,38	0
56	MG	1A	4099	1/1	0.89	0.21	40,40,40,40	0
56	MG	2a	3139	1/1	0.89	0.09	70,70,70,70	0
56	MG	2A	3771	1/1	0.89	0.10	62,62,62,62	0
56	MG	1A	3981	1/1	0.89	0.18	60,60,60,60	0
56	MG	2A	3338	1/1	0.89	0.18	62,62,62,62	0
56	MG	2A	3041	1/1	0.89	0.12	70,70,70,70	0
56	MG	1A	3964	1/1	0.89	0.07	33,33,33,33	0
56	MG	1A	3129	1/1	0.89	0.27	47,47,47,47	0
56	MG	1A	3565	1/1	0.89	0.11	58,58,58,58	0
56	MG	1A	3976	1/1	0.89	0.14	47,47,47,47	0
56	MG	2A	3473	1/1	0.89	0.14	60,60,60,60	0
56	MG	2A	3257	1/1	0.89	0.16	62,62,62,62	0
56	MG	2a	3024	1/1	0.89	0.16	59,59,59,59	0
56	MG	1A	3970	1/1	0.89	0.16	20,20,20,20	0
56	MG	2A	3619	1/1	0.89	0.12	36,36,36,36	0
56	MG	2a	3008	1/1	0.89	0.13	57,57,57,57	0
56	MG	1A	3490	1/1	0.89	0.23	35,35,35,35	0
56	MG	1A	3398	1/1	0.89	0.20	23,23,23,23	0
56	MG	1A	3091	1/1	0.89	0.13	50,50,50,50	0
56	MG	1A	3484	1/1	0.89	0.25	59,59,59,59	0
56	MG	1A	3420	1/1	0.89	0.15	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3839	1/1	0.89	0.10	35,35,35,35	0
56	MG	1A	3306	1/1	0.89	0.21	41,41,41,41	0
56	MG	1A	3029	1/1	0.89	0.14	23,23,23,23	0
56	MG	2D	309	1/1	0.89	0.20	35,35,35,35	0
56	MG	2a	3056	1/1	0.89	0.11	57,57,57,57	0
56	MG	1A	3390	1/1	0.89	0.23	36,36,36,36	0
56	MG	2A	3885	1/1	0.89	0.24	59,59,59,59	0
56	MG	1A	3646	1/1	0.89	0.16	30,30,30,30	0
56	MG	2A	3183	1/1	0.89	0.20	52,52,52,52	0
56	MG	2A	3689	1/1	0.89	0.09	59,59,59,59	0
56	MG	1B	227	1/1	0.89	0.14	60,60,60,60	0
56	MG	1A	3159	1/1	0.89	0.30	30,30,30,30	0
56	MG	1A	3696	1/1	0.89	0.14	20,20,20,20	0
56	MG	1A	3446	1/1	0.89	0.17	52,52,52,52	0
56	MG	1a	1680	1/1	0.89	0.15	63,63,63,63	0
56	MG	1a	1786	1/1	0.89	0.10	73,73,73,73	0
56	MG	1A	4019	1/1	0.89	0.14	22,22,22,22	0
56	MG	2A	3442	1/1	0.89	0.21	57,57,57,57	0
56	MG	15	102	1/1	0.89	0.32	42,42,42,42	0
56	MG	2A	3845	1/1	0.89	0.09	44,44,44,44	0
56	MG	1A	3538	1/1	0.89	0.18	50,50,50,50	0
56	MG	1A	3712	1/1	0.89	0.07	54,54,54,54	0
56	MG	1a	1695	1/1	0.89	0.27	52,52,52,52	0
56	MG	2A	3312	1/1	0.89	0.16	50,50,50,50	0
56	MG	1a	1671	1/1	0.89	0.12	49,49,49,49	0
56	MG	1a	1827	1/1	0.89	0.15	52,52,52,52	0
56	MG	2A	3581	1/1	0.89	0.11	46,46,46,46	0
56	MG	2A	3152	1/1	0.89	0.28	71,71,71,71	0
56	MG	2A	3089	1/1	0.89	0.14	61,61,61,61	0
56	MG	2A	3686	1/1	0.89	0.18	53,53,53,53	0
56	MG	2F	303	1/1	0.89	0.40	48,48,48,48	0
56	MG	1a	1720	1/1	0.89	0.28	51,51,51,51	0
56	MG	1A	3419	1/1	0.89	0.11	32,32,32,32	0
56	MG	1a	1665	1/1	0.89	0.21	51,51,51,51	0
56	MG	1A	3957	1/1	0.89	0.08	50,50,50,50	0
56	MG	1A	3613	1/1	0.89	0.15	42,42,42,42	0
56	MG	2A	3781	1/1	0.89	0.09	57,57,57,57	0
56	MG	2A	3326	1/1	0.89	0.24	61,61,61,61	0
56	MG	1a	1654	1/1	0.89	0.16	71,71,71,71	0
56	MG	1A	3314	1/1	0.89	0.23	48,48,48,48	0
56	MG	2a	3036	1/1	0.89	0.15	72,72,72,72	0
56	MG	1A	3416	1/1	0.89	0.22	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3456	1/1	0.89	0.11	61,61,61,61	0
56	MG	2A	3670	1/1	0.89	0.34	47,47,47,47	0
56	MG	1B	236	1/1	0.89	0.14	49,49,49,49	0
56	MG	2A	3206	1/1	0.89	0.32	53,53,53,53	0
56	MG	1a	1732	1/1	0.89	0.20	64,64,64,64	0
56	MG	1A	3822	1/1	0.89	0.09	25,25,25,25	0
56	MG	1A	3379	1/1	0.89	0.15	48,48,48,48	0
56	MG	1A	3473	1/1	0.89	0.42	65,65,65,65	0
56	MG	2A	3643	1/1	0.89	0.11	62,62,62,62	0
56	MG	2A	3408	1/1	0.89	0.40	52,52,52,52	0
56	MG	2A	3115	1/1	0.89	0.09	41,41,41,41	0
56	MG	1A	3555	1/1	0.89	0.21	23,23,23,23	0
56	MG	2A	3198	1/1	0.89	0.15	68,68,68,68	0
56	MG	2a	3105	1/1	0.89	0.12	45,45,45,45	0
56	MG	1A	3063	1/1	0.89	0.16	43,43,43,43	0
56	MG	2a	3220	1/1	0.89	0.06	63,63,63,63	0
56	MG	2A	3575	1/1	0.89	0.20	65,65,65,65	0
56	MG	2A	3465	1/1	0.89	0.11	48,48,48,48	0
56	MG	2a	3214	1/1	0.89	0.08	74,74,74,74	0
56	MG	1A	3956	1/1	0.89	0.23	45,45,45,45	0
56	MG	1A	3940	1/1	0.89	0.14	28,28,28,28	0
56	MG	2A	3254	1/1	0.89	0.17	63,63,63,63	0
56	MG	1x	103	1/1	0.89	0.15	48,48,48,48	0
56	MG	2A	3627	1/1	0.89	0.13	44,44,44,44	0
56	MG	2F	301	1/1	0.89	0.35	46,46,46,46	0
56	MG	1A	3315	1/1	0.89	0.14	51,51,51,51	0
56	MG	2w	103	1/1	0.89	0.07	64,64,64,64	0
56	MG	1A	3650	1/1	0.89	0.20	49,49,49,49	0
56	MG	1W	201	1/1	0.89	0.29	49,49,49,49	0
56	MG	2A	3189	1/1	0.89	0.20	60,60,60,60	0
56	MG	1A	3246	1/1	0.89	0.27	50,50,50,50	0
56	MG	1A	3479	1/1	0.89	0.14	53,53,53,53	0
56	MG	2A	3341	1/1	0.89	0.31	66,66,66,66	0
56	MG	2A	3583	1/1	0.89	0.08	61,61,61,61	0
56	MG	2A	3873	1/1	0.89	0.40	75,75,75,75	0
56	MG	2A	3603	1/1	0.89	0.09	60,60,60,60	0
56	MG	1A	3401	1/1	0.89	0.28	35,35,35,35	0
56	MG	1A	3006	1/1	0.89	0.21	47,47,47,47	0
56	MG	2A	3491	1/1	0.89	0.14	50,50,50,50	0
56	MG	2A	3149	1/1	0.89	0.13	63,63,63,63	0
56	MG	1A	3451	1/1	0.89	0.31	42,42,42,42	0
56	MG	2x	102	1/1	0.89	0.10	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3263	1/1	0.89	0.11	64,64,64,64	0
56	MG	1A	4026	1/1	0.89	0.12	35,35,35,35	0
56	MG	1A	3344	1/1	0.89	0.19	53,53,53,53	0
56	MG	1A	4002	1/1	0.89	0.12	31,31,31,31	0
56	MG	1A	3447	1/1	0.89	0.19	51,51,51,51	0
56	MG	1A	3891	1/1	0.89	0.21	21,21,21,21	0
56	MG	2A	3834	1/1	0.89	0.15	48,48,48,48	0
56	MG	1A	3552	1/1	0.89	0.18	27,27,27,27	0
56	MG	1A	3486	1/1	0.89	0.18	44,44,44,44	0
56	MG	2B	209	1/1	0.89	0.17	59,59,59,59	0
56	MG	2A	3788	1/1	0.89	0.19	51,51,51,51	0
56	MG	18	105	1/1	0.90	0.14	45,45,45,45	0
56	MG	2A	3238	1/1	0.90	0.22	45,45,45,45	0
56	MG	2A	3384	1/1	0.90	0.27	62,62,62,62	0
56	MG	1A	3791	1/1	0.90	0.24	63,63,63,63	0
56	MG	20	102	1/1	0.90	0.18	65,65,65,65	0
56	MG	2A	3811	1/1	0.90	0.16	54,54,54,54	0
56	MG	1A	3428	1/1	0.90	0.09	56,56,56,56	0
56	MG	2A	3075	1/1	0.90	0.23	48,48,48,48	0
56	MG	2E	301	1/1	0.90	0.15	49,49,49,49	0
56	MG	2A	3578	1/1	0.90	0.15	54,54,54,54	0
56	MG	1A	3967	1/1	0.90	0.12	46,46,46,46	0
56	MG	2A	3561	1/1	0.90	0.15	36,36,36,36	0
56	MG	1A	3316	1/1	0.90	0.21	40,40,40,40	0
56	MG	2a	3028	1/1	0.90	0.09	62,62,62,62	0
56	MG	2A	3046	1/1	0.90	0.13	48,48,48,48	0
56	MG	1A	3366	1/1	0.90	0.26	40,40,40,40	0
56	MG	2A	3761	1/1	0.90	0.18	62,62,62,62	0
56	MG	2A	3569	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3783	1/1	0.90	0.15	58,58,58,58	0
56	MG	2A	3680	1/1	0.90	0.24	54,54,54,54	0
56	MG	2A	3249	1/1	0.90	0.30	55,55,55,55	0
56	MG	2A	3132	1/1	0.90	0.15	36,36,36,36	0
56	MG	1a	1636	1/1	0.90	0.12	49,49,49,49	0
56	MG	2a	3017	1/1	0.90	0.10	71,71,71,71	0
56	MG	1A	4085	1/1	0.90	0.17	17,17,17,17	0
56	MG	2A	3222	1/1	0.90	0.35	61,61,61,61	0
56	MG	2D	302	1/1	0.90	0.16	55,55,55,55	0
56	MG	2A	3027	1/1	0.90	0.18	71,71,71,71	0
56	MG	1A	3290	1/1	0.90	0.18	40,40,40,40	0
56	MG	1G	201	1/1	0.90	0.20	43,43,43,43	0
56	MG	1A	3403	1/1	0.90	0.27	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3081	1/1	0.90	0.14	60,60,60,60	0
56	MG	2A	3317	1/1	0.90	0.45	49,49,49,49	0
56	MG	1A	3253	1/1	0.90	0.13	54,54,54,54	0
56	MG	2A	3256	1/1	0.90	0.11	68,68,68,68	0
56	MG	1A	3878	1/1	0.90	0.41	30,30,30,30	0
56	MG	2A	3586	1/1	0.90	0.09	60,60,60,60	0
56	MG	1A	3898	1/1	0.90	0.19	32,32,32,32	0
56	MG	2A	3065	1/1	0.90	0.16	68,68,68,68	0
56	MG	1A	3971	1/1	0.90	0.31	32,32,32,32	0
56	MG	1A	3393	1/1	0.90	0.21	43,43,43,43	0
56	MG	1F	309	1/1	0.90	0.16	53,53,53,53	0
56	MG	1A	3604	1/1	0.90	0.17	27,27,27,27	0
56	MG	2A	3594	1/1	0.90	0.18	66,66,66,66	0
56	MG	1A	3025	1/1	0.90	0.15	30,30,30,30	0
56	MG	2D	303	1/1	0.90	0.33	42,42,42,42	0
56	MG	1a	1676	1/1	0.90	0.10	72,72,72,72	0
56	MG	1A	3406	1/1	0.90	0.33	43,43,43,43	0
56	MG	2A	3815	1/1	0.90	0.07	73,73,73,73	0
56	MG	1A	4071	1/1	0.90	0.14	51,51,51,51	0
56	MG	1O	201	1/1	0.90	0.16	57,57,57,57	0
56	MG	2A	3446	1/1	0.90	0.14	63,63,63,63	0
56	MG	1A	3363	1/1	0.90	0.20	51,51,51,51	0
56	MG	1A	3942	1/1	0.90	0.13	51,51,51,51	0
56	MG	1A	3641	1/1	0.90	0.14	22,22,22,22	0
56	MG	2A	3215	1/1	0.90	0.14	56,56,56,56	0
56	MG	2A	3301	1/1	0.90	0.17	57,57,57,57	0
56	MG	2a	3207	1/1	0.90	0.08	62,62,62,62	0
56	MG	1A	3409	1/1	0.90	0.26	41,41,41,41	0
56	MG	1A	3609	1/1	0.90	0.20	25,25,25,25	0
56	MG	2a	3132	1/1	0.90	0.14	54,54,54,54	0
56	MG	2a	3162	1/1	0.90	0.07	82,82,82,82	0
56	MG	2a	3059	1/1	0.90	0.08	80,80,80,80	0
56	MG	1A	4065	1/1	0.90	0.13	36,36,36,36	0
56	MG	1A	3718	1/1	0.90	0.19	31,31,31,31	0
56	MG	2A	3782	1/1	0.90	0.08	55,55,55,55	0
56	MG	2A	3786	1/1	0.90	0.12	51,51,51,51	0
56	MG	1T	203	1/1	0.90	0.13	53,53,53,53	0
56	MG	1A	3010	1/1	0.90	0.20	36,36,36,36	0
56	MG	1a	1758	1/1	0.90	0.12	32,32,32,32	0
56	MG	1A	3168	1/1	0.90	0.48	40,40,40,40	0
56	MG	1A	3376	1/1	0.90	0.37	44,44,44,44	0
56	MG	16	102	1/1	0.90	0.43	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3866	1/1	0.90	0.14	22,22,22,22	0
56	MG	1A	3724	1/1	0.90	0.09	53,53,53,53	0
56	MG	2A	3387	1/1	0.90	0.25	62,62,62,62	0
56	MG	2a	3093	1/1	0.90	0.20	53,53,53,53	0
56	MG	1A	3916	1/1	0.90	0.17	22,22,22,22	0
56	MG	2A	3070	1/1	0.90	0.28	56,56,56,56	0
56	MG	1A	3308	1/1	0.90	0.17	32,32,32,32	0
56	MG	2A	3727	1/1	0.90	0.15	61,61,61,61	0
56	MG	1A	4013	1/1	0.90	0.07	62,62,62,62	0
56	MG	1A	3443	1/1	0.90	0.20	49,49,49,49	0
56	MG	1A	3424	1/1	0.90	0.17	48,48,48,48	0
56	MG	2A	3837	1/1	0.90	0.07	66,66,66,66	0
56	MG	2l	204	1/1	0.90	0.12	72,72,72,72	0
56	MG	1A	3654	1/1	0.90	0.14	37,37,37,37	0
56	MG	2A	3572	1/1	0.90	0.15	51,51,51,51	0
56	MG	1A	3748	1/1	0.90	0.16	47,47,47,47	0
56	MG	1a	1622	1/1	0.90	0.10	40,40,40,40	0
56	MG	2a	3102	1/1	0.90	0.11	54,54,54,54	0
56	MG	2A	3284	1/1	0.90	0.29	59,59,59,59	0
56	MG	1a	1699	1/1	0.90	0.30	47,47,47,47	0
56	MG	1A	3081	1/1	0.90	0.15	27,27,27,27	0
56	MG	2A	3748	1/1	0.90	0.42	68,68,68,68	0
56	MG	1x	107	1/1	0.90	0.23	49,49,49,49	0
56	MG	2A	3212	1/1	0.90	0.25	66,66,66,66	0
56	MG	2A	3380	1/1	0.90	0.13	75,75,75,75	0
56	MG	1D	306	1/1	0.90	0.30	33,33,33,33	0
56	MG	1A	3051	1/1	0.90	0.28	31,31,31,31	0
56	MG	1a	1815	1/1	0.90	0.19	66,66,66,66	0
56	MG	1a	1819	1/1	0.90	0.21	68,68,68,68	0
56	MG	2A	3777	1/1	0.90	0.23	47,47,47,47	0
56	MG	2A	3219	1/1	0.90	0.09	52,52,52,52	0
56	MG	2A	3879	1/1	0.90	0.11	47,47,47,47	0
56	MG	2A	3541	1/1	0.90	0.09	49,49,49,49	0
56	MG	2A	3329	1/1	0.90	0.14	60,60,60,60	0
56	MG	2A	3274	1/1	0.90	0.17	59,59,59,59	0
56	MG	1A	3662	1/1	0.90	0.15	19,19,19,19	0
56	MG	1T	204	1/1	0.90	0.10	59,59,59,59	0
56	MG	1A	3365	1/1	0.90	0.09	55,55,55,55	0
56	MG	2A	3635	1/1	0.90	0.29	61,61,61,61	0
56	MG	1A	3586	1/1	0.90	0.36	31,31,31,31	0
56	MG	1a	1795	1/1	0.90	0.20	64,64,64,64	0
56	MG	1A	3055	1/1	0.90	0.15	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3601	1/1	0.90	0.42	43,43,43,43	0
56	MG	2l	201	1/1	0.90	0.25	55,55,55,55	0
56	MG	2A	3445	1/1	0.90	0.28	60,60,60,60	0
56	MG	2A	3472	1/1	0.90	0.15	64,64,64,64	0
56	MG	2A	3630	1/1	0.90	0.21	42,42,42,42	0
56	MG	1A	3663	1/1	0.90	0.17	21,21,21,21	0
56	MG	2a	3011	1/1	0.90	0.12	66,66,66,66	0
56	MG	2a	3194	1/1	0.90	0.14	55,55,55,55	0
56	MG	2A	3881	1/1	0.90	0.15	62,62,62,62	0
56	MG	1a	1775	1/1	0.90	0.12	65,65,65,65	0
56	MG	2A	3359	1/1	0.90	0.39	51,51,51,51	0
56	MG	1A	4017	1/1	0.90	0.07	39,39,39,39	0
56	MG	1a	1626	1/1	0.90	0.20	52,52,52,52	0
56	MG	1x	115	1/1	0.90	0.17	64,64,64,64	0
56	MG	2a	3085	1/1	0.90	0.16	73,73,73,73	0
56	MG	2A	3553	1/1	0.90	0.12	49,49,49,49	0
56	MG	1A	3491	1/1	0.90	0.13	38,38,38,38	0
56	MG	2A	3624	1/1	0.90	0.14	40,40,40,40	0
56	MG	15	104	1/1	0.90	0.24	42,42,42,42	0
56	MG	2A	3732	1/1	0.90	0.10	72,72,72,72	0
