



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:15 am BST

PDB ID : 5HCP
Title : Crystal structure of antimicrobial peptide Metalnikowin bound to the *Thermus thermophilus* 70S ribosome
Authors : Gagnon, M.G.; Roy, R.N.; Lomakin, I.B.; Florin, T.; Mankin, A.S.; Steitz, T.A.
Deposited on : 2016-01-04
Resolution : 2.89 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
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

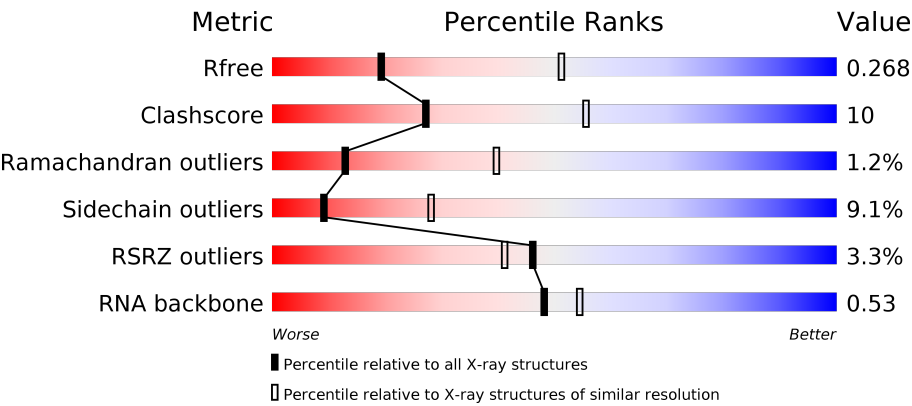
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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.








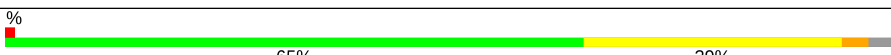
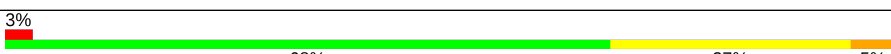


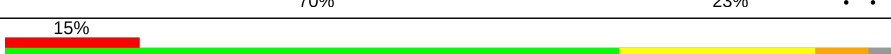
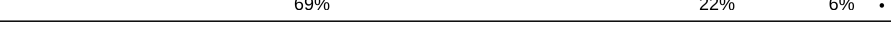
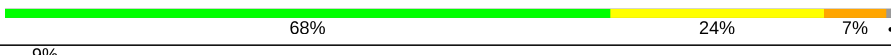




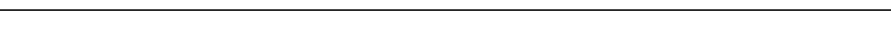





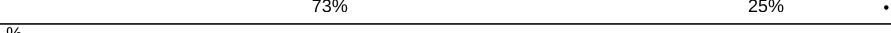


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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>59%</div><div>29%</div><div>5%</div><div>6%</div></div>
1	2A	2915	<div><div>2%</div><div></div><div>51%</div><div>38%</div><div>7%</div><div></div></div>
2	1B	121	<div><div></div><div>73%</div><div>26%</div><div></div></div>
2	2B	121	<div><div>2%</div><div></div><div>43%</div><div>45%</div><div>11%</div><div></div></div>


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	















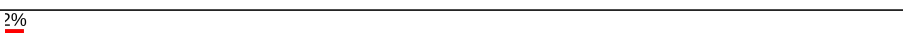




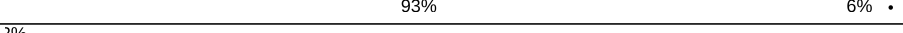
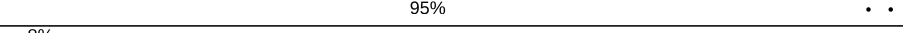




Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1x	77	
54	2x	77	
55	1z	15	
55	2z	15	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	12	3001	-	-	-	X
56	MG	1A	3007	-	-	-	X
56	MG	1A	3320	-	-	-	X
56	MG	1A	3333	-	-	-	X
56	MG	1A	3384	-	-	-	X
56	MG	1A	3411	-	-	-	X
56	MG	1A	3901	-	-	-	X
56	MG	1A	3916	-	-	-	X
56	MG	1A	4027	-	-	-	X
56	MG	1A	4054	-	-	-	X
56	MG	1F	304	-	-	-	X
56	MG	1T	206	-	-	-	X
56	MG	1a	1639	-	-	-	X
56	MG	1a	1756	-	-	-	X
56	MG	1a	1757	-	-	-	X
56	MG	2A	3093	-	-	-	X
56	MG	2a	3001	-	-	-	X
56	MG	2a	3039	-	-	-	X
56	MG	2a	3043	-	-	-	X
56	MG	2a	3138	-	-	-	X
56	MG	2a	3254	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 288976 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	2746	Total	C	N	O	P	0	0	0
			59154	26327	11077	19005	2745			
1	2A	2790	Total	C	N	O	P	0	0	0
			60091	26746	11243	19313	2789			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1146	476	831	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2142	1352	426	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
			1425	914	256	251	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	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
			1085	693	189	202	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	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
			1139	709	231	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			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	186	Total	C	N	O	S	0	0	0
			1470	937	262	269	2			
21	2Z	186	Total	C	N	O	S	0	0	0
			1454	929	256	267	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	75	Total	C	N	O	S	0	0	0
			598	370	127	100	1			
22	20	75	Total	C	N	O	S	0	0	0
			598	370	127	100	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
			558	352	102	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	1477	Total	C	N	O	P	0	0	0
			31750	14131	5883	10259	1477			
32	2a	1483	Total	C	N	O	P	0	0	0
			31877	14188	5905	10301	1483			

- 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
			1786	1136	321	325	4			
33	2b	231	Total	C	N	O	S	0	0	0
			1697	1079	292	321	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
			1480	932	281	266	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1412	883	269	259	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
			1618	1013	312	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1630	1022	321	280	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
			1095	695	203	193	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
			806	511	143	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			817	516	146	152	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
			1183	732	232	213	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1167	728	220	213	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
			1074	681	202	189	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
			976	620	189	167			
40	2i	127	Total	C	N	O	0	0	0
			932	589	177	166			

- 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
			682	424	130	128			
41	2j	96	Total	C	N	O	0	0	0
			678	424	126	128			

- 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
			826	513	156	154	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
			829	516	155	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
			920	579	181	159	1			
43	2l	122	Total	C	N	O	S	0	0	0
			918	576	182	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	118	Total	C	N	O	S	0	0	0
			923	569	191	161	2			
44	2m	116	Total	C	N	O	S	0	0	0
			903	555	187	159	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			482	306	100	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			459	291	93	71	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
			715	447	140	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
			671	424	133	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
			811	519	148	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	84	Total	C	N	O	S	0	0	0
			642	409	119	112	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
			712	435	152	123	2			
51	2t	96	Total	C	N	O	S	0	0	0
			731	449	156	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
			187	116	42	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	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			
53	2v	5	Total	C	N	O	P	0	0	0
			109	49	22	33	5			

- Molecule 54 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
54	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 55 is a protein called Metalnikowin-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	1z	12	Total	C	N	O	0	0	0
			105	66	22	17			
55	2z	13	Total	C	N	O	0	0	0
			112	71	23	18			

- 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	2	Total	Mg	0	0
			2	2		
56	1z	1	Total	Mg	0	0
			1	1		
56	2d	2	Total	Mg	0	0
			2	2		
56	1T	6	Total	Mg	0	0
			6	6		
56	1N	7	Total	Mg	0	0
			7	7		
56	1u	1	Total	Mg	0	0
			1	1		
56	18	3	Total	Mg	0	0
			3	3		
56	1o	3	Total	Mg	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2l	5	Total 5	Mg 5	0	0
56	1Y	1	Total 1	Mg 1	0	0
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1P	6	Total 6	Mg 6	0	0
56	2B	10	Total 10	Mg 10	0	0
56	1q	3	Total 3	Mg 3	0	0
56	23	1	Total 1	Mg 1	0	0
56	1k	1	Total 1	Mg 1	0	0
56	1E	12	Total 12	Mg 12	0	0
56	2z	1	Total 1	Mg 1	0	0
56	1b	1	Total 1	Mg 1	0	0
56	25	1	Total 1	Mg 1	0	0
56	2F	4	Total 4	Mg 4	0	0
56	16	4	Total 4	Mg 4	0	0
56	28	3	Total 3	Mg 3	0	0
56	2e	2	Total 2	Mg 2	0	0
56	1W	6	Total 6	Mg 6	0	0
56	1A	1090	Total 1090	Mg 1090	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2P	1	Total Mg 1 1	0	0
56	1X	1	Total Mg 1 1	0	0
56	12	1	Total Mg 1 1	0	0
56	20	1	Total Mg 1 1	0	0
56	1p	2	Total Mg 2 2	0	0
56	2T	1	Total Mg 1 1	0	0
56	1D	13	Total Mg 13 13	0	0
56	2N	1	Total Mg 1 1	0	0
56	1e	3	Total Mg 3 3	0	0
56	2G	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	1V	2	Total Mg 2 2	0	0
56	2X	1	Total Mg 1 1	0	0
56	2v	1	Total Mg 1 1	0	0
56	1a	309	Total Mg 309 309	0	0
56	2Q	5	Total Mg 5 5	0	0
56	15	3	Total Mg 3 3	0	0
56	1x	10	Total Mg 10 10	0	0
56	1R	6	Total Mg 6 6	0	0
56	1m	1	Total Mg 1 1	0	0
56	2U	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1G	3	Total 3 Mg 3	0	0
56	2O	3	Total 3 Mg 3	0	0
56	11	3	Total 3 Mg 3	0	0
56	1d	2	Total 2 Mg 2	0	0
56	2r	1	Total 1 Mg 1	0	0
56	1H	4	Total 4 Mg 4	0	0
56	2q	3	Total 3 Mg 3	0	0
56	2Y	1	Total 1 Mg 1	0	0
56	1v	1	Total 1 Mg 1	0	0
56	2x	7	Total 7 Mg 7	0	0
56	2R	2	Total 2 Mg 2	0	0
56	1Z	2	Total 2 Mg 2	0	0
56	2D	5	Total 5 Mg 5	0	0
56	14	1	Total 1 Mg 1	0	0
56	1U	6	Total 6 Mg 6	0	0
56	1O	3	Total 3 Mg 3	0	0
56	1r	3	Total 3 Mg 3	0	0
56	19	5	Total 5 Mg 5	0	0
56	1l	2	Total 2 Mg 2	0	0
56	1F	8	Total 8 Mg 8	0	0
56	10	6	Total 6 Mg 6	0	0

Continued on next page...

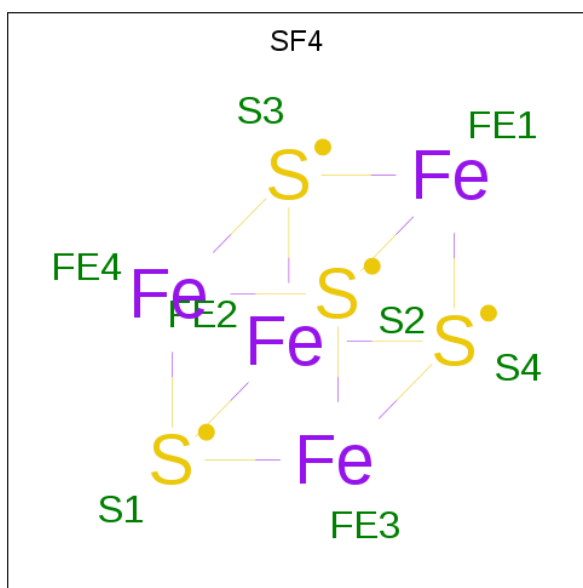
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2t	1	Total 1	Mg 1	0	0
56	1Q	9	Total 9	Mg 9	0	0
56	2A	561	Total 561	Mg 561	0	0
56	1h	2	Total 2	Mg 2	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	1B	30	Total 30	Mg 30	0	0
56	2a	255	Total 255	Mg 255	0	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total 1	Zn 1	0	0
57	14	1	Total 1	Zn 1	0	0
57	1n	1	Total 1	Zn 1	0	0
57	15	1	Total 1	Zn 1	0	0
57	29	1	Total 1	Zn 1	0	0
57	19	1	Total 1	Zn 1	0	0
57	26	1	Total 1	Zn 1	0	0
57	25	1	Total 1	Zn 1	0	0
57	24	1	Total 1	Zn 1	0	0
57	2n	1	Total 1	Zn 1	0	0
57	2Y	1	Total 1	Zn 1	0	0
57	16	1	Total 1	Zn 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	1d	1	Total	Fe	S	0	0
			8	4	4		
58	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1A	2412	Total	O	0	0
			2412	2412		
59	1B	46	Total	O	0	0
			46	46		
59	1D	25	Total	O	0	0
			25	25		
59	1E	30	Total	O	0	0
			30	30		
59	1F	21	Total	O	0	0
			21	21		
59	1G	8	Total	O	0	0
			8	8		
59	1H	4	Total	O	0	0
			4	4		
59	1I	3	Total	O	0	0
			3	3		
59	1N	8	Total	O	0	0
			8	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1O	5	Total 5	O 5	0	0
59	1P	25	Total 25	O 25	0	0
59	1Q	13	Total 13	O 13	0	0
59	1R	18	Total 18	O 18	0	0
59	1S	2	Total 2	O 2	0	0
59	1T	13	Total 13	O 13	0	0
59	1U	18	Total 18	O 18	0	0
59	1V	5	Total 5	O 5	0	0
59	1W	14	Total 14	O 14	0	0
59	1X	5	Total 5	O 5	0	0
59	1Y	1	Total 1	O 1	0	0
59	1Z	6	Total 6	O 6	0	0
59	10	8	Total 8	O 8	0	0
59	11	7	Total 7	O 7	0	0
59	12	2	Total 2	O 2	0	0
59	13	3	Total 3	O 3	0	0
59	15	7	Total 7	O 7	0	0
59	16	11	Total 11	O 11	0	0
59	17	9	Total 9	O 9	0	0
59	18	16	Total 16	O 16	0	0
59	19	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1a	394	Total 394	O 394	0	0
59	1b	1	Total 1	O 1	0	0
59	1c	1	Total 1	O 1	0	0
59	1d	3	Total 3	O 3	0	0
59	1e	4	Total 4	O 4	0	0
59	1f	1	Total 1	O 1	0	0
59	1h	2	Total 2	O 2	0	0
59	1j	1	Total 1	O 1	0	0
59	1k	2	Total 2	O 2	0	0
59	1l	3	Total 3	O 3	0	0
59	1m	1	Total 1	O 1	0	0
59	1p	1	Total 1	O 1	0	0
59	1q	1	Total 1	O 1	0	0
59	1s	1	Total 1	O 1	0	0
59	1u	1	Total 1	O 1	0	0
59	1v	3	Total 3	O 3	0	0
59	1x	10	Total 10	O 10	0	0
59	1z	5	Total 5	O 5	0	0
59	2A	824	Total 824	O 824	0	0
59	2B	9	Total 9	O 9	0	0
59	2D	18	Total 18	O 18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2E	11	Total 11	O 11	0	0
59	2F	6	Total 6	O 6	0	0
59	2N	2	Total 2	O 2	0	0
59	2O	1	Total 1	O 1	0	0
59	2P	6	Total 6	O 6	0	0
59	2R	1	Total 1	O 1	0	0
59	2T	1	Total 1	O 1	0	0
59	2U	3	Total 3	O 3	0	0
59	2W	1	Total 1	O 1	0	0
59	2X	3	Total 3	O 3	0	0
59	2Y	2	Total 2	O 2	0	0
59	2Z	5	Total 5	O 5	0	0
59	20	2	Total 2	O 2	0	0
59	21	1	Total 1	O 1	0	0
59	23	2	Total 2	O 2	0	0
59	25	1	Total 1	O 1	0	0
59	27	1	Total 1	O 1	0	0
59	28	4	Total 4	O 4	0	0
59	2a	329	Total 329	O 329	0	0
59	2c	1	Total 1	O 1	0	0
59	2d	1	Total 1	O 1	0	0

Continued on next page...

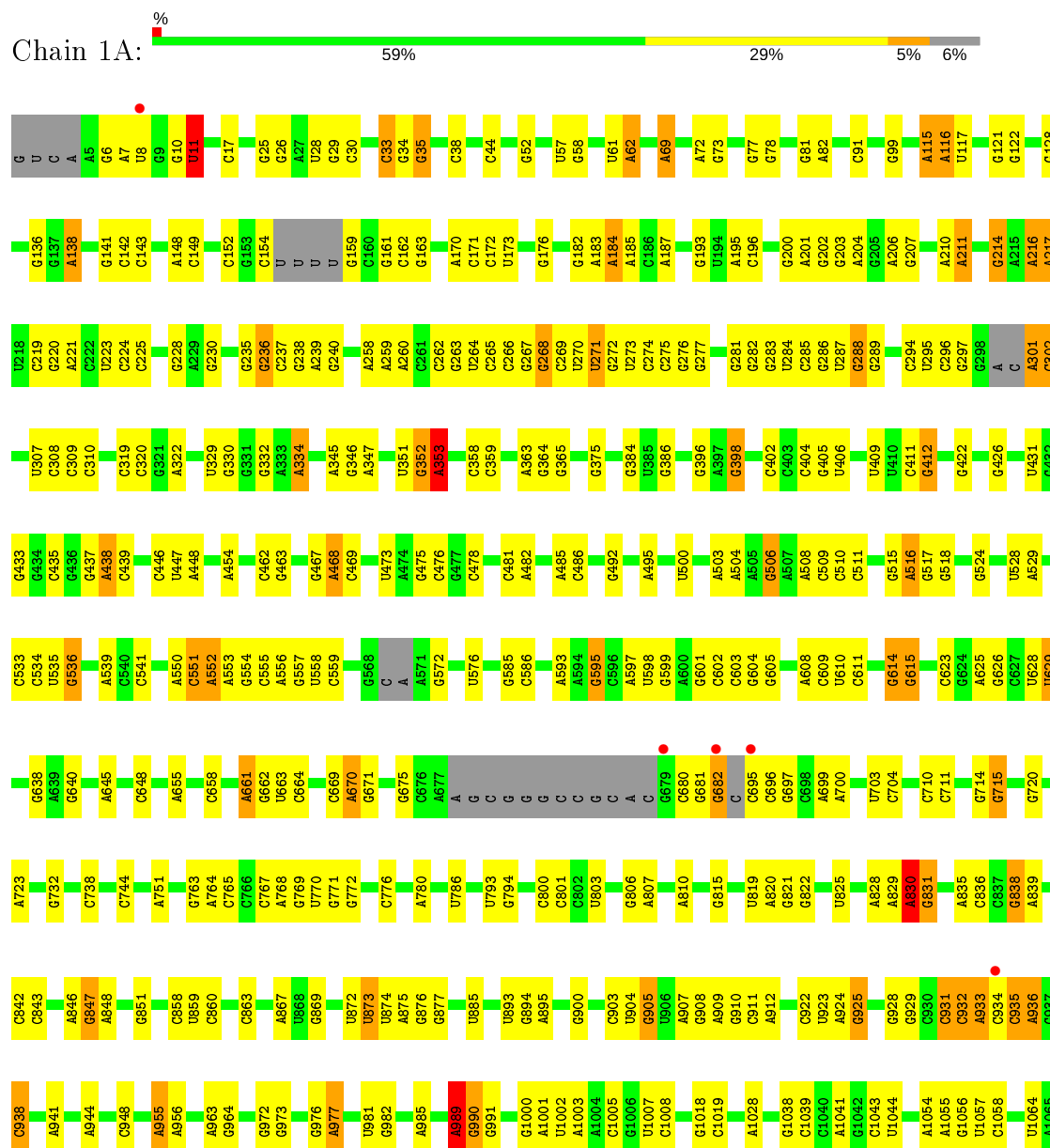
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2e	4	Total 4	O 4	0	0
59	2g	1	Total 1	O 1	0	0
59	2i	2	Total 2	O 2	0	0
59	2l	2	Total 2	O 2	0	0
59	2m	1	Total 1	O 1	0	0
59	2o	1	Total 1	O 1	0	0
59	2p	2	Total 2	O 2	0	0
59	2q	1	Total 1	O 1	0	0
59	2t	4	Total 4	O 4	0	0
59	2u	1	Total 1	O 1	0	0
59	2x	6	Total 6	O 6	0	0
59	2z	2	Total 2	O 2	0	0

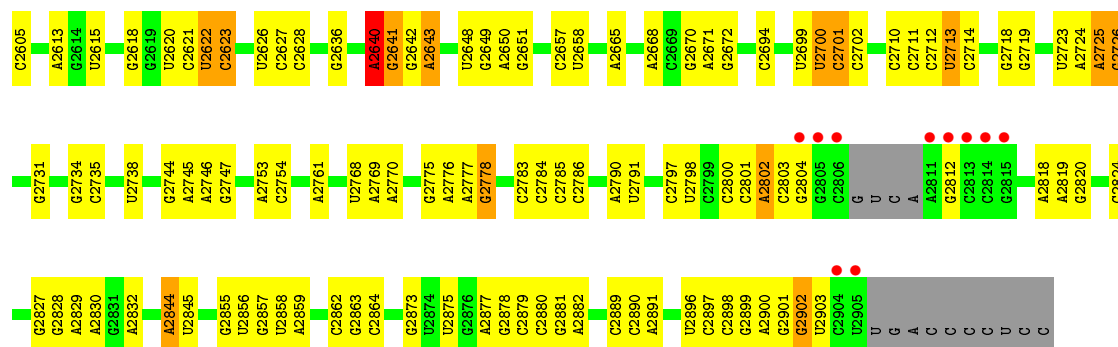
3 Residue-property plots

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.