56	MG	2a	3114	1/1	0.90	0.11	65,65,65,65	0
56	MG	1a	1765	1/1	0.91	0.16	51,51,51,51	0
56	MG	1A	3994	1/1	0.91	0.07	70,70,70,70	0
56	MG	2A	3526	1/1	0.91	0.09	30,30,30,30	0
56	MG	1A	3467	1/1	0.91	0.13	46,46,46,46	0
56	MG	1A	3532	1/1	0.91	0.21	52,52,52,52	0
56	MG	2a	3203	1/1	0.91	0.14	63,63,63,63	0
56	MG	1Z	301	1/1	0.91	0.23	48,48,48,48	0
56	MG	2A	3521	1/1	0.91	0.11	38,38,38,38	0
56	MG	1a	1603	1/1	0.91	0.27	61,61,61,61	0
56	MG	1A	3582	1/1	0.91	0.18	30,30,30,30	0
56	MG	2A	3342	1/1	0.91	0.10	55,55,55,55	0
56	MG	2A	3754	1/1	0.91	0.43	67,67,67,67	0
56	MG	1A	3796	1/1	0.91	0.18	20,20,20,20	0
56	MG	2A	3636	1/1	0.91	0.47	55,55,55,55	0
56	MG	2A	3319	1/1	0.91	0.15	53,53,53,53	0
56	MG	2A	3496	1/1	0.91	0.08	55,55,55,55	0
56	MG	2A	3504	1/1	0.91	0.16	49,49,49,49	0
56	MG	1a	1728	1/1	0.91	0.21	51,51,51,51	0
56	MG	2A	3091	1/1	0.91	0.29	48,48,48,48	0
56	MG	1A	4029	1/1	0.91	0.12	50,50,50,50	0
56	MG	1A	3124	1/1	0.91	0.18	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3861	1/1	0.91	0.27	61,61,61,61	0
56	MG	2A	3723	1/1	0.91	0.11	51,51,51,51	0
56	MG	1a	1617	1/1	0.91	0.15	53,53,53,53	0
56	MG	1a	1718	1/1	0.91	0.14	53,53,53,53	0
56	MG	1A	3213	1/1	0.91	0.21	44,44,44,44	0
56	MG	2y	101	1/1	0.91	0.19	60,60,60,60	0
56	MG	1A	3271	1/1	0.91	0.24	44,44,44,44	0
56	MG	1a	1645	1/1	0.91	0.14	52,52,52,52	0
56	MG	1w	104	1/1	0.91	0.17	72,72,72,72	0
56	MG	1A	3499	1/1	0.91	0.16	44,44,44,44	0
56	MG	2A	3390	1/1	0.91	0.24	54,54,54,54	0
56	MG	1A	3972	1/1	0.91	0.15	43,43,43,43	0
56	MG	2A	3164	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3370	1/1	0.91	0.14	40,40,40,40	0
56	MG	2A	3281	1/1	0.91	0.07	70,70,70,70	0
56	MG	2A	3685	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3466	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	3483	1/1	0.91	0.11	59,59,59,59	0
56	MG	1A	3539	1/1	0.91	0.32	45,45,45,45	0
56	MG	2A	3286	1/1	0.91	0.16	56,56,56,56	0
56	MG	2A	3458	1/1	0.91	0.14	53,53,53,53	0
56	MG	1A	4050	1/1	0.91	0.09	46,46,46,46	0
56	MG	18	103	1/1	0.91	0.13	22,22,22,22	0
56	MG	2A	3298	1/1	0.91	0.12	57,57,57,57	0
56	MG	2A	3093	1/1	0.91	0.23	37,37,37,37	0
56	MG	2A	3832	1/1	0.91	0.15	38,38,38,38	0
56	MG	1A	3427	1/1	0.91	0.18	43,43,43,43	0
56	MG	1A	3671	1/1	0.91	0.11	29,29,29,29	0
56	MG	1A	3524	1/1	0.91	0.20	51,51,51,51	0
56	MG	1E	308	1/1	0.91	0.12	31,31,31,31	0
56	MG	1A	3906	1/1	0.91	0.08	49,49,49,49	0
56	MG	1A	3812	1/1	0.91	0.11	54,54,54,54	0
56	MG	2a	3190	1/1	0.91	0.09	77,77,77,77	0
56	MG	2A	3878	1/1	0.91	0.23	38,38,38,38	0
56	MG	1I	201	1/1	0.91	0.14	61,61,61,61	0
56	MG	2a	3072	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	3191	1/1	0.91	0.09	43,43,43,43	0
56	MG	1A	3737	1/1	0.91	0.11	41,41,41,41	0
56	MG	2A	3357	1/1	0.91	0.13	50,50,50,50	0
56	MG	1w	112	1/1	0.91	0.12	53,53,53,53	0
56	MG	2F	304	1/1	0.91	0.18	54,54,54,54	0
56	MG	2a	3208	1/1	0.91	0.08	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3740	1/1	0.91	0.13	49,49,49,49	0
56	MG	1a	1719	1/1	0.91	0.11	41,41,41,41	0
56	MG	1a	1630	1/1	0.91	0.17	60,60,60,60	0
56	MG	2A	3736	1/1	0.91	0.24	57,57,57,57	0
56	MG	2A	3401	1/1	0.91	0.22	54,54,54,54	0
56	MG	2A	3488	1/1	0.91	0.15	56,56,56,56	0
56	MG	1A	4030	1/1	0.91	0.08	61,61,61,61	0
56	MG	2B	211	1/1	0.91	0.17	75,75,75,75	0
56	MG	1E	310	1/1	0.91	0.16	61,61,61,61	0
56	MG	1A	3487	1/1	0.91	0.12	44,44,44,44	0
56	MG	1A	3500	1/1	0.91	0.18	37,37,37,37	0
56	MG	2a	3224	1/1	0.91	0.12	61,61,61,61	0
56	MG	1A	3521	1/1	0.91	0.10	47,47,47,47	0
56	MG	2B	204	1/1	0.91	0.18	61,61,61,61	0
56	MG	2A	3454	1/1	0.91	0.17	50,50,50,50	0
56	MG	1S	203	1/1	0.91	0.14	66,66,66,66	0
56	MG	2A	3275	1/1	0.91	0.12	59,59,59,59	0
56	MG	1A	3328	1/1	0.91	0.19	48,48,48,48	0
56	MG	2A	3511	1/1	0.91	0.12	58,58,58,58	0
56	MG	1A	3758	1/1	0.91	0.16	40,40,40,40	0
56	MG	2A	3269	1/1	0.91	0.13	53,53,53,53	0
56	MG	2A	3449	1/1	0.91	0.21	56,56,56,56	0
56	MG	1a	1602	1/1	0.91	0.17	61,61,61,61	0
56	MG	2A	3527	1/1	0.91	0.16	44,44,44,44	0
56	MG	1V	207	1/1	0.91	0.12	52,52,52,52	0
56	MG	1W	204	1/1	0.91	0.12	34,34,34,34	0
56	MG	1A	3140	1/1	0.91	0.26	40,40,40,40	0
56	MG	1A	3485	1/1	0.91	0.24	42,42,42,42	0
56	MG	1A	3541	1/1	0.91	0.17	43,43,43,43	0
56	MG	1A	3285	1/1	0.91	0.32	26,26,26,26	0
56	MG	2A	3280	1/1	0.91	0.15	57,57,57,57	0
56	MG	1A	3680	1/1	0.91	0.27	38,38,38,38	0
56	MG	2A	3595	1/1	0.91	0.23	65,65,65,65	0
56	MG	2A	3178	1/1	0.91	0.09	48,48,48,48	0
56	MG	1a	1686	1/1	0.91	0.14	62,62,62,62	0
56	MG	1T	202	1/1	0.91	0.16	45,45,45,45	0
56	MG	2A	3514	1/1	0.91	0.13	67,67,67,67	0
56	MG	1A	3291	1/1	0.91	0.12	32,32,32,32	0
56	MG	2a	3126	1/1	0.91	0.12	66,66,66,66	0
56	MG	2A	3144	1/1	0.91	0.21	54,54,54,54	0
56	MG	1a	1631	1/1	0.91	0.12	33,33,33,33	0
56	MG	1A	3536	1/1	0.91	0.12	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3606	1/1	0.91	0.18	62,62,62,62	0
56	MG	1a	1833	1/1	0.91	0.23	43,43,43,43	0
56	MG	2a	3158	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3545	1/1	0.91	0.15	46,46,46,46	0
56	MG	1A	3273	1/1	0.91	0.28	35,35,35,35	0
56	MG	1A	3309	1/1	0.91	0.18	38,38,38,38	0
56	MG	2A	3475	1/1	0.91	0.32	56,56,56,56	0
56	MG	1A	3350	1/1	0.91	0.33	51,51,51,51	0
56	MG	10	101	1/1	0.91	0.13	38,38,38,38	0
56	MG	2a	3110	1/1	0.91	0.10	62,62,62,62	0
56	MG	2A	3066	1/1	0.91	0.09	51,51,51,51	0
56	MG	1a	1675	1/1	0.91	0.20	64,64,64,64	0
56	MG	1A	3775	1/1	0.91	0.18	21,21,21,21	0
56	MG	2B	214	1/1	0.91	0.19	62,62,62,62	0
56	MG	2a	3152	1/1	0.91	0.20	70,70,70,70	0
56	MG	2A	3427	1/1	0.91	0.23	42,42,42,42	0
56	MG	1A	3977	1/1	0.91	0.21	59,59,59,59	0
56	MG	2a	3223	1/1	0.91	0.18	64,64,64,64	0
56	MG	1A	3195	1/1	0.91	0.15	55,55,55,55	0
56	MG	2A	3542	1/1	0.91	0.10	46,46,46,46	0
56	MG	1A	3965	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3961	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3768	1/1	0.91	0.15	38,38,38,38	0
56	MG	2A	3816	1/1	0.91	0.29	68,68,68,68	0
56	MG	23	102	1/1	0.91	0.18	45,45,45,45	0
56	MG	2a	3032	1/1	0.91	0.18	65,65,65,65	0
56	MG	1A	3715	1/1	0.91	0.17	48,48,48,48	0
56	MG	2A	3574	1/1	0.91	0.14	46,46,46,46	0
56	MG	2A	3231	1/1	0.91	0.23	50,50,50,50	0
56	MG	2A	3841	1/1	0.91	0.09	47,47,47,47	0
56	MG	1v	101	1/1	0.91	0.14	65,65,65,65	0
56	MG	2a	3076	1/1	0.91	0.08	53,53,53,53	0
56	MG	2a	3159	1/1	0.91	0.07	56,56,56,56	0
56	MG	1A	3399	1/1	0.91	0.19	48,48,48,48	0
56	MG	2A	3090	1/1	0.91	0.30	45,45,45,45	0
56	MG	2x	104	1/1	0.91	0.10	62,62,62,62	0
56	MG	2A	3773	1/1	0.91	0.23	73,73,73,73	0
56	MG	1V	202	1/1	0.91	0.30	39,39,39,39	0
56	MG	1A	3189	1/1	0.91	0.65	47,47,47,47	0
56	MG	1a	1674	1/1	0.91	0.17	53,53,53,53	0
56	MG	2a	3169	1/1	0.91	0.10	77,77,77,77	0
56	MG	1B	206	1/1	0.91	0.14	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3369	1/1	0.91	0.12	44,44,44,44	0
56	MG	1A	3056	1/1	0.91	0.16	45,45,45,45	0
56	MG	2A	3398	1/1	0.91	0.17	58,58,58,58	0
56	MG	1A	3459	1/1	0.91	0.12	49,49,49,49	0
56	MG	2A	3081	1/1	0.91	0.41	52,52,52,52	0
56	MG	1Q	207	1/1	0.91	0.09	44,44,44,44	0
56	MG	2A	3810	1/1	0.91	0.32	78,78,78,78	0
56	MG	1a	1809	1/1	0.91	0.13	72,72,72,72	0
56	MG	2A	3690	1/1	0.91	0.08	40,40,40,40	0
56	MG	1a	1643	1/1	0.91	0.15	51,51,51,51	0
56	MG	1l	105	1/1	0.91	0.19	53,53,53,53	0
56	MG	2A	3671	1/1	0.91	0.08	59,59,59,59	0
56	MG	2D	304	1/1	0.91	0.54	57,57,57,57	0
56	MG	2A	3701	1/1	0.91	0.13	58,58,58,58	0
56	MG	1Q	208	1/1	0.91	0.41	47,47,47,47	0
56	MG	2A	3765	1/1	0.91	0.11	53,53,53,53	0
56	MG	2a	3078	1/1	0.91	0.22	50,50,50,50	0
56	MG	2A	3226	1/1	0.91	0.52	57,57,57,57	0
56	MG	2A	3694	1/1	0.91	0.12	50,50,50,50	0
56	MG	2a	3240	1/1	0.91	0.14	67,67,67,67	0
56	MG	2A	3632	1/1	0.91	0.12	39,39,39,39	0
56	MG	1a	1763	1/1	0.91	0.14	62,62,62,62	0
56	MG	2A	3784	1/1	0.91	0.32	64,64,64,64	0
56	MG	1A	3951	1/1	0.91	0.10	42,42,42,42	0
56	MG	1A	3867	1/1	0.92	0.11	55,55,55,55	0
56	MG	2d	301	1/1	0.92	0.09	65,65,65,65	0
56	MG	1A	3454	1/1	0.92	0.59	39,39,39,39	0
56	MG	1A	3531	1/1	0.92	0.45	47,47,47,47	0
56	MG	1A	3727	1/1	0.92	0.16	39,39,39,39	0
56	MG	2A	3519	1/1	0.92	0.13	33,33,33,33	0
56	MG	2A	3010	1/1	0.92	0.17	46,46,46,46	0
56	MG	2A	3645	1/1	0.92	0.14	37,37,37,37	0
56	MG	2A	3857	1/1	0.92	0.22	66,66,66,66	0
56	MG	2A	3529	1/1	0.92	0.16	52,52,52,52	0
56	MG	1A	3986	1/1	0.92	0.24	70,70,70,70	0
56	MG	1a	1792	1/1	0.92	0.08	60,60,60,60	0
56	MG	17	104	1/1	0.92	0.15	37,37,37,37	0
56	MG	1a	1802	1/1	0.92	0.13	63,63,63,63	0
56	MG	2P	202	1/1	0.92	0.16	47,47,47,47	0
56	MG	1w	106	1/1	0.92	0.06	61,61,61,61	0
56	MG	2A	3849	1/1	0.92	0.08	63,63,63,63	0
56	MG	2A	3351	1/1	0.92	0.33	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3312	1/1	0.92	0.10	34,34,34,34	0
56	MG	1A	3515	1/1	0.92	0.18	47,47,47,47	0
56	MG	2A	3156	1/1	0.92	0.13	54,54,54,54	0
56	MG	2Z	301	1/1	0.92	0.10	72,72,72,72	0
56	MG	1A	3112	1/1	0.92	0.24	35,35,35,35	0
56	MG	1A	3597	1/1	0.92	0.19	49,49,49,49	0
56	MG	2a	3021	1/1	0.92	0.07	69,69,69,69	0
56	MG	1A	3380	1/1	0.92	0.18	48,48,48,48	0
56	MG	2B	203	1/1	0.92	0.18	60,60,60,60	0
56	MG	1A	3809	1/1	0.92	0.17	39,39,39,39	0
56	MG	1A	3700	1/1	0.92	0.18	25,25,25,25	0
56	MG	2A	3814	1/1	0.92	0.25	60,60,60,60	0
56	MG	2B	208	1/1	0.92	0.10	59,59,59,59	0
56	MG	17	106	1/1	0.92	0.21	25,25,25,25	0
56	MG	1A	3417	1/1	0.92	0.18	48,48,48,48	0
56	MG	1A	4041	1/1	0.92	0.11	42,42,42,42	0
56	MG	1A	3936	1/1	0.92	0.09	14,14,14,14	0
56	MG	1A	3327	1/1	0.92	0.24	36,36,36,36	0
56	MG	2A	3535	1/1	0.92	0.14	51,51,51,51	0
56	MG	1E	302	1/1	0.92	0.21	47,47,47,47	0
56	MG	2A	3785	1/1	0.92	0.08	53,53,53,53	0
56	MG	2a	3058	1/1	0.92	0.10	74,74,74,74	0
56	MG	1D	312	1/1	0.92	0.21	37,37,37,37	0
56	MG	2A	3061	1/1	0.92	0.27	63,63,63,63	0
56	MG	2A	3034	1/1	0.92	0.17	56,56,56,56	0
56	MG	2A	3556	1/1	0.92	0.18	50,50,50,50	0
56	MG	2A	3300	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3201	1/1	0.92	0.27	70,70,70,70	0
56	MG	17	105	1/1	0.92	0.21	37,37,37,37	0
56	MG	1A	3463	1/1	0.92	0.45	47,47,47,47	0
56	MG	1A	3580	1/1	0.92	0.35	29,29,29,29	0
56	MG	2A	3795	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	3167	1/1	0.92	0.14	38,38,38,38	0
56	MG	1A	3352	1/1	0.92	0.42	41,41,41,41	0
56	MG	1U	205	1/1	0.92	0.65	38,38,38,38	0
56	MG	1a	1777	1/1	0.92	0.18	59,59,59,59	0
56	MG	1A	3016	1/1	0.92	0.20	45,45,45,45	0
56	MG	25	101	1/1	0.92	0.16	58,58,58,58	0
56	MG	2A	3681	1/1	0.92	0.15	54,54,54,54	0
56	MG	2A	3410	1/1	0.92	0.27	70,70,70,70	0
56	MG	1A	3206	1/1	0.92	0.18	42,42,42,42	0
56	MG	2A	3600	1/1	0.92	0.16	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3565	1/1	0.92	0.18	68,68,68,68	0
56	MG	1A	3059	1/1	0.92	0.24	47,47,47,47	0
56	MG	1a	1678	1/1	0.92	0.30	59,59,59,59	0
56	MG	2a	3083	1/1	0.92	0.45	65,65,65,65	0
56	MG	2A	3718	1/1	0.92	0.16	41,41,41,41	0
56	MG	2A	3016	1/1	0.92	0.17	57,57,57,57	0
56	MG	1A	4022	1/1	0.92	0.08	31,31,31,31	0
56	MG	2a	3026	1/1	0.92	0.36	60,60,60,60	0
56	MG	1A	4055	1/1	0.92	0.07	41,41,41,41	0
56	MG	1A	3188	1/1	0.92	0.08	37,37,37,37	0
56	MG	2y	104	1/1	0.92	0.13	50,50,50,50	0
56	MG	1A	3574	1/1	0.92	0.24	40,40,40,40	0
56	MG	1a	1662	1/1	0.92	0.17	60,60,60,60	0
56	MG	2a	3219	1/1	0.92	0.12	68,68,68,68	0
56	MG	1A	3005	1/1	0.92	0.15	37,37,37,37	0
56	MG	2a	3063	1/1	0.92	0.11	63,63,63,63	0