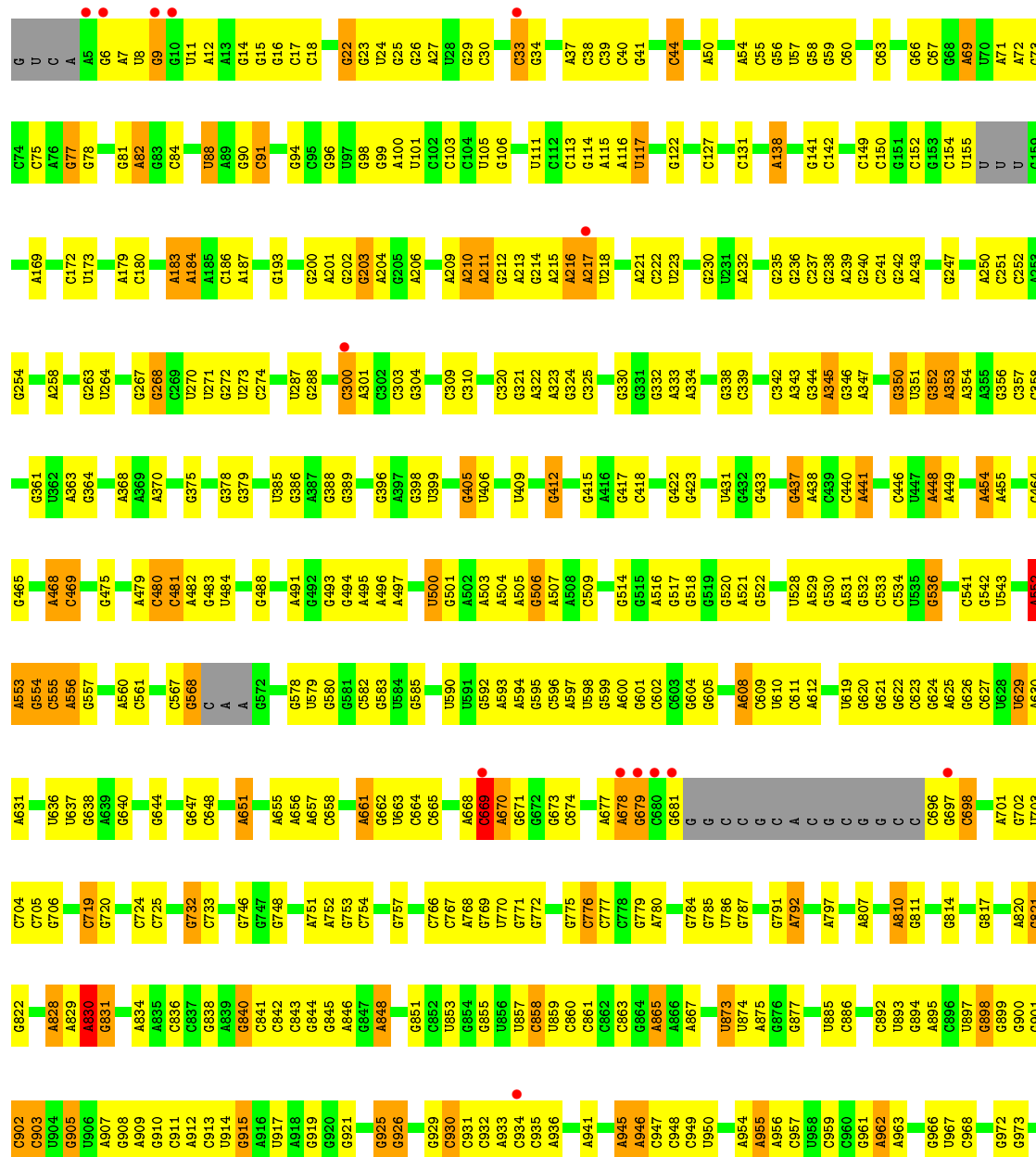
• Molecule 1: 23S Ribosomal RNA



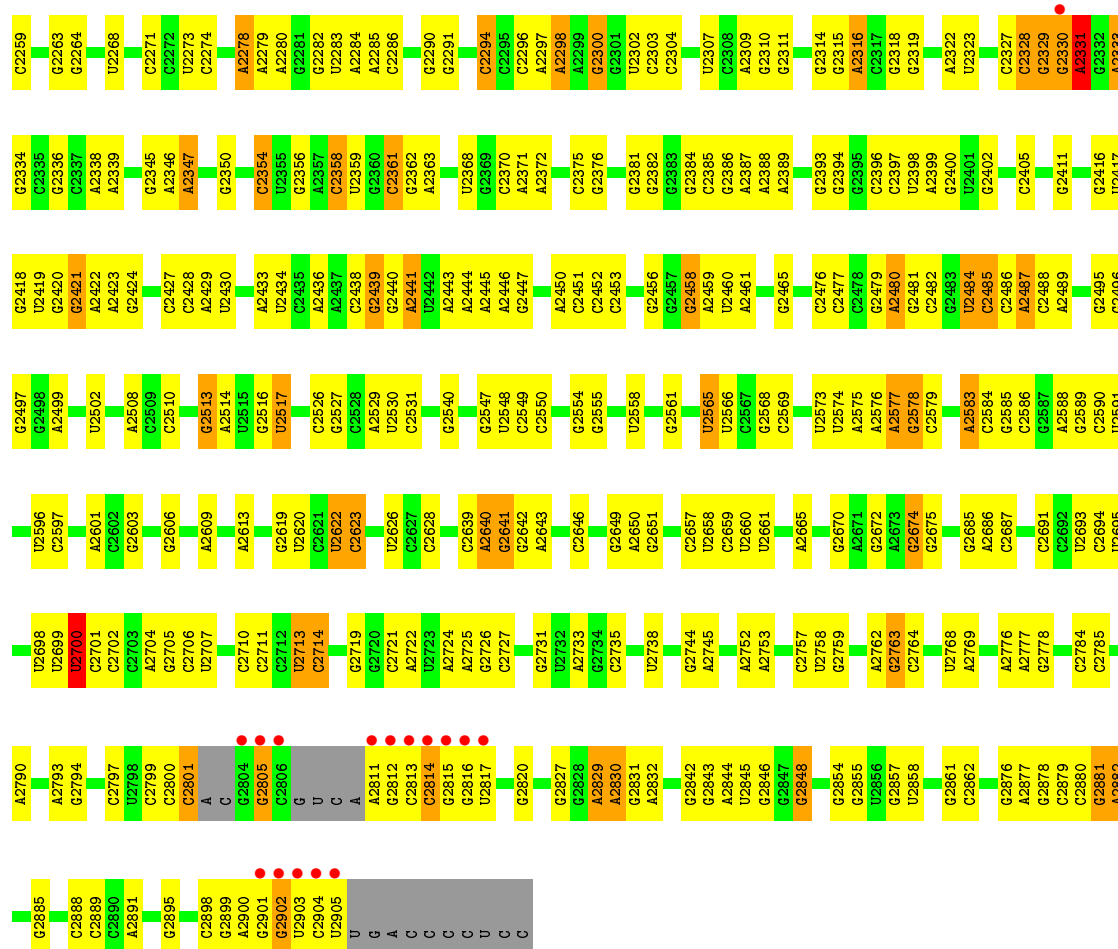
G2505	G2400	G2287	C	G	C2047	A1933	C1812	G1688	C1578	U1476	G1354	C1229	A1066
G2509	U2401	G2288	A	G	A2052	A1934	A1813	G1691	G	A1479	G1355	G1230	G1067
C2510	G2516	A2289	C	A	U1935	G1935	A1816	C1692	A	U1479	U1358	U1231	U1088
U2511	C2404	G2290	C	U	G2063	U1936	A1816	C1693	C	C1482	C1359	U1232	G1069
C2512	C2405	G2291	C	A	A2054	A1939	A1821	C1694	G	U1490	C1360	G1235	U1070
C2513	U2417	C2294	U	G	C2057	A1940	G1822	A1700	G1583	A1490	A1366	U1249	A1071
U2514	U2417	C2294	U	G	G2058	C1941	U1826	A1700	G1587	A1495	A1366	C1245	A1072
U2515	G2516	A2298	G	G	G2059	U1826	C1827	C1704	A1588	G1496	A1366	C1246	A1073
C2516	U2517	G2290	G	G	C2060	A1948	C1828	C1704	A1591	A1495	G1377	G1247	A1074
C2518	C2429	U2302	G	G	C2061	A1949	U1828	C1709	G1592	G1501	G1378	G1248	G1075
C2523	A2433	C2303	G	A	U2062	G1950	G1839	C1710	C1593	G1502	G1379	U1249	A1077
G2524	U2434	U2307	C	C	C2064	G1951	C1830	A1711	C1593	G1502	U1380	U1249	U1078
U2529	C2435	G2315	U	U	U1952	A1953	G1831	A1711	C1593	G1502	A1381	A1254	C1086
U2530	A2436	A2316	G	G	G1954	A1958	A1832	A1715	C1603	G1505	U1397	A1257	U1086
C2531	U2440	G2319	U	U	G2074	A1959	A1833	A1716	A1604	G1507	U1402	A1264	A1090
C2540	A2441	A2320	G	G	A2075	U1960	A1845	U1717	A1612	C1508	U1403	A1264	A1091
A2541	U2442	A2321	A	A	C2076	U1960	G1846	G1720	A1613	C1509	A1404	G1281	G1092
A2542	A2443	A2322	C	C	A2078	U1976	G1846	A1723	G1614	C1510	A1405	A1282	A1093
G2543	A2444	U2323	C	C	A2080	U1976	G1846	A1723	G1615	G1511	A1405	G1283	G1157
A2544	A2445	U2323	C	C	A2081	U1976	G1846	A1723	G1616	G1512	G1409	G1284	G1158
A2545	A2446	U2323	C	C	G2082	U1979	G1846	C1729	G1617	C1513	A1410	U1285	G1159
G2554	U2449	G2330	C	C	A2083	U1984	G1854	C1730	A1618	C1514	U1285	A1286	G1170
G2555	A2450	A2331	C	C	C2086	G1985	A1855	U1734	C1620	A1517	G1416	U1294	A1173
G2556	A2451	G2332	G	G	C2087	G1986	G1856	A1735	C1623	A1518	U1417	U1295	A1174
C2561	C2452	U2336	U	U	C2088	A1987	C1857	A1746	A1624	G1519	C1421	G1296	G1175
G2562	A2453	G2337	C	C	G2090	G1988	A1858	U1738	A1625	G1520	G1426	G1297	G1176
U2563	U2454	U2338	C	C	G2091	G1989	G1859	U1739	A1626	G1521	A1424	A1298	G1179
U2564	G2455	A2339	C	C	A2092	A1990	C1862	C1740	G1627	G1524	G1425	A1298	G1180
U2565	G2456	U2340	C	C	G2093	A1991	G1863	A1744	C1630	G1528	G1426	G1301	G1183
C2566	A2457	G2341	G	G	U2094	A1992	C1868	G1745	A1631	G1529	A1429	G1305	G1184
C2567	U2460	G2342	U	U	U2096	A1993	C1869	A1746	A1632	G1530	G1430	C1306	U1185
G2568	U2345	U2244	G	G	U2100	A2007	C1873	A1747	C1633	A1531	U1439	G1311	U1186
C2569	A2346	G2245	G	G	G2101	U2012	A1877	A1766	C1634	G1532	U1440	U1312	A1187
U2573	G2347	G2246	G	G	U2107	G2013	A1878	U1767	G1638	G1536	U1441	U1313	A1188
A2575	U2348	G2248	G	G	G2108	U2014	G1879	G1776	G1639	A1540	U1450	A1314	G1198
U2576	C2354	G2249	A	A	G2114	G2018	A1889	G1783	U1647	A1541	U1451	G1315	C1199
A2577	U2355	G2250	G	G	G2114	C2019	G1889	U1792	A1648	A1541	G1452	G1316	G1199
U2578	G2356	U2254	G	G	G2121	C2020	G1889	G1793	C1649	U1548	G1453	A1317	A1200
C2579	A2357	U2255	C	C	U2123	G2024	G1889	G1794	A1654	C1549	A1457	U1318	G1200
A2583	G2358	G2256	G	G	U2124	G2024	G1889	A1792	A1655	A1552	G1458	A1319	C1211
C2584	U2361	G2257	C	C	G2124	G2031	C1907	G1799	A1655	A1554	G1461	A1321	U1210
G2585	C2367	C2259	C	C	G	U2032	C1907	G1799	A1655	A1554	G1461	A1321	C1211
C2586	U2368	C2259	C	C	G	G2033	C1907	G1799	A1655	A1554	G1461	A1321	C1211
G2587	G2383	C2275	G	G	C	A2034	A1910	G1802	A1659	A1555	C1462	U1337	G1215
A2588	U2391	A2279	U	U	C	A2035	A1910	A1803	A1662	U1565	U1465	C1342	G1216
G2593	C2392	A2280	A	A	C	G2042	G1920	A1805	A1663	G1566	G1467	C1343	A1218
A2601	G2393	U2283	A	A	C	U2043	A1921	G1806	A1680	G1570	U1472	U1345	U1219
U2604	G2394	A2284	U	U	C	G2044	G1924	G1809	U1685	G1575	C1473	A1346	A1221
	C2396	A2285	A	A	U	U2045	G1927	A1810	C1686	C1576	A1474	U1347	A1222
		C2286	C	C	A	C2046	G1927	C1811	A1687	C1577	C1475	G1348	A1223



• Molecule 1: 23S Ribosomal RNA

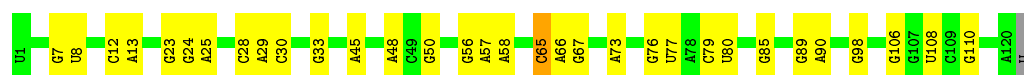


G	A2041	A1934	U1835	U1734	C1630	U1534	C1444	C1359	G1280	G1194	C1121	U1057
C	C2042	C1936	A1845	A1735	A1631	A1535	C1447	C1361	C1195	C1122	U1123	C1058
C	U2043	U1936	A1846	A1735	G1638	G1538	C1448	U1361	C1199	U1123	C1122	U1059
A	G2044	A1937	G1846	U1739	G1639	C1538	C1449	C1363	G1199	G1124	C1125	G1060
A	G2045	U1938	G1847	C1740	C1639	U1542	U1450	G1363	A1200	U1126	G1126	G1061
C	C2046	U1938	G1942	G1741	C1643	C1543	U1451	G1364	G1205	U1127	U1127	G1062
U	G2047	G1943	G1943	G1741	C1644	C1452	U1451	G1369	G1206	U1128	U1128	G1063
C	C2048	G1943	G1945	A1744	C1644	C1452	C1453	G1369	C1206	U1129	U1129	U1064
C	U2049	G1945	G1856	G1745	A1648	U1549	C1453	G1369	A1065	A1129	A1129	A1065
A	G2050	A1948	G1857	G1745	C1648	C1549	C1456	C1372	G1209	A1130	A1130	A1066
A	A2051	A1949	G1858	A1746	C1649	U1549	C1457	G1373	U1210	A1131	A1131	G1067
C	A2052	G1950	A1859	A1747	C1649	A1552	G1458	U1374	G1211	A1132	A1132	U1068
C	G2053	C1950	C1860	G1747	C1652	A1553	C1458	C1375	G1212	A1133	G1133	G1069
C	A2054	G1951	G1861	G1765	A1653	A1554	G1459	G1376	G1213	A1134	A1134	C1070
C	G2055	A1952	C1862	A1766	A1654	A1555	G1461	G1377	G1214	U1135	U1135	U1071
U	G2056	G1953	C1863	A1766	A1654	A1555	G1461	G1377	G1214	U1135	U1135	U1071
C	G2057	G1954	C1864	U1767	A1655	A1556	C1462	G1378	G1215	G1136	G1136	A1072
C	G2058	G1954	C1864	U1767	A1655	A1556	C1462	G1378	G1215	G1136	G1136	A1072
U	G2059	G1954	C1864	U1767	A1655	A1556	C1462	G1378	G1215	G1136	G1136	A1072
C	C2060	A1958	C1874	A1769	A1659	U1560	U1465	G1379	G	A1140	A1140	A1073
G	C2061	A1959	C1874	A1769	A1659	U1560	U1465	G1379	G	A1140	A1140	A1073
G	U2062	C2061	A1877	C1770	C1660	G1567	G1466	U1380	A	A1141	A1141	G1076
C	C2063	U1967	A1878	C1771	A1661	U1568	G1467	G1382	U	A1077	A1077	U1002
A	C2064	C1968	G1879	G1786	G1669	G1570	G1470	C1306	G	A1143	A1143	U1078
C	G2067	A1973	G1880	U1787	G1670	G1571	G1471	A1307	A	U1146	U1146	G1082
C	C2068	A1973	G1880	U1787	G1670	G1571	G1471	A1307	A	U1146	U1146	G1082
U	C2076	U1976	A1883	G1788	G1671	U1572	A1472	G1393	C1222	C1147	C1147	C1083
C	C2077	A1981	A1884	A1789	G1672	A1573	C1473	A1394	C1224	C1148	C1148	G1084
U	A2078	G1981	G1887	A1792	G1673	U1574	G1474	U1397	C1225	C1149	C1149	C1085
C	A2079	G1988	G1888	G1793	G1674	U1575	C1475	U1398	A1226	G1151	G1151	C1086
A	A2080	A1889	C1795	U1796	U1674	U1576	U1476	A1399	A1310	U1150	U1150	C1087
C	A2081	G1990	C1797	U1796	U1674	U1576	U1476	A1399	A1310	U1150	U1150	C1087
C	C2082	C1988	U1798	U1798	G1681	G1583	G1480	G1400	G1315	C1154	C1154	C1088
C	A2083	U1994	G1799	U1798	C1682	G1584	G1481	G1401	G1316	G1155	G1155	C1089
C	G2088	A1991	U1994	U1799	A1683	G1585	G1488	G1402	U1317	A1156	A1156	A1091
C	A2089	A1992	U1994	U1799	A1683	G1585	G1488	G1402	U1317	A1156	A1156	A1091
C	U2090	A1993	U1994	U1799	A1683	G1585	G1488	G1402	U1317	A1156	A1156	A1091
C	C2091	U2012	G1999	U1809	C1690	A1591	G1493	C1407	G1237	G1160	G1160	C1097
C	A2092	G2013	G1999	U1809	C1690	A1591	G1493	C1407	G1237	G1160	G1160	C1097
U	C2093	U2014	C1902	U1810	C1694	C1593	G1496	G1409	G1328	C1161	C1161	C1098
C	U2095	C2017	C1903	C1811	C1694	C1593	G1496	A1410	C1241	G1167	G1167	A1029
C	U2096	C2017	C1903	C1811	C1694	C1593	G1496	A1410	C1241	G1167	G1167	A1029
G	U2100	C2018	C1906	C1812	A1700	A1499	A1499	G1413	U1243	G1170	G1170	A1035
G	U2101	G2019	C1907	C1813	A1701	U1500	U1500	G1414	U1243	A1171	A1171	A1036
U	A2103	C2021	A1910	C1820	A1702	C1601	G1501	A1332	C1244	G1103	G1103	C1037
C	G2108	G2023	G1912	G1822	C1703	C1603	G1416	U1337	C1245	G1104	G1104	G1038
G	G2115	C2026	C1915	C1823	C1704	A1604	A1506	A1248	U1249	A1174	A1174	G1039
G	C2116	A2027	C1916	C1824	C1704	A1604	A1506	A1248	U1249	U1175	U1175	C1039
C	U2117	G2030	G1920	U1827	A1715	G1605	G1507	U1337	U1249	G1176	G1176	C1040
A	U2118	G2030	G1920	U1827	A1715	G1605	G1507	U1337	U1249	G1176	G1176	C1040
G	U2119	A2034	A1921	U1828	C1716	A1619	C1513	C1338	A1177	A1177	A1177	A1041
G	U2120	A2035	A1921	U1828	C1716	A1619	C1513	C1338	A1177	A1177	A1177	A1041
C	G2121	C2036	G1924	G1829	U1717	G1619	A1517	A1423	U1256	U1178	U1178	C1042
C	C2122	A2037	G1925	G1830	G1718	A1620	C1509	A1424	A1257	G1179	G1179	G1043
C	U2123	C2027	C1916	C1825	G1713	G1614	G1511	G1425	A1257	G1180	G1180	U1044
C	U2118	G2030	G1920	U1827	A1715	G1615	C1512	G1426	C1262	G1181	G1181	C1043
G	U2119	A2034	A1921	U1828	C1716	A1619	C1513	A1429	C1262	G1182	G1182	G1047
G	U2120	A2035	A1921	U1828	C1716	A1619	C1513	A1429	C1262	G1182	G1182	G1047
C	G2121	C2036	G1924	G1829	U1717	G1619	A1517	A1429	C1262	G1182	G1182	G1047
C	C2124	U2038	G1926	G1831	G1719	A1625	G1528	G1430	C1266	G1183	G1183	G1048
C	G2125	G2039	G1927	C1832	G1720	A1626	G1529	G1434	U1185	U1185	U1185	C1049
C	G2126	G2040	G1927	C1833	G1720	A1626	G1529	G1434	G1274	U1186	U1186	C1050
C	G2127	G2041	G1927	C1834	G1720	A1626	G1529	G1434	G1275	A1187	A1187	C1051
C	G2128	G2042	G1927	C1835	G1720	A1626	G1529	G1434	G1277	A1188	A1188	C1052
C	G2129	G2043	G1927	C1836	G1720	A1626	G1529	G1434	G1277	A1189	A1189	C1053
C	G2130	G2044	G1927	C1837	G1720	A1626	G1529	G1434	G1277	A1190	A1190	C1054
C	G2131	G2045	G1927	C1838	G1720	A1626	G1529	G1434	G1277	A1191	A1191	C1055
C	G2132	G2046	G1927	C1839	G1720	A1626	G1529	G1434	G1277	A1192	A1192	C1056
C	G2133	G2047	G1927	C1840	G1720	A1626	G1529	G1434	G1277	A1193	A1193	C1057
C	G2134	G2048	G1927	C1841	G1720	A1626	G1529	G1434	G1277	A1194	A1194	C1058



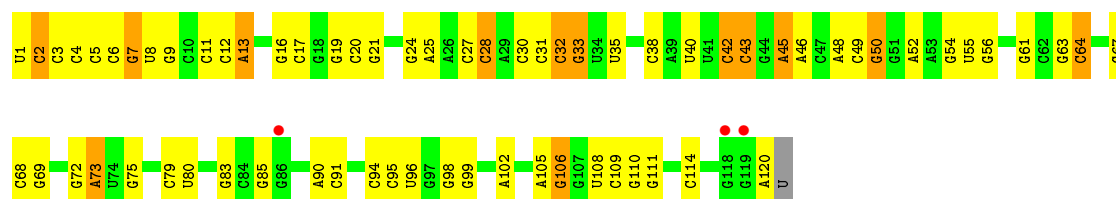
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 73% 26% ..



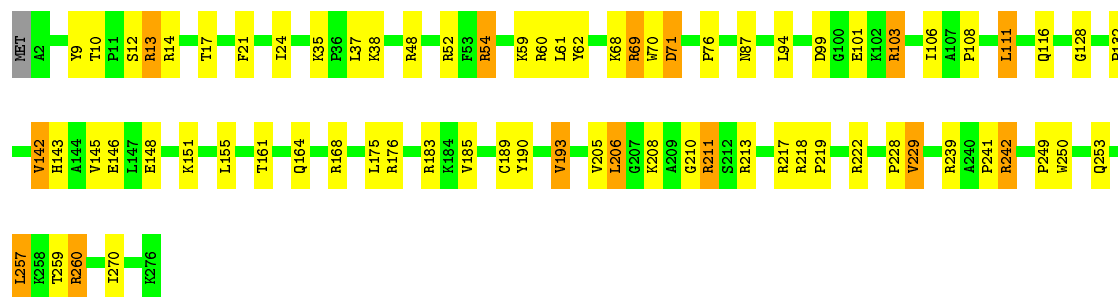
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 2% 43% 45% 11% .