56	MG	2A	3433	1/1	0.92	0.22	49,49,49,49	0
56	MG	1A	3860	1/1	0.92	0.19	36,36,36,36	0
56	MG	1a	1635	1/1	0.92	0.09	55,55,55,55	0
56	MG	1A	3080	1/1	0.92	0.17	47,47,47,47	0
56	MG	1B	230	1/1	0.92	0.07	61,61,61,61	0
56	MG	2a	3198	1/1	0.92	0.11	62,62,62,62	0
56	MG	1A	3973	1/1	0.92	0.20	50,50,50,50	0
56	MG	1A	3289	1/1	0.92	0.11	49,49,49,49	0
56	MG	2A	3111	1/1	0.92	0.18	59,59,59,59	0
56	MG	2A	3213	1/1	0.92	0.15	61,61,61,61	0
56	MG	1A	3084	1/1	0.92	0.15	33,33,33,33	0
56	MG	2a	3230	1/1	0.92	0.29	65,65,65,65	0
56	MG	2a	3092	1/1	0.92	0.09	77,77,77,77	0
56	MG	2A	3015	1/1	0.92	0.13	39,39,39,39	0
56	MG	2A	3422	1/1	0.92	0.10	42,42,42,42	0
56	MG	1A	3265	1/1	0.92	0.20	43,43,43,43	0
56	MG	1a	1681	1/1	0.92	0.21	56,56,56,56	0
56	MG	1A	3789	1/1	0.92	0.09	43,43,43,43	0
56	MG	2A	3365	1/1	0.92	0.27	54,54,54,54	0
56	MG	1U	209	1/1	0.92	0.79	44,44,44,44	0
56	MG	1A	3026	1/1	0.92	0.13	45,45,45,45	0
56	MG	1a	1823	1/1	0.92	0.06	59,59,59,59	0
56	MG	1A	3896	1/1	0.92	0.24	60,60,60,60	0
56	MG	2a	3108	1/1	0.92	0.07	65,65,65,65	0
56	MG	1A	3437	1/1	0.92	0.10	53,53,53,53	0
56	MG	1A	3744	1/1	0.92	0.13	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1S	201	1/1	0.92	0.66	40,40,40,40	0
56	MG	1A	4090	1/1	0.92	0.23	53,53,53,53	0
56	MG	2A	3533	1/1	0.92	0.14	60,60,60,60	0
56	MG	1w	111	1/1	0.92	0.07	69,69,69,69	0
56	MG	1A	3325	1/1	0.92	0.23	26,26,26,26	0
56	MG	1A	3368	1/1	0.92	0.16	37,37,37,37	0
56	MG	1A	3562	1/1	0.92	0.27	43,43,43,43	0
56	MG	1W	205	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3548	1/1	0.92	0.37	46,46,46,46	0
56	MG	1A	3357	1/1	0.92	0.17	48,48,48,48	0
56	MG	1A	3235	1/1	0.92	0.14	59,59,59,59	0
56	MG	2A	3278	1/1	0.92	0.09	65,65,65,65	0
56	MG	1A	3897	1/1	0.92	0.11	56,56,56,56	0
56	MG	2a	3112	1/1	0.92	0.32	62,62,62,62	0
56	MG	1A	3284	1/1	0.92	0.58	35,35,35,35	0
56	MG	1A	3683	1/1	0.92	0.21	20,20,20,20	0
56	MG	2A	3052	1/1	0.92	0.09	63,63,63,63	0
56	MG	1A	3882	1/1	0.92	0.18	44,44,44,44	0
56	MG	1A	4079	1/1	0.92	0.23	53,53,53,53	0
56	MG	1x	113	1/1	0.92	0.10	65,65,65,65	0
56	MG	2A	3764	1/1	0.92	0.08	44,44,44,44	0
56	MG	2A	3579	1/1	0.92	0.19	45,45,45,45	0
56	MG	2A	3464	1/1	0.92	0.15	63,63,63,63	0
56	MG	1A	3589	1/1	0.92	0.17	35,35,35,35	0
56	MG	2B	201	1/1	0.92	0.16	66,66,66,66	0
56	MG	1a	1736	1/1	0.92	0.18	46,46,46,46	0
56	MG	2A	3537	1/1	0.92	0.11	56,56,56,56	0
56	MG	1B	224	1/1	0.92	0.21	52,52,52,52	0
56	MG	1A	3590	1/1	0.92	0.14	26,26,26,26	0
56	MG	2A	3362	1/1	0.92	0.18	43,43,43,43	0
56	MG	2A	3440	1/1	0.92	0.18	61,61,61,61	0
56	MG	1A	3163	1/1	0.92	0.24	48,48,48,48	0
56	MG	1A	3851	1/1	0.92	0.17	11,11,11,11	0
56	MG	1a	1778	1/1	0.92	0.14	55,55,55,55	0
56	MG	1a	1637	1/1	0.92	0.29	54,54,54,54	0
56	MG	1A	3926	1/1	0.92	0.12	28,28,28,28	0
56	MG	2a	3195	1/1	0.92	0.18	52,52,52,52	0
56	MG	1A	3640	1/1	0.92	0.28	49,49,49,49	0
56	MG	1a	1625	1/1	0.92	0.15	55,55,55,55	0
56	MG	1A	3043	1/1	0.92	0.23	33,33,33,33	0
56	MG	1A	3705	1/1	0.92	0.23	28,28,28,28	0
56	MG	20	103	1/1	0.92	0.25	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3656	1/1	0.92	0.15	59,59,59,59	0
56	MG	1A	3602	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3243	1/1	0.92	0.42	33,33,33,33	0
56	MG	2A	3340	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	3773	1/1	0.92	0.11	46,46,46,46	0
56	MG	2A	3289	1/1	0.92	0.52	61,61,61,61	0
56	MG	1A	3408	1/1	0.92	0.40	32,32,32,32	0
56	MG	1A	3465	1/1	0.92	0.68	48,48,48,48	0
56	MG	2i	201	1/1	0.92	0.08	62,62,62,62	0
56	MG	2A	3524	1/1	0.92	0.38	69,69,69,69	0
56	MG	1a	1618	1/1	0.92	0.21	49,49,49,49	0
56	MG	2A	3719	1/1	0.92	0.08	60,60,60,60	0
56	MG	2A	3108	1/1	0.92	0.12	65,65,65,65	0
56	MG	1A	3849	1/1	0.92	0.11	52,52,52,52	0
56	MG	2R	202	1/1	0.92	0.12	47,47,47,47	0
56	MG	2A	3438	1/1	0.92	0.25	56,56,56,56	0
56	MG	2A	3166	1/1	0.92	0.14	50,50,50,50	0
56	MG	1A	3761	1/1	0.92	0.18	36,36,36,36	0
56	MG	1A	3258	1/1	0.92	0.35	25,25,25,25	0
56	MG	1A	3513	1/1	0.92	0.16	63,63,63,63	0
56	MG	1a	1670	1/1	0.92	0.09	60,60,60,60	0
56	MG	2A	3374	1/1	0.92	0.08	57,57,57,57	0
56	MG	2a	3104	1/1	0.92	0.21	54,54,54,54	0
56	MG	2E	304	1/1	0.92	0.08	43,43,43,43	0
56	MG	2a	3123	1/1	0.92	0.23	68,68,68,68	0
56	MG	2A	3095	1/1	0.92	0.07	59,59,59,59	0
56	MG	1A	3848	1/1	0.92	0.13	54,54,54,54	0
56	MG	1A	3050	1/1	0.92	0.21	21,21,21,21	0
56	MG	1A	3214	1/1	0.92	0.11	57,57,57,57	0
56	MG	2A	3240	1/1	0.92	0.14	51,51,51,51	0
56	MG	2A	3763	1/1	0.92	0.09	60,60,60,60	0
56	MG	1A	3929	1/1	0.92	0.17	39,39,39,39	0
56	MG	1A	3230	1/1	0.92	0.14	36,36,36,36	0
56	MG	1a	1821	1/1	0.92	0.05	53,53,53,53	0
56	MG	1A	3542	1/1	0.92	0.23	37,37,37,37	0
56	MG	1a	1829	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3499	1/1	0.92	0.16	47,47,47,47	0
56	MG	1A	3632	1/1	0.92	0.16	34,34,34,34	0
56	MG	1A	3815	1/1	0.92	0.15	28,28,28,28	0
56	MG	15	105	1/1	0.92	0.18	49,49,49,49	0
56	MG	1A	3707	1/1	0.92	0.17	25,25,25,25	0
56	MG	2A	3469	1/1	0.92	0.19	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3025	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3781	1/1	0.92	0.17	41,41,41,41	0
56	MG	1A	3257	1/1	0.92	0.17	58,58,58,58	0
56	MG	1A	3764	1/1	0.92	0.17	14,14,14,14	0
56	MG	2A	3324	1/1	0.92	0.36	49,49,49,49	0
56	MG	1B	213	1/1	0.92	0.13	56,56,56,56	0
56	MG	1A	3678	1/1	0.92	0.16	23,23,23,23	0
56	MG	2A	3415	1/1	0.93	0.12	62,62,62,62	0
56	MG	1a	1755	1/1	0.93	0.08	88,88,88,88	0
56	MG	2A	3245	1/1	0.93	0.26	47,47,47,47	0
56	MG	2A	3749	1/1	0.93	0.23	58,58,58,58	0
56	MG	1A	3603	1/1	0.93	0.18	39,39,39,39	0
56	MG	1A	3616	1/1	0.93	0.15	19,19,19,19	0
56	MG	2E	302	1/1	0.93	0.13	61,61,61,61	0
56	MG	1A	3130	1/1	0.93	0.18	29,29,29,29	0
56	MG	2y	105	1/1	0.93	0.07	76,76,76,76	0
56	MG	1A	3320	1/1	0.93	0.19	46,46,46,46	0
56	MG	2A	3842	1/1	0.93	0.16	42,42,42,42	0
56	MG	1A	3462	1/1	0.93	0.58	54,54,54,54	0
56	MG	1a	1750	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3268	1/1	0.93	0.17	35,35,35,35	0
56	MG	2A	3180	1/1	0.93	0.27	47,47,47,47	0
56	MG	2A	3141	1/1	0.93	0.17	39,39,39,39	0
56	MG	1A	4009	1/1	0.93	0.21	23,23,23,23	0
56	MG	2A	3790	1/1	0.93	0.08	61,61,61,61	0
56	MG	1N	202	1/1	0.93	0.12	42,42,42,42	0
56	MG	2a	3091	1/1	0.93	0.19	62,62,62,62	0
56	MG	2A	3261	1/1	0.93	0.15	59,59,59,59	0
56	MG	2A	3489	1/1	0.93	0.31	62,62,62,62	0
56	MG	2A	3609	1/1	0.93	0.16	29,29,29,29	0
56	MG	2A	3498	1/1	0.93	0.18	58,58,58,58	0
56	MG	2A	3807	1/1	0.93	0.11	65,65,65,65	0
56	MG	2A	3836	1/1	0.93	0.14	62,62,62,62	0
56	MG	1A	3302	1/1	0.93	0.31	52,52,52,52	0
56	MG	2A	3555	1/1	0.93	0.18	27,27,27,27	0
56	MG	1A	3387	1/1	0.93	0.18	48,48,48,48	0
56	MG	2A	3677	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3321	1/1	0.93	0.11	48,48,48,48	0
56	MG	1a	1771	1/1	0.93	0.12	40,40,40,40	0
56	MG	2a	3150	1/1	0.93	0.12	76,76,76,76	0
56	MG	2A	3096	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3995	1/1	0.93	0.06	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3794	1/1	0.93	0.09	65,65,65,65	0
56	MG	2A	3620	1/1	0.93	0.14	64,64,64,64	0
56	MG	1A	3772	1/1	0.93	0.17	28,28,28,28	0
56	MG	2A	3840	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3441	1/1	0.93	0.14	41,41,41,41	0
56	MG	2A	3023	1/1	0.93	0.59	51,51,51,51	0
56	MG	1A	3288	1/1	0.93	0.21	34,34,34,34	0
56	MG	2A	3621	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	3218	1/1	0.93	0.14	34,34,34,34	0
56	MG	2a	3039	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3024	1/1	0.93	0.11	43,43,43,43	0
56	MG	1A	3301	1/1	0.93	0.26	24,24,24,24	0
56	MG	1A	3657	1/1	0.93	0.10	44,44,44,44	0
56	MG	1U	212	1/1	0.93	0.12	37,37,37,37	0
56	MG	2A	3887	1/1	0.93	0.15	56,56,56,56	0
56	MG	2A	3607	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3306	1/1	0.93	0.12	50,50,50,50	0
56	MG	2A	3293	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3877	1/1	0.93	0.25	30,30,30,30	0
56	MG	2A	3437	1/1	0.93	0.23	56,56,56,56	0
56	MG	1E	306	1/1	0.93	0.15	26,26,26,26	0
56	MG	2A	3102	1/1	0.93	0.15	59,59,59,59	0
56	MG	2A	3852	1/1	0.93	0.11	53,53,53,53	0
56	MG	1A	3107	1/1	0.93	0.10	27,27,27,27	0
56	MG	2A	3460	1/1	0.93	0.14	57,57,57,57	0
56	MG	28	101	1/1	0.93	0.28	66,66,66,66	0
56	MG	2a	3200	1/1	0.93	0.13	77,77,77,77	0
56	MG	1A	3993	1/1	0.93	0.14	27,27,27,27	0
56	MG	2A	3013	1/1	0.93	0.30	50,50,50,50	0
56	MG	17	108	1/1	0.93	0.15	45,45,45,45	0
56	MG	1A	3911	1/1	0.93	0.08	55,55,55,55	0
56	MG	2A	3658	1/1	0.93	0.11	69,69,69,69	0
56	MG	1A	3735	1/1	0.93	0.13	45,45,45,45	0
56	MG	2a	3241	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	3267	1/1	0.93	0.27	40,40,40,40	0
56	MG	2A	3039	1/1	0.93	0.14	65,65,65,65	0
56	MG	2A	3453	1/1	0.93	0.15	52,52,52,52	0
56	MG	2A	3190	1/1	0.93	0.12	67,67,67,67	0
56	MG	2A	3444	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3866	1/1	0.93	0.16	38,38,38,38	0
56	MG	1A	4054	1/1	0.93	0.48	53,53,53,53	0
56	MG	2A	3576	1/1	0.93	0.10	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2B	218	1/1	0.93	0.20	67,67,67,67	0
56	MG	2a	3109	1/1	0.93	0.23	72,72,72,72	0
56	MG	1A	3807	1/1	0.93	0.39	27,27,27,27	0
56	MG	2A	3113	1/1	0.93	0.24	59,59,59,59	0
56	MG	2A	3259	1/1	0.93	0.14	60,60,60,60	0
56	MG	2A	3363	1/1	0.93	0.28	51,51,51,51	0
56	MG	2I	202	1/1	0.93	0.08	64,64,64,64	0
56	MG	1A	3978	1/1	0.93	0.15	36,36,36,36	0
56	MG	1A	3608	1/1	0.93	0.18	39,39,39,39	0
56	MG	1A	3453	1/1	0.93	0.43	31,31,31,31	0
56	MG	2A	3378	1/1	0.93	0.66	55,55,55,55	0
56	MG	2A	3165	1/1	0.93	0.22	65,65,65,65	0
56	MG	2A	3610	1/1	0.93	0.06	41,41,41,41	0
56	MG	1A	3133	1/1	0.93	0.32	35,35,35,35	0
56	MG	2A	3757	1/1	0.93	0.08	66,66,66,66	0
56	MG	1A	3260	1/1	0.93	0.15	47,47,47,47	0
56	MG	2a	3164	1/1	0.93	0.17	58,58,58,58	0
56	MG	1P	202	1/1	0.93	0.36	23,23,23,23	0
56	MG	18	102	1/1	0.93	0.44	41,41,41,41	0
56	MG	1A	3668	1/1	0.93	0.14	21,21,21,21	0
56	MG	1A	3587	1/1	0.93	0.35	35,35,35,35	0
56	MG	2A	3487	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3212	1/1	0.93	0.11	35,35,35,35	0
56	MG	2B	220	1/1	0.93	0.12	65,65,65,65	0
56	MG	2A	3588	1/1	0.93	0.15	37,37,37,37	0
56	MG	1A	3864	1/1	0.93	0.14	52,52,52,52	0
56	MG	15	103	1/1	0.93	0.30	33,33,33,33	0
56	MG	2A	3693	1/1	0.93	0.13	62,62,62,62	0
56	MG	1A	3436	1/1	0.93	0.22	49,49,49,49	0
56	MG	1a	1740	1/1	0.93	0.18	43,43,43,43	0
56	MG	2a	3111	1/1	0.93	0.10	63,63,63,63	0
56	MG	2A	3652	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3044	1/1	0.93	0.13	29,29,29,29	0
56	MG	1A	3272	1/1	0.93	0.17	22,22,22,22	0
56	MG	1D	308	1/1	0.93	0.19	36,36,36,36	0
56	MG	1A	3197	1/1	0.93	0.22	38,38,38,38	0
56	MG	1A	3629	1/1	0.93	0.08	29,29,29,29	0
56	MG	2A	3709	1/1	0.93	0.23	48,48,48,48	0
56	MG	1A	3829	1/1	0.93	0.26	32,32,32,32	0
56	MG	1a	1684	1/1	0.93	0.20	63,63,63,63	0
56	MG	1A	3232	1/1	0.93	0.09	56,56,56,56	0
56	MG	2A	3772	1/1	0.93	0.07	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3103	1/1	0.93	0.16	58,58,58,58	0
56	MG	2A	3237	1/1	0.93	0.46	44,44,44,44	0
56	MG	1A	4087	1/1	0.93	0.11	53,53,53,53	0
56	MG	1f	201	1/1	0.93	0.20	44,44,44,44	0
59	ZN	2n	501	1/1	0.93	0.08	107,107,107,107	0
56	MG	1a	1621	1/1	0.93	0.09	51,51,51,51	0
56	MG	1A	3939	1/1	0.93	0.17	21,21,21,21	0
56	MG	2A	3078	1/1	0.93	0.14	59,59,59,59	0
56	MG	2A	3054	1/1	0.93	0.10	63,63,63,63	0
56	MG	2A	3742	1/1	0.93	0.09	72,72,72,72	0
56	MG	1A	3551	1/1	0.93	0.15	50,50,50,50	0
56	MG	2a	3019	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3592	1/1	0.93	0.20	22,22,22,22	0
56	MG	1A	3832	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3596	1/1	0.93	0.16	29,29,29,29	0
56	MG	2A	3354	1/1	0.93	0.10	62,62,62,62	0
56	MG	1D	304	1/1	0.93	0.20	35,35,35,35	0
56	MG	2A	3336	1/1	0.93	0.60	62,62,62,62	0
56	MG	2A	3628	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3806	1/1	0.93	0.10	26,26,26,26	0
56	MG	2a	3144	1/1	0.93	0.15	65,65,65,65	0
56	MG	2a	3229	1/1	0.93	0.23	61,61,61,61	0
56	MG	1B	223	1/1	0.93	0.21	51,51,51,51	0
56	MG	2A	3868	1/1	0.93	0.14	70,70,70,70	0
56	MG	2A	3244	1/1	0.93	0.23	43,43,43,43	0
56	MG	1a	1785	1/1	0.93	0.08	65,65,65,65	0
56	MG	2A	3235	1/1	0.93	0.27	44,44,44,44	0
56	MG	1A	3331	1/1	0.93	0.30	43,43,43,43	0
56	MG	1A	3371	1/1	0.93	0.21	46,46,46,46	0
56	MG	2x	105	1/1	0.93	0.09	67,67,67,67	0
56	MG	1A	4098	1/1	0.93	0.11	50,50,50,50	0
56	MG	2A	3559	1/1	0.93	0.12	53,53,53,53	0
56	MG	2a	3192	1/1	0.93	0.12	56,56,56,56	0
56	MG	10	103	1/1	0.93	0.15	32,32,32,32	0
56	MG	1A	3676	1/1	0.93	0.16	16,16,16,16	0
56	MG	1A	3600	1/1	0.93	0.41	39,39,39,39	0
56	MG	1A	3881	1/1	0.93	0.19	36,36,36,36	0
56	MG	2A	3563	1/1	0.93	0.13	36,36,36,36	0
56	MG	1A	3529	1/1	0.93	0.37	28,28,28,28	0
56	MG	1A	3966	1/1	0.93	0.14	36,36,36,36	0
56	MG	2A	3345	1/1	0.93	0.12	39,39,39,39	0
56	MG	2A	3134	1/1	0.93	0.20	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3560	1/1	0.93	0.14	51,51,51,51	0
56	MG	1A	3581	1/1	0.93	0.18	15,15,15,15	0
56	MG	1a	1832	1/1	0.93	0.14	55,55,55,55	0
56	MG	1B	221	1/1	0.93	0.20	56,56,56,56	0
56	MG	1A	3915	1/1	0.93	0.15	26,26,26,26	0
56	MG	1V	203	1/1	0.93	0.32	26,26,26,26	0
56	MG	1A	3242	1/1	0.93	0.23	22,22,22,22	0
56	MG	1A	3377	1/1	0.93	0.17	47,47,47,47	0
56	MG	1a	1767	1/1	0.93	0.10	67,67,67,67	0
56	MG	1A	3883	1/1	0.93	0.09	66,66,66,66	0
56	MG	2A	3050	1/1	0.93	0.20	57,57,57,57	0
56	MG	2A	3589	1/1	0.93	0.07	44,44,44,44	0
56	MG	2A	3055	1/1	0.93	0.26	53,53,53,53	0
56	MG	1a	1794	1/1	0.93	0.08	60,60,60,60	0
56	MG	1a	1770	1/1	0.93	0.10	49,49,49,49	0
56	MG	2A	3318	1/1	0.93	0.72	50,50,50,50	0
56	MG	1B	225	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	4011	1/1	0.93	0.27	65,65,65,65	0
56	MG	1A	3264	1/1	0.93	0.17	36,36,36,36	0
56	MG	1A	3938	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3858	1/1	0.93	0.23	43,43,43,43	0
56	MG	2A	3076	1/1	0.93	0.21	31,31,31,31	0
56	MG	2A	3478	1/1	0.93	0.10	43,43,43,43	0
56	MG	1A	3205	1/1	0.93	0.11	46,46,46,46	0
56	MG	1A	3481	1/1	0.93	0.22	40,40,40,40	0
56	MG	1A	3658	1/1	0.93	0.11	42,42,42,42	0
56	MG	1x	105	1/1	0.93	0.13	49,49,49,49	0
56	MG	2A	3573	1/1	0.93	0.19	62,62,62,62	0
56	MG	2A	3371	1/1	0.93	0.06	64,64,64,64	0
56	MG	1a	1650	1/1	0.93	0.12	56,56,56,56	0
56	MG	25	102	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3651	1/1	0.93	0.12	37,37,37,37	0
56	MG	1A	3953	1/1	0.93	0.05	50,50,50,50	0
56	MG	1A	3558	1/1	0.93	0.25	54,54,54,54	0
56	MG	1A	4064	1/1	0.93	0.16	34,34,34,34	0
56	MG	2A	3482	1/1	0.93	0.49	42,42,42,42	0
56	MG	2a	3012	1/1	0.93	0.11	70,70,70,70	0
56	MG	1A	3262	1/1	0.93	0.19	59,59,59,59	0
56	MG	1A	3594	1/1	0.93	0.18	55,55,55,55	0
56	MG	1A	3425	1/1	0.93	0.20	60,60,60,60	0
56	MG	2A	3747	1/1	0.93	0.19	66,66,66,66	0
56	MG	2a	3161	1/1	0.93	0.06	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3633	1/1	0.93	0.12	28,28,28,28	0
56	MG	1A	3736	1/1	0.93	0.08	38,38,38,38	0
56	MG	2a	3232	1/1	0.93	0.14	63,63,63,63	0
56	MG	1A	3353	1/1	0.94	0.24	33,33,33,33	0
56	MG	1R	203	1/1	0.94	0.24	46,46,46,46	0
56	MG	2A	3277	1/1	0.94	0.10	58,58,58,58	0
56	MG	2A	3158	1/1	0.94	0.45	56,56,56,56	0
56	MG	2A	3644	1/1	0.94	0.41	43,43,43,43	0
56	MG	1A	3482	1/1	0.94	0.23	43,43,43,43	0
56	MG	2A	3678	1/1	0.94	0.13	76,76,76,76	0
56	MG	2A	3196	1/1	0.94	0.10	62,62,62,62	0
56	MG	1B	222	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3894	1/1	0.94	0.17	21,21,21,21	0
56	MG	1A	3729	1/1	0.94	0.07	32,32,32,32	0
56	MG	1A	3052	1/1	0.94	0.13	40,40,40,40	0
56	MG	1A	3347	1/1	0.94	0.51	41,41,41,41	0
56	MG	2a	3040	1/1	0.94	0.10	77,77,77,77	0
56	MG	1A	3414	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3728	1/1	0.94	0.19	44,44,44,44	0
56	MG	1a	1707	1/1	0.94	0.20	57,57,57,57	0
56	MG	1A	3381	1/1	0.94	0.10	52,52,52,52	0
56	MG	1B	217	1/1	0.94	0.24	47,47,47,47	0
56	MG	2A	3547	1/1	0.94	0.17	34,34,34,34	0
56	MG	1A	3374	1/1	0.94	0.14	30,30,30,30	0
56	MG	2A	3220	1/1	0.94	0.12	52,52,52,52	0
56	MG	2D	310	1/1	0.94	0.18	56,56,56,56	0
56	MG	2A	3157	1/1	0.94	0.87	44,44,44,44	0
56	MG	2A	3349	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3780	1/1	0.94	0.14	34,34,34,34	0
56	MG	2A	3593	1/1	0.94	0.18	46,46,46,46	0
56	MG	1n	101	1/1	0.94	0.16	54,54,54,54	0
56	MG	1a	1632	1/1	0.94	0.14	58,58,58,58	0
56	MG	27	101	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3850	1/1	0.94	0.19	47,47,47,47	0
56	MG	2A	3073	1/1	0.94	0.51	52,52,52,52	0
56	MG	1a	1768	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	4058	1/1	0.94	0.27	28,28,28,28	0
56	MG	2A	3597	1/1	0.94	0.23	58,58,58,58	0
56	MG	2A	3067	1/1	0.94	0.11	30,30,30,30	0
56	MG	1A	3324	1/1	0.94	0.22	39,39,39,39	0
56	MG	2a	3141	1/1	0.94	0.08	68,68,68,68	0
56	MG	2B	206	1/1	0.94	0.21	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3522	1/1	0.94	0.31	53,53,53,53	0
56	MG	1a	1663	1/1	0.94	0.23	52,52,52,52	0
56	MG	2A	3083	1/1	0.94	0.19	57,57,57,57	0
56	MG	1A	3304	1/1	0.94	0.32	21,21,21,21	0
56	MG	2A	3571	1/1	0.94	0.09	42,42,42,42	0
56	MG	1A	3708	1/1	0.94	0.07	45,45,45,45	0
56	MG	1E	304	1/1	0.94	0.19	34,34,34,34	0
56	MG	2a	3033	1/1	0.94	0.12	81,81,81,81	0
56	MG	1A	3611	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3396	1/1	0.94	0.28	26,26,26,26	0
56	MG	2A	3557	1/1	0.94	0.13	59,59,59,59	0
56	MG	1A	3557	1/1	0.94	0.16	47,47,47,47	0
56	MG	1a	1649	1/1	0.94	0.18	44,44,44,44	0
56	MG	1w	107	1/1	0.94	0.16	69,69,69,69	0
56	MG	1A	3194	1/1	0.94	0.35	33,33,33,33	0
56	MG	2A	3733	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3199	1/1	0.94	0.14	50,50,50,50	0
56	MG	2A	3316	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3855	1/1	0.94	0.14	20,20,20,20	0
56	MG	1l	103	1/1	0.94	0.21	36,36,36,36	0
56	MG	2A	3485	1/1	0.94	0.63	44,44,44,44	0
56	MG	2a	3228	1/1	0.94	0.25	62,62,62,62	0
56	MG	2a	3181	1/1	0.94	0.15	64,64,64,64	0
56	MG	2A	3042	1/1	0.94	0.10	44,44,44,44	0
56	MG	1b	302	1/1	0.94	0.17	71,71,71,71	0
56	MG	1D	311	1/1	0.94	0.20	50,50,50,50	0
56	MG	2B	205	1/1	0.94	0.15	66,66,66,66	0
56	MG	2A	3079	1/1	0.94	0.35	46,46,46,46	0
56	MG	1A	3518	1/1	0.94	0.29	54,54,54,54	0
56	MG	1A	4015	1/1	0.94	0.13	29,29,29,29	0
56	MG	1a	1782	1/1	0.94	0.08	79,79,79,79	0
56	MG	2A	3420	1/1	0.94	0.10	60,60,60,60	0
56	MG	1A	3134	1/1	0.94	0.36	41,41,41,41	0
56	MG	1A	3496	1/1	0.94	0.18	25,25,25,25	0
56	MG	1A	3181	1/1	0.94	0.17	39,39,39,39	0
56	MG	1A	3117	1/1	0.94	0.26	35,35,35,35	0
56	MG	1A	3217	1/1	0.94	0.12	39,39,39,39	0
56	MG	2A	3140	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3751	1/1	0.94	0.11	67,67,67,67	0
56	MG	1A	3588	1/1	0.94	0.38	36,36,36,36	0
56	MG	1A	3022	1/1	0.94	0.18	34,34,34,34	0
56	MG	1A	3192	1/1	0.94	0.22	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3887	1/1	0.94	0.18	31,31,31,31	0
56	MG	2A	3062	1/1	0.94	0.18	66,66,66,66	0
56	MG	2A	3227	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3598	1/1	0.94	0.33	35,35,35,35	0
56	MG	1A	3185	1/1	0.94	0.14	37,37,37,37	0
56	MG	1A	3999	1/1	0.94	0.17	39,39,39,39	0
56	MG	2A	3403	1/1	0.94	0.31	57,57,57,57	0
56	MG	1A	3413	1/1	0.94	0.11	37,37,37,37	0
56	MG	11	101	1/1	0.94	0.59	33,33,33,33	0
56	MG	2A	3057	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3015	1/1	0.94	0.15	39,39,39,39	0
56	MG	2B	210	1/1	0.94	0.15	67,67,67,67	0
56	MG	2A	3047	1/1	0.94	0.10	24,24,24,24	0
56	MG	2A	3739	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3826	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3143	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3215	1/1	0.94	0.15	39,39,39,39	0
56	MG	2A	3058	1/1	0.94	0.11	52,52,52,52	0
56	MG	2A	3208	1/1	0.94	0.13	53,53,53,53	0
56	MG	2A	3722	1/1	0.94	0.13	40,40,40,40	0
56	MG	1A	3853	1/1	0.94	0.15	55,55,55,55	0
56	MG	17	102	1/1	0.94	0.11	32,32,32,32	0
56	MG	2A	3492	1/1	0.94	0.38	58,58,58,58	0
56	MG	1A	3008	1/1	0.94	0.21	26,26,26,26	0
56	MG	1a	1741	1/1	0.94	0.24	60,60,60,60	0
56	MG	2A	3649	1/1	0.94	0.08	68,68,68,68	0
56	MG	2a	3119	1/1	0.94	0.08	69,69,69,69	0
56	MG	1A	3694	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3044	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	3762	1/1	0.94	0.20	21,21,21,21	0
56	MG	1a	1830	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3576	1/1	0.94	0.23	43,43,43,43	0
56	MG	2a	3035	1/1	0.94	0.32	76,76,76,76	0
56	MG	1a	1619	1/1	0.94	0.22	52,52,52,52	0
56	MG	2A	3246	1/1	0.94	0.26	49,49,49,49	0
56	MG	1A	3793	1/1	0.94	0.21	56,56,56,56	0
56	MG	2A	3385	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3192	1/1	0.94	0.14	60,60,60,60	0
56	MG	1A	3803	1/1	0.94	0.09	26,26,26,26	0
56	MG	2A	3001	1/1	0.94	0.14	55,55,55,55	0
56	MG	1A	3769	1/1	0.94	0.19	25,25,25,25	0
56	MG	2A	3560	1/1	0.94	0.12	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3430	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3662	1/1	0.94	0.09	59,59,59,59	0
56	MG	1a	1804	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	3092	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3082	1/1	0.94	0.17	43,43,43,43	0
56	MG	1a	1799	1/1	0.94	0.20	46,46,46,46	0
56	MG	1A	3893	1/1	0.94	0.18	21,21,21,21	0
56	MG	1B	235	1/1	0.94	0.22	47,47,47,47	0
56	MG	2A	3696	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3054	1/1	0.94	0.19	42,42,42,42	0
56	MG	2w	104	1/1	0.94	0.08	69,69,69,69	0
56	MG	2a	3065	1/1	0.94	0.05	77,77,77,77	0
56	MG	1a	1724	1/1	0.94	0.28	49,49,49,49	0
56	MG	1A	3319	1/1	0.94	0.24	51,51,51,51	0
56	MG	2A	3360	1/1	0.94	0.09	56,56,56,56	0
56	MG	1A	3299	1/1	0.94	0.07	30,30,30,30	0
56	MG	1A	3910	1/1	0.94	0.21	51,51,51,51	0
56	MG	1l	201	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3148	1/1	0.94	0.13	51,51,51,51	0
56	MG	1w	101	1/1	0.94	0.19	65,65,65,65	0
56	MG	2A	3211	1/1	0.94	0.19	45,45,45,45	0
56	MG	1A	3902	1/1	0.94	0.19	43,43,43,43	0
56	MG	1A	3711	1/1	0.94	0.16	48,48,48,48	0
56	MG	1A	4040	1/1	0.94	0.30	47,47,47,47	0
56	MG	1V	205	1/1	0.94	0.20	29,29,29,29	0
56	MG	2U	202	1/1	0.94	0.79	58,58,58,58	0
56	MG	1A	3337	1/1	0.94	0.15	37,37,37,37	0
56	MG	1A	3111	1/1	0.94	0.16	37,37,37,37	0
56	MG	1A	4077	1/1	0.94	0.16	27,27,27,27	0
56	MG	2a	3030	1/1	0.94	0.19	63,63,63,63	0
56	MG	2A	3133	1/1	0.94	0.46	55,55,55,55	0
56	MG	1a	1716	1/1	0.94	0.15	49,49,49,49	0
56	MG	2A	3884	1/1	0.94	0.10	61,61,61,61	0
56	MG	1A	3852	1/1	0.94	0.20	39,39,39,39	0
56	MG	1A	3738	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3903	1/1	0.94	0.15	45,45,45,45	0
56	MG	1A	3909	1/1	0.94	0.17	49,49,49,49	0
56	MG	1a	1652	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	4025	1/1	0.94	0.18	40,40,40,40	0