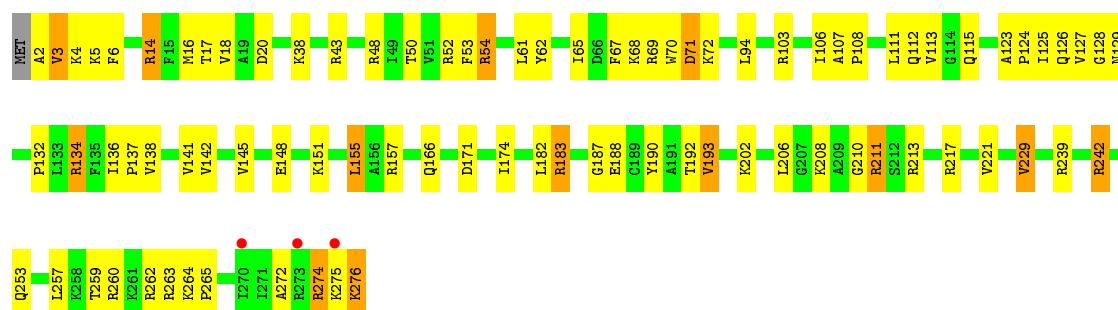


• Molecule 3: 50S ribosomal protein L2

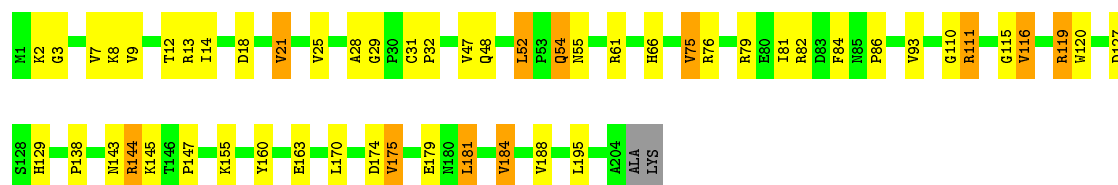
Chain 1D: 73% 21% 5%



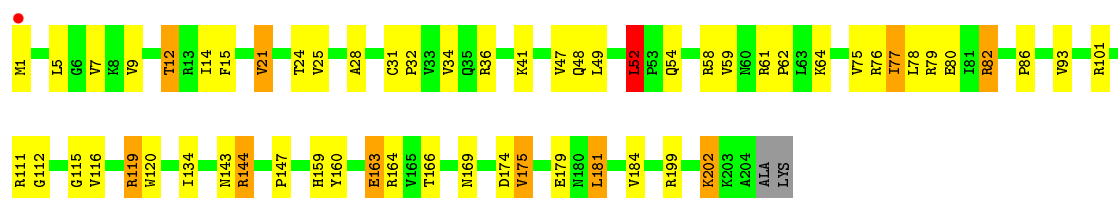
- Molecule 3: 50S ribosomal protein L2



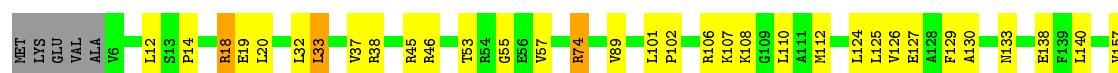
- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3



- Molecule 5: 50S ribosomal protein L4

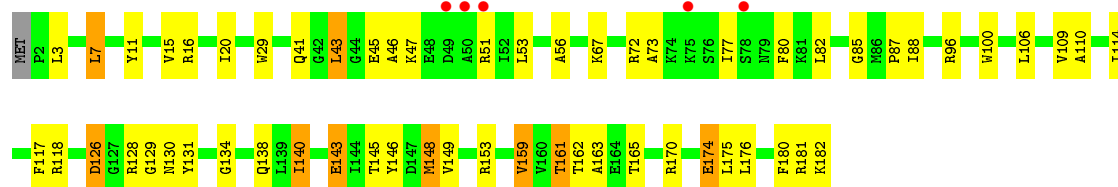




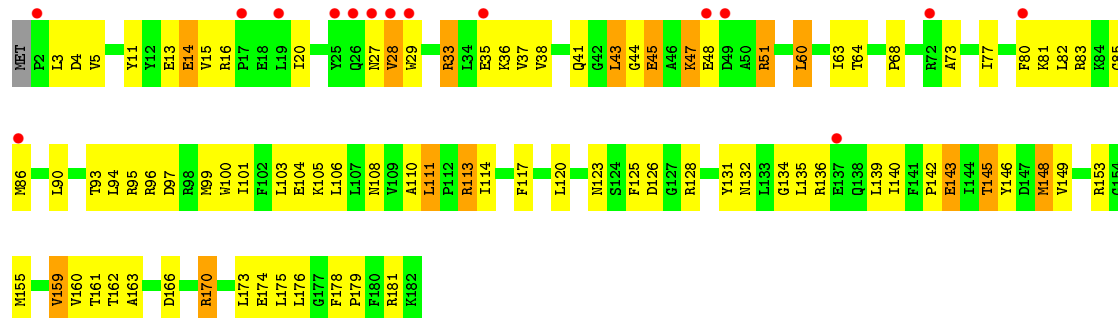
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5

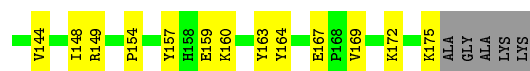


- Molecule 6: 50S ribosomal protein L5

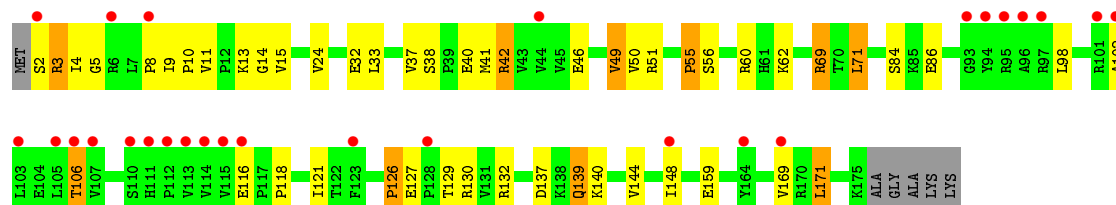


- Molecule 7: 50S ribosomal protein L6

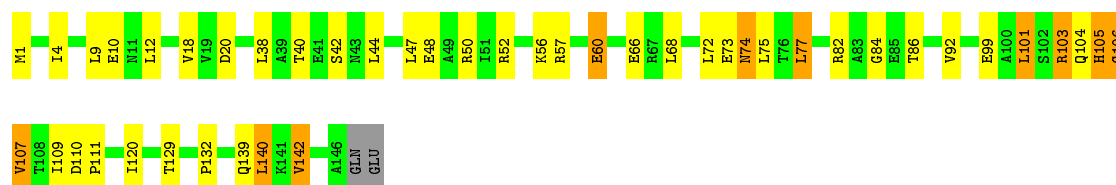




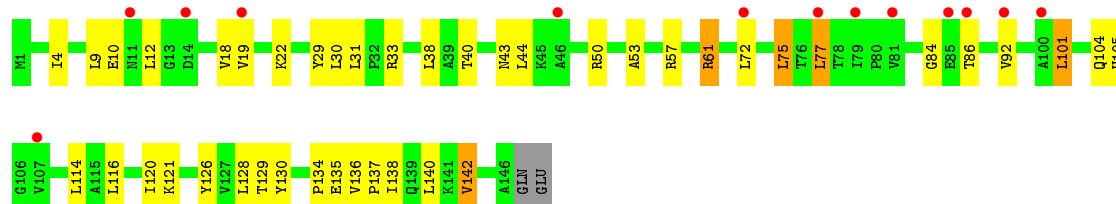
• Molecule 7: 50S ribosomal protein L6



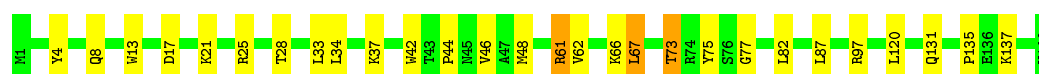
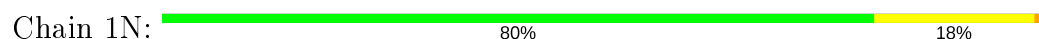
• Molecule 8: 50S ribosomal protein L9



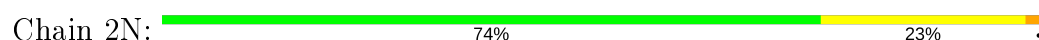
• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13





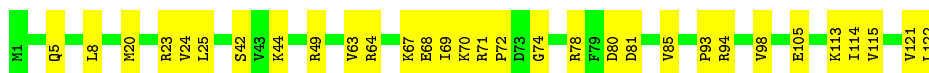
- Molecule 10: 50S ribosomal protein L14

Chain 1O: 75% 21% .



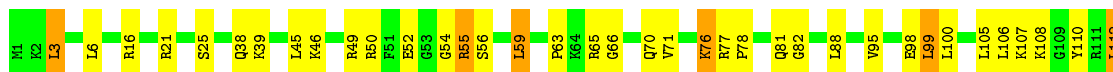
- Molecule 10: 50S ribosomal protein L14

Chain 2O: 75% 25% .



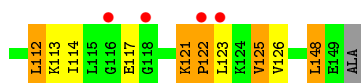
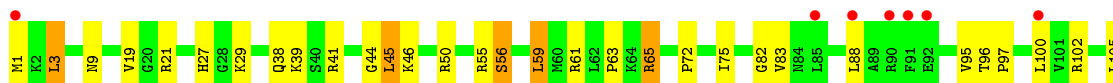
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 67% 27% 6% .



- Molecule 11: 50S ribosomal protein L15

Chain 2P: 7% 72% 21% 7% .

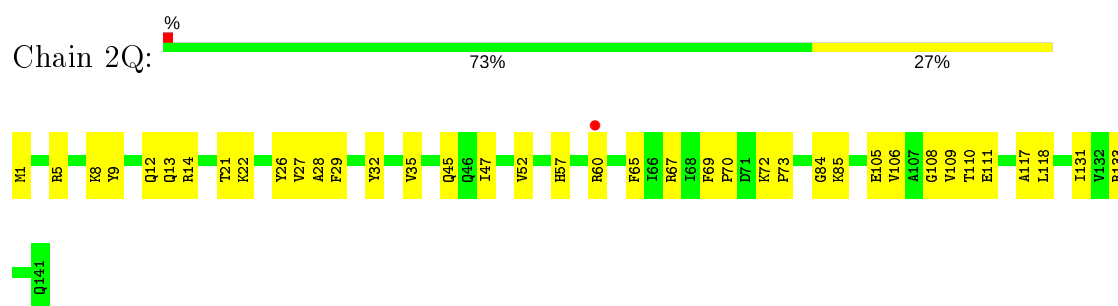


- Molecule 12: 50S ribosomal protein L16

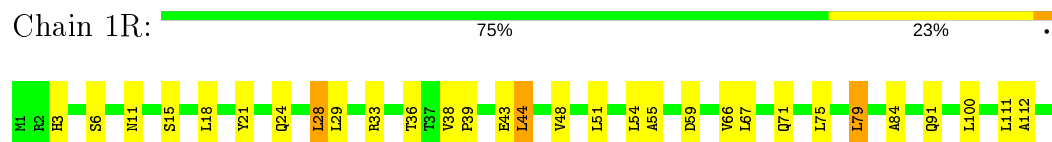
Chain 1Q: % 73% 25% .



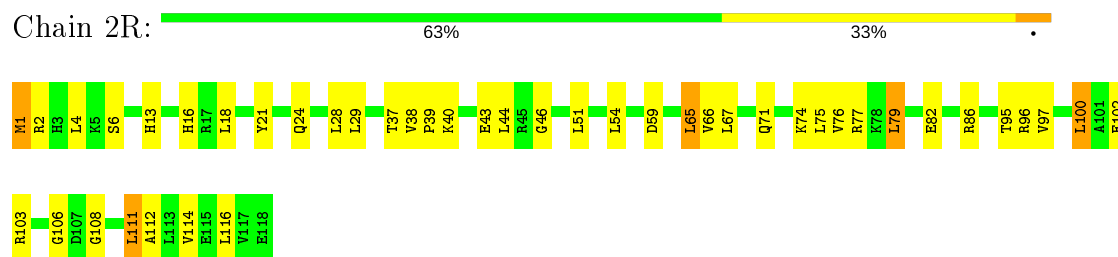
- Molecule 12: 50S ribosomal protein L16



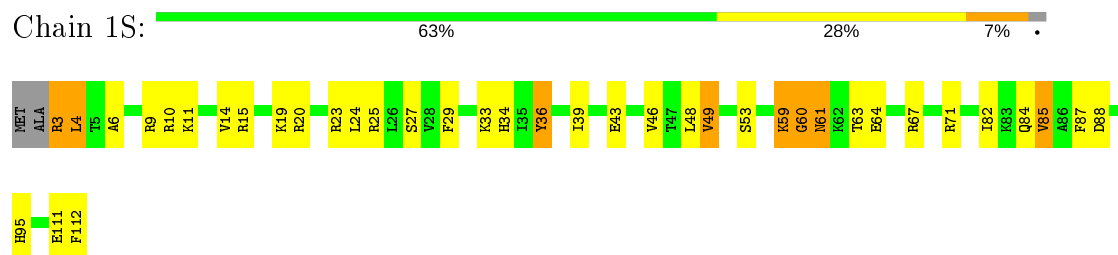
- Molecule 13: 50S ribosomal protein L17



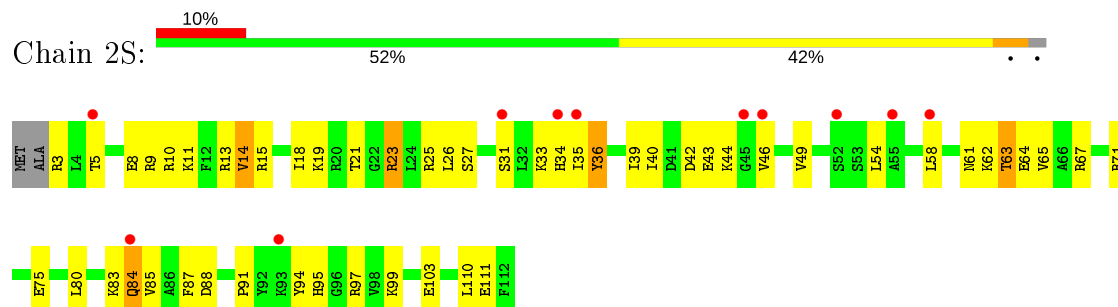
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

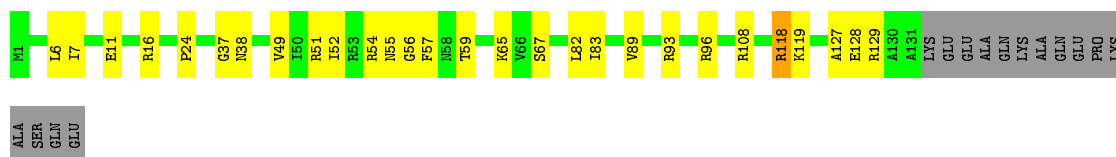


- Molecule 14: 50S ribosomal protein L18



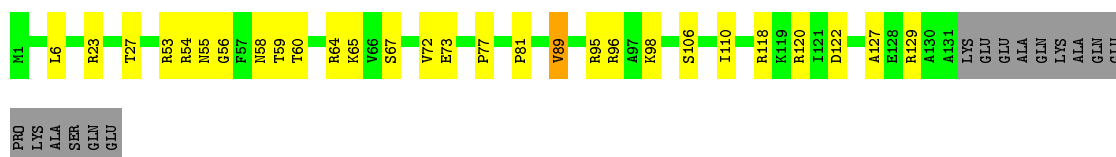
- Molecule 15: 50S ribosomal protein L19





- Molecule 15: 50S ribosomal protein L19

Chain 2T: 71% 18% 10%



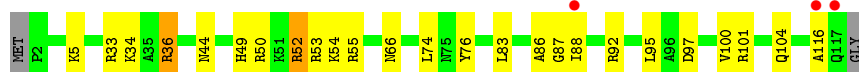
- Molecule 16: 50S ribosomal protein L20

Chain 1U: 78% 17% 5%



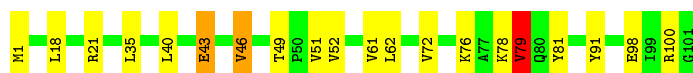
- Molecule 16: 50S ribosomal protein L20

Chain 2U: 3% 77% 19%



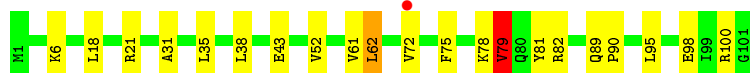
- Molecule 17: 50S ribosomal protein L21

Chain 1V: 80% 17% 3%



- Molecule 17: 50S ribosomal protein L21

Chain 2V: 79% 19% 2%



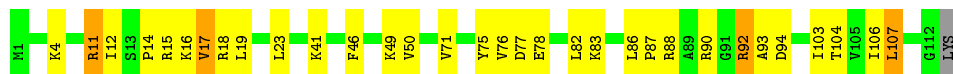
- Molecule 18: 50S ribosomal protein L22

Chain 1W: 78% 19% 3%




- Molecule 18: 50S ribosomal protein L22

Chain 2W:  71% 25% ..




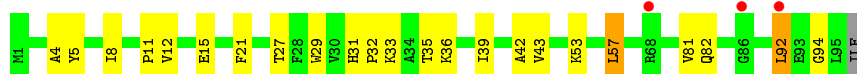
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  77% 21% ..



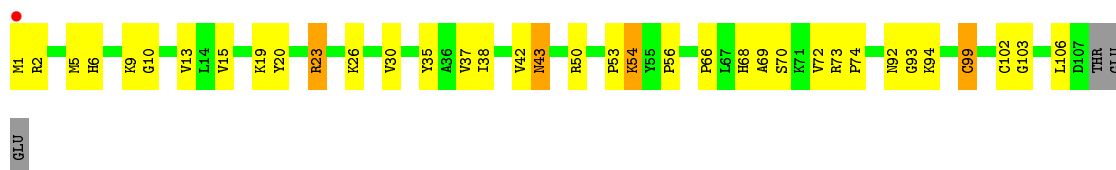
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  3% 75% 22% ..



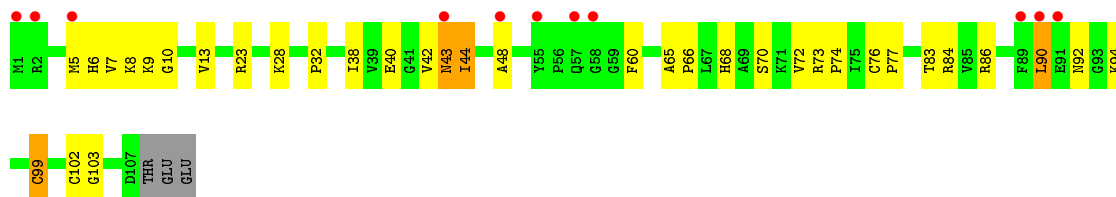
- Molecule 20: 50S ribosomal protein L24

Chain 1Y:  % 65% 29% ..



- Molecule 20: 50S ribosomal protein L24

Chain 2Y:  10% 65% 28% ..



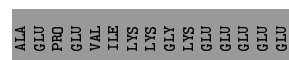
- Molecule 21: 50S ribosomal protein L25

Chain 1Z:  65% 23% 10%

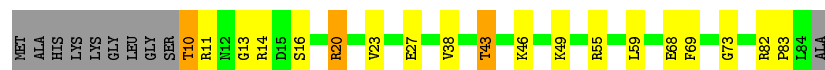




- Molecule 21: 50S ribosomal protein L25



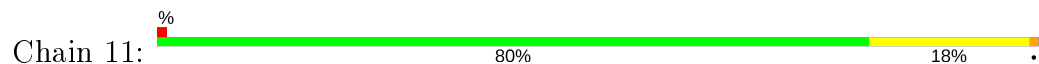
- Molecule 22: 50S ribosomal protein L27



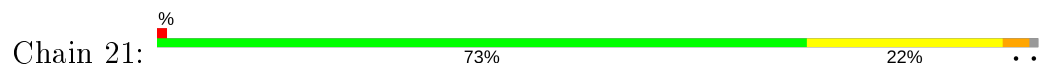
- Molecule 22: 50S ribosomal protein L27



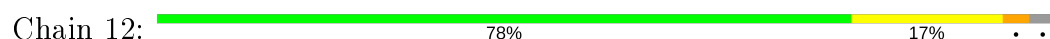
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

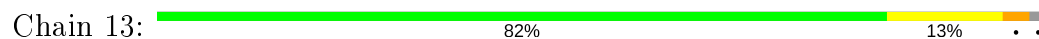




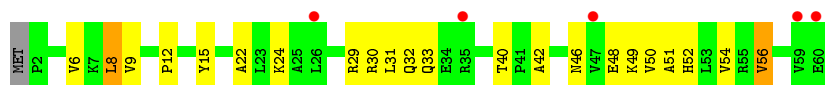
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



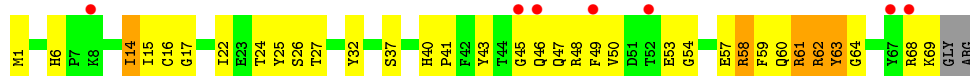
- Molecule 25: 50S ribosomal protein L30



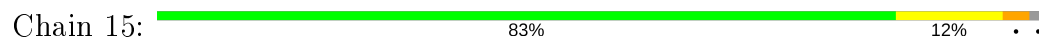
- Molecule 26: 50S ribosomal protein L31



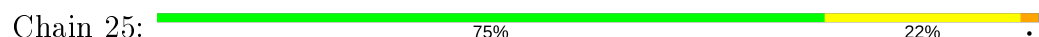
- Molecule 26: 50S ribosomal protein L31

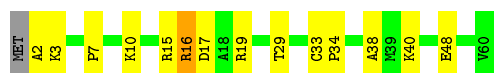


- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32





- Molecule 28: 50S ribosomal protein L33

Chain 16: 76% 17% 6%



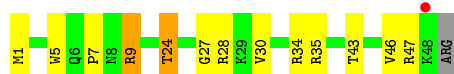
- Molecule 28: 50S ribosomal protein L33

Chain 26: 70% 22% 6%



- Molecule 29: 50S ribosomal protein L34

Chain 17: 2% 71% 22%



- Molecule 29: 50S ribosomal protein L34

Chain 27: 6% 63% 33%



- Molecule 30: 50S ribosomal protein L35

Chain 18: 69% 29%



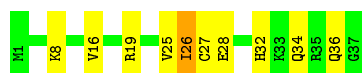
- Molecule 30: 50S ribosomal protein L35

Chain 28: 2% 62% 34%



- Molecule 31: 50S ribosomal protein L36

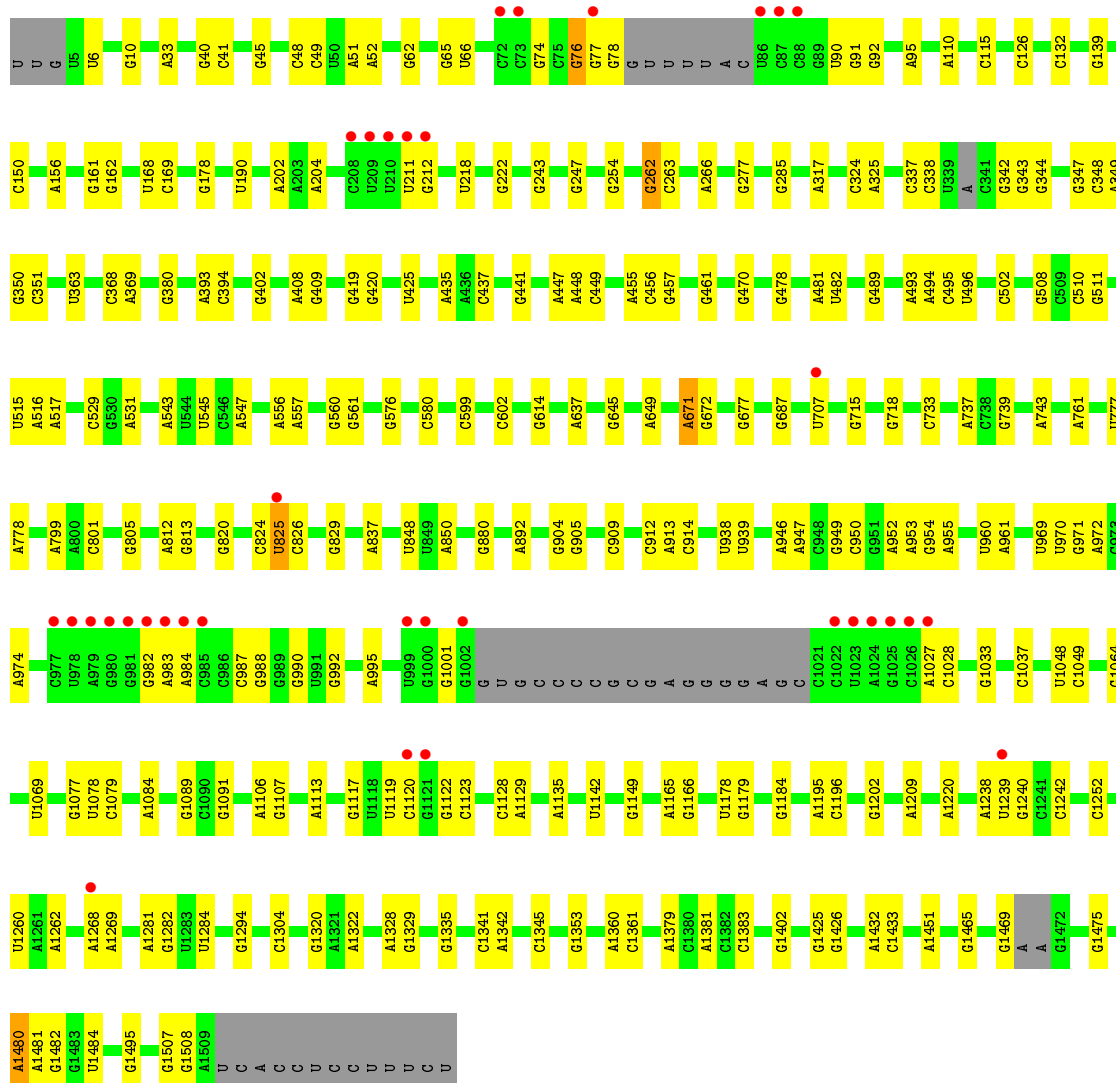
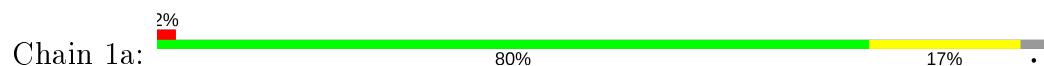
Chain 19: 73% 24%