56	MG	1A	3423	1/1	0.94	0.14	42,42,42,42	0
56	MG	1A	3905	1/1	0.94	0.26	23,23,23,23	0
56	MG	2I	101	1/1	0.94	0.57	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1756	1/1	0.94	0.17	54,54,54,54	0
56	MG	2A	3038	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	3817	1/1	0.94	0.59	39,39,39,39	0
56	MG	1A	3102	1/1	0.94	0.15	46,46,46,46	0
56	MG	1b	301	1/1	0.94	0.18	74,74,74,74	0
56	MG	2A	3393	1/1	0.94	0.16	40,40,40,40	0
56	MG	2a	3113	1/1	0.94	0.11	56,56,56,56	0
56	MG	1A	3759	1/1	0.94	0.16	15,15,15,15	0
56	MG	1A	3944	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3086	1/1	0.94	0.47	28,28,28,28	0
56	MG	2A	3728	1/1	0.94	0.11	64,64,64,64	0
56	MG	2A	3209	1/1	0.94	0.16	43,43,43,43	0
56	MG	2a	3057	1/1	0.94	0.11	65,65,65,65	0
56	MG	1A	3090	1/1	0.94	0.23	30,30,30,30	0
56	MG	2A	3481	1/1	0.94	0.78	60,60,60,60	0
56	MG	1A	3757	1/1	0.94	0.17	50,50,50,50	0
56	MG	1A	3429	1/1	0.94	0.13	44,44,44,44	0
56	MG	1A	3914	1/1	0.94	0.18	19,19,19,19	0
56	MG	1a	1687	1/1	0.94	0.13	50,50,50,50	0
56	MG	2a	3206	1/1	0.94	0.17	62,62,62,62	0
56	MG	1A	3469	1/1	0.94	0.19	33,33,33,33	0
56	MG	2x	101	1/1	0.94	0.15	60,60,60,60	0
56	MG	1A	3245	1/1	0.94	0.13	43,43,43,43	0
56	MG	2A	3513	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3636	1/1	0.94	0.14	16,16,16,16	0
56	MG	1A	3573	1/1	0.94	0.16	34,34,34,34	0
56	MG	18	106	1/1	0.94	0.14	26,26,26,26	0
56	MG	1A	3865	1/1	0.94	0.10	65,65,65,65	0
56	MG	1a	1640	1/1	0.94	0.14	69,69,69,69	0
56	MG	1A	3343	1/1	0.94	0.25	47,47,47,47	0
56	MG	2A	3119	1/1	0.94	0.22	36,36,36,36	0
56	MG	2A	3185	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3857	1/1	0.94	0.22	36,36,36,36	0
56	MG	2k	201	1/1	0.94	0.16	55,55,55,55	0
56	MG	1A	3814	1/1	0.94	0.18	63,63,63,63	0
56	MG	2A	3867	1/1	0.94	0.12	35,35,35,35	0
56	MG	2l	203	1/1	0.94	0.12	61,61,61,61	0
56	MG	2A	3512	1/1	0.94	0.08	58,58,58,58	0
56	MG	1A	3310	1/1	0.94	0.23	40,40,40,40	0
57	CLM	2A	3888	20/20	0.94	0.32	38,45,57,61	0
56	MG	1A	3313	1/1	0.94	0.20	39,39,39,39	0
56	MG	2B	207	1/1	0.94	0.17	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4048	1/1	0.94	0.09	34,34,34,34	0
56	MG	1A	3835	1/1	0.94	0.14	33,33,33,33	0
56	MG	1A	3098	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3638	1/1	0.94	0.29	55,55,55,55	0
56	MG	2a	3218	1/1	0.94	0.14	74,74,74,74	0
56	MG	1A	3175	1/1	0.94	0.28	30,30,30,30	0
56	MG	1A	3623	1/1	0.94	0.17	26,26,26,26	0
56	MG	1B	220	1/1	0.94	0.14	32,32,32,32	0
56	MG	2A	3006	1/1	0.94	0.17	54,54,54,54	0
56	MG	1A	3464	1/1	0.94	0.10	46,46,46,46	0
56	MG	2A	3775	1/1	0.94	0.09	66,66,66,66	0
56	MG	1a	1614	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3392	1/1	0.94	0.13	58,58,58,58	0
56	MG	2A	3741	1/1	0.94	0.09	42,42,42,42	0
56	MG	2a	3013	1/1	0.94	0.15	58,58,58,58	0
56	MG	1E	314	1/1	0.94	0.20	30,30,30,30	0
56	MG	1A	3649	1/1	0.94	0.14	29,29,29,29	0
56	MG	17	107	1/1	0.94	0.10	49,49,49,49	0
56	MG	23	103	1/1	0.94	0.24	55,55,55,55	0
56	MG	1A	3567	1/1	0.94	0.18	29,29,29,29	0
56	MG	1A	3813	1/1	0.94	0.17	40,40,40,40	0
56	MG	2A	3870	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3203	1/1	0.94	0.15	24,24,24,24	0
56	MG	28	103	1/1	0.94	0.17	42,42,42,42	0
56	MG	1A	4044	1/1	0.94	0.08	43,43,43,43	0
56	MG	2A	3539	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3221	1/1	0.94	0.16	46,46,46,46	0
56	MG	1A	3568	1/1	0.94	0.20	30,30,30,30	0
56	MG	1A	3093	1/1	0.94	0.16	51,51,51,51	0
56	MG	1A	4021	1/1	0.94	0.19	32,32,32,32	0
56	MG	1A	3624	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3612	1/1	0.94	0.20	51,51,51,51	0
56	MG	1A	3035	1/1	0.94	0.14	39,39,39,39	0
56	MG	1A	3615	1/1	0.94	0.12	33,33,33,33	0
56	MG	2a	3133	1/1	0.94	0.20	66,66,66,66	0
56	MG	2A	3135	1/1	0.94	0.16	51,51,51,51	0
56	MG	1a	1701	1/1	0.94	0.24	53,53,53,53	0
56	MG	2A	3060	1/1	0.94	0.20	46,46,46,46	0
56	MG	2A	3468	1/1	0.94	0.26	51,51,51,51	0
56	MG	2A	3412	1/1	0.94	0.19	53,53,53,53	0
56	MG	2a	3177	1/1	0.94	0.25	65,65,65,65	0
56	MG	1A	4005	1/1	0.94	0.08	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3407	1/1	0.94	0.06	57,57,57,57	0
56	MG	1P	203	1/1	0.94	0.21	25,25,25,25	0
56	MG	1A	3449	1/1	0.94	0.35	32,32,32,32	0
56	MG	1A	3435	1/1	0.94	0.25	42,42,42,42	0
56	MG	2A	3210	1/1	0.94	0.11	61,61,61,61	0
56	MG	1A	3920	1/1	0.94	0.20	65,65,65,65	0
59	ZN	2Y	501	1/1	0.94	0.15	81,81,81,81	0
56	MG	1a	1743	1/1	0.95	0.12	61,61,61,61	0
56	MG	2a	3215	1/1	0.95	0.09	59,59,59,59	0
56	MG	2A	3118	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3069	1/1	0.95	0.24	28,28,28,28	0
56	MG	2r	101	1/1	0.95	0.06	65,65,65,65	0
56	MG	1a	1651	1/1	0.95	0.22	61,61,61,61	0
56	MG	2A	3756	1/1	0.95	0.12	55,55,55,55	0
56	MG	1A	3156	1/1	0.95	0.38	39,39,39,39	0
56	MG	2a	3186	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	4093	1/1	0.95	0.12	38,38,38,38	0
56	MG	2V	203	1/1	0.95	0.30	57,57,57,57	0
56	MG	1a	1751	1/1	0.95	0.11	52,52,52,52	0
56	MG	1B	203	1/1	0.95	0.16	33,33,33,33	0
56	MG	1A	3298	1/1	0.95	0.14	36,36,36,36	0
56	MG	1A	3755	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3089	1/1	0.95	0.12	41,41,41,41	0
56	MG	2A	3426	1/1	0.95	0.18	42,42,42,42	0
56	MG	1A	3088	1/1	0.95	0.17	37,37,37,37	0
56	MG	1a	1605	1/1	0.95	0.19	55,55,55,55	0
56	MG	1a	1773	1/1	0.95	0.12	54,54,54,54	0
57	CLM	1A	4102	20/20	0.95	0.28	18,29,44,60	0
56	MG	1A	3184	1/1	0.95	0.10	64,64,64,64	0
56	MG	2A	3872	1/1	0.95	0.16	48,48,48,48	0
56	MG	1A	3846	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3415	1/1	0.95	0.18	40,40,40,40	0
56	MG	1A	3452	1/1	0.95	0.44	38,38,38,38	0
56	MG	1A	3330	1/1	0.95	0.24	46,46,46,46	0
56	MG	2A	3825	1/1	0.95	0.07	43,43,43,43	0
56	MG	1a	1634	1/1	0.95	0.25	66,66,66,66	0
56	MG	2A	3125	1/1	0.95	0.07	58,58,58,58	0
56	MG	1a	1705	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3318	1/1	0.95	0.30	43,43,43,43	0
56	MG	2A	3882	1/1	0.95	0.15	42,42,42,42	0
56	MG	2A	3729	1/1	0.95	0.09	68,68,68,68	0
56	MG	2a	3160	1/1	0.95	0.28	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	13	103	1/1	0.95	0.18	39,39,39,39	0
56	MG	1A	3249	1/1	0.95	0.14	42,42,42,42	0
56	MG	1x	116	1/1	0.95	0.14	65,65,65,65	0
56	MG	2A	3502	1/1	0.95	0.23	55,55,55,55	0
56	MG	1A	3721	1/1	0.95	0.17	27,27,27,27	0
56	MG	1a	1745	1/1	0.95	0.12	54,54,54,54	0
56	MG	1A	3152	1/1	0.95	0.14	29,29,29,29	0
56	MG	2A	3639	1/1	0.95	0.15	42,42,42,42	0
56	MG	2A	3218	1/1	0.95	0.54	35,35,35,35	0
56	MG	13	102	1/1	0.95	0.15	38,38,38,38	0
56	MG	2A	3303	1/1	0.95	0.48	71,71,71,71	0
56	MG	1X	105	1/1	0.95	0.17	29,29,29,29	0
56	MG	1A	3113	1/1	0.95	0.41	37,37,37,37	0
56	MG	1A	3359	1/1	0.95	0.23	58,58,58,58	0
56	MG	1A	3164	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3584	1/1	0.95	0.14	32,32,32,32	0
56	MG	2A	3523	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3834	1/1	0.95	0.26	32,32,32,32	0
56	MG	2a	3155	1/1	0.95	0.10	70,70,70,70	0
56	MG	2A	3584	1/1	0.95	0.12	59,59,59,59	0
56	MG	2A	3510	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3031	1/1	0.95	0.09	48,48,48,48	0
56	MG	1B	205	1/1	0.95	0.13	47,47,47,47	0
56	MG	2A	3101	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3450	1/1	0.95	0.09	56,56,56,56	0
56	MG	11	102	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	3760	1/1	0.95	0.19	45,45,45,45	0
56	MG	1A	3819	1/1	0.95	0.14	44,44,44,44	0
56	MG	2A	3233	1/1	0.95	0.12	33,33,33,33	0
56	MG	1A	3554	1/1	0.95	0.27	41,41,41,41	0
56	MG	1U	208	1/1	0.95	0.29	30,30,30,30	0
56	MG	1A	3186	1/1	0.95	0.22	37,37,37,37	0
56	MG	1A	4023	1/1	0.95	0.18	30,30,30,30	0
56	MG	1A	4088	1/1	0.95	0.17	21,21,21,21	0
56	MG	1A	3474	1/1	0.95	0.25	32,32,32,32	0
56	MG	2a	3226	1/1	0.95	0.15	50,50,50,50	0
56	MG	1A	3527	1/1	0.95	0.28	32,32,32,32	0
56	MG	1A	3269	1/1	0.95	0.12	29,29,29,29	0
56	MG	1A	3843	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3426	1/1	0.95	0.15	44,44,44,44	0
56	MG	1B	209	1/1	0.95	0.17	47,47,47,47	0
56	MG	2A	3724	1/1	0.95	0.13	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1B	204	1/1	0.95	0.29	42,42,42,42	0
56	MG	1A	3511	1/1	0.95	0.21	36,36,36,36	0
56	MG	2A	3646	1/1	0.95	0.30	59,59,59,59	0
56	MG	1A	3741	1/1	0.95	0.24	37,37,37,37	0
56	MG	2A	3154	1/1	0.95	0.12	52,52,52,52	0
56	MG	2a	3097	1/1	0.95	0.19	49,49,49,49	0
56	MG	2A	3020	1/1	0.95	0.39	39,39,39,39	0
56	MG	1m	3001	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3975	1/1	0.95	0.08	50,50,50,50	0
56	MG	1A	3345	1/1	0.95	0.13	46,46,46,46	0
56	MG	2A	3441	1/1	0.95	0.14	60,60,60,60	0
56	MG	2a	3222	1/1	0.95	0.19	55,55,55,55	0
56	MG	10	106	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3782	1/1	0.95	0.24	48,48,48,48	0
56	MG	1A	3637	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3139	1/1	0.95	0.22	36,36,36,36	0
56	MG	1A	3278	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3153	1/1	0.95	0.11	41,41,41,41	0
56	MG	2A	3311	1/1	0.95	0.26	59,59,59,59	0
56	MG	2A	3647	1/1	0.95	0.17	64,64,64,64	0
56	MG	2A	3641	1/1	0.95	0.14	38,38,38,38	0
56	MG	2A	3871	1/1	0.95	0.14	39,39,39,39	0
56	MG	1a	1734	1/1	0.95	0.14	53,53,53,53	0
56	MG	1A	3070	1/1	0.95	0.14	12,12,12,12	0
56	MG	2A	3500	1/1	0.95	0.15	55,55,55,55	0
56	MG	1x	101	1/1	0.95	0.20	38,38,38,38	0
56	MG	1w	105	1/1	0.95	0.33	62,62,62,62	0
56	MG	2A	3389	1/1	0.95	0.20	36,36,36,36	0
56	MG	1A	3240	1/1	0.95	0.19	34,34,34,34	0
56	MG	1a	1694	1/1	0.95	0.06	56,56,56,56	0
56	MG	2A	3068	1/1	0.95	0.34	61,61,61,61	0
56	MG	1a	1601	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	3599	1/1	0.95	0.16	42,42,42,42	0
56	MG	1D	309	1/1	0.95	0.34	20,20,20,20	0
56	MG	1A	3072	1/1	0.95	0.39	31,31,31,31	0
56	MG	1A	3918	1/1	0.95	0.30	28,28,28,28	0
56	MG	2A	3776	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3788	1/1	0.95	0.07	35,35,35,35	0
56	MG	2P	204	1/1	0.95	0.26	57,57,57,57	0
56	MG	1A	3673	1/1	0.95	0.17	17,17,17,17	0
56	MG	1A	3895	1/1	0.95	0.15	18,18,18,18	0
56	MG	2A	3430	1/1	0.95	0.22	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3829	1/1	0.95	0.09	45,45,45,45	0
56	MG	1A	3118	1/1	0.95	0.18	22,22,22,22	0
56	MG	1A	3619	1/1	0.95	0.20	41,41,41,41	0
56	MG	1A	4078	1/1	0.95	0.10	24,24,24,24	0
56	MG	1A	3198	1/1	0.95	0.13	35,35,35,35	0
56	MG	2a	3125	1/1	0.95	0.09	64,64,64,64	0
56	MG	2A	3026	1/1	0.95	0.52	53,53,53,53	0
56	MG	2A	3591	1/1	0.95	0.18	46,46,46,46	0
56	MG	2a	3004	1/1	0.95	0.21	51,51,51,51	0
56	MG	1A	3540	1/1	0.95	0.13	45,45,45,45	0
56	MG	2A	3434	1/1	0.95	0.33	46,46,46,46	0
56	MG	1A	3648	1/1	0.95	0.15	30,30,30,30	0
56	MG	2A	3629	1/1	0.95	0.13	36,36,36,36	0
56	MG	1a	1820	1/1	0.95	0.07	68,68,68,68	0
56	MG	2A	3633	1/1	0.95	0.08	40,40,40,40	0
56	MG	1w	103	1/1	0.95	0.20	64,64,64,64	0
56	MG	1A	3516	1/1	0.95	0.25	40,40,40,40	0
56	MG	1A	3274	1/1	0.95	0.15	38,38,38,38	0
56	MG	2A	3105	1/1	0.95	0.34	57,57,57,57	0
56	MG	1A	3033	1/1	0.95	0.45	24,24,24,24	0
56	MG	1A	3166	1/1	0.95	0.27	34,34,34,34	0
56	MG	1A	3421	1/1	0.95	0.18	32,32,32,32	0
56	MG	1A	3193	1/1	0.95	0.49	30,30,30,30	0
56	MG	1a	1749	1/1	0.95	0.21	33,33,33,33	0
56	MG	1G	202	1/1	0.95	0.21	51,51,51,51	0
56	MG	1A	3535	1/1	0.95	0.11	57,57,57,57	0
56	MG	1A	4096	1/1	0.95	0.17	46,46,46,46	0
56	MG	2a	3074	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3507	1/1	0.95	0.18	44,44,44,44	0
56	MG	1A	3492	1/1	0.95	0.15	33,33,33,33	0
56	MG	2A	3659	1/1	0.95	0.14	58,58,58,58	0
56	MG	1P	208	1/1	0.95	0.29	42,42,42,42	0
56	MG	2A	3124	1/1	0.95	0.05	66,66,66,66	0
56	MG	1Q	204	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3222	1/1	0.95	0.26	29,29,29,29	0
56	MG	1A	3444	1/1	0.95	0.34	43,43,43,43	0
56	MG	2a	3185	1/1	0.95	0.16	52,52,52,52	0
56	MG	2A	3544	1/1	0.95	0.12	35,35,35,35	0
56	MG	2y	102	1/1	0.95	0.40	74,74,74,74	0
56	MG	2A	3580	1/1	0.95	0.16	45,45,45,45	0
56	MG	2A	3707	1/1	0.95	0.15	36,36,36,36	0
56	MG	2T	203	1/1	0.95	0.15	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3665	1/1	0.95	0.10	61,61,61,61	0
56	MG	1N	206	1/1	0.95	0.22	37,37,37,37	0
56	MG	2A	3195	1/1	0.95	0.12	44,44,44,44	0
56	MG	1a	1608	1/1	0.95	0.20	45,45,45,45	0
56	MG	2A	3117	1/1	0.95	0.10	55,55,55,55	0
56	MG	1A	3520	1/1	0.95	0.24	56,56,56,56	0
56	MG	2a	3010	1/1	0.95	0.19	60,60,60,60	0
56	MG	1A	3356	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3946	1/1	0.95	0.09	40,40,40,40	0
56	MG	2A	3846	1/1	0.95	0.16	62,62,62,62	0
56	MG	1A	4072	1/1	0.95	0.13	48,48,48,48	0
56	MG	2a	3088	1/1	0.95	0.15	55,55,55,55	0
56	MG	1a	1688	1/1	0.95	0.11	63,63,63,63	0
56	MG	1A	3389	1/1	0.95	0.33	23,23,23,23	0
56	MG	1A	3104	1/1	0.95	0.18	25,25,25,25	0
56	MG	1a	1738	1/1	0.95	0.09	57,57,57,57	0
56	MG	2A	3672	1/1	0.95	0.09	51,51,51,51	0
56	MG	2a	3044	1/1	0.95	0.24	56,56,56,56	0
56	MG	1A	3837	1/1	0.95	0.11	51,51,51,51	0
56	MG	1X	104	1/1	0.95	0.36	61,61,61,61	0
56	MG	2A	3017	1/1	0.95	0.17	36,36,36,36	0
56	MG	2A	3634	1/1	0.95	0.51	56,56,56,56	0
56	MG	2A	3760	1/1	0.95	0.13	54,54,54,54	0
56	MG	1a	1735	1/1	0.95	0.16	53,53,53,53	0
56	MG	2A	3327	1/1	0.95	0.17	51,51,51,51	0
56	MG	1A	3840	1/1	0.95	0.12	22,22,22,22	0
56	MG	2A	3654	1/1	0.95	0.18	57,57,57,57	0
56	MG	1A	3410	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3969	1/1	0.95	0.13	42,42,42,42	0
56	MG	1A	3774	1/1	0.95	0.16	19,19,19,19	0
56	MG	1A	3351	1/1	0.95	0.71	47,47,47,47	0
56	MG	1A	3397	1/1	0.95	0.30	30,30,30,30	0
56	MG	2A	3774	1/1	0.95	0.14	64,64,64,64	0
56	MG	2a	3237	1/1	0.95	0.21	61,61,61,61	0
56	MG	1A	4097	1/1	0.95	0.17	35,35,35,35	0
56	MG	1a	1624	1/1	0.95	0.11	62,62,62,62	0
56	MG	1a	1769	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3388	1/1	0.95	0.06	62,62,62,62	0
56	MG	1A	3210	1/1	0.95	0.25	35,35,35,35	0
56	MG	1A	3138	1/1	0.95	0.17	28,28,28,28	0
56	MG	19	101	1/1	0.95	0.27	34,34,34,34	0
56	MG	1A	3950	1/1	0.95	0.15	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3168	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3876	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3795	1/1	0.95	0.20	19,19,19,19	0
56	MG	1A	3810	1/1	0.95	0.16	25,25,25,25	0
56	MG	1a	1737	1/1	0.95	0.30	62,62,62,62	0
56	MG	2A	3272	1/1	0.95	0.15	56,56,56,56	0
56	MG	1A	3460	1/1	0.95	0.28	40,40,40,40	0
56	MG	2A	3276	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	3075	1/1	0.95	0.18	21,21,21,21	0
59	ZN	14	102	1/1	0.95	0.13	87,87,87,87	0
56	MG	1A	3502	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	3348	1/1	0.95	0.29	41,41,41,41	0
56	MG	1A	3847	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3803	1/1	0.95	0.13	81,81,81,81	0
56	MG	1Y	203	1/1	0.95	0.19	47,47,47,47	0
56	MG	2A	3028	1/1	0.95	0.16	48,48,48,48	0
59	ZN	29	501	1/1	0.95	0.11	72,72,72,72	0
56	MG	1A	3372	1/1	0.95	0.38	43,43,43,43	0
56	MG	2A	3699	1/1	0.95	0.07	70,70,70,70	0
56	MG	2A	3305	1/1	0.95	0.12	54,54,54,54	0
56	MG	1A	3087	1/1	0.95	0.36	35,35,35,35	0
56	MG	1A	3904	1/1	0.95	0.16	32,32,32,32	0
56	MG	1A	3067	1/1	0.95	0.16	32,32,32,32	0
56	MG	1A	3763	1/1	0.95	0.15	22,22,22,22	0
56	MG	2A	3827	1/1	0.95	0.09	62,62,62,62	0
56	MG	1a	1682	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3144	1/1	0.95	0.18	42,42,42,42	0
56	MG	2A	3110	1/1	0.95	0.15	61,61,61,61	0
56	MG	1A	3082	1/1	0.95	0.24	33,33,33,33	0
56	MG	2V	202	1/1	0.95	0.52	48,48,48,48	0
56	MG	2A	3518	1/1	0.95	0.16	53,53,53,53	0
56	MG	1A	3106	1/1	0.95	0.17	26,26,26,26	0
56	MG	1a	1613	1/1	0.95	0.22	49,49,49,49	0
56	MG	1A	3216	1/1	0.95	0.33	32,32,32,32	0
56	MG	1A	3595	1/1	0.95	0.14	34,34,34,34	0
56	MG	1A	3830	1/1	0.95	0.18	48,48,48,48	0
56	MG	1A	3362	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3146	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	3229	1/1	0.95	0.38	32,32,32,32	0
56	MG	1A	3009	1/1	0.95	0.12	17,17,17,17	0
56	MG	1A	3183	1/1	0.95	0.21	48,48,48,48	0
56	MG	2A	3084	1/1	0.95	0.13	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3663	1/1	0.95	0.13	54,54,54,54	0
56	MG	2a	3234	1/1	0.95	0.16	60,60,60,60	0
56	MG	1E	315	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3868	1/1	0.95	0.12	35,35,35,35	0
56	MG	1A	3525	1/1	0.95	0.27	31,31,31,31	0
56	MG	1A	3509	1/1	0.95	0.18	31,31,31,31	0
56	MG	1B	226	1/1	0.95	0.06	69,69,69,69	0
56	MG	2A	3049	1/1	0.95	0.13	54,54,54,54	0
56	MG	2A	3142	1/1	0.95	0.14	43,43,43,43	0
56	MG	1a	1612	1/1	0.95	0.09	62,62,62,62	0
56	MG	2a	3204	1/1	0.95	0.14	65,65,65,65	0
56	MG	1A	3805	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3076	1/1	0.96	0.15	20,20,20,20	0
56	MG	1A	3472	1/1	0.96	0.23	33,33,33,33	0
56	MG	2A	3097	1/1	0.96	0.15	45,45,45,45	0
56	MG	2f	201	1/1	0.96	0.11	48,48,48,48	0
56	MG	1A	3831	1/1	0.96	0.17	37,37,37,37	0
56	MG	1a	1744	1/1	0.96	0.15	54,54,54,54	0
56	MG	1A	3642	1/1	0.96	0.12	14,14,14,14	0
56	MG	1A	3884	1/1	0.96	0.32	28,28,28,28	0
56	MG	1A	3094	1/1	0.96	0.15	20,20,20,20	0
56	MG	1A	3688	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3514	1/1	0.96	0.24	64,64,64,64	0
56	MG	1A	3011	1/1	0.96	0.21	31,31,31,31	0
56	MG	2A	3669	1/1	0.96	0.55	59,59,59,59	0
56	MG	1A	3959	1/1	0.96	0.23	46,46,46,46	0
56	MG	1A	3250	1/1	0.96	0.23	36,36,36,36	0
56	MG	2a	3191	1/1	0.96	0.13	71,71,71,71	0
56	MG	1a	1783	1/1	0.96	0.12	57,57,57,57	0
56	MG	2A	3035	1/1	0.96	0.20	36,36,36,36	0
56	MG	1A	3105	1/1	0.96	0.33	30,30,30,30	0
56	MG	2a	3130	1/1	0.96	0.08	68,68,68,68	0
56	MG	2A	3009	1/1	0.96	0.12	38,38,38,38	0
56	MG	1U	210	1/1	0.96	0.23	25,25,25,25	0
56	MG	2A	3655	1/1	0.96	0.08	56,56,56,56	0
56	MG	2A	3451	1/1	0.96	0.26	37,37,37,37	0
56	MG	1A	3287	1/1	0.96	0.12	43,43,43,43	0
56	MG	2a	3134	1/1	0.96	0.10	58,58,58,58	0
56	MG	1A	3383	1/1	0.96	0.33	31,31,31,31	0
56	MG	2A	3697	1/1	0.96	0.21	72,72,72,72	0
56	MG	13	101	1/1	0.96	0.10	26,26,26,26	0
56	MG	1A	3886	1/1	0.96	0.14	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3445	1/1	0.96	0.18	36,36,36,36	0
56	MG	2A	3813	1/1	0.96	0.15	53,53,53,53	0
56	MG	1P	205	1/1	0.96	0.16	16,16,16,16	0
56	MG	2a	3018	1/1	0.96	0.12	61,61,61,61	0
56	MG	1A	3630	1/1	0.96	0.15	29,29,29,29	0
56	MG	1A	3544	1/1	0.96	0.23	37,37,37,37	0
56	MG	1A	3890	1/1	0.96	0.10	33,33,33,33	0
56	MG	18	104	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3068	1/1	0.96	0.18	48,48,48,48	0
56	MG	1A	3295	1/1	0.96	0.18	22,22,22,22	0
56	MG	2A	3325	1/1	0.96	0.33	57,57,57,57	0
56	MG	1A	3863	1/1	0.96	0.17	34,34,34,34	0
56	MG	2A	3355	1/1	0.96	0.12	51,51,51,51	0
56	MG	2a	3073	1/1	0.96	0.13	50,50,50,50	0
56	MG	2A	3179	1/1	0.96	0.21	65,65,65,65	0
56	MG	1A	4003	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3020	1/1	0.96	0.18	33,33,33,33	0
56	MG	2A	3204	1/1	0.96	0.18	47,47,47,47	0
56	MG	1A	3099	1/1	0.96	0.23	16,16,16,16	0
56	MG	2a	3116	1/1	0.96	0.15	53,53,53,53	0
56	MG	1A	3666	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3252	1/1	0.96	0.18	37,37,37,37	0
56	MG	17	103	1/1	0.96	0.11	22,22,22,22	0
56	MG	2A	3045	1/1	0.96	0.20	53,53,53,53	0
56	MG	2A	3558	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3145	1/1	0.96	0.21	21,21,21,21	0
56	MG	1A	3912	1/1	0.96	0.37	31,31,31,31	0
56	MG	1A	3126	1/1	0.96	0.47	34,34,34,34	0
56	MG	1a	1723	1/1	0.96	0.21	46,46,46,46	0
56	MG	1A	4008	1/1	0.96	0.39	33,33,33,33	0
56	MG	1a	1761	1/1	0.96	0.14	51,51,51,51	0
56	MG	2a	3124	1/1	0.96	0.23	55,55,55,55	0
56	MG	2A	3587	1/1	0.96	0.20	56,56,56,56	0
56	MG	2A	3007	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	4086	1/1	0.96	0.16	28,28,28,28	0
56	MG	1A	3679	1/1	0.96	0.16	34,34,34,34	0
56	MG	1X	102	1/1	0.96	0.16	35,35,35,35	0
56	MG	2A	3294	1/1	0.96	0.31	67,67,67,67	0
56	MG	1a	1727	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	3169	1/1	0.96	0.14	49,49,49,49	0
56	MG	1E	311	1/1	0.96	0.23	52,52,52,52	0
56	MG	1A	4066	1/1	0.96	0.16	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3652	1/1	0.96	0.15	31,31,31,31	0
56	MG	2a	3029	1/1	0.96	0.38	40,40,40,40	0
56	MG	1A	3828	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	3100	1/1	0.96	0.11	41,41,41,41	0
56	MG	2A	3673	1/1	0.96	0.15	57,57,57,57	0
56	MG	1A	3553	1/1	0.96	0.35	45,45,45,45	0
56	MG	1A	3824	1/1	0.96	0.15	30,30,30,30	0
56	MG	1A	3030	1/1	0.96	0.27	32,32,32,32	0
56	MG	1A	3550	1/1	0.96	0.16	40,40,40,40	0
56	MG	1A	3311	1/1	0.96	0.19	40,40,40,40	0
56	MG	1F	307	1/1	0.96	0.25	30,30,30,30	0
56	MG	2A	3394	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3549	1/1	0.96	0.28	30,30,30,30	0
56	MG	1A	3176	1/1	0.96	0.23	27,27,27,27	0
56	MG	2A	3100	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3149	1/1	0.96	0.25	29,29,29,29	0
56	MG	1A	3745	1/1	0.96	0.14	14,14,14,14	0
56	MG	1A	3137	1/1	0.96	0.20	27,27,27,27	0
56	MG	2U	203	1/1	0.96	0.41	54,54,54,54	0
56	MG	1a	1831	1/1	0.96	0.22	43,43,43,43	0
56	MG	1A	3943	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3172	1/1	0.96	0.23	36,36,36,36	0
56	MG	1Q	203	1/1	0.96	0.24	24,24,24,24	0
56	MG	1e	202	1/1	0.96	0.23	59,59,59,59	0
56	MG	1A	3110	1/1	0.96	0.16	26,26,26,26	0
56	MG	1A	3014	1/1	0.96	0.18	22,22,22,22	0
56	MG	2a	3071	1/1	0.96	0.18	62,62,62,62	0
56	MG	2a	3217	1/1	0.96	0.12	72,72,72,72	0
56	MG	1A	3293	1/1	0.96	0.23	42,42,42,42	0
56	MG	1P	201	1/1	0.96	0.26	25,25,25,25	0
56	MG	2A	3436	1/1	0.96	0.17	41,41,41,41	0
56	MG	2A	3471	1/1	0.96	0.19	32,32,32,32	0
56	MG	1A	3120	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	3751	1/1	0.96	0.18	42,42,42,42	0
56	MG	1S	202	1/1	0.96	0.16	51,51,51,51	0
56	MG	2A	3631	1/1	0.96	0.14	39,39,39,39	0
56	MG	1A	3530	1/1	0.96	0.12	40,40,40,40	0
56	MG	18	101	1/1	0.96	0.26	37,37,37,37	0
56	MG	1A	3248	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3064	1/1	0.96	0.20	32,32,32,32	0
56	MG	1A	3277	1/1	0.96	0.33	44,44,44,44	0
56	MG	2A	3615	1/1	0.96	0.13	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3023	1/1	0.96	0.08	15,15,15,15	0
56	MG	1A	3659	1/1	0.96	0.19	24,24,24,24	0
56	MG	2a	3239	1/1	0.96	0.05	66,66,66,66	0
56	MG	2A	3018	1/1	0.96	0.21	49,49,49,49	0
56	MG	1A	3179	1/1	0.96	0.13	29,29,29,29	0
56	MG	2A	3528	1/1	0.96	0.18	59,59,59,59	0
56	MG	2T	204	1/1	0.96	0.17	54,54,54,54	0
56	MG	1D	303	1/1	0.96	0.13	17,17,17,17	0
56	MG	1A	3872	1/1	0.96	0.25	33,33,33,33	0
56	MG	2A	3109	1/1	0.96	0.19	39,39,39,39	0
56	MG	1A	3570	1/1	0.96	0.21	29,29,29,29	0
56	MG	2A	3854	1/1	0.96	0.11	35,35,35,35	0
56	MG	1a	1739	1/1	0.96	0.36	77,77,77,77	0
56	MG	2A	3106	1/1	0.96	0.10	36,36,36,36	0
56	MG	2A	3224	1/1	0.96	0.09	49,49,49,49	0