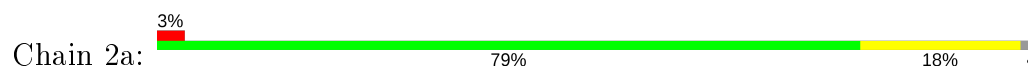
- Molecule 31: 50S ribosomal protein L36

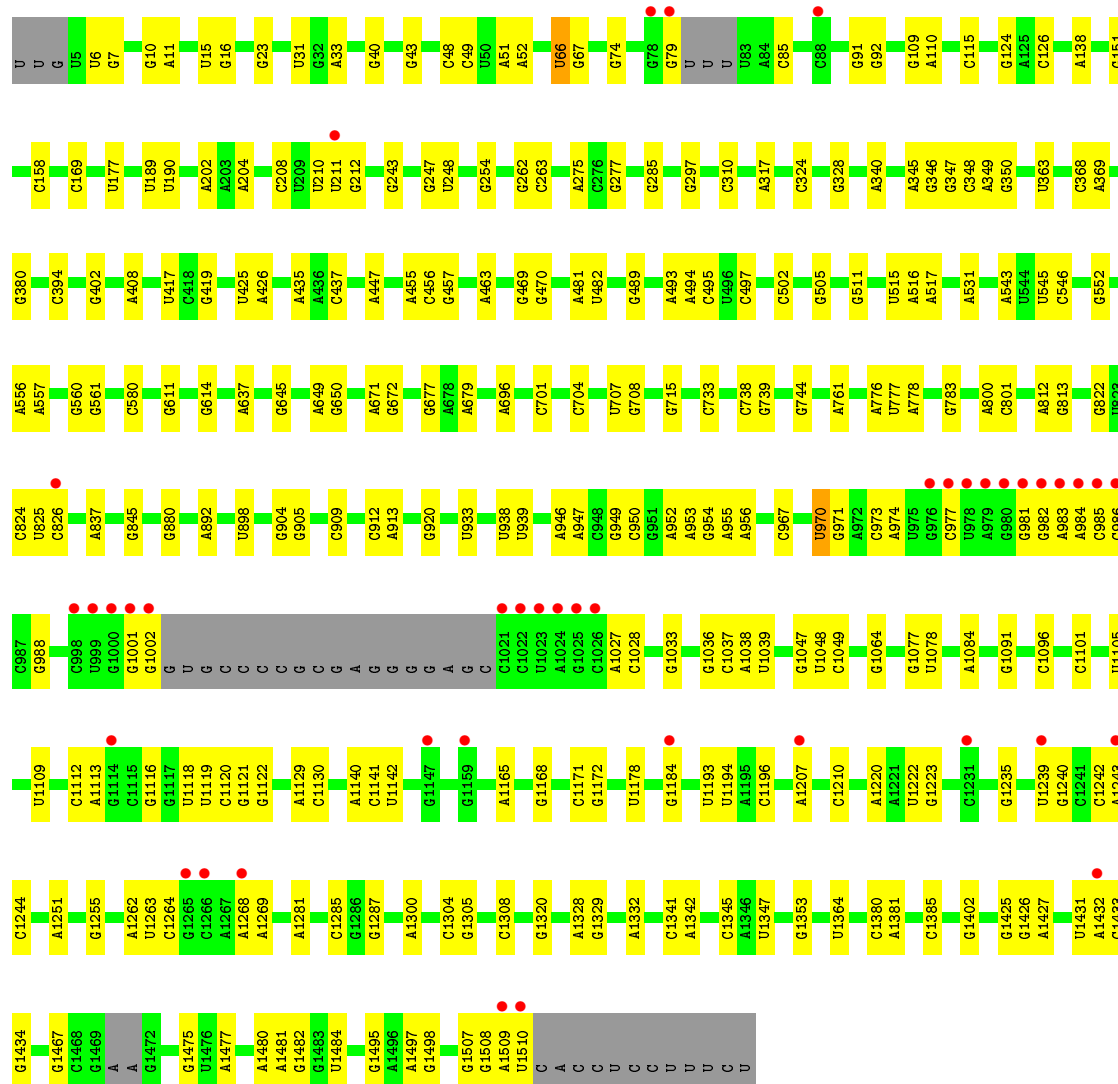


- Molecule 32: 16S Ribosomal RNA

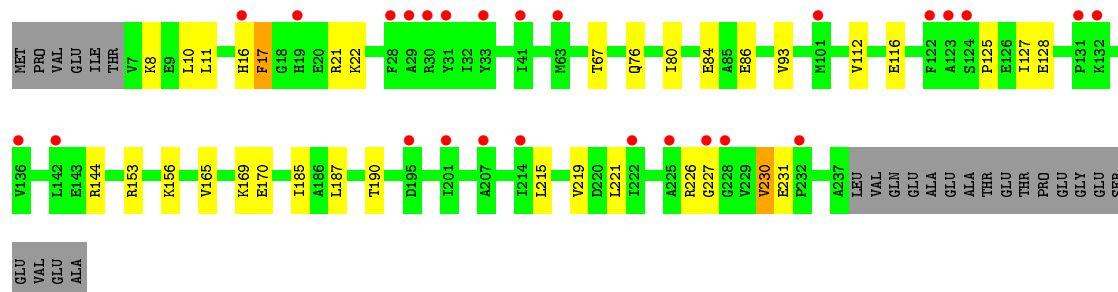
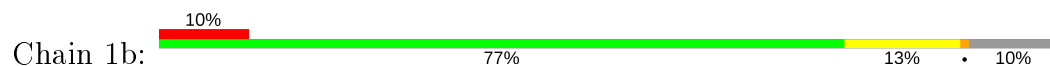


- Molecule 32: 16S Ribosomal RNA

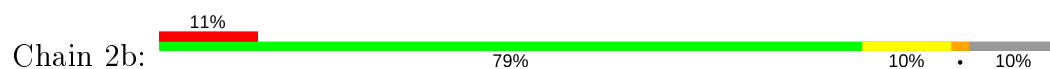


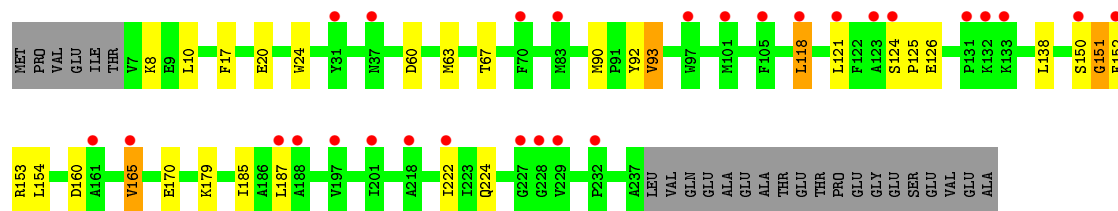


• Molecule 33: 30S ribosomal protein S2

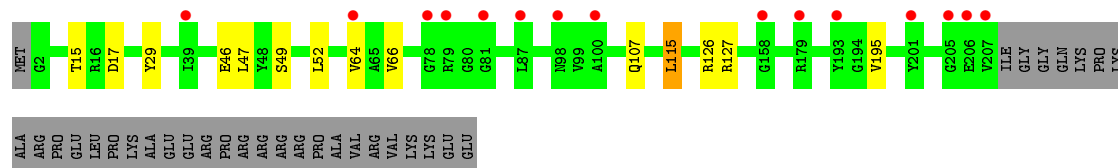
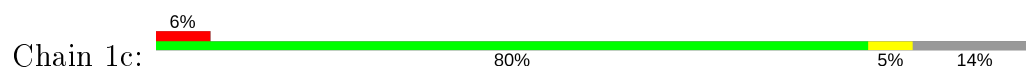


• Molecule 33: 30S ribosomal protein S2

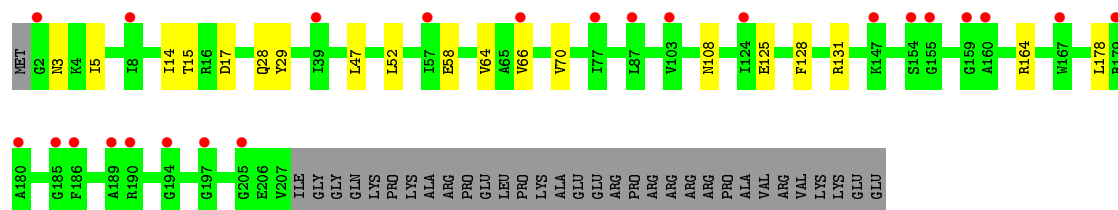
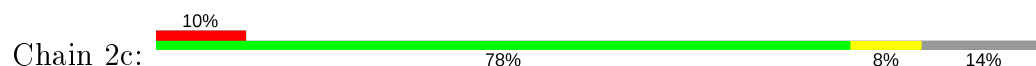




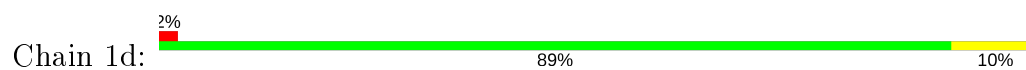
• Molecule 34: 30S ribosomal protein S3



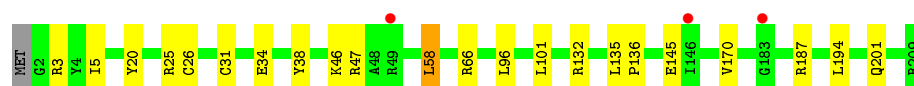
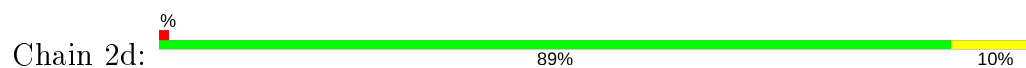
• Molecule 34: 30S ribosomal protein S3



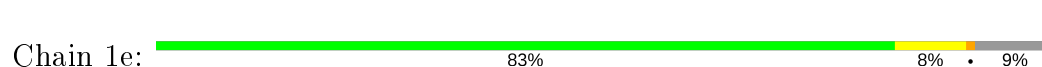
• Molecule 35: 30S ribosomal protein S4



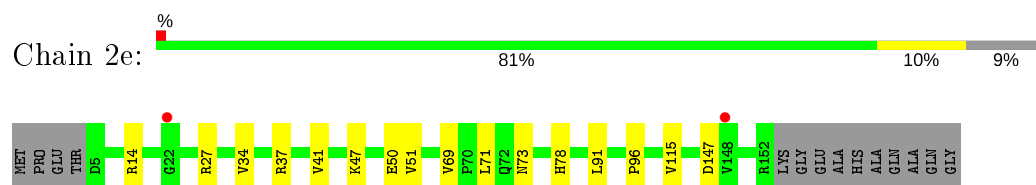
• Molecule 35: 30S ribosomal protein S4



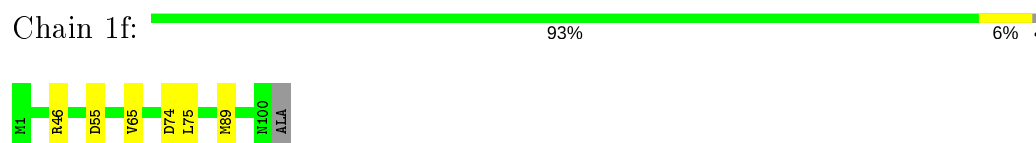
• Molecule 36: 30S ribosomal protein S5



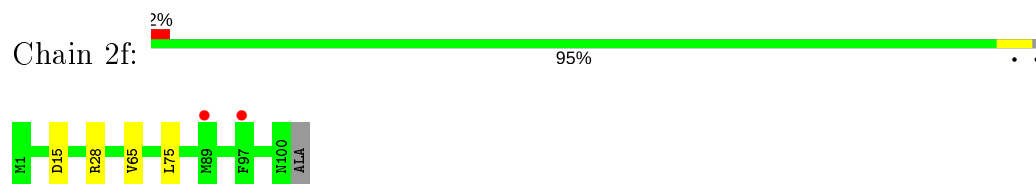
- Molecule 36: 30S ribosomal protein S5



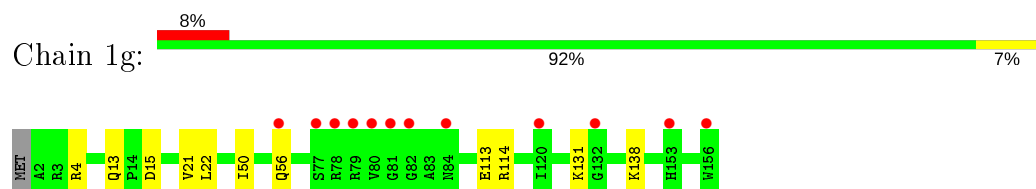
- Molecule 37: 30S ribosomal protein S6



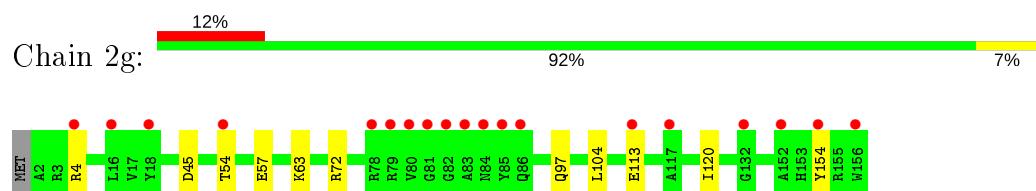
- Molecule 37: 30S ribosomal protein S6



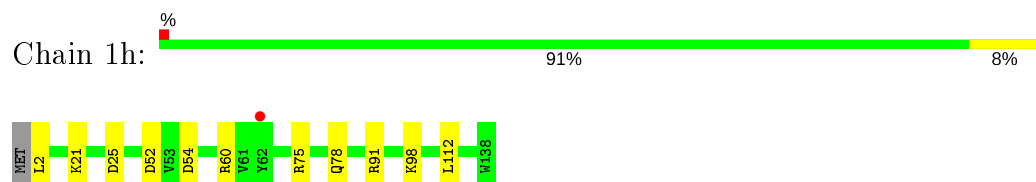
- Molecule 38: 30S ribosomal protein S7



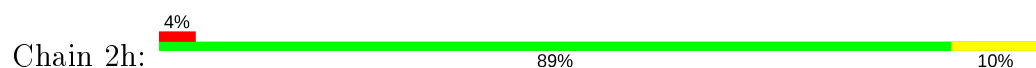
- Molecule 38: 30S ribosomal protein S7

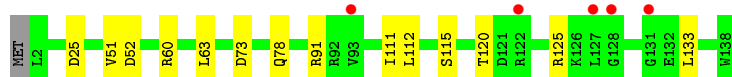


- Molecule 39: 30S ribosomal protein S8

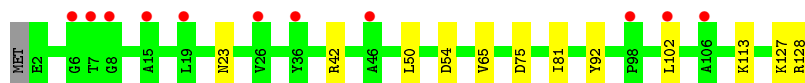
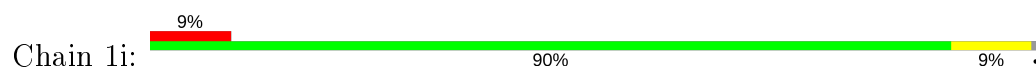


- Molecule 39: 30S ribosomal protein S8

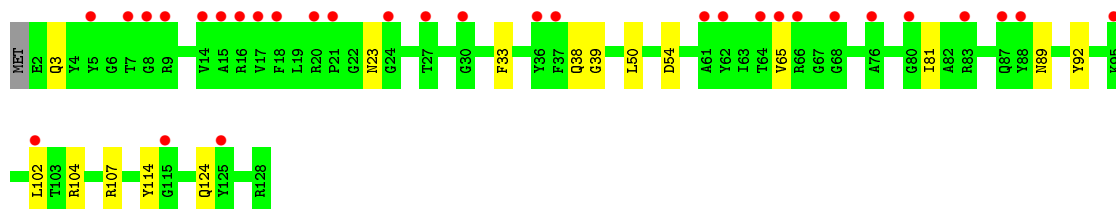
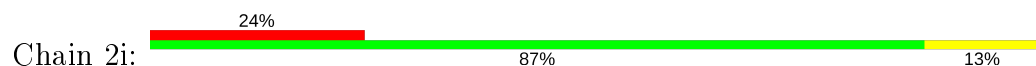




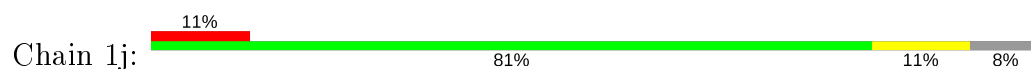
- Molecule 40: 30S ribosomal protein S9



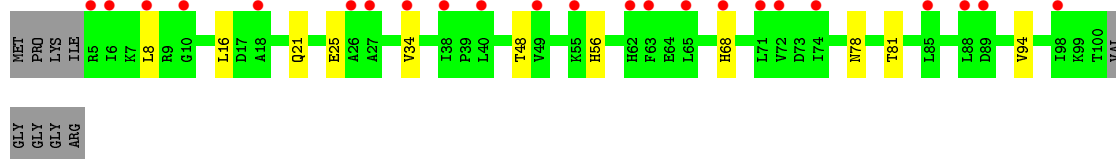
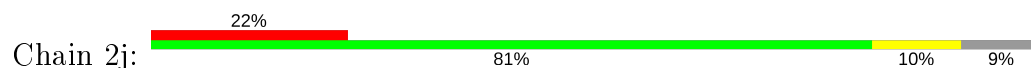
- Molecule 40: 30S ribosomal protein S9



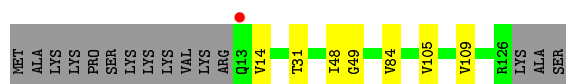
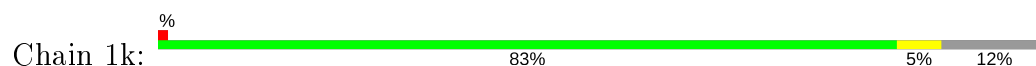
- Molecule 41: 30S ribosomal protein S10



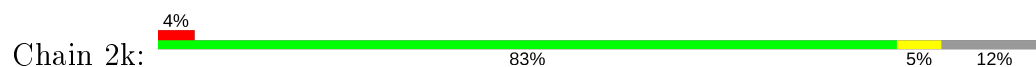
- Molecule 41: 30S ribosomal protein S10

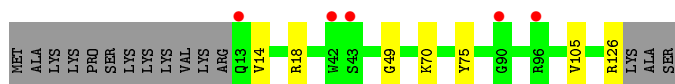


- Molecule 42: 30S ribosomal protein S11

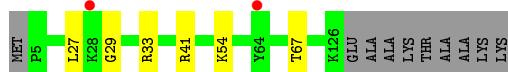
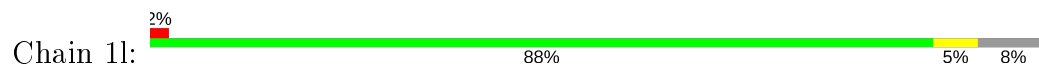


- Molecule 42: 30S ribosomal protein S11

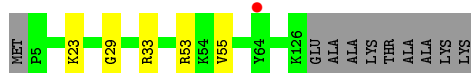
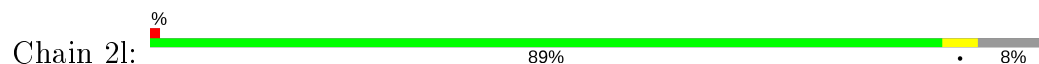




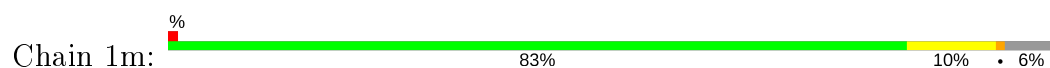
- Molecule 43: 30S ribosomal protein S12



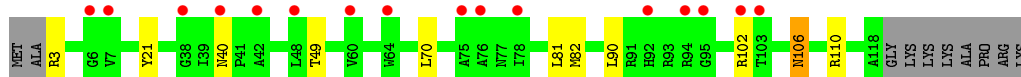
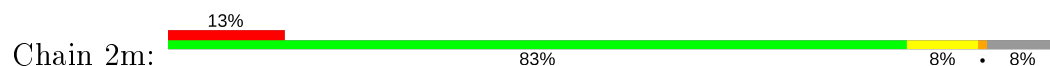
- Molecule 43: 30S ribosomal protein S12



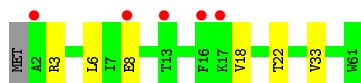
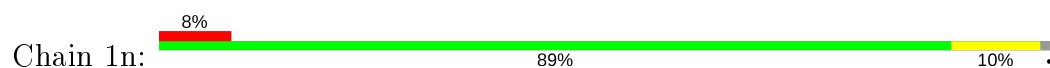
- Molecule 44: 30S ribosomal protein S13



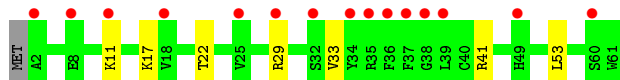
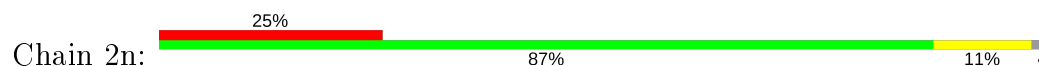
- Molecule 44: 30S ribosomal protein S13



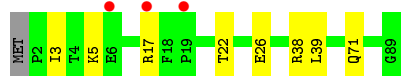
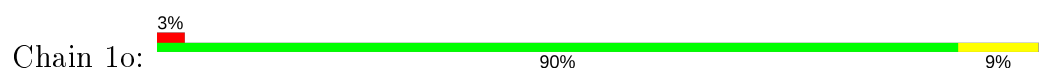
- Molecule 45: 30S ribosomal protein S14 type Z



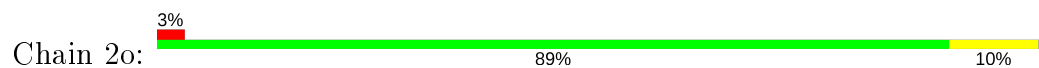
- Molecule 45: 30S ribosomal protein S14 type Z



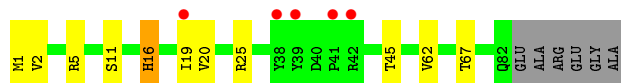
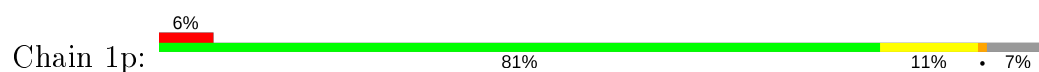
- Molecule 46: 30S ribosomal protein S15



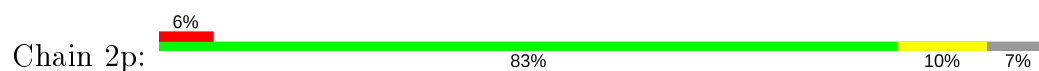
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



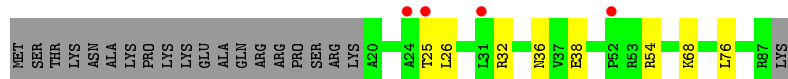
- Molecule 48: 30S ribosomal protein S17



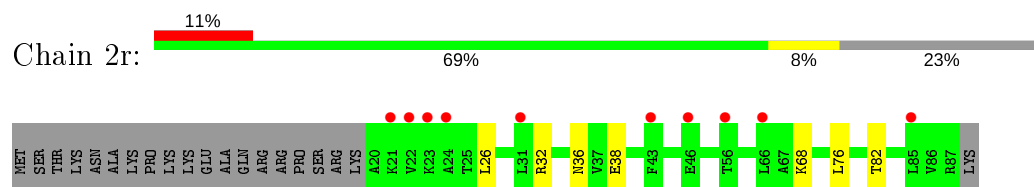
- Molecule 48: 30S ribosomal protein S17



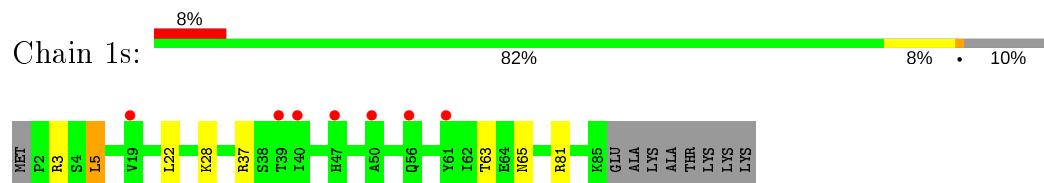
- Molecule 49: 30S ribosomal protein S18



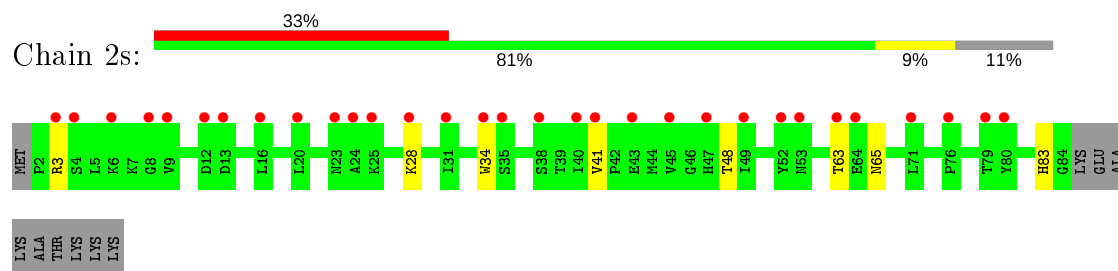
- Molecule 49: 30S ribosomal protein S18



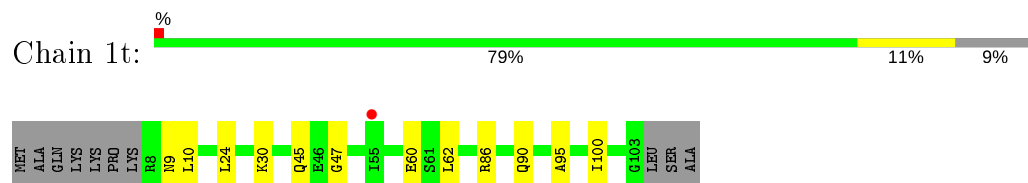
- Molecule 50: 30S ribosomal protein S19



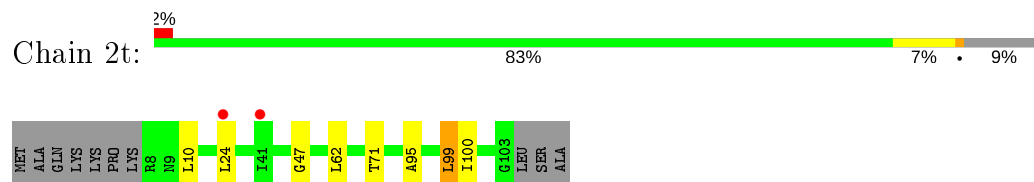
- Molecule 50: 30S ribosomal protein S19



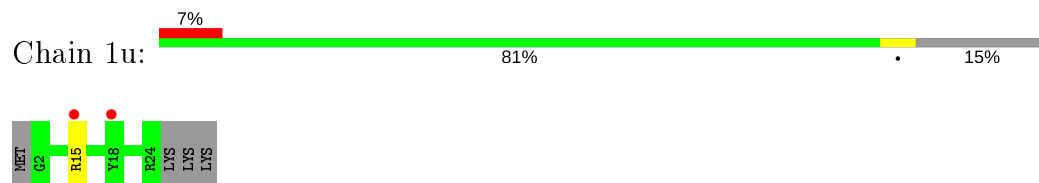
- Molecule 51: 30S ribosomal protein S20



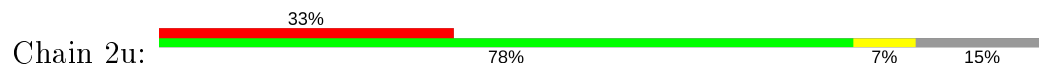
- Molecule 51: 30S ribosomal protein S20

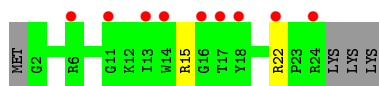


- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx

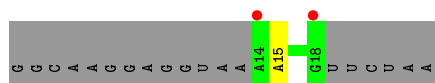




- Molecule 53: mRNA



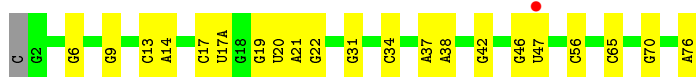
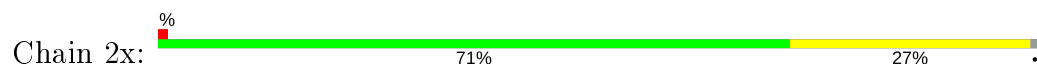
- Molecule 53: mRNA



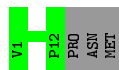
- Molecule 54: P-site tRNA



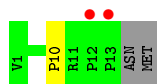
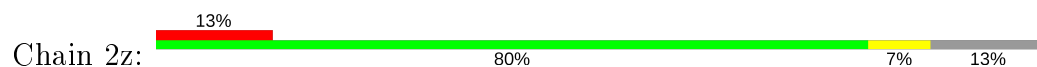
- Molecule 54: P-site tRNA



- Molecule 55: Metalnikowin-1



- Molecule 55: Metalnikowin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.87Å 450.49Å 623.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.89 49.85 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.85-2.89) 98.6 (49.85-2.89)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.268 0.212 , 0.268	Depositor DCC
R_{free} test set	64043 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	288976	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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, ZN, SF4, MG, 5MC, 4SU, 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	0.60	4/66249 (0.0%)	0.96	66/103407 (0.1%)
1	2A	0.47	1/67298 (0.0%)	0.95	48/105044 (0.0%)
2	1B	0.45	0/2877	0.86	0/4488
2	2B	0.52	0/2878	0.97	1/4490 (0.0%)
3	1D	0.41	0/2186	0.58	0/2944
3	2D	0.36	0/2192	0.58	0/2951
4	1E	0.44	0/1592	0.58	0/2149
4	2E	0.37	0/1592	0.58	0/2149
5	1F	0.41	0/1619	0.57	0/2193
5	2F	0.35	0/1615	0.57	0/2188
6	1G	0.32	0/1450	0.53	0/1959
6	2G	0.35	0/1449	0.57	0/1958
7	1H	0.35	0/1356	0.54	0/1834
7	2H	0.31	0/1356	0.51	0/1834
8	1I	0.31	0/1100	0.56	0/1501
8	2I	0.31	0/1076	0.56	0/1471
9	1N	0.41	0/1144	0.54	0/1543
9	2N	0.34	0/1144	0.55	0/1543
10	1O	0.42	0/943	0.57	0/1269
10	2O	0.37	0/943	0.59	1/1269 (0.1%)
11	1P	0.38	0/1156	0.60	1/1537 (0.1%)
11	2P	0.36	0/1152	0.58	0/1533
12	1Q	0.41	0/1143	0.53	0/1527
12	2Q	0.36	0/1143	0.59	0/1527
13	1R	0.42	0/982	0.65	0/1312
13	2R	0.32	0/982	0.57	0/1312
14	1S	0.35	0/887	0.60	0/1180
14	2S	0.32	0/880	0.54	0/1172
15	1T	0.39	0/1105	0.59	0/1477
15	2T	0.33	0/1097	0.53	0/1468
16	1U	0.44	0/977	0.56	0/1301
16	2U	0.33	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	1V	0.42	0/782	0.58	0/1049
17	2V	0.36	0/782	0.53	0/1049
18	1W	0.45	0/897	0.58	0/1205
18	2W	0.37	0/897	0.57	0/1205
19	1X	0.41	0/764	0.55	0/1025
19	2X	0.37	0/764	0.58	1/1025 (0.1%)
20	1Y	0.40	0/819	0.59	0/1095
20	2Y	0.33	0/819	0.54	0/1095
21	1Z	0.32	0/1502	0.51	0/2041
21	2Z	0.34	0/1486	0.54	0/2022
22	10	0.42	0/606	0.59	0/808
22	20	0.36	0/606	0.55	0/808
23	11	0.41	0/762	0.54	0/1014
23	21	0.35	0/762	0.53	0/1014
24	12	0.35	0/590	0.52	0/781
24	22	0.33	0/590	0.47	0/781
25	13	0.40	0/474	0.56	0/635
25	23	0.33	0/469	0.58	0/630
26	14	0.38	0/571	0.67	0/768
26	24	0.34	0/545	0.65	0/737
27	15	0.41	0/469	0.58	0/635
27	25	0.35	0/469	0.59	0/635
28	16	0.43	0/460	0.53	0/613
28	26	0.37	0/456	0.53	0/608
29	17	0.41	0/426	0.58	0/561
29	27	0.38	0/426	0.54	0/561
30	18	0.42	0/525	0.60	0/691
30	28	0.36	0/525	0.55	0/691
31	19	0.42	0/310	0.54	0/407
31	29	0.36	0/310	0.54	0/407
32	1a	0.40	0/35537	0.89	8/55456 (0.0%)
32	2a	0.38	0/35680	0.88	19/55681 (0.0%)
33	1b	0.31	0/1820	0.56	0/2468
33	2b	2.72	8/1728 (0.5%)	0.70	3/2352 (0.1%)
34	1c	0.28	0/1504	0.49	1/2047 (0.0%)
34	2c	0.33	0/1435	0.55	0/1960
35	1d	0.31	0/1648	0.54	0/2222
35	2d	0.30	0/1659	0.54	1/2230 (0.0%)
36	1e	0.31	0/1145	0.55	0/1543
36	2e	0.30	0/1111	0.58	0/1504
37	1f	0.31	0/819	0.51	0/1111
37	2f	0.31	0/830	0.52	0/1125
38	1g	0.30	0/1198	0.48	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	2g	0.31	0/1185	0.49	0/1602
39	1h	0.30	0/1108	0.52	0/1494
39	2h	0.29	0/1094	0.51	0/1478
40	1i	0.31	0/995	0.55	0/1339
40	2i	0.33	0/949	0.58	0/1284
41	1j	0.31	0/695	0.56	0/950
41	2j	0.30	0/690	0.55	0/943
42	1k	0.31	0/840	0.52	0/1138
42	2k	0.29	0/844	0.50	0/1145
43	1l	0.32	0/936	0.53	0/1263
43	2l	0.33	0/934	0.59	1/1262 (0.1%)
44	1m	0.29	0/933	0.56	0/1254
44	2m	0.31	0/913	0.52	0/1230
45	1n	0.33	0/491	0.57	0/653
45	2n	0.33	0/467	0.49	0/624
46	1o	0.31	0/726	0.56	0/970
46	2o	0.31	0/739	0.50	0/985
47	1p	0.29	0/686	0.52	0/926
47	2p	0.31	0/693	0.53	0/935
48	1q	0.32	0/824	0.55	1/1105 (0.1%)
48	2q	0.30	0/836	0.48	0/1117
49	1r	0.30	0/560	0.50	0/746
49	2r	0.30	0/560	0.52	0/746
50	1s	0.29	0/657	0.56	1/890 (0.1%)
50	2s	0.32	0/661	0.60	0/893
51	1t	0.28	0/714	0.61	0/948
51	2t	0.29	0/733	0.52	0/969
52	1u	0.24	0/191	0.46	0/252
52	2u	0.30	0/203	0.52	0/266
53	1v	0.64	0/122	1.10	0/188
53	2v	0.53	0/122	0.94	0/188
54	1x	0.57	2/1725 (0.1%)	1.14	18/2689 (0.7%)
54	2x	0.54	1/1725 (0.1%)	1.14	14/2689 (0.5%)
55	1z	0.38	0/109	0.70	0/148
55	2z	0.35	0/117	0.64	0/160
All	All	0.50	16/306294 (0.0%)	0.85	185/458208 (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
5	2F	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	2b	92	TYR	CD1-CE1	59.23	2.28	1.39
33	2b	92	TYR	CD2-CE2	53.18	2.19	1.39
33	2b	92	TYR	CE1-CZ	41.65	1.92	1.38
33	2b	92	TYR	CE2-CZ	41.39	1.92	1.38
33	2b	92	TYR	CG-CD1	33.82	1.83	1.39
33	2b	92	TYR	CG-CD2	32.39	1.81	1.39
33	2b	151	GLY	N-CA	22.82	1.80	1.46
33	2b	150	SER	C-N	10.50	1.51	1.33
1	1A	552	A	N9-C4	-7.88	1.33	1.37
1	1A	1187	A	N9-C4	-7.20	1.33	1.37
1	2A	552	A	N9-C4	-6.75	1.33	1.37
1	1A	1066	A	N9-C4	-6.05	1.34	1.37
54	1x	22	G	N7-C5	5.76	1.42	1.39
54	1x	14	A	C8-N7	-5.24	1.27	1.31
1	1A	2298	A	N9-C4	-5.13	1.34	1.37
54	2x	22	G	N7-C5	5.01	1.42	1.39

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	2b	150	SER	C-N-CA	16.39	156.71	122.30
1	1A	552	A	C2-N3-C4	-11.05	105.07	110.60
54	1x	46	G	C6-N1-C2	-10.06	119.06	125.10
1	1A	1066	A	C2-N3-C4	-9.89	105.66	110.60
54	2x	46	G	C6-N1-C2	-9.72	119.27	125.10
1	2A	552	A	C2-N3-C4	-8.87	106.16	110.60
1	1A	552	A	N3-C4-C5	8.78	132.94	126.80
33	2b	151	GLY	N-CA-C	8.74	134.95	113.10
1	1A	552	A	N3-C4-N9	-8.51	120.59	127.40
54	1x	14	A	C5-N7-C8	8.50	108.15	103.90
54	2x	14	A	C4-C5-C6	8.45	121.23	117.00
1	1A	1187	A	C2-N3-C4	-8.39	106.41	110.60
1	1A	989	A	C5-N7-C8	-8.31	99.75	103.90
54	2x	14	A	C5-N7-C8	8.19	107.99	103.90
1	1A	847	G	O5'-P-OP2	-7.93	98.57	105.70
32	2a	1141	C	C2-N1-C1'	7.89	127.48	118.80
1	1A	2083	A	O4'-C1'-N9	7.54	114.23	108.20
54	1x	22	G	C5-N7-C8	-7.48	100.56	104.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2083	A	C2-N3-C4	-7.47	106.87	110.60
1	1A	1067	G	N3-C4-N9	-7.41	121.56	126.00
1	1A	214	G	O4'-C1'-N9	7.40	114.12	108.20
1	2A	552	A	N3-C4-C5	7.39	131.97	126.80
54	2x	22	G	C5-N7-C8	-7.35	100.62	104.30
1	1A	1187	A	N3-C4-C5	7.33	131.93	126.80
32	1a	825	U	C5-C6-N1	7.32	126.36	122.70
1	1A	138	A	N7-C8-N9	7.28	117.44	113.80
54	1x	22	G	N3-C4-N9	-7.15	121.71	126.00
54	1x	14	A	C4-C5-C6	7.13	120.56	117.00
1	1A	989	A	N7-C8-N9	7.07	117.34	113.80
19	2X	57	LEU	CA-CB-CG	6.99	131.37	115.30
54	2x	46	G	C5-C6-N1	6.97	114.98	111.50
1	1A	536	G	O4'-C1'-N9	6.93	113.75	108.20
32	2a	738	C	C2-N1-C1'	6.91	126.40	118.80
43	2l	29	GLY	N-CA-C	-6.87	95.92	113.10
54	1x	46	G	C5-C6-N1	6.84	114.92	111.50
54	1x	22	G	N1-C6-O6	-6.77	115.84	119.90
54	2x	22	G	C4-C5-C6	-6.67	114.80	118.80
1	1A	1066	A	N1-C2-N3	6.64	132.62	129.30
54	1x	22	G	C4-C5-C6	-6.63	114.82	118.80
1	1A	138	A	C5-N7-C8	-6.59	100.60	103.90
1	1A	1685	U	O5'-P-OP2	-6.57	99.79	105.70
1	1A	977	A	C5-N7-C8	-6.55	100.62	103.90
1	2A	2583	A	C8-N9-C4	6.52	108.41	105.80
1	1A	1044	U	O5'-P-OP2	-6.47	99.88	105.70
32	2a	738	C	N1-C2-O2	6.40	122.74	118.90
32	2a	1141	C	N1-C2-O2	6.40	122.74	118.90
1	2A	138	A	N7-C8-N9	6.40	117.00	113.80
54	1x	14	A	C5-C6-N1	-6.37	114.52	117.70
1	1A	353	A	C2-N3-C4	-6.36	107.42	110.60
1	1A	2212	G	C5-C6-O6	-6.32	124.81	128.60
1	1A	1694	C	O5'-P-OP1	-6.31	100.02	105.70
1	1A	989	A	C8-N9-C4	-6.31	103.28	105.80
1	1A	1153	U	C2-N1-C1'	6.28	125.23	117.70
54	1x	22	G	C8-N9-C1'	6.26	135.13	127.00
1	2A	830	A	O4'-C1'-N9	6.24	113.19	108.20
1	1A	1294	U	O5'-P-OP1	-6.16	100.16	105.70
1	1A	409	U	C2-N1-C1'	-6.13	110.34	117.70
32	2a	1207	A	C5-C6-N6	6.13	128.60	123.70
1	2A	409	U	O4'-C1'-N1	6.12	113.10	108.20
1	1A	2013	G	P-O3'-C3'	6.11	127.03	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1067	G	N3-C2-N2	-6.10	115.63	119.90
1	2A	138	A	C8-N9-C4	-6.10	103.36	105.80
32	1a	150	C	N1-C2-O2	6.10	122.56	118.90
1	2A	552	A	N3-C4-N9	-6.08	122.54	127.40
1	1A	11	U	C2-N1-C1'	6.07	124.98	117.70
1	1A	1806	G	O5'-P-OP2	-6.05	100.25	105.70
1	2A	2484	U	C2-N1-C1'	6.04	124.94	117.70
32	2a	1207	A	N1-C6-N6	-6.03	114.98	118.60
1	1A	1066	A	C5-N7-C8	-5.95	100.93	103.90
1	1A	2057	C	O5'-P-OP1	-5.89	100.40	105.70
10	2O	8	LEU	CA-CB-CG	5.89	128.84	115.30
1	1A	138	A	C8-N9-C4	-5.89	103.44	105.80
1	1A	551	C	N3-C2-O2	-5.88	117.79	121.90
1	1A	2035	A	C8-N9-C4	5.87	108.15	105.80
32	2a	66	U	P-O3'-C3'	5.87	126.75	119.70
54	2x	46	G	N3-C2-N2	-5.87	115.79	119.90
54	2x	22	G	C8-N9-C1'	5.86	134.62	127.00
54	2x	46	G	C5-C6-O6	-5.85	125.09	128.60
1	2A	300	C	C2-N1-C1'	5.79	125.17	118.80
1	2A	536	G	O4'-C1'-N9	5.78	112.82	108.20
54	1x	14	A	C8-N9-C1'	-5.78	117.30	127.70
1	1A	1187	A	N3-C4-N9	-5.74	122.81	127.40
32	2a	982	G	C8-N9-C4	-5.73	104.11	106.40
32	2a	1141	C	C6-N1-C2	-5.68	118.03	120.30
1	2A	989	A	N1-C6-N6	5.66	122.00	118.60
54	1x	22	G	N7-C8-N9	5.66	115.93	113.10
1	1A	1297	G	O4'-C1'-N9	-5.66	103.68	108.20
1	2A	1248	A	O4'-C1'-N9	5.63	112.70	108.20
1	1A	1744	A	C2-N3-C4	-5.63	107.79	110.60
1	2A	2271	C	C6-N1-C2	-5.62	118.05	120.30
1	1A	1248	A	O4'-C1'-N9	5.62	112.69	108.20
1	2A	1109	C	C2-N1-C1'	5.62	124.98	118.80
54	2x	22	G	N3-C4-N9	-5.61	122.63	126.00
1	2A	989	A	O4'-C1'-N9	5.60	112.68	108.20
35	2d	58	LEU	CA-CB-CG	5.59	128.16	115.30
1	1A	2857	G	O4'-C1'-N9	5.59	112.67	108.20
1	2A	873	U	N3-C2-O2	5.57	126.10	122.20
1	2A	300	C	N1-C2-O2	5.55	122.23	118.90
1	2A	2484	U	N1-C2-O2	5.55	126.69	122.80
1	1A	138	A	O4'-C1'-N9	5.53	112.62	108.20
54	1x	22	G	C6-C5-N7	5.52	133.71	130.40
1	2A	1358	U	C2-N1-C1'	5.52	124.33	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2013	G	P-O3'-C3'	5.51	126.32	119.70
1	2A	1359	C	C2-N1-C1'	5.50	124.85	118.80
1	2A	1820	C	P-O3'-C3'	5.50	126.30	119.70
1	1A	2222	C	N3-C2-O2	-5.50	118.05	121.90
1	2A	1659	A	O5'-P-OP1	-5.49	100.76	105.70
1	2A	829	A	C2-N3-C4	5.48	113.34	110.60
1	1A	1218	A	OP1-P-O3'	5.48	117.25	105.20
54	1x	22	G	N9-C4-C5	5.46	107.58	105.40
54	2x	14	A	C8-N9-C1'	-5.46	117.88	127.70
32	2a	982	G	N3-C4-C5	-5.41	125.89	128.60
1	2A	88	U	C2-N1-C1'	5.40	124.18	117.70
1	1A	30	C	O5'-P-OP1	-5.40	100.84	105.70
32	2a	671	A	P-O3'-C3'	5.38	126.16	119.70
1	2A	2759	G	N1-C6-O6	5.38	123.13	119.90
1	1A	989	A	C2-N3-C4	-5.38	107.91	110.60
1	2A	2268	U	N3-C2-O2	5.36	125.95	122.20
1	2A	1114	A	P-O3'-C3'	5.36	126.13	119.70
1	1A	1358	U	C2-N1-C1'	5.36	124.13	117.70
1	2A	1248	A	N1-C6-N6	5.35	121.81	118.60
1	1A	1693	G	O4'-C1'-N9	-5.35	103.92	108.20
1	2A	1676	C	N3-C2-O2	5.34	125.64	121.90
54	2x	14	A	C4-N9-C1'	5.33	135.90	126.30
11	1P	99	LEU	CA-CB-CG	5.31	127.50	115.30
1	1A	977	A	O4'-C1'-N9	5.30	112.44	108.20
1	2A	1604	A	P-O3'-C3'	5.29	126.05	119.70
1	2A	2700	U	P-O3'-C3'	5.28	126.04	119.70
54	1x	14	A	C4-N9-C1'	5.28	135.81	126.30
1	1A	977	A	C4-C5-N7	5.27	113.33	110.70
54	1x	46	G	C5-C6-O6	-5.27	125.44	128.60
1	2A	2583	A	N7-C8-N9	-5.27	111.17	113.80
32	2a	1141	C	C6-N1-C1'	-5.26	114.49	120.80
32	1a	825	U	C6-N1-C2	-5.26	117.85	121.00
1	1A	1218	A	P-O3'-C3'	5.25	126.00	119.70
1	1A	1066	A	N7-C8-N9	5.24	116.42	113.80
32	2a	738	C	N3-C2-O2	-5.24	118.23	121.90
1	1A	2512	C	C6-N1-C2	5.24	122.40	120.30
54	1x	46	G	N3-C2-N2	-5.23	116.24	119.90
32	2a	1141	C	N3-C2-O2	-5.22	118.24	121.90
1	1A	552	A	C4-N9-C1'	-5.22	116.90	126.30
1	2A	2331	A	C2-N3-C4	5.22	113.21	110.60
1	2A	719	C	N1-C2-O2	-5.21	115.77	118.90
1	2A	202	G	O4'-C1'-N9	5.21	112.37	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1676	C	N1-C2-O2	-5.21	115.78	118.90
2	2B	42	C	P-O3'-C3'	5.20	125.94	119.70
32	2a	933	U	C2-N3-C4	5.20	130.12	127.00
1	2A	792	A	O4'-C1'-N9	5.19	112.36	108.20
1	2A	1404	A	C2-N3-C4	5.18	113.19	110.60
1	2A	2530	U	N3-C2-O2	5.18	125.82	122.20
54	2x	14	A	C5-C6-N1	-5.17	115.11	117.70
1	1A	1439	U	O5'-P-OP1	-5.17	101.05	105.70
1	2A	2458	G	C4-N9-C1'	-5.16	119.79	126.50
1	1A	830	A	P-O3'-C3'	5.14	125.87	119.70
1	1A	2640	A	O4'-C1'-N9	5.14	112.31	108.20
48	1q	98	LEU	CA-CB-CG	5.13	127.11	115.30
54	2x	22	G	C4-N9-C1'	-5.13	119.83	126.50
32	1a	969	U	P-O3'-C3'	5.13	125.86	119.70
32	2a	982	G	C4-N9-C1'	5.12	133.16	126.50
1	2A	669	C	C2-N1-C1'	5.12	124.43	118.80
1	1A	794	G	O4'-C1'-N9	5.11	112.29	108.20
1	1A	202	G	O4'-C1'-N9	5.10	112.28	108.20
1	2A	2814	C	C6-N1-C2	-5.10	118.26	120.30
1	2A	636	U	N3-C2-O2	-5.09	118.64	122.20
32	1a	76	G	N3-C4-N9	5.08	129.05	126.00
1	1A	1153	U	C5-C6-N1	5.08	125.24	122.70
1	1A	2449	U	OP2-P-O3'	5.08	116.38	105.20
1	2A	111	U	C2-N1-C1'	5.07	123.79	117.70
1	2A	830	A	P-O3'-C3'	5.06	125.78	119.70
32	1a	671	A	P-O3'-C3'	5.06	125.77	119.70
50	1s	5	LEU	CA-CB-CG	5.05	126.93	115.30
1	1A	552	A	C8-N9-C1'	5.05	136.80	127.70
33	2b	118	LEU	CA-CB-CG	5.05	126.92	115.30
54	1x	14	A	C4-C5-N7	-5.05	108.18	110.70
1	1A	1281	G	C8-N9-C4	5.04	108.42	106.40
34	1c	115	LEU	CA-CB-CG	5.04	126.90	115.30
32	1a	262	G	P-O3'-C3'	5.04	125.74	119.70
1	2A	1690	C	C2-N1-C1'	5.04	124.34	118.80
32	2a	970	U	P-O3'-C3'	5.03	125.74	119.70
1	1A	586	C	N1-C2-O2	-5.03	115.88	118.90
1	1A	1066	A	N3-C4-N9	-5.03	123.38	127.40
1	1A	905	G	N3-C4-C5	5.01	131.11	128.60
32	2a	1385	C	C6-N1-C2	-5.01	118.30	120.30
32	2a	109	G	P-O3'-C3'	5.01	125.71	119.70
32	1a	1480	A	N7-C8-N9	5.01	116.30	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2F	20	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	59154	0	29827	662	0
1	2A	60091	0	30297	897	0
2	1B	2572	0	1306	22	0
2	2B	2573	0	1306	49	0
3	1D	2136	0	2218	61	0
3	2D	2142	0	2229	63	0
4	1E	1559	0	1617	36	0
4	2E	1559	0	1618	41	0
5	1F	1584	0	1625	29	0
5	2F	1580	0	1619	45	0
6	1G	1425	0	1443	36	0
6	2G	1424	0	1434	68	0
7	1H	1330	0	1407	30	0
7	2H	1330	0	1407	33	0
8	1I	1085	0	1114	28	0
8	2I	1061	0	1080	25	0
9	1N	1117	0	1184	16	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	18	0
10	2O	933	0	996	21	0
11	1P	1139	0	1223	38	0
11	2P	1135	0	1212	40	0
12	1Q	1122	0	1178	28	0
12	2Q	1122	0	1179	26	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	27	0
14	1S	877	0	938	30	0
14	2S	870	0	923	36	0
15	1T	1091	0	1151	18	0
15	2T	1083	0	1136	21	0
16	1U	959	0	1019	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	2U	959	0	1018	19	0
17	1V	771	0	830	10	0
17	2V	771	0	830	13	0
18	1W	886	0	940	15	0
18	2W	886	0	940	23	0
19	1X	750	0	814	16	0
19	2X	750	0	814	18	0
20	1Y	806	0	881	25	0
20	2Y	806	0	881	26	0
21	1Z	1470	0	1478	29	0
21	2Z	1454	0	1452	35	0
22	10	598	0	614	15	0
22	20	598	0	614	14	0
23	11	755	0	826	14	0
23	21	755	0	826	19	0
24	12	588	0	643	9	0
24	22	588	0	643	13	0
25	13	469	0	518	5	0
25	23	464	0	514	15	0
26	14	558	0	544	23	0
26	24	532	0	503	23	0
27	15	455	0	465	9	0
27	25	455	0	465	14	0
28	16	453	0	473	11	0
28	26	449	0	469	11	0
29	17	418	0	467	9	0
29	27	418	0	467	13	0
30	18	517	0	582	14	0
30	28	517	0	582	21	0
31	19	307	0	335	7	0
31	29	307	0	335	9	0
32	1a	31750	0	16028	0	0
32	2a	31877	0	16088	0	0
33	1b	1786	0	1744	0	0
33	2b	1697	0	1574	0	0
34	1c	1480	0	1400	0	0
34	2c	1412	0	1246	0	0
35	1d	1618	0	1579	0	1
35	2d	1630	0	1633	0	0
36	1e	1129	0	1185	0	0
36	2e	1095	0	1124	0	0
37	1f	806	0	793	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	2f	817	0	808	0	1
38	1g	1183	0	1165	0	0
38	2g	1167	0	1119	0	0
39	1h	1088	0	1126	0	0
39	2h	1074	0	1100	0	0
40	1i	976	0	973	0	0
40	2i	932	0	891	0	0
41	1j	682	0	598	0	0
41	2j	678	0	612	0	0
42	1k	826	0	829	0	0
42	2k	829	0	825	0	0
43	1l	920	0	958	0	0
43	2l	918	0	947	0	0
44	1m	923	0	962	0	0
44	2m	903	0	923	0	0
45	1n	482	0	507	0	0
45	2n	459	0	467	0	0
46	1o	715	0	729	0	0
46	2o	728	0	760	0	0
47	1p	671	0	679	0	0
47	2p	677	0	686	0	0
48	1q	811	0	858	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	642	0	629	0	0
50	2s	646	0	644	0	0
51	1t	712	0	759	0	0
51	2t	731	0	807	0	0
52	1u	187	0	186	0	0
52	2u	199	0	208	0	0
53	1v	109	0	54	0	0
53	2v	109	0	55	0	0
54	1x	1625	0	829	0	0
54	2x	1625	0	829	0	0
55	1z	105	0	108	0	0
55	2z	112	0	115	0	0
56	10	6	0	0	0	0
56	11	3	0	0	0	0
56	12	1	0	0	0	0
56	13	2	0	0	0	0
56	14	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	15	3	0	0	0	0
56	16	4	0	0	0	0
56	17	2	0	0	0	0
56	18	3	0	0	0	0
56	19	5	0	0	0	0
56	1A	1090	0	0	0	0
56	1B	30	0	0	0	0
56	1D	13	0	0	0	0
56	1E	12	0	0	0	0
56	1F	8	0	0	0	0
56	1G	3	0	0	0	0
56	1H	4	0	0	0	0
56	1N	7	0	0	0	0
56	1O	3	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	9	0	0	0	0
56	1R	6	0	0	0	0
56	1T	6	0	0	0	0
56	1U	6	0	0	0	0
56	1V	2	0	0	0	0
56	1W	6	0	0	0	0
56	1X	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1Z	2	0	0	0	0
56	1a	309	0	0	0	0
56	1b	1	0	0	0	0
56	1d	2	0	0	0	0
56	1e	3	0	0	0	0
56	1f	1	0	0	0	0
56	1h	2	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	1	0	0	0	0
56	1n	1	0	0	0	0
56	1o	3	0	0	0	0
56	1p	2	0	0	0	0
56	1q	3	0	0	0	0
56	1r	3	0	0	0	0
56	1t	1	0	0	0	0
56	1u	1	0	0	0	0
56	1v	1	0	0	0	0
56	1x	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1z	1	0	0	0	0
56	20	1	0	0	0	0
56	23	1	0	0	0	0
56	25	1	0	0	0	0
56	28	3	0	0	0	0
56	2A	561	0	0	0	0
56	2B	10	0	0	0	0
56	2D	5	0	0	0	0
56	2E	4	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	3	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	5	0	0	0	0
56	2R	2	0	0	0	0
56	2T	1	0	0	0	0
56	2U	1	0	0	0	0
56	2X	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	255	0	0	0	0
56	2d	2	0	0	0	0
56	2e	2	0	0	0	0
56	2f	1	0	0	0	0
56	2l	5	0	0	0	0
56	2q	3	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	2x	7	0	0	0	0
56	2z	1	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	1	0	0	0	0
57	26	1	0	0	0	0
57	29	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1d	8	0	0	0	0
58	2d	8	0	0	0	0
59	10	8	0	0	2	0
59	11	7	0	0	0	0
59	12	2	0	0	0	0
59	13	3	0	0	0	0
59	15	7	0	0	1	0
59	16	11	0	0	2	0
59	17	9	0	0	0	0
59	18	16	0	0	0	0
59	19	3	0	0	1	0
59	1A	2412	0	0	135	0
59	1B	46	0	0	5	0
59	1D	25	0	0	2	0
59	1E	30	0	0	5	0
59	1F	21	0	0	1	0
59	1G	8	0	0	0	0
59	1H	4	0	0	0	0
59	1I	3	0	0	2	0
59	1N	8	0	0	0	0
59	1O	5	0	0	0	0
59	1P	25	0	0	3	0
59	1Q	13	0	0	3	0
59	1R	18	0	0	1	0
59	1S	2	0	0	0	0
59	1T	13	0	0	2	0
59	1U	18	0	0	1	0
59	1V	5	0	0	1	0
59	1W	14	0	0	1	0
59	1X	5	0	0	0	0
59	1Y	1	0	0	0	0
59	1Z	6	0	0	1	0
59	1a	394	0	0	0	0
59	1b	1	0	0	0	0
59	1c	1	0	0	0	0
59	1d	3	0	0	0	0
59	1e	4	0	0	0	0
59	1f	1	0	0	0	0
59	1h	2	0	0	0	0
59	1j	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1k	2	0	0	0	0
59	1l	3	0	0	0	0
59	1m	1	0	0	0	0
59	1p	1	0	0	0	0
59	1q	1	0	0	0	0
59	1s	1	0	0	0	0
59	1u	1	0	0	0	0
59	1v	3	0	0	0	0
59	1x	10	0	0	0	0
59	1z	5	0	0	0	0
59	20	2	0	0	0	0
59	21	1	0	0	0	0
59	23	2	0	0	0	0
59	25	1	0	0	0	0
59	27	1	0	0	0	0
59	28	4	0	0	0	0
59	2A	824	0	0	85	0
59	2B	9	0	0	0	0
59	2D	18	0	0	0	0
59	2E	11	0	0	0	0
59	2F	6	0	0	0	0
59	2N	2	0	0	0	0
59	2O	1	0	0	0	0
59	2P	6	0	0	0	0
59	2R	1	0	0	0	0
59	2T	1	0	0	0	0
59	2U	3	0	0	0	0
59	2W	1	0	0	0	0
59	2X	3	0	0	1	0
59	2Y	2	0	0	1	0
59	2Z	5	0	0	1	0
59	2a	329	0	0	0	0
59	2c	1	0	0	0	0
59	2d	1	0	0	0	0
59	2e	4	0	0	0	0
59	2g	1	0	0	0	0
59	2i	2	0	0	0	0
59	2l	2	0	0	0	0
59	2m	1	0	0	0	0
59	2o	1	0	0	0	0
59	2p	2	0	0	0	0
59	2q	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2t	4	0	0	0	0
59	2u	1	0	0	0	0
59	2x	6	0	0	0	0
59	2z	2	0	0	0	0
All	All	288976	0	189961	2587	1

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 10.