56	MG	2A	3404	1/1	0.96	0.21	45,45,45,45	0
56	MG	1A	3899	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3670	1/1	0.96	0.19	28,28,28,28	0
56	MG	1A	3078	1/1	0.96	0.17	31,31,31,31	0
56	MG	1A	3180	1/1	0.96	0.35	35,35,35,35	0
56	MG	1D	301	1/1	0.96	0.13	34,34,34,34	0
56	MG	2a	3016	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3432	1/1	0.96	0.29	36,36,36,36	0
56	MG	1A	3655	1/1	0.96	0.07	58,58,58,58	0
56	MG	1A	3384	1/1	0.96	0.14	41,41,41,41	0
56	MG	2a	3067	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3941	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3653	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3344	1/1	0.96	0.51	48,48,48,48	0
56	MG	2A	3304	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3710	1/1	0.96	0.15	51,51,51,51	0
56	MG	1A	3779	1/1	0.96	0.12	18,18,18,18	0
56	MG	1x	118	1/1	0.96	0.14	58,58,58,58	0
56	MG	2a	3103	1/1	0.96	0.21	62,62,62,62	0
56	MG	1A	3875	1/1	0.96	0.39	35,35,35,35	0
56	MG	2A	3752	1/1	0.96	0.22	54,54,54,54	0
56	MG	1D	313	1/1	0.96	0.35	34,34,34,34	0
56	MG	1D	302	1/1	0.96	0.18	36,36,36,36	0
56	MG	1A	3695	1/1	0.96	0.11	25,25,25,25	0
56	MG	1A	3115	1/1	0.96	0.09	32,32,32,32	0
56	MG	1a	1628	1/1	0.96	0.22	47,47,47,47	0
56	MG	2A	3024	1/1	0.96	0.42	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3007	1/1	0.96	0.26	26,26,26,26	0
56	MG	1A	3455	1/1	0.96	0.27	28,28,28,28	0
56	MG	2a	3048	1/1	0.96	0.19	58,58,58,58	0
56	MG	2A	3730	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3756	1/1	0.96	0.13	45,45,45,45	0
56	MG	2A	3172	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3634	1/1	0.96	0.17	52,52,52,52	0
56	MG	1a	1616	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3259	1/1	0.96	0.18	38,38,38,38	0
56	MG	2A	3313	1/1	0.96	0.07	57,57,57,57	0
56	MG	1B	202	1/1	0.96	0.33	47,47,47,47	0
56	MG	1A	4010	1/1	0.96	0.17	28,28,28,28	0
56	MG	1A	3275	1/1	0.96	0.17	31,31,31,31	0
56	MG	2a	3042	1/1	0.96	0.20	60,60,60,60	0
56	MG	2P	201	1/1	0.96	0.34	58,58,58,58	0
56	MG	1A	3674	1/1	0.96	0.16	22,22,22,22	0
56	MG	1D	307	1/1	0.96	0.26	44,44,44,44	0
56	MG	1A	3501	1/1	0.96	0.13	28,28,28,28	0
56	MG	1w	108	1/1	0.96	0.11	74,74,74,74	0
56	MG	1A	3556	1/1	0.96	0.31	41,41,41,41	0
56	MG	1A	3182	1/1	0.96	0.22	49,49,49,49	0
56	MG	2A	3012	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3395	1/1	0.96	0.23	40,40,40,40	0
56	MG	1A	3150	1/1	0.96	0.17	31,31,31,31	0
56	MG	2A	3534	1/1	0.96	0.10	41,41,41,41	0
56	MG	1m	3002	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	3233	1/1	0.96	0.14	30,30,30,30	0
56	MG	1A	3701	1/1	0.96	0.18	23,23,23,23	0
56	MG	1a	1697	1/1	0.96	0.28	49,49,49,49	0
56	MG	1A	3571	1/1	0.96	0.53	29,29,29,29	0
56	MG	2A	3616	1/1	0.96	0.10	63,63,63,63	0
56	MG	2A	3666	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3925	1/1	0.96	0.17	39,39,39,39	0
56	MG	2A	3590	1/1	0.96	0.15	64,64,64,64	0
56	MG	15	101	1/1	0.96	0.34	31,31,31,31	0
56	MG	1a	1702	1/1	0.96	0.29	53,53,53,53	0
56	MG	2A	3617	1/1	0.96	0.20	59,59,59,59	0
56	MG	1a	1639	1/1	0.96	0.19	56,56,56,56	0
56	MG	1A	3013	1/1	0.96	0.35	26,26,26,26	0
56	MG	1T	201	1/1	0.96	0.23	47,47,47,47	0
56	MG	1A	3255	1/1	0.96	0.19	29,29,29,29	0
56	MG	2A	3738	1/1	0.96	0.10	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2F	305	1/1	0.96	0.33	43,43,43,43	0
56	MG	2a	3146	1/1	0.96	0.08	68,68,68,68	0
56	MG	2A	3530	1/1	0.96	0.17	49,49,49,49	0
56	MG	2A	3769	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3036	1/1	0.96	0.08	28,28,28,28	0
56	MG	2A	3021	1/1	0.96	0.17	55,55,55,55	0
56	MG	1A	3900	1/1	0.96	0.16	20,20,20,20	0
56	MG	17	101	1/1	0.96	0.19	31,31,31,31	0
56	MG	1V	204	1/1	0.96	0.36	32,32,32,32	0
56	MG	1A	3546	1/1	0.96	0.22	43,43,43,43	0
56	MG	1E	309	1/1	0.96	0.37	47,47,47,47	0
56	MG	2A	3197	1/1	0.96	0.22	55,55,55,55	0
56	MG	1A	3908	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3794	1/1	0.96	0.19	48,48,48,48	0
56	MG	1A	3095	1/1	0.96	0.29	44,44,44,44	0
56	MG	1A	3231	1/1	0.96	0.11	33,33,33,33	0
56	MG	2A	3797	1/1	0.96	0.08	40,40,40,40	0
56	MG	2A	3517	1/1	0.96	0.09	46,46,46,46	0
56	MG	1B	239	1/1	0.96	0.15	30,30,30,30	0
56	MG	1a	1633	1/1	0.96	0.21	52,52,52,52	0
56	MG	16	101	1/1	0.96	0.19	41,41,41,41	0
56	MG	2A	3131	1/1	0.96	0.08	75,75,75,75	0
56	MG	2A	3290	1/1	0.96	0.13	36,36,36,36	0
56	MG	2A	3174	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3201	1/1	0.96	0.15	22,22,22,22	0
56	MG	2A	3424	1/1	0.96	0.22	49,49,49,49	0
56	MG	2A	3126	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3200	1/1	0.96	0.13	33,33,33,33	0
56	MG	2e	201	1/1	0.96	0.14	64,64,64,64	0
56	MG	2D	301	1/1	0.96	0.32	47,47,47,47	0
56	MG	2A	3874	1/1	0.96	0.05	66,66,66,66	0
56	MG	1A	3754	1/1	0.96	0.15	18,18,18,18	0
56	MG	2V	201	1/1	0.96	0.56	69,69,69,69	0
56	MG	2A	3865	1/1	0.96	0.07	51,51,51,51	0
56	MG	2a	3115	1/1	0.96	0.14	61,61,61,61	0
56	MG	1A	3178	1/1	0.96	0.17	17,17,17,17	0
56	MG	1A	4075	1/1	0.96	0.30	48,48,48,48	0
56	MG	2A	3549	1/1	0.96	0.14	47,47,47,47	0
56	MG	1Q	201	1/1	0.97	0.62	42,42,42,42	0
56	MG	1A	3811	1/1	0.97	0.12	49,49,49,49	0
56	MG	2a	3038	1/1	0.97	0.23	53,53,53,53	0
56	MG	2a	3205	1/1	0.97	0.06	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3119	1/1	0.97	0.26	23,23,23,23	0
56	MG	1x	114	1/1	0.97	0.21	51,51,51,51	0
56	MG	2a	3075	1/1	0.97	0.22	57,57,57,57	0
56	MG	1F	310	1/1	0.97	0.14	41,41,41,41	0
56	MG	2A	3550	1/1	0.97	0.17	57,57,57,57	0
56	MG	1a	1713	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3862	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3064	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3691	1/1	0.97	0.16	24,24,24,24	0
56	MG	1A	3031	1/1	0.97	0.28	31,31,31,31	0
56	MG	2A	3835	1/1	0.97	0.14	34,34,34,34	0
56	MG	2A	3161	1/1	0.97	0.39	64,64,64,64	0
56	MG	23	101	1/1	0.97	0.22	54,54,54,54	0
56	MG	2A	3137	1/1	0.97	0.34	40,40,40,40	0
56	MG	1A	4020	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3839	1/1	0.97	0.16	43,43,43,43	0
56	MG	1A	3305	1/1	0.97	0.31	34,34,34,34	0
56	MG	2a	3121	1/1	0.97	0.12	54,54,54,54	0
56	MG	1A	3085	1/1	0.97	0.18	23,23,23,23	0
56	MG	2A	3477	1/1	0.97	0.14	23,23,23,23	0
56	MG	1A	3677	1/1	0.97	0.12	23,23,23,23	0
56	MG	1A	3841	1/1	0.97	0.21	39,39,39,39	0
56	MG	1A	3859	1/1	0.97	0.37	38,38,38,38	0
56	MG	1A	3239	1/1	0.97	0.18	25,25,25,25	0
56	MG	2A	3346	1/1	0.97	0.08	67,67,67,67	0
56	MG	1U	202	1/1	0.97	0.20	27,27,27,27	0
56	MG	2A	3598	1/1	0.97	0.15	42,42,42,42	0
56	MG	1O	202	1/1	0.97	0.42	47,47,47,47	0
59	ZN	1n	102	1/1	0.97	0.15	66,66,66,66	0
56	MG	2A	3582	1/1	0.97	0.10	39,39,39,39	0
56	MG	2a	3090	1/1	0.97	0.20	66,66,66,66	0
56	MG	2a	3211	1/1	0.97	0.14	50,50,50,50	0
56	MG	1A	3040	1/1	0.97	0.15	30,30,30,30	0
56	MG	1x	106	1/1	0.97	0.21	52,52,52,52	0
56	MG	1A	3407	1/1	0.97	0.13	36,36,36,36	0
56	MG	2a	3099	1/1	0.97	0.16	52,52,52,52	0
56	MG	1A	3714	1/1	0.97	0.14	14,14,14,14	0
56	MG	1A	3825	1/1	0.97	0.16	34,34,34,34	0
56	MG	1F	305	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	3158	1/1	0.97	0.31	60,60,60,60	0
56	MG	2A	3675	1/1	0.97	0.06	57,57,57,57	0
56	MG	1a	1615	1/1	0.97	0.07	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3520	1/1	0.97	0.11	49,49,49,49	0
56	MG	2A	3151	1/1	0.97	0.21	60,60,60,60	0
56	MG	1U	206	1/1	0.97	0.16	33,33,33,33	0
56	MG	1Z	303	1/1	0.97	0.20	42,42,42,42	0
56	MG	1A	3880	1/1	0.97	0.09	60,60,60,60	0
56	MG	1V	201	1/1	0.97	0.45	30,30,30,30	0
56	MG	1E	307	1/1	0.97	0.22	57,57,57,57	0
56	MG	1A	3579	1/1	0.97	0.26	21,21,21,21	0
56	MG	1A	3161	1/1	0.97	0.18	22,22,22,22	0
56	MG	2A	3704	1/1	0.97	0.19	44,44,44,44	0
56	MG	2A	3229	1/1	0.97	0.47	33,33,33,33	0
56	MG	1A	4084	1/1	0.97	0.24	14,14,14,14	0
56	MG	1A	3049	1/1	0.97	0.23	39,39,39,39	0
56	MG	2N	201	1/1	0.97	0.08	35,35,35,35	0
56	MG	1A	3720	1/1	0.97	0.19	44,44,44,44	0
56	MG	1O	204	1/1	0.97	0.14	46,46,46,46	0
56	MG	2a	3087	1/1	0.97	0.10	59,59,59,59	0
56	MG	1A	3752	1/1	0.97	0.14	37,37,37,37	0
56	MG	2A	3170	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	3778	1/1	0.97	0.16	20,20,20,20	0
56	MG	1A	3032	1/1	0.97	0.28	26,26,26,26	0
56	MG	1A	3154	1/1	0.97	0.43	39,39,39,39	0
56	MG	1a	1757	1/1	0.97	0.12	35,35,35,35	0
56	MG	2A	3413	1/1	0.97	0.19	55,55,55,55	0
56	MG	2A	3626	1/1	0.97	0.17	33,33,33,33	0
56	MG	2A	3683	1/1	0.97	0.10	64,64,64,64	0
56	MG	1A	3254	1/1	0.97	0.17	36,36,36,36	0
56	MG	2A	3241	1/1	0.97	0.24	62,62,62,62	0
56	MG	2A	3755	1/1	0.97	0.07	54,54,54,54	0
56	MG	1A	3495	1/1	0.97	0.23	47,47,47,47	0
56	MG	1A	3593	1/1	0.97	0.34	27,27,27,27	0
56	MG	1A	3466	1/1	0.97	0.17	36,36,36,36	0
56	MG	2m	201	1/1	0.97	0.12	73,73,73,73	0
56	MG	2A	3501	1/1	0.97	0.07	58,58,58,58	0
56	MG	2A	3366	1/1	0.97	0.14	60,60,60,60	0
56	MG	2A	3112	1/1	0.97	0.11	51,51,51,51	0
60	SF4	2d	302	8/8	0.97	0.15	59,73,81,82	0
56	MG	2A	3667	1/1	0.97	0.10	57,57,57,57	0
56	MG	1R	202	1/1	0.97	0.42	36,36,36,36	0
56	MG	1A	3034	1/1	0.97	0.30	23,23,23,23	0
56	MG	1A	3280	1/1	0.97	0.15	21,21,21,21	0
56	MG	1a	1776	1/1	0.97	0.10	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3221	1/1	0.97	0.08	55,55,55,55	0
56	MG	1B	219	1/1	0.97	0.28	34,34,34,34	0
56	MG	1A	3783	1/1	0.97	0.15	17,17,17,17	0
56	MG	1A	3931	1/1	0.97	0.08	40,40,40,40	0
56	MG	1B	218	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3227	1/1	0.97	0.26	37,37,37,37	0
56	MG	1A	3672	1/1	0.97	0.10	35,35,35,35	0
56	MG	2A	3745	1/1	0.97	0.09	50,50,50,50	0
56	MG	2A	3184	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3746	1/1	0.97	0.25	46,46,46,46	0
56	MG	2A	3187	1/1	0.97	0.21	56,56,56,56	0
56	MG	1A	3375	1/1	0.97	0.15	42,42,42,42	0
56	MG	1A	3543	1/1	0.97	0.38	34,34,34,34	0
56	MG	1A	3952	1/1	0.97	0.18	39,39,39,39	0
56	MG	2A	3167	1/1	0.97	0.15	39,39,39,39	0
56	MG	1a	1717	1/1	0.97	0.06	64,64,64,64	0
56	MG	1A	3281	1/1	0.97	0.26	31,31,31,31	0
56	MG	2A	3880	1/1	0.97	0.12	52,52,52,52	0
56	MG	1A	3656	1/1	0.97	0.18	34,34,34,34	0
56	MG	1A	3842	1/1	0.97	0.18	31,31,31,31	0
56	MG	2A	3653	1/1	0.97	0.21	61,61,61,61	0
56	MG	1A	3190	1/1	0.97	0.25	25,25,25,25	0
56	MG	1A	3638	1/1	0.97	0.08	40,40,40,40	0
56	MG	1F	306	1/1	0.97	0.25	23,23,23,23	0
56	MG	2A	3778	1/1	0.97	0.11	58,58,58,58	0
56	MG	1A	3698	1/1	0.97	0.21	28,28,28,28	0
56	MG	1x	108	1/1	0.97	0.20	62,62,62,62	0
56	MG	1A	3620	1/1	0.97	0.10	52,52,52,52	0
56	MG	1A	3204	1/1	0.97	0.16	29,29,29,29	0
56	MG	1A	3731	1/1	0.97	0.14	24,24,24,24	0
56	MG	2a	3069	1/1	0.97	0.23	62,62,62,62	0
56	MG	1A	3790	1/1	0.97	0.17	19,19,19,19	0
56	MG	2A	3431	1/1	0.97	0.20	49,49,49,49	0
56	MG	1A	4045	1/1	0.97	0.12	17,17,17,17	0
56	MG	2A	3705	1/1	0.97	0.16	51,51,51,51	0
56	MG	1A	3021	1/1	0.97	0.10	21,21,21,21	0
56	MG	1a	1764	1/1	0.97	0.11	58,58,58,58	0
56	MG	1A	3142	1/1	0.97	0.21	14,14,14,14	0
56	MG	2A	3037	1/1	0.97	0.08	68,68,68,68	0
56	MG	2a	3184	1/1	0.97	0.11	57,57,57,57	0
56	MG	1a	1704	1/1	0.97	0.29	60,60,60,60	0
56	MG	2a	3210	1/1	0.97	0.09	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3132	1/1	0.97	0.26	33,33,33,33	0
56	MG	1W	202	1/1	0.97	0.15	50,50,50,50	0
56	MG	2A	3032	1/1	0.97	0.20	47,47,47,47	0
56	MG	1A	3669	1/1	0.97	0.14	19,19,19,19	0
56	MG	2A	3330	1/1	0.97	0.13	60,60,60,60	0