All (2587) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:598:U:OP1	59:1A:4101:HOH:O	1.83	0.94
4:1E:110:GLY:O	59:1E:401:HOH:O	1.86	0.92
15:2T:55:ASN:H	15:2T:59:THR:HG22	1.36	0.91
1:2A:786:U:OP2	59:2A:3601:HOH:O	1.89	0.90
15:1T:16:ARG:NH2	15:1T:83:ILE:O	2.03	0.90
1:1A:2123:U:H3	1:1A:2208:G:H1	1.12	0.90
1:1A:2330:G:N7	59:1A:4115:HOH:O	2.05	0.88
1:2A:1649:C:OP2	59:2A:3602:HOH:O	1.91	0.87
1:2A:621:G:N7	59:2A:3614:HOH:O	2.07	0.87
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.39	0.87
1:1A:786:U:OP2	59:1A:4102:HOH:O	1.92	0.86
1:1A:893:U:O4	1:1A:977:A:N6	2.09	0.85
2:2B:20:C:H42	2:2B:63:G:H1	1.25	0.84
1:1A:2466:G:OP2	59:1A:4103:HOH:O	1.94	0.84
1:2A:1256:G:N2	1:2A:1257:A:N7	5.80	0.84
1:1A:1355:G:OP2	29:17:9:ARG:NH1	2.11	0.83
1:1A:2510:C:OP1	59:1A:4104:HOH:O	1.95	0.83
29:17:24:THR:HG22	29:17:27:GLY:H	1.41	0.83
1:2A:1083:C:H42	1:2A:1162:G:H1	1.24	0.83
31:19:19:ARG:NH2	59:19:5001:HOH:O	2.10	0.83
1:1A:2699:U:O4	59:1A:4107:HOH:O	1.97	0.83
1:1A:2586:C:OP2	59:1A:4106:HOH:O	1.96	0.83
1:2A:1188:A:OP1	9:2N:25:ARG:NH2	2.12	0.82
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.13	0.82
1:2A:1981:A:N7	59:2A:3623:HOH:O	2.11	0.81
12:1Q:58:PHE:O	12:1Q:60:ARG:NH1	2.13	0.81
1:1A:1828:U:H5'	3:1D:259:THR:HG22	1.62	0.81
22:10:11:ARG:O	22:10:14:ARG:NH2	2.13	0.81
2:2B:16:G:N2	2:2B:68:C:N3	2.28	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2067:G:H5'	27:25:19:ARG:HA	1.62	0.81
27:25:16:ARG:HH11	27:25:16:ARG:HG2	1.46	0.81
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.43	0.81
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.63	0.80
1:1A:972:G:N7	59:1A:4152:HOH:O	2.13	0.80
1:2A:1036:C:OP2	59:2A:3603:HOH:O	2.00	0.80
1:1A:1100:G:N2	1:1A:1149:C:O2	2.15	0.80
1:1A:1155:G:H21	1:1A:1156:A:H2	1.26	0.79
1:1A:2298:A:H62	1:1A:2355:U:H3	1.28	0.79
12:2Q:27:VAL:O	12:2Q:29:PHE:N	2.13	0.79
1:2A:1109:C:H42	1:2A:1119:G:H1	1.29	0.79
1:1A:838:G:O6	59:1A:4109:HOH:O	2.00	0.79
1:2A:1735:A:H62	1:2A:1744:A:H2	1.26	0.79
1:1A:1068:U:OP2	59:1A:4108:HOH:O	1.99	0.79
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.65	0.78
1:2A:1316:G:OP2	59:2A:3605:HOH:O	2.02	0.78
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.49	0.77
6:2G:80:PHE:O	6:2G:82:LEU:N	2.16	0.77
1:2A:1248:A:H2	1:2A:1286:A:H62	1.31	0.77
28:26:14:THR:OG1	28:26:48:VAL:O	2.02	0.77
12:2Q:29:PHE:O	21:2Z:122:ARG:NH2	2.17	0.77
1:2A:186:C:OP2	59:2A:3604:HOH:O	2.01	0.77
1:1A:1735:A:H62	1:1A:1744:A:H2	1.30	0.77
21:1Z:1:MET:N	59:1Z:401:HOH:O	2.07	0.77
20:1Y:54:LYS:HA	20:1Y:56:PRO:HD3	1.67	0.76
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.68	0.76
1:1A:771:G:N1	59:1A:4121:HOH:O	2.16	0.76
1:1A:2694:C:O2	10:1O:70:LYS:NZ	2.17	0.76
1:1A:682:G:H1	1:1A:695:C:H42	1.33	0.76
1:2A:2848:G:H5'	13:2R:46:GLY:HA2	1.66	0.76
1:1A:2510:C:OP2	59:1A:4111:HOH:O	2.03	0.76
4:2E:199:ARG:HH12	4:2E:202:LYS:HE3	1.51	0.76
1:2A:1355:G:OP2	29:27:9:ARG:NH1	2.18	0.75
1:2A:702:G:O6	59:2A:3608:HOH:O	2.04	0.75
1:2A:831:G:OP2	59:2A:3606:HOH:O	2.03	0.75
26:14:53:GLU:HB3	26:14:54:GLY:HA2	1.67	0.75
1:2A:2603:G:OP2	59:2A:3607:HOH:O	2.03	0.75
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.19	0.75
1:1A:1647:U:O4	59:1A:4110:HOH:O	2.03	0.75
1:2A:1991:A:OP1	59:2A:3611:HOH:O	2.05	0.75
1:1A:1518:A:OP2	59:1A:4114:HOH:O	2.05	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:20:27:GLU:HG3	22:20:68:GLU:HA	1.68	0.75
1:1A:2024:G:OP2	59:1A:4113:HOH:O	2.04	0.74
1:2A:1377:G:OP1	59:2A:3609:HOH:O	2.04	0.74
1:1A:2844:A:N3	59:1A:4188:HOH:O	2.20	0.74
1:1A:1378:C:OP1	59:1A:4112:HOH:O	2.04	0.74
1:1A:1038:G:OP1	16:1U:50:ARG:NH2	2.21	0.74
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.68	0.74
1:2A:1361:U:H2'	1:2A:1362:A:H8	1.50	0.74
14:2S:84:GLN:HA	14:2S:111:GLU:HB2	1.69	0.74
1:2A:2517:U:OP1	4:2E:144:ARG:NH2	2.20	0.74
1:1A:2898:C:OP2	59:1A:4119:HOH:O	2.06	0.74
1:2A:929:G:N3	1:2A:948:C:O2'	31.27	0.74
1:1A:929:G:O6	1:1A:938:C:N4	2.21	0.74
1:2A:900:G:H2'	1:2A:901:G:H8	1.52	0.74
4:2E:179:GLU:HB3	4:2E:181:LEU:HD22	1.69	0.74
1:1A:2456:G:OP1	5:1F:74:ARG:NH2	2.21	0.73
1:1A:1000:G:OP2	12:1Q:14:ARG:NH2	2.21	0.73
1:1A:655:A:OP1	11:1P:65:ARG:NH1	2.20	0.73
1:2A:1116:G:H1	1:2A:1124:C:H42	15.91	0.73
1:2A:1823:C:OP1	59:2A:3612:HOH:O	2.05	0.73
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.70	0.73
1:1A:772:G:N2	59:1A:4121:HOH:O	2.15	0.73
1:1A:1070:G:O2'	59:1A:4108:HOH:O	2.07	0.73
12:1Q:32:TYR:OH	12:1Q:111:GLU:OE1	2.04	0.73
1:2A:2513:G:N7	59:2A:3657:HOH:O	2.22	0.73
1:2A:323:A:OP1	20:2Y:86:ARG:NH2	2.20	0.73
1:1A:2014:U:OP2	59:1A:4122:HOH:O	2.07	0.73
1:1A:550:A:OP1	59:1A:4117:HOH:O	2.06	0.73
1:1A:723:A:OP1	59:1A:4120:HOH:O	2.06	0.73
1:2A:828:A:OP2	59:2A:3610:HOH:O	2.05	0.73
1:2A:2043:U:OP1	59:2A:3615:HOH:O	2.07	0.73
1:2A:655:A:OP1	11:2P:65:ARG:NH1	2.22	0.73
1:2A:1039:C:OP1	16:2U:53:ARG:NH2	2.21	0.73
1:2A:117:U:OP2	59:2A:3616:HOH:O	2.07	0.73
1:1A:2079:A:N7	59:1A:4200:HOH:O	2.21	0.72
1:1A:593:A:O2'	17:1V:78:LYS:NZ	2.21	0.72
1:2A:2588:A:H5'	27:25:3:LYS:HD2	1.71	0.72
1:2A:673:G:H4'	30:28:46:ARG:HH22	1.53	0.72
1:2A:1360:C:OP2	59:2A:3609:HOH:O	2.05	0.72
1:2A:677:A:O2'	59:2A:3613:HOH:O	2.06	0.72
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1007:U:OP2	59:1A:4123:HOH:O	2.07	0.72
1:2A:1108:G:N2	1:2A:1121:C:O2	2.16	0.72
1:1A:535:U:OP2	59:1A:4118:HOH:O	2.06	0.72
1:2A:1406:G:OP1	10:2O:49:ARG:NH1	111.39	0.72
1:2A:2310:G:H2'	1:2A:2311:G:H8	1.54	0.72
4:1E:127:ASP:OD2	59:1E:402:HOH:O	2.08	0.72
1:1A:751:A:OP2	59:1A:4121:HOH:O	2.06	0.72
1:1A:991:G:OP1	59:1A:4126:HOH:O	2.08	0.72
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.72	0.72
7:1H:43:VAL:HG12	7:1H:52:VAL:HG22	1.72	0.71
1:1A:2719:G:H1'	13:1R:71:GLN:HE22	1.55	0.71
2:2B:17:C:O2	2:2B:67:G:N2	2.20	0.71
3:2D:276:LYS:H	3:2D:276:LYS:HD3	1.52	0.71
1:2A:1648:A:OP1	59:2A:3602:HOH:O	2.07	0.71
1:1A:1354:G:H4'	29:17:7:PRO:HB2	1.70	0.71
1:1A:353:A:H2	1:1A:1254:A:HO2'	1.37	0.71
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.73	0.71
1:2A:1214:G:H1	1:2A:1224:C:H42	1.39	0.71
1:2A:267:G:HO2'	1:2A:268:G:H8	1.37	0.71
18:2W:92:ARG:NH2	18:2W:94:ASP:OD1	2.23	0.71
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.23	0.71
1:2A:396:G:N7	59:2A:3668:HOH:O	2.23	0.71
1:1A:2100:U:OP1	23:11:21:ARG:NH2	2.23	0.71
1:2A:665:C:O2'	1:2A:2361:C:OP1	2.06	0.71
1:2A:1002:U:OP2	12:2Q:14:ARG:NH1	2.23	0.71
1:1A:1360:C:OP2	59:1A:4124:HOH:O	2.08	0.71
1:1A:847:G:O6	5:1F:53:THR:OG1	2.09	0.71
1:2A:2606:G:N7	59:2A:3670:HOH:O	2.23	0.71
1:2A:343:A:O2'	1:2A:345:A:OP2	2.06	0.70
8:1I:77:LEU:HB3	8:1I:142:VAL:HG13	1.73	0.70
1:2A:2800:C:OP1	4:2E:61:ARG:NH2	2.24	0.70
1:1A:2650:A:OP2	59:1A:4131:HOH:O	2.09	0.70
1:1A:478:C:OP1	59:1A:4125:HOH:O	2.08	0.70
1:1A:830:A:OP2	59:1A:4129:HOH:O	2.09	0.70
1:1A:710:C:O2'	59:1A:4127:HOH:O	2.08	0.70
1:1A:932:C:H2'	1:1A:933:A:H5''	1.72	0.70
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.72	0.70
1:2A:183:A:N7	59:2A:3604:HOH:O	2.25	0.70
1:1A:2718:G:OP2	59:1A:4128:HOH:O	2.09	0.70
24:22:64:LEU:HD11	24:22:68:ARG:HH21	1.56	0.70
1:2A:1360:C:N4	1:2A:1382:G:O6	2.20	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1401:G:O6	59:2A:3617:HOH:O	2.08	0.70
1:2A:396:G:OP2	59:2A:3619:HOH:O	2.09	0.70
1:2A:1828:U:H5'	3:2D:259:THR:HG22	1.71	0.70
12:2Q:26:TYR:O	12:2Q:67:ARG:NH1	2.22	0.70
7:2H:9:ILE:HB	7:2H:50:VAL:HB	1.73	0.70
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.74	0.70
20:2Y:44:ILE:HD13	20:2Y:44:ILE:H	1.55	0.70
1:1A:2339:A:H2'	1:1A:2340:G:C8	2.27	0.70
1:2A:1310:A:OP2	59:2A:3618:HOH:O	2.09	0.70
6:2G:33:ARG:HH11	6:2G:33:ARG:HB2	1.56	0.70
1:1A:1067:G:N2	1:1A:1068:U:O4	2.25	0.69
1:1A:2502:U:OP2	59:1A:4132:HOH:O	2.09	0.69
59:1E:401:HOH:O	13:1R:3:HIS:NE2	2.24	0.69
1:2A:1682:C:OP2	59:2A:3621:HOH:O	2.10	0.69
6:2G:15:VAL:HG13	6:2G:175:LEU:HD23	1.74	0.69
1:2A:609:C:OP2	11:2P:21:ARG:NH2	2.25	0.69
1:1A:1043:C:OP1	59:1A:4133:HOH:O	2.10	0.69
1:1A:396:G:OP2	59:1A:4135:HOH:O	2.10	0.69
1:1A:38:C:O2	5:1F:46:ARG:NH2	2.24	0.69
11:2P:59:LEU:HD21	30:28:10:ALA:HA	1.73	0.69
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.56	0.69
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.26	0.69
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.74	0.69
1:2A:1613:A:OP2	59:2A:3622:HOH:O	2.11	0.69
1:1A:1064:U:HO2'	1:1A:1066:A:H2	1.40	0.69
1:1A:1680:A:OP2	59:1A:4130:HOH:O	2.09	0.69
1:2A:179:A:N1	59:2A:3676:HOH:O	2.24	0.69
1:2A:679:G:O6	1:2A:698:C:N4	2.16	0.69
1:2A:1035:A:OP2	59:2A:3603:HOH:O	2.10	0.69
1:2A:1512:G:HO2'	1:2A:1592:C:HO2'	1.30	0.69
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.74	0.69
1:1A:1619:G:OP2	59:1A:4136:HOH:O	2.11	0.69
16:2U:44:ASN:HD21	17:2V:75:PHE:HB3	1.57	0.69
25:13:3:ARG:NH1	25:13:60:GLU:OE1	2.23	0.69
1:2A:1240:C:H2'	1:2A:1241:G:H8	1.58	0.69
1:1A:138:A:H8	1:1A:1453:C:HO2'	1.41	0.69
1:2A:2733:A:OP1	59:2A:3625:HOH:O	2.11	0.69
17:1V:98:GLU:OE2	17:1V:100:ARG:NH1	2.25	0.69
1:2A:1010:G:OP1	59:2A:3620:HOH:O	2.09	0.69
1:1A:2573:U:H1'	10:1O:23:ARG:HH11	1.56	0.69
1:2A:2284:A:H2'	1:2A:2285:A:C8	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1663:A:OP2	59:1A:4137:HOH:O	2.11	0.69
1:2A:2643:A:HO2'	1:2A:2820:G:HO2'	1.35	0.69
6:2G:135:LEU:HB2	6:2G:155:MET:HG2	1.75	0.69
1:1A:1218:A:H4'	1:1A:1219:U:OP1	1.94	0.68
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.74	0.68
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.25	0.68
1:1A:1430:G:O2'	1:1A:1441:U:O2	2.08	0.68
1:1A:258:A:H2'	1:1A:259:A:C8	3.12	0.68
1:2A:1066:A:H62	1:2A:1185:U:H3	1.39	0.68
1:2A:596:C:OP1	59:2A:3624:HOH:O	2.11	0.68
1:2A:60:C:H42	1:2A:90:G:H1	1.41	0.68
1:2A:1064:U:H3	1:2A:1187:A:H62	1.38	0.68
1:2A:1716:C:OP1	59:2A:3627:HOH:O	2.11	0.68
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.66	0.68
1:2A:957:C:OP1	12:2Q:8:LYS:NZ	2.26	0.68
4:1E:181:LEU:HD21	15:1T:6:LEU:HD12	1.75	0.68
1:1A:1188:A:OP1	9:1N:25:ARG:NH2	2.26	0.68
2:1B:23:G:O6	59:1B:301:HOH:O	2.07	0.68
1:2A:2053:G:N7	59:2A:3693:HOH:O	2.27	0.68
1:2A:2226:G:H5''	1:2A:2227:G:N7	2.09	0.68
1:2A:552:A:O2'	1:2A:553:A:H5'	1.94	0.68
23:11:21:ARG:HD3	23:11:35:THR:HG21	1.75	0.68
1:2A:330:G:N1	1:2A:333:A:OP2	2.25	0.68
1:1A:1229:C:OP2	59:1A:4138:HOH:O	2.11	0.68
1:2A:1026:A:OP1	59:2A:3629:HOH:O	2.12	0.68
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.25	0.68
1:1A:2480:A:OP2	59:1A:4139:HOH:O	2.12	0.67
1:1A:426:G:N7	59:1A:4258:HOH:O	2.27	0.67
1:2A:2888:C:OP2	59:2A:3628:HOH:O	2.11	0.67
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.75	0.67
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.76	0.67
1:1A:807:A:OP1	59:1A:4144:HOH:O	2.12	0.67
1:2A:1958:A:OP1	59:2A:3630:HOH:O	2.12	0.67
1:1A:1951:G:O2'	1:1A:1989:G:O6	2.09	0.67
1:1A:780:A:N3	59:1A:4214:HOH:O	2.27	0.67
1:1A:1479:A:H61	1:1A:1604:A:H62	1.40	0.67
1:1A:1813:A:N7	59:1A:4240:HOH:O	2.25	0.67
1:1A:2493:G:OP2	59:1A:4142:HOH:O	2.12	0.67
8:1I:104:GLN:HG3	8:1I:105:HIS:HD2	1.59	0.67
15:1T:51:ARG:NH1	59:1T:301:HOH:O	2.24	0.67
1:2A:903:C:OP2	22:20:77:ARG:NH2	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:867:A:H2'	1:2A:990:G:H5''	1.77	0.67
1:1A:541:C:OP1	27:15:16:ARG:NH2	2.27	0.67
1:2A:2316:A:H5''	6:2G:134:GLY:HA3	1.74	0.67
1:1A:1358:U:OP1	59:1A:4148:HOH:O	2.13	0.67
1:1A:2013:G:N7	59:1A:4260:HOH:O	2.28	0.67
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.76	0.67
1:1A:271:U:H4'	8:1I:50:ARG:HH12	1.57	0.67
26:24:62:ARG:O	26:24:64:GLY:N	2.27	0.67
1:2A:69:A:H5''	1:2A:71:A:C8	2.29	0.67
2:2B:13:A:N1	2:2B:69:G:O2'	2.22	0.67
1:1A:2670:G:O2'	7:1H:175:LYS:NZ	2.28	0.67
1:2A:2694:C:OP1	15:2T:53:ARG:NH2	2.21	0.67
1:1A:2563:U:OP2	59:1A:4143:HOH:O	2.12	0.67
1:1A:302:C:H42	1:1A:384:G:H1	1.42	0.67
1:1A:1845:A:OP2	3:1D:54:ARG:NH2	2.27	0.67
1:2A:1088:C:O2'	1:2A:1093:A:O2'	2.11	0.67
1:2A:622:G:N2	1:2A:627:C:O3'	2.28	0.67
1:1A:1211:C:O2'	59:1A:4146:HOH:O	2.13	0.67
1:1A:909:A:N6	59:1A:4261:HOH:O	2.28	0.67
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.28	0.67
1:2A:560:A:H2'	1:2A:561:C:C6	2.30	0.67
6:2G:63:ILE:HA	6:2G:143:GLU:HG3	1.75	0.67
1:1A:2443:A:OP2	59:1A:4141:HOH:O	2.12	0.66
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	1.77	0.66
1:1A:609:C:OP2	11:1P:21:ARG:NH2	2.28	0.66
2:1B:58:A:OP2	59:1B:302:HOH:O	2.14	0.66
1:1A:1514:C:OP1	59:1A:4140:HOH:O	2.12	0.66
1:1A:2123:U:O2	1:1A:2208:G:N2	2.26	0.66
1:2A:1306:C:OP2	18:2W:83:LYS:NZ	2.25	0.66
1:2A:1499:A:OP2	59:2A:3632:HOH:O	2.13	0.66
11:1P:25:SER:O	59:1P:301:HOH:O	2.12	0.66
7:2H:3:ARG:HH22	7:2H:5:GLY:H	1.42	0.66
22:10:16:SER:O	59:10:201:HOH:O	2.14	0.66
1:1A:2083:A:OP1	59:1A:4153:HOH:O	2.14	0.66
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.61	0.66
4:1E:145:LYS:NZ	59:1E:403:HOH:O	2.24	0.66
1:2A:2846:G:N7	59:2A:3695:HOH:O	2.27	0.66
1:2A:2356:G:OP2	28:26:38:LYS:NZ	2.29	0.66
16:2U:49:HIS:HA	16:2U:52:ARG:HG2	1.77	0.66
1:1A:1530:G:N2	1:1A:1549:C:O2	2.17	0.66
1:1A:553:A:O3'	59:1A:4150:HOH:O	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1377:G:OP1	59:1A:4124:HOH:O	2.14	0.66
1:1A:1813:A:OP1	59:1A:4151:HOH:O	2.13	0.66
1:1A:2518:C:OP2	59:1A:4155:HOH:O	2.14	0.66
1:1A:81:G:OP1	59:1A:4145:HOH:O	2.13	0.66
6:1G:161:THR:HG23	6:1G:163:ALA:H	1.61	0.66
1:2A:1282:A:OP1	59:2A:3631:HOH:O	2.13	0.66
1:1A:2323:U:H5'	6:1G:88:ILE:HD11	1.77	0.65
1:1A:2383:G:N3	59:1A:4268:HOH:O	2.29	0.65
4:1E:179:GLU:HB3	4:1E:181:LEU:HD22	1.78	0.65
1:2A:2079:A:N7	59:2A:3706:HOH:O	2.30	0.65
8:2I:77:LEU:HB3	8:2I:142:VAL:HG13	1.76	0.65
1:1A:345:A:OP1	5:1F:168:ARG:NH1	2.29	0.65
1:1A:2700:U:H4'	1:1A:2701:C:H5'	1.78	0.65
1:1A:534:C:OP1	59:1A:4118:HOH:O	2.13	0.65
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.79	0.65
1:2A:206:A:OP2	59:2A:3633:HOH:O	2.14	0.65
1:2A:2376:G:O6	30:28:43:GLN:NE2	2.20	0.65
1:2A:663:U:H2'	1:2A:664:C:C6	2.32	0.65
1:2A:842:C:H2'	1:2A:843:C:C6	2.32	0.65
17:2V:6:LYS:HB2	17:2V:38:LEU:HD21	1.77	0.65
1:1A:1316:G:OP2	59:1A:4156:HOH:O	2.14	0.65
1:2A:82:A:N1	1:2A:96:G:O2'	2.23	0.65
2:2B:16:G:H1	2:2B:68:C:H42	1.43	0.65
2:2B:83:G:H1	2:2B:94:C:H42	1.45	0.65
1:1A:236:G:OP2	59:1A:4157:HOH:O	2.14	0.65
8:1I:82:ARG:NH1	59:1I:5002:HOH:O	2.29	0.65
1:2A:2368:U:OP1	22:20:20:ARG:NH1	2.29	0.65
1:1A:1314:A:N7	59:1A:4278:HOH:O	2.30	0.65
1:1A:1517:A:OP2	59:1A:4154:HOH:O	2.14	0.65
7:2H:118:PRO:HG2	7:2H:121:ILE:HG13	1.79	0.65
1:1A:1354:G:O6	59:1A:4149:HOH:O	2.13	0.65
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.79	0.65
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.79	0.65
3:1D:239:ARG:NH2	59:1D:403:HOH:O	2.29	0.65
2:2B:55:U:H1'	6:2G:29:TRP:HE1	1.60	0.65
6:1G:145:THR:OG1	6:1G:148:MET:SD	2.53	0.65
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.11	0.65
1:2A:1625:A:N7	59:2A:3703:HOH:O	2.29	0.65
1:2A:2513:G:OP2	59:2A:3634:HOH:O	2.14	0.65
8:2I:114:LEU:HD11	8:2I:128:LEU:HD13	1.78	0.65
1:1A:1000:G:O6	59:1A:4134:HOH:O	2.10	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2642:G:OP2	59:1A:4160:HOH:O	2.15	0.64
1:1A:2494:C:N3	12:1Q:124:LYS:NZ	2.45	0.64
1:1A:2444:A:OP2	59:1A:4163:HOH:O	2.15	0.64
1:1A:260:A:N7	1:1A:282:G:N2	2.45	0.64
17:1V:21:ARG:HG2	17:1V:91:TYR:CD1	2.32	0.64
1:1A:2429:A:N7	59:1A:4281:HOH:O	2.30	0.64
17:1V:78:LYS:O	59:1V:301:HOH:O	2.13	0.64
11:2P:97:PRO:HD3	11:2P:126:VAL:O	1.97	0.64
1:1A:2007:A:OP1	59:1A:4159:HOH:O	2.15	0.64
5:1F:18:ARG:NH2	5:1F:127:GLU:OE2	2.31	0.64
6:2G:13:GLU:O	6:2G:15:VAL:N	2.31	0.64
1:2A:2829:A:OP1	13:2R:2:ARG:NH2	2.31	0.64
1:2A:2307:U:OP2	14:2S:9:ARG:NH2	2.31	0.64
16:2U:92:ARG:HA	16:2U:95:LEU:HB2	1.80	0.64
1:1A:358:C:H4'	20:1Y:73:ARG:HD3	1.79	0.64
2:2B:45:A:O4'	6:2G:95:ARG:NH1	2.30	0.64
1:2A:661:A:H8	11:2P:117:GLU:HG3	1.63	0.64
1:1A:237:C:O2	30:18:12:LYS:NZ	2.26	0.64
1:1A:2775:G:OP2	59:1A:4161:HOH:O	2.15	0.64
1:1A:710:C:OP2	59:1A:4162:HOH:O	2.15	0.64
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.62	0.64
1:2A:600:A:OP2	59:2A:3635:HOH:O	2.15	0.64
1:2A:1830:C:OP2	3:2D:183:ARG:NH2	2.31	0.64
6:2G:41:GLN:HE22	6:2G:153:ARG:HB3	1.63	0.64
1:1A:2657:C:OP2	1:1A:2744:G:O2'	2.14	0.63
3:1D:108:PRO:HD2	3:1D:111:LEU:HG	1.80	0.63
1:2A:2583:A:OP1	1:2A:2585:G:O2'	2.15	0.63
26:14:58:ARG:O	26:14:61:ARG:N	2.31	0.63
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.79	0.63
8:1I:132:PRO:O	59:1I:5001:HOH:O	2.15	0.63
14:1S:59:LYS:HE3	14:1S:60:GLY:H	1.63	0.63
26:24:46:GLN:O	26:24:48:ARG:N	2.32	0.63
1:2A:2226:G:H3'	1:2A:2227:G:C8	2.33	0.63
1:2A:2623:C:OP2	27:25:2:ALA:N	2.31	0.63
21:2Z:151:HIS:ND1	21:2Z:168:GLU:O	2.32	0.63
4:2E:111:ARG:HG3	4:2E:160:TYR:CD2	2.33	0.63
1:2A:590:U:O4	59:2A:3626:HOH:O	2.11	0.63
1:2A:989:A:OP2	59:2A:3636:HOH:O	2.15	0.63
1:1A:1220:G:H1'	1:1A:1221:A:H5'	1.79	0.63
1:1A:2648:U:OP2	59:1A:4164:HOH:O	2.16	0.63
26:24:60:GLN:HA	26:24:62:ARG:HG2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1739:U:O2'	3:2D:14:ARG:NH2	2.32	0.63
1:1A:1450:U:H2'	1:1A:1451:U:C6	2.34	0.63
1:2A:1361:U:H2'	1:2A:1362:A:C8	2.32	0.63
1:2A:1845:A:OP2	3:2D:54:ARG:NH2	2.30	0.63
1:2A:2251:C:H2'	1:2A:2252:A:H8	1.62	0.63
2:2B:19:G:H1	2:2B:64:C:H42	1.44	0.63
1:2A:720:G:H1'	5:2F:74:ARG:HD3	1.81	0.62
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.81	0.62
19:1X:60:ARG:HH22	29:17:47:ARG:HH22	1.47	0.62
1:1A:1153:U:HO2'	1:1A:1154:C:H6	1.47	0.62
1:1A:648:C:O2'	1:1A:703:U:OP1	2.16	0.62
1:1A:296:C:H2'	1:1A:297:G:H8	1.64	0.62
23:21:76:ARG:NH1	23:21:97:LEU:O	2.30	0.62
1:2A:2858:U:OP2	15:2T:95:ARG:NH1	2.33	0.62
1:2A:907:A:N3	2:2B:79:C:O2'	2.32	0.62
4:2E:181:LEU:HD21	15:2T:6:LEU:HD12	1.81	0.62
1:1A:1540:A:H2'	1:1A:1541:A:C8	2.35	0.62
6:1G:41:GLN:HE22	6:1G:153:ARG:HB3	1.64	0.62
1:2A:2100:U:O3'	23:21:35:THR:OG1	2.18	0.62
1:2A:917:U:OP1	12:2Q:5:ARG:HG2	1.99	0.62
10:2O:64:ARG:NH1	10:2O:81:ASP:OD1	2.33	0.62
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.82	0.62
1:1A:1502:G:OP2	59:1A:4168:HOH:O	2.16	0.62
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.15	0.62
1:2A:152:C:OP2	23:21:92:LYS:NZ	2.32	0.62
1:2A:78:G:H1	1:2A:103:C:H42	1.46	0.62
1:1A:595:G:N1	1:1A:2052:A:OP2	2.29	0.62
6:2G:35:GLU:HG2	6:2G:36:LYS:HE2	1.82	0.62
1:2A:1056:G:OP2	16:2U:66:ASN:ND2	2.33	0.62
15:2T:56:GLY:O	15:2T:59:THR:HG23	2.00	0.62
1:2A:63:C:O2'	1:2A:481:C:N3	2.29	0.61
1:1A:1715:A:OP2	59:1A:4170:HOH:O	2.16	0.61
1:2A:1570:G:H2'	1:2A:1571:G:C8	2.35	0.61
1:2A:1910:A:H2'	1:2A:1911:A:C8	2.35	0.61
3:2D:123:ALA:HB1	3:2D:129:ASN:HD22	1.65	0.61
1:1A:1541:A:N3	1:1A:1623:C:O2'	2.31	0.61
1:1A:610:U:H2'	1:1A:611:C:C6	2.35	0.61
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.80	0.61
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.80	0.61
1:1A:1359:C:OP1	59:1A:4124:HOH:O	2.16	0.61
1:1A:2043:U:O2'	1:1A:2628:C:H5'	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:645:A:OP2	11:1P:108:LYS:NZ	2.33	0.61
1:2A:1022:G:OP2	59:2A:3640:HOH:O	2.16	0.61
1:2A:2061:C:OP2	9:2N:109:LYS:NZ	2.28	0.61
1:2A:475:G:N7	59:2A:3717:HOH:O	2.31	0.61
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.83	0.61
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.33	0.61
1:1A:81:G:H1	1:1A:99:G:HO2'	1.47	0.61
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	1.81	0.61
1:1A:1210:U:H2'	1:1A:1211:C:C6	2.35	0.61
10:1O:71:ARG:NH2	10:1O:105:GLU:OE1	2.32	0.61
1:2A:1813:A:OP1	59:2A:3601:HOH:O	2.16	0.61
1:2A:2762:A:OP2	7:2H:62:LYS:NZ	2.32	0.61
11:2P:121:LYS:O	11:2P:123:LEU:N	2.33	0.61
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	1.82	0.61
1:1A:699:A:H2'	1:1A:700:A:C8	3.59	0.61
11:1P:54:GLY:O	59:1P:302:HOH:O	2.16	0.61
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.16	0.61
1:2A:1092:G:H1'	1:2A:1155:G:H22	1.65	0.61
1:2A:2012:U:H2'	1:2A:2013:G:H5''	1.83	0.61
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.81	0.61
1:1A:2368:U:OP1	22:10:20:ARG:NH1	2.33	0.61
18:1W:14:PRO:HG2	18:1W:78:GLU:HG2	1.82	0.61
6:2G:83:ARG:N	6:2G:86:MET:SD	2.64	0.61
1:1A:2493:G:OP1	59:1A:4169:HOH:O	2.16	0.61
1:2A:2338:A:H2'	1:2A:2339:A:C8	2.35	0.61
4:1E:120:TRP:CE3	4:1E:155:LYS:HD3	2.36	0.60
1:2A:2027:C:OP2	59:2A:3643:HOH:O	2.17	0.60
26:14:16:CYS:SG	26:14:17:GLY:N	2.74	0.60
1:2A:1212:U:O2	1:2A:1227:G:N2	2.34	0.60
26:14:68:ARG:HH21	26:14:68:ARG:HA	1.66	0.60
24:12:21:LEU:HD13	24:12:64:LEU:HA	1.82	0.60
1:2A:1240:C:H2'	1:2A:1241:G:C8	2.35	0.60
1:2A:50:A:OP2	1:2A:114:G:N1	2.27	0.60
8:2I:104:GLN:HG3	8:2I:105:HIS:CD2	2.35	0.60
1:2A:2573:U:H1'	10:2O:23:ARG:HD3	1.82	0.60
11:2P:56:SER:HB2	11:2P:61:ARG:HD2	1.83	0.60
1:1A:1739:U:O2'	3:1D:14:ARG:NH2	2.34	0.60
1:2A:1029:A:H5''	1:2A:1030:C:H5	1.67	0.60
2:2B:90:A:C5	2:2B:91:C:H1'	2.36	0.60
14:2S:39:ILE:HB	14:2S:49:VAL:HG22	1.84	0.60
1:1A:405:G:OP1	59:1A:4165:HOH:O	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:90:LYS:NZ	7:1H:159:GLU:OE1	2.31	0.60
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.00	0.60
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.34	0.60
1:1A:909:A:OP2	59:1A:4173:HOH:O	2.16	0.60
26:24:14:ILE:HG22	26:24:22:ILE:HD13	1.82	0.60
18:2W:14:PRO:HG2	18:2W:78:GLU:HG2	1.83	0.60
21:2Z:131:ARG:NH2	59:2Z:402:HOH:O	2.34	0.60
11:1P:121:LYS:O	11:1P:123:LEU:N	2.35	0.60
18:1W:15:ARG:NH1	59:1W:3101:HOH:O	2.29	0.60
1:2A:807:A:N7	59:2A:3713:HOH:O	2.31	0.60
5:2F:124:LEU:HB3	5:2F:193:VAL:HG22	1.83	0.60
1:2A:2694:C:O2	10:2O:70:LYS:NZ	2.25	0.60
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.66	0.59
1:2A:1050:C:H2'	1:2A:1051:C:C6	2.37	0.59
1:2A:733:C:OP2	59:2A:3639:HOH:O	2.16	0.59
1:1A:1511:G:O2'	1:1A:1591:A:N1	2.31	0.59
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.20	0.59
1:1A:172:C:H2'	1:1A:173:U:C6	2.38	0.59
3:2D:68:LYS:HD2	3:2D:70:TRP:CZ2	2.37	0.59
28:16:6:ARG:NH2	59:16:5001:HOH:O	2.35	0.59
1:2A:1359:C:OP1	59:2A:3609:HOH:O	2.16	0.59
1:2A:2405:C:OP2	30:28:30:ARG:NH1	2.35	0.59
1:2A:1064:U:HO2'	1:2A:1066:A:H2	1.50	0.59
11:2P:121:LYS:HD2	11:2P:122:PRO:HD2	1.84	0.59
1:2A:885:U:H2'	1:2A:886:C:C6	2.37	0.59
3:2D:145:VAL:HB	3:2D:155:LEU:HB2	1.85	0.59
1:2A:1297:G:OP1	16:2U:36:ARG:NH2	2.35	0.59
1:1A:1833:A:O2'	3:1D:259:THR:HG21	2.02	0.59
1:1A:2032:U:OP1	18:1W:42:ARG:NH1	2.35	0.59
1:2A:2124:C:O2	1:2A:2207:G:N2	2.21	0.59
1:2A:2226:G:H8	1:2A:2227:G:N7	2.01	0.59
1:2A:1423:A:OP1	29:27:10:ARG:NH2	2.35	0.59
1:2A:1311:G:O5'	18:2W:15:ARG:NH2	2.36	0.59
1:2A:1894:U:OP1	1:2A:2421:G:O2'	2.20	0.59
1:2A:2482:C:N4	1:2A:2487:A:O2'	2.36	0.59
12:1Q:32:TYR:CE1	12:1Q:133:ARG:HG3	2.38	0.59
15:1T:54:ARG:HA	15:1T:59:THR:HG22	1.85	0.59
1:2A:105:U:H2'	1:2A:106:G:C8	2.38	0.59
1:2A:346:G:HO2'	1:2A:1249:U:H3	1.51	0.59
28:16:13:CYS:SG	28:16:47:THR:HG21	2.43	0.59
1:1A:1612:A:OP1	3:1D:211:ARG:NH1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.84	0.59
21:1Z:154:ASP:OD1	21:1Z:154:ASP:N	2.36	0.59
28:26:9:LEU:HA	28:26:54:ILE:HB	1.84	0.59
1:2A:105:U:H2'	1:2A:106:G:H8	1.67	0.59
7:2H:38:SER:HB3	7:2H:41:MET:HG2	1.85	0.59
1:1A:1853:G:OP1	3:1D:54:ARG:NH1	2.36	0.58
1:2A:1098:C:H42	1:2A:1151:G:H1	1.51	0.58
1:2A:330:G:N2	1:2A:333:A:O5'	2.34	0.58
1:2A:57:U:H2'	1:2A:58:G:C8	5.31	0.58
1:2A:608:A:N1	1:2A:855:G:O2'	2.32	0.58
1:1A:2463:C:OP2	59:1A:4176:HOH:O	2.17	0.58
21:1Z:157:LEU:HD11	21:1Z:163:LEU:HD13	1.85	0.58
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.36	0.58
1:2A:493:G:N7	29:27:39:ARG:NH2	2.50	0.58
1:2A:947:C:H2'	1:2A:948:C:C6	2.38	0.58
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.76	0.58
1:1A:2338:A:H2'	1:1A:2339:A:C8	2.38	0.58
1:1A:2441:A:H2'	1:1A:2441:A:N3	2.18	0.58
1:1A:2636:G:OP1	59:1A:4171:HOH:O	2.16	0.58
1:1A:276:G:N7	59:1A:4300:HOH:O	2.32	0.58
1:1A:2803:C:H2'	1:1A:2804:G:H8	1.67	0.58
1:2A:1093:A:H61	1:2A:1157:G:HO2'	1.50	0.58
1:2A:2719:G:H1'	13:2R:71:GLN:HE22	1.68	0.58
1:2A:746:G:O6	59:2A:3637:HOH:O	2.16	0.58
1:1A:1520:C:H2'	1:1A:1521:G:C8	2.39	0.58
1:1A:57:U:H2'	1:1A:58:G:C8	5.76	0.58
1:1A:629:U:OP1	5:1F:102:PRO:HA	2.04	0.58
19:1X:11:PRO:HB3	19:1X:92:LEU:HD11	1.85	0.58
27:25:16:ARG:NH1	27:25:16:ARG:HG2	2.17	0.58
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.39	0.58
1:2A:1912:G:O6	59:2A:3641:HOH:O	2.16	0.58
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	1.85	0.58
1:1A:2801:C:O2	1:1A:2902:G:N2	2.30	0.58
1:1A:1184:C:O3'	9:1N:25:ARG:NH1	2.37	0.58
11:1P:126:VAL:HG12	11:1P:148:LEU:HD13	1.84	0.58
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.84	0.58
18:2W:86:LEU:HD12	18:2W:87:PRO:HD2	1.86	0.58
1:1A:1723:A:OP1	59:1A:4177:HOH:O	2.17	0.58
1:2A:1110:U:O2	1:2A:1119:G:N2	2.37	0.58
1:2A:2578:G:H2'	1:2A:2579:C:C6	2.38	0.58
1:2A:2657:C:OP2	1:2A:2744:G:O2'	2.15	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:661:A:OP1	11:1P:133:SER:OG	2.18	0.58
1:2A:346:G:H5'	5:2F:169:ASN:HD21	1.69	0.58
1:2A:2100:U:OP1	23:21:21:ARG:NH2	2.36	0.57
3:2D:112:GLN:N	3:2D:115:GLN:OE1	2.36	0.57
10:2O:80:ASP:OD1	15:2T:64:ARG:NH2	2.37	0.57
1:1A:57:U:H2'	1:1A:58:G:H8	5.76	0.57
1:1A:893:U:OP2	59:1A:4172:HOH:O	2.16	0.57
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.86	0.57
4:2E:199:ARG:NH1	4:2E:202:LYS:HE3	2.16	0.57
18:2W:18:ARG:HG3	18:2W:76:VAL:HB	1.86	0.57
1:1A:481:C:H4'	59:1A:5923:HOH:O	2.03	0.57
1:2A:1625:A:H2'	1:2A:1626:A:C8	2.39	0.57
1:2A:1734:U:O2	1:2A:1746:A:H5'	2.04	0.57
1:2A:590:U:H5''	1:2A:989:A:N1	2.19	0.57
1:2A:598:U:OP1	59:2A:3644:HOH:O	2.17	0.57
1:2A:929:G:N2	1:2A:948:C:O2	27.97	0.57
6:2G:41:GLN:HG3	6:2G:60:LEU:HD21	1.85	0.57
1:1A:1846:G:O6	3:1D:35:LYS:NZ	2.31	0.57
1:1A:2244:U:H2'	1:1A:2245:G:C8	2.40	0.57
1:1A:182:G:OP2	59:1A:4178:HOH:O	2.18	0.57
1:1A:682:G:N2	1:1A:695:C:N3	2.47	0.57
1:2A:1194:G:H2'	1:2A:1195:C:C6	2.39	0.57
1:2A:1231:G:H5'	17:2V:81:TYR:CE1	2.40	0.57
1:1A:2124:C:N3	1:1A:2207:G:O6	2.37	0.57
1:1A:301:A:O2'	1:1A:302:C:OP1	2.23	0.57
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.33	0.57
1:2A:75:C:H42	1:2A:106:G:H1	1.52	0.57
1:2A:2832:A:OP1	4:2E:159:HIS:NE2	2.38	0.57
1:1A:720:G:OP2	59:1A:4175:HOH:O	2.17	0.57
15:2T:65:LYS:HE2	15:2T:67:SER:HB3	1.86	0.57
18:2W:4:LYS:HB2	18:2W:106:ILE:HG12	1.87	0.57
1:1A:353:A:H2	1:1A:1254:A:O2'	1.88	0.57
1:1A:924:A:H2'	1:1A:925:G:H5'	1.87	0.57
1:2A:1992:A:OP2	3:2D:242:ARG:NH2	2.38	0.57
1:2A:2830:A:H2'	1:2A:2831:G:C8	2.40	0.57
6:2G:36:LYS:HG2	6:2G:160:VAL:HB	1.85	0.57
1:1A:1552:A:HO2'	1:1A:1553:A:H8	1.52	0.57
1:1A:2012:U:H2'	1:1A:2013:G:H5''	1.86	0.57
9:1N:17:ASP:O	9:1N:21:LYS:NZ	2.28	0.57
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.39	0.57
1:2A:2310:G:H2'	1:2A:2311:G:C8	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2858:U:H4'	1:2A:2877:A:C2	2.40	0.57
1:2A:29:G:N2	1:2A:534:C:O2	2.35	0.57
20:2Y:9:LYS:NZ	20:2Y:28:LYS:O	2.37	0.57
13:1R:11:ASN:ND2	59:1R:301:HOH:O	2.38	0.57
1:2A:17:C:H2'	1:2A:18:C:H6	1.70	0.57
1:2A:2622:U:C4	27:25:3:LYS:HG2	2.40	0.57
1:2A:324:G:N2	1:2A:339:C:O2	2.36	0.57
1:2A:1828:U:H5'	3:2D:259:THR:CG2	2.34	0.57
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.40	0.57
1:1A:230:G:C8	30:18:5:LYS:HG2	2.40	0.56
1:1A:2315:G:H22	1:1A:2323:U:H3	1.52	0.56
6:1G:118:ARG:O	6:1G:181:ARG:HB3	2.05	0.56
14:1S:39:ILE:HB	14:1S:49:VAL:HG13	1.87	0.56
1:2A:1135:U:H2'	1:2A:1136:G:C8	2.40	0.56
1:2A:2044:G:H5'	1:2A:2628:C:H4'	1.87	0.56
1:2A:1232:U:H4'	17:2V:79:VAL:HG22	1.87	0.56
1:1A:552:A:C2	1:1A:2063:A:H2'	2.40	0.56
6:1G:7:LEU:HD13	6:1G:100:TRP:HE3	1.70	0.56
1:2A:1973:A:OP1	10:2O:42:SER:OG	2.21	0.56
1:2A:1309:G:H2'	1:2A:2035:A:N6	2.20	0.56
1:2A:542:G:H2'	1:2A:543:U:C6	2.41	0.56
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.05	0.56
6:2G:5:VAL:HG23	6:2G:104:GLU:OE2	2.04	0.56
7:1H:3:ARG:HG2	7:1H:6:ARG:HG2	1.86	0.56
14:1S:43:GLU:OE1	14:1S:43:GLU:N	6.03	0.56
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.86	0.56
1:2A:1685:U:H2'	1:2A:1686:C:H5''	1.86	0.56
1:2A:2704:A:H2'	1:2A:2705:G:H8	1.70	0.56
1:2A:2558:U:O2	10:2O:23:ARG:NH1	2.35	0.56
20:2Y:83:THR:HG21	20:2Y:99:CYS:HB2	1.87	0.56
1:1A:601:G:H2'	1:1A:602:C:C6	2.40	0.56
18:1W:18:ARG:HG3	18:1W:76:VAL:HB	1.88	0.56
1:2A:1067:G:N7	1:2A:1184:C:N4	2.54	0.56
1:2A:1820:C:H5''	1:2A:1821:A:OP1	2.06	0.56
1:2A:1873:C:H5'	3:2D:253:GLN:NE2	2.19	0.56
11:2P:19:VAL:HG12	11:2P:27:HIS:HB3	1.86	0.56
1:1A:550:A:O2'	1:1A:2064:C:O2	2.23	0.56
11:1P:113:LYS:NZ	59:1P:304:HOH:O	2.37	0.56
2:2B:50:G:OP1	14:2S:63:THR:N	2.38	0.56
21:2Z:134:PRO:O	21:2Z:136:PHE:N	2.36	0.56
1:1A:869:G:OP1	59:1A:4180:HOH:O	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:114:ILE:HA	6:1G:140:ILE:HD11	1.88	0.56
1:2A:2017:C:H4'	1:2A:2018:G:OP1	2.04	0.56
1:2A:2441:A:OP2	59:2A:3645:HOH:O	2.17	0.56
1:1A:1889:A:N6	1:1A:1904:G:O2'	2.39	0.56
8:1I:72:LEU:C	8:1I:74:ASN:H	2.07	0.56
1:2A:1154:C:H2'	1:2A:1155:G:C8	3.94	0.56
6:2G:37:VAL:HG22	6:2G:159:VAL:HB	1.88	0.56
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.23	0.56
24:12:29:LYS:HG2	24:12:57:ILE:HD13	1.86	0.56
1:1A:1426:G:C8	15:1T:118:ARG:HG2	88.41	0.56
12:1Q:118:LEU:HD12	12:1Q:131:ILE:HG23	1.86	0.56
2:2B:32:C:H2'	2:2B:33:G:O4'	2.05	0.56
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.69	0.56
5:1F:89:VAL:O	59:1F:401:HOH:O	2.18	0.56
1:2A:1638:G:H2'	1:2A:1639:G:C8	2.41	0.56
59:2A:3929:HOH:O	18:2W:11:ARG:HD3	2.04	0.56
1:1A:173:U:H4'	1:1A:206:A:H4'	1.88	0.56
1:1A:206:A:C2	1:1A:223:U:H4'	2.41	0.56
1:2A:1184:C:O3'	9:2N:25:ARG:NH1	2.39	0.56
1:2A:2091:G:H2'	1:2A:2092:A:H8	1.69	0.56
1:2A:2095:U:H2'	1:2A:2096:U:C6	2.41	0.56
1:2A:2641:G:H2'	1:2A:2642:G:C8	2.41	0.56
1:2A:2797:C:OP1	4:2E:41:LYS:NZ	2.29	0.56
1:2A:454:A:H3'	1:2A:455:A:H8	1.71	0.56
1:1A:2019:G:OP1	59:1A:4181:HOH:O	2.18	0.56
6:1G:129:GLY:O	6:1G:161:THR:HG22	2.05	0.56
1:2A:1098:C:H2'	1:2A:1099:A:H5'	1.87	0.56
1:2A:2043:U:O2'	1:2A:2628:C:H5'	2.06	0.56
1:1A:2824:C:H5'	27:15:29:THR:HG21	1.87	0.55
4:1E:111:ARG:HG3	4:1E:160:TYR:CD2	2.41	0.55
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.86	0.55
10:1O:18:LYS:HB2	10:1O:45:GLU:HB2	1.87	0.55
1:2A:976:G:H4'	1:2A:977:A:O5'	2.06	0.55
5:2F:20:LEU:HD13	5:2F:21:ALA:H	1.71	0.55
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.06	0.55
1:1A:1198:C:OP1	16:1U:92:ARG:NH1	2.38	0.55
1:1A:185:A:N6	1:1A:2441:A:O2'	2.39	0.55
1:1A:235:G:H4'	1:1A:412:G:C5	2.41	0.55
1:1A:2803:C:H2'	1:1A:2804:G:C8	2.41	0.55
11:1P:95:VAL:HG22	11:1P:125:VAL:HB	1.89	0.55
1:2A:1570:G:H2'	1:2A:1571:G:H8	1.70	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1741:G:N7	3:2D:14:ARG:NH2	2.49	0.55
1:2A:668:A:H4'	1:2A:669:C:C5	2.41	0.55
23:11:3:LYS:HB2	23:11:61:ARG:HH11	1.71	0.55
1:1A:1828:U:H5''	3:1D:260:ARG:HB3	1.89	0.55
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.71	0.55
1:1A:508:A:OP1	20:1Y:50:ARG:NH2	2.39	0.55
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.40	0.55
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.39	0.55
1:1A:1039:C:OP1	16:1U:53:ARG:NH2	2.39	0.55
1:1A:1054:A:OP2	9:1N:37:LYS:NZ	2.25	0.55
1:1A:1520:C:H2'	1:1A:1521:G:H8	1.69	0.55
1:1A:2761:A:OP1	7:1H:3:ARG:NH2	2.27	0.55
14:2S:99:LYS:NZ	14:2S:103:GLU:OE2	2.23	0.55
21:2Z:179:ASP:HB3	21:2Z:182:LYS:HB2	1.89	0.55
1:1A:2618:G:O6	59:1A:4167:HOH:O	2.16	0.55
12:1Q:60:ARG:H	12:1Q:60:ARG:NH1	2.04	0.55
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HB	1.87	0.55
1:1A:1248:A:H2	1:1A:1286:A:H62	1.54	0.55
1:1A:138:A:H8	1:1A:1453:C:O2'	1.89	0.55
1:1A:1475:C:H2'	1:1A:1476:U:C6	2.41	0.55
1:2A:1067:G:N2	1:2A:1068:U:O4	2.40	0.55
1:2A:2362:G:HO2'	1:2A:2363:A:H8	1.55	0.55
1:2A:2660:U:H2'	1:2A:2661:U:C6	2.42	0.55
2:2B:54:G:H21	6:2G:29:TRP:HZ2	1.54	0.55
16:2U:44:ASN:ND2	17:2V:75:PHE:HB3	2.21	0.55
21:2Z:152:ALA:O	21:2Z:155:LEU:HB2	2.06	0.55
1:1A:509:C:H2'	1:1A:510:C:C6	2.41	0.55
1:1A:628:U:H4'	1:1A:704:C:H4'	1.89	0.55
4:1E:54:GLN:HE21	4:1E:55:ASN:H	1.55	0.55
1:2A:1713:G:O2'	1:2A:2012:U:O4	2.14	0.55
1:2A:1174:A:N6	1:2A:2502:U:OP1	2.40	0.55
1:1A:1920:G:N3	1:1A:1920:G:H2'	2.21	0.55
1:1A:2347:A:H61	22:10:43:THR:CG2	2.19	0.55
1:1A:2800:C:O2'	1:1A:2818:A:N3	2.35	0.55
1:2A:1059:U:H2'	1:2A:1060:G:C8	2.42	0.55
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.72	0.55
4:2E:54:GLN:HE21	4:2E:58:ARG:HB2	1.72	0.55
26:14:63:TYR:N	26:14:64:GLY:HA2	2.20	0.55
1:2A:1403:G:N1	1:2A:1417:U:OP2	2.33	0.55
1:2A:56:G:O2'	1:2A:71:A:N1	2.35	0.55
1:2A:885:U:H2'	1:2A:886:C:H6	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:71:ASP:HB3	3:2D:103:ARG:NH2	2.21	0.55
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.89	0.55
1:1A:1603:C:OP2	1:1A:1604:A:O2'	2.18	0.55
1:2A:263:G:H2'	1:2A:264:U:C6	2.41	0.55
3:2D:20:ASP:N	3:2D:20:ASP:OD1	2.37	0.55
1:2A:2799:C:H1'	4:2E:62:PRO:HG3	1.89	0.55
7:2H:11:VAL:HG13	7:2H:15:VAL:HG22	1.87	0.55
1:1A:1425:G:O2'	1:1A:1426:G:OP1	4.91	0.54
1:1A:6:G:O6	59:1A:4174:HOH:O	2.17	0.54
1:1A:714:G:H5'	1:1A:715:G:OP2	2.07	0.54
12:1Q:59:ARG:HA	12:1Q:60:ARG:NH2	2.21	0.54
1:2A:1116:G:H1'	1:2A:1134:G:C8	2.41	0.54
1:2A:1833:A:H4'	3:2D:259:THR:HG23	1.89	0.54
1:2A:841:C:H2'	1:2A:842:C:C6	2.42	0.54
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.89	0.54
8:2I:120:ILE:HG21	8:2I:126:TYR:CE2	2.41	0.54
1:2A:1426:G:O2'	15:2T:122:ASP:OD2	93.50	0.54
26:14:26:SER:OG	26:14:27:THR:N	2.40	0.54
2:2B:83:G:H4'	25:23:52:HIS:CG	2.43	0.54
1:2A:483:G:C8	29:27:37:LYS:HG2	2.41	0.54
1:2A:1227:G:O3'	25:23:29:ARG:NH1	2.40	0.54
6:2G:103:LEU:HD23	6:2G:106:LEU:HD23	1.89	0.54
11:2P:88:LEU:HD11	11:2P:114:ILE:HD12	1.87	0.54
1:2A:661:A:H5''	11:2P:117:GLU:HG2	1.90	0.54
1:1A:1092:G:H1'	1:1A:1155:G:N2	2.21	0.54
1:1A:149:C:N3	1:1A:163:G:N1	5.78	0.54
1:2A:1154:C:H3'	1:2A:1155:G:C8	2.42	0.54
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.72	0.54
26:14:58:ARG:HB3	26:14:58:ARG:NH1	2.22	0.54
1:1A:1992:A:OP1	59:1A:4179:HOH:O	2.18	0.54
1:1A:2354:C:OP1	59:1A:4182:HOH:O	2.18	0.54
1:2A:1103:G:H2'	1:2A:1104:G:C8	2.42	0.54
1:2A:2735:C:H5''	13:2R:1:MET:HE3	1.89	0.54
1:2A:894:G:H2'	1:2A:895:A:C8	2.43	0.54
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.89	0.54
1:1A:2797:C:H2'	1:1A:2798:U:O4'	2.08	0.54
31:29:27:CYS:SG	31:29:28:GLU:N	2.81	0.54
1:2A:1457:A:H2'	1:2A:1458:G:C8	2.43	0.54
1:2A:555:C:H4'	1:2A:556:A:H5''	1.88	0.54
2:2B:114:C:H4'	14:2S:46:VAL:HG22	1.89	0.54
7:2H:3:ARG:NH2	7:2H:5:GLY:H	2.04	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1295:G:OP2	11:2P:21:