56	MG	1A	3122	1/1	0.97	0.30	37,37,37,37	0
56	MG	1X	101	1/1	0.97	0.23	32,32,32,32	0
56	MG	1A	3614	1/1	0.97	0.17	35,35,35,35	0
56	MG	1A	3211	1/1	0.97	0.43	34,34,34,34	0
56	MG	1U	203	1/1	0.97	0.32	28,28,28,28	0
56	MG	2U	201	1/1	0.97	0.26	54,54,54,54	0
56	MG	2A	3177	1/1	0.97	0.17	35,35,35,35	0
56	MG	2A	3411	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3146	1/1	0.97	0.35	25,25,25,25	0
56	MG	1A	3448	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3386	1/1	0.97	0.30	30,30,30,30	0
56	MG	1B	231	1/1	0.97	0.21	39,39,39,39	0
56	MG	1A	3038	1/1	0.97	0.21	30,30,30,30	0
56	MG	2A	3851	1/1	0.97	0.10	39,39,39,39	0
56	MG	2A	3668	1/1	0.97	0.19	54,54,54,54	0
56	MG	2A	3435	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3028	1/1	0.97	0.17	21,21,21,21	0
56	MG	1X	103	1/1	0.97	0.31	37,37,37,37	0
56	MG	1A	3135	1/1	0.97	0.11	23,23,23,23	0
56	MG	1A	3833	1/1	0.97	0.15	55,55,55,55	0
56	MG	1O	105	1/1	0.97	0.13	53,53,53,53	0
56	MG	2A	3695	1/1	0.97	0.08	60,60,60,60	0
56	MG	1O	203	1/1	0.97	0.14	40,40,40,40	0
56	MG	2A	3648	1/1	0.97	0.15	47,47,47,47	0
56	MG	1a	1811	1/1	0.97	0.10	38,38,38,38	0
56	MG	2a	3189	1/1	0.97	0.10	57,57,57,57	0
56	MG	2A	3425	1/1	0.97	0.14	43,43,43,43	0
56	MG	1A	3913	1/1	0.97	0.50	34,34,34,34	0
56	MG	1a	1647	1/1	0.97	0.27	55,55,55,55	0
56	MG	2A	3266	1/1	0.97	0.21	59,59,59,59	0
56	MG	1A	3610	1/1	0.97	0.20	44,44,44,44	0
56	MG	1A	3935	1/1	0.97	0.14	40,40,40,40	0
56	MG	2A	3791	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3326	1/1	0.97	0.18	48,48,48,48	0
56	MG	1R	201	1/1	0.97	0.23	32,32,32,32	0
56	MG	1A	3046	1/1	0.97	0.16	28,28,28,28	0
56	MG	1a	1774	1/1	0.97	0.14	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3559	1/1	0.97	0.21	54,54,54,54	0
56	MG	2q	202	1/1	0.97	0.13	72,72,72,72	0
56	MG	2A	3423	1/1	0.97	0.17	35,35,35,35	0
56	MG	1A	3294	1/1	0.97	0.13	41,41,41,41	0
56	MG	1A	3507	1/1	0.97	0.27	42,42,42,42	0
56	MG	1A	3628	1/1	0.97	0.12	51,51,51,51	0
56	MG	2A	3128	1/1	0.97	0.12	42,42,42,42	0
56	MG	1a	1733	1/1	0.97	0.31	53,53,53,53	0
56	MG	1A	3647	1/1	0.97	0.15	30,30,30,30	0
56	MG	1A	4069	1/1	0.97	0.14	20,20,20,20	0
56	MG	1A	3071	1/1	0.97	0.21	29,29,29,29	0
56	MG	2A	3604	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3283	1/1	0.97	0.44	33,33,33,33	0
56	MG	1A	3508	1/1	0.97	0.18	23,23,23,23	0
56	MG	2F	306	1/1	0.97	0.60	51,51,51,51	0
56	MG	1A	3583	1/1	0.97	0.11	44,44,44,44	0
56	MG	1x	102	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	3569	1/1	0.97	0.22	42,42,42,42	0
56	MG	2A	3720	1/1	0.97	0.13	48,48,48,48	0
56	MG	1A	3037	1/1	0.97	0.16	32,32,32,32	0
60	SF4	1d	302	8/8	0.97	0.14	68,78,85,86	0
56	MG	2A	3651	1/1	0.97	0.20	44,44,44,44	0
56	MG	1A	3476	1/1	0.97	0.13	40,40,40,40	0
56	MG	1A	3236	1/1	0.97	0.47	30,30,30,30	0
56	MG	1A	3027	1/1	0.97	0.13	71,71,71,71	0
56	MG	1A	3177	1/1	0.98	0.20	25,25,25,25	0
56	MG	1A	4057	1/1	0.98	0.21	23,23,23,23	0
56	MG	1a	1653	1/1	0.98	0.14	56,56,56,56	0
56	MG	1A	3153	1/1	0.98	0.13	26,26,26,26	0
56	MG	1A	3687	1/1	0.98	0.16	27,27,27,27	0
56	MG	1A	3307	1/1	0.98	0.17	26,26,26,26	0
58	K	2A	3889	1/1	0.98	0.09	36,36,36,36	0
56	MG	2a	3212	1/1	0.98	0.13	59,59,59,59	0
56	MG	1A	3012	1/1	0.98	0.20	28,28,28,28	0
56	MG	1A	3873	1/1	0.98	0.16	35,35,35,35	0
56	MG	1A	3057	1/1	0.98	0.18	28,28,28,28	0
56	MG	2A	3122	1/1	0.98	0.24	53,53,53,53	0
56	MG	1A	4007	1/1	0.98	0.12	15,15,15,15	0
56	MG	2A	3505	1/1	0.98	0.17	57,57,57,57	0
56	MG	1A	3223	1/1	0.98	0.08	46,46,46,46	0
56	MG	1A	3141	1/1	0.98	0.18	26,26,26,26	0
56	MG	1a	1825	1/1	0.98	0.23	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1h	201	1/1	0.98	0.10	58,58,58,58	0
56	MG	1A	3385	1/1	0.98	0.18	27,27,27,27	0
56	MG	1A	3354	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3879	1/1	0.98	0.21	36,36,36,36	0
56	MG	1A	3702	1/1	0.98	0.12	8,8,8,8	0
56	MG	2a	3171	1/1	0.98	0.12	64,64,64,64	0
56	MG	1A	3621	1/1	0.98	0.21	27,27,27,27	0
56	MG	1A	3125	1/1	0.98	0.47	34,34,34,34	0
56	MG	1B	232	1/1	0.98	0.11	50,50,50,50	0
56	MG	1N	204	1/1	0.98	0.39	42,42,42,42	0
56	MG	2A	3232	1/1	0.98	0.15	60,60,60,60	0
56	MG	1B	216	1/1	0.98	0.16	47,47,47,47	0
56	MG	1V	206	1/1	0.98	0.10	29,29,29,29	0
56	MG	2A	3567	1/1	0.98	0.10	54,54,54,54	0
56	MG	1a	1664	1/1	0.98	0.08	60,60,60,60	0
56	MG	1U	204	1/1	0.98	0.17	22,22,22,22	0
56	MG	1A	3716	1/1	0.98	0.19	31,31,31,31	0
56	MG	1a	1708	1/1	0.98	0.27	58,58,58,58	0
56	MG	1A	3439	1/1	0.98	0.19	44,44,44,44	0
56	MG	2A	3717	1/1	0.98	0.04	51,51,51,51	0
56	MG	1A	3097	1/1	0.98	0.32	35,35,35,35	0
56	MG	1A	3517	1/1	0.98	0.24	44,44,44,44	0
56	MG	1D	305	1/1	0.98	0.30	29,29,29,29	0
56	MG	2A	3577	1/1	0.98	0.16	57,57,57,57	0
56	MG	1A	3743	1/1	0.98	0.12	22,22,22,22	0
56	MG	2a	3129	1/1	0.98	0.24	49,49,49,49	0
56	MG	1F	302	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3723	1/1	0.98	0.17	40,40,40,40	0
56	MG	1a	1742	1/1	0.98	0.12	55,55,55,55	0
56	MG	2A	3139	1/1	0.98	0.13	34,34,34,34	0
56	MG	1A	3196	1/1	0.98	0.11	38,38,38,38	0
56	MG	1A	3856	1/1	0.98	0.14	16,16,16,16	0
56	MG	1A	3199	1/1	0.98	0.21	20,20,20,20	0
56	MG	1U	211	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3457	1/1	0.98	0.21	25,25,25,25	0
56	MG	1F	301	1/1	0.98	0.16	27,27,27,27	0
56	MG	2A	3548	1/1	0.98	0.18	35,35,35,35	0
56	MG	2A	3092	1/1	0.98	0.10	48,48,48,48	0
56	MG	2E	303	1/1	0.98	0.12	36,36,36,36	0
56	MG	1W	203	1/1	0.98	0.17	31,31,31,31	0
56	MG	1A	3173	1/1	0.98	0.32	34,34,34,34	0
56	MG	1a	1725	1/1	0.98	0.16	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3682	1/1	0.98	0.13	74,74,74,74	0
56	MG	1A	4091	1/1	0.98	0.20	31,31,31,31	0
56	MG	1A	3219	1/1	0.98	0.30	32,32,32,32	0
56	MG	1A	3730	1/1	0.98	0.16	19,19,19,19	0
56	MG	1A	3804	1/1	0.98	0.17	22,22,22,22	0
56	MG	1A	3631	1/1	0.98	0.11	14,14,14,14	0
56	MG	2a	3235	1/1	0.98	0.06	66,66,66,66	0
56	MG	1E	312	1/1	0.98	0.13	39,39,39,39	0
56	MG	2A	3455	1/1	0.98	0.17	61,61,61,61	0
56	MG	1A	3749	1/1	0.98	0.11	30,30,30,30	0
56	MG	1A	3355	1/1	0.98	0.49	25,25,25,25	0
56	MG	2A	3877	1/1	0.98	0.24	49,49,49,49	0
56	MG	1A	3162	1/1	0.98	0.81	31,31,31,31	0
56	MG	1A	4080	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3066	1/1	0.98	0.13	29,29,29,29	0
56	MG	2Q	201	1/1	0.98	0.13	49,49,49,49	0
56	MG	2A	3642	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3244	1/1	0.98	0.16	42,42,42,42	0
56	MG	2A	3863	1/1	0.98	0.12	28,28,28,28	0
56	MG	2B	219	1/1	0.98	0.14	62,62,62,62	0
56	MG	1Q	202	1/1	0.98	0.36	34,34,34,34	0
56	MG	1A	3174	1/1	0.98	0.26	27,27,27,27	0
56	MG	2a	3079	1/1	0.98	0.09	56,56,56,56	0
56	MG	1A	3047	1/1	0.98	0.20	23,23,23,23	0
59	ZN	25	106	1/1	0.98	0.20	57,57,57,57	0
56	MG	1A	3003	1/1	0.98	0.16	19,19,19,19	0
56	MG	1A	3591	1/1	0.98	0.29	35,35,35,35	0
56	MG	2A	3843	1/1	0.98	0.16	35,35,35,35	0
56	MG	2A	3223	1/1	0.98	0.10	45,45,45,45	0
56	MG	1A	3704	1/1	0.98	0.10	21,21,21,21	0
56	MG	1A	3821	1/1	0.98	0.13	26,26,26,26	0
56	MG	1A	3266	1/1	0.98	0.11	40,40,40,40	0
56	MG	1Y	202	1/1	0.98	0.12	68,68,68,68	0
56	MG	1A	3786	1/1	0.98	0.09	24,24,24,24	0
56	MG	1A	3442	1/1	0.98	0.40	36,36,36,36	0
56	MG	1A	3827	1/1	0.98	0.15	39,39,39,39	0
56	MG	1B	201	1/1	0.98	0.29	48,48,48,48	0
56	MG	1A	3171	1/1	0.98	0.18	44,44,44,44	0
56	MG	1P	204	1/1	0.98	0.47	23,23,23,23	0
56	MG	2A	3260	1/1	0.98	0.16	57,57,57,57	0
56	MG	1a	1828	1/1	0.98	0.25	42,42,42,42	0
56	MG	1A	3077	1/1	0.98	0.12	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3536	1/1	0.98	0.17	57,57,57,57	0
56	MG	2A	3328	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3073	1/1	0.98	0.16	14,14,14,14	0
56	MG	2A	3744	1/1	0.98	0.21	44,44,44,44	0
56	MG	2A	3322	1/1	0.98	0.10	48,48,48,48	0
56	MG	1l	202	1/1	0.98	0.19	41,41,41,41	0
56	MG	2A	3758	1/1	0.98	0.11	64,64,64,64	0
56	MG	1A	3128	1/1	0.98	0.18	36,36,36,36	0
56	MG	1A	3108	1/1	0.98	0.25	36,36,36,36	0
56	MG	1A	3792	1/1	0.98	0.15	45,45,45,45	0
56	MG	28	102	1/1	0.98	0.10	48,48,48,48	0
56	MG	1a	1610	1/1	0.98	0.11	23,23,23,23	0
56	MG	2A	3708	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3874	1/1	0.98	0.20	27,27,27,27	0
56	MG	1a	1629	1/1	0.98	0.15	54,54,54,54	0
56	MG	1F	303	1/1	0.98	0.23	28,28,28,28	0
56	MG	2D	305	1/1	0.98	0.14	33,33,33,33	0
56	MG	1A	3187	1/1	0.98	0.17	31,31,31,31	0
56	MG	2A	3725	1/1	0.98	0.09	34,34,34,34	0
56	MG	1A	3241	1/1	0.98	0.34	30,30,30,30	0
56	MG	1A	3160	1/1	0.98	0.33	26,26,26,26	0
56	MG	2A	3258	1/1	0.98	0.08	67,67,67,67	0
56	MG	2A	3188	1/1	0.98	0.11	43,43,43,43	0
56	MG	1A	3820	1/1	0.98	0.09	18,18,18,18	0
56	MG	1A	3818	1/1	0.98	0.11	42,42,42,42	0
56	MG	2B	215	1/1	0.98	0.15	69,69,69,69	0
56	MG	1A	3042	1/1	0.98	0.28	22,22,22,22	0
56	MG	1A	3692	1/1	0.98	0.14	55,55,55,55	0
56	MG	2A	3127	1/1	0.98	0.29	65,65,65,65	0
56	MG	1A	3001	1/1	0.99	0.13	39,39,39,39	0
56	MG	2a	3055	1/1	0.99	0.12	60,60,60,60	0
56	MG	1a	1816	1/1	0.99	0.14	53,53,53,53	0
56	MG	1A	4063	1/1	0.99	0.12	46,46,46,46	0
56	MG	2a	3128	1/1	0.99	0.06	44,44,44,44	0
56	MG	2A	3019	1/1	0.99	0.11	30,30,30,30	0
56	MG	1A	3645	1/1	0.99	0.21	20,20,20,20	0
56	MG	1A	3660	1/1	0.99	0.20	31,31,31,31	0
56	MG	2A	3080	1/1	0.99	0.15	56,56,56,56	0
56	MG	2A	3545	1/1	0.99	0.13	35,35,35,35	0
56	MG	1A	3785	1/1	0.99	0.15	37,37,37,37	0
56	MG	1A	3225	1/1	0.99	0.19	39,39,39,39	0
56	MG	1A	3622	1/1	0.99	0.14	22,22,22,22	0

Continued on next page...

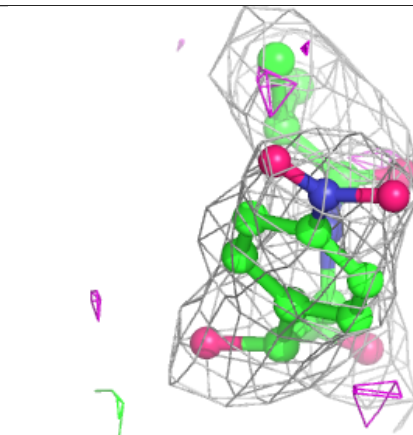
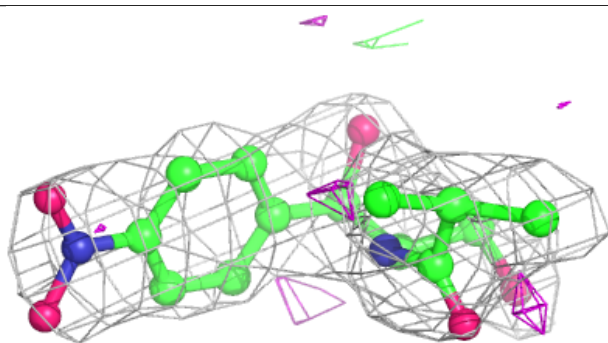
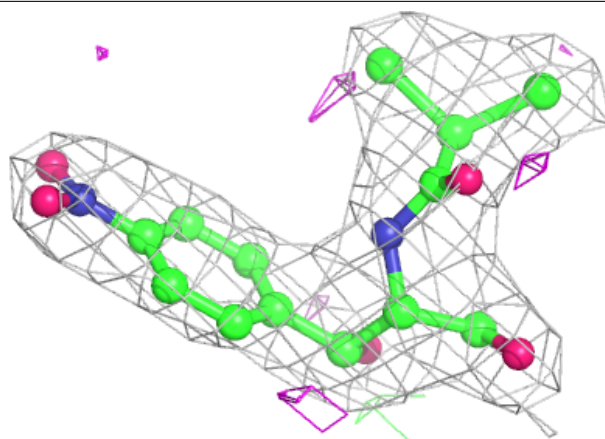
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3079	1/1	0.99	0.23	26,26,26,26	0
56	MG	1a	1648	1/1	0.99	0.11	48,48,48,48	0
56	MG	1a	1644	1/1	0.99	0.12	39,39,39,39	0
56	MG	2a	3022	1/1	0.99	0.06	43,43,43,43	0
56	MG	2A	3147	1/1	0.99	0.29	31,31,31,31	0
56	MG	1A	3919	1/1	0.99	0.16	30,30,30,30	0
56	MG	1B	210	1/1	0.99	0.20	51,51,51,51	0
56	MG	1U	207	1/1	0.99	0.13	29,29,29,29	0
56	MG	2A	3429	1/1	0.99	0.31	53,53,53,53	0
56	MG	1A	3228	1/1	0.99	0.21	32,32,32,32	0
56	MG	1A	3045	1/1	0.99	0.12	28,28,28,28	0
56	MG	1A	3719	1/1	0.99	0.13	47,47,47,47	0
59	ZN	15	106	1/1	0.99	0.20	38,38,38,38	0
56	MG	2a	3094	1/1	0.99	0.22	62,62,62,62	0
56	MG	1A	3373	1/1	0.99	0.10	43,43,43,43	0
59	ZN	19	102	1/1	0.99	0.22	40,40,40,40	0
59	ZN	1Y	204	1/1	0.99	0.19	53,53,53,53	0
56	MG	1A	3036	1/1	0.99	0.16	15,15,15,15	0
56	MG	1A	3618	1/1	0.99	0.20	26,26,26,26	0
56	MG	2A	3625	1/1	0.99	0.14	57,57,57,57	0
56	MG	1A	3286	1/1	0.99	0.37	42,42,42,42	0
56	MG	27	102	1/1	0.99	0.26	34,34,34,34	0
56	MG	1B	238	1/1	0.99	0.12	37,37,37,37	0
56	MG	2A	3307	1/1	0.99	0.17	54,54,54,54	0
58	K	1A	4103	1/1	0.99	0.10	21,21,21,21	0
56	MG	2A	3660	1/1	0.99	0.09	33,33,33,33	0
56	MG	1E	305	1/1	0.99	0.31	32,32,32,32	0
59	ZN	26	501	1/1	0.99	0.17	64,64,64,64	0
59	ZN	16	104	1/1	0.99	0.21	37,37,37,37	0
56	MG	2A	3288	1/1	0.99	0.24	36,36,36,36	0
56	MG	1A	3127	1/1	1.00	0.14	42,42,42,42	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

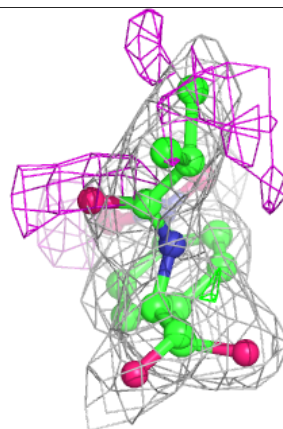
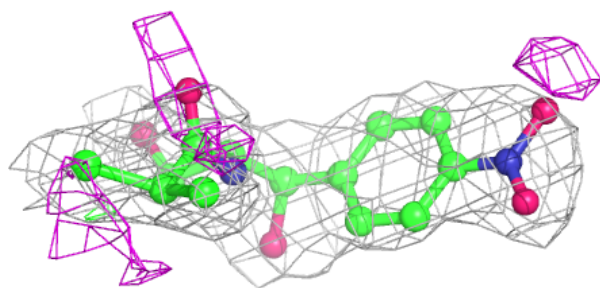
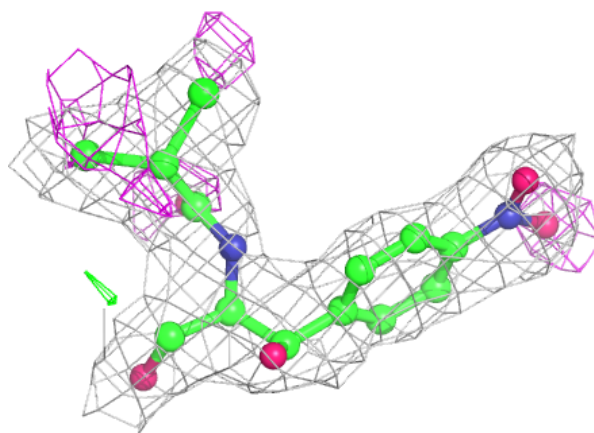
Electron density around CLM 2A 3888:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLM 1A 4102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.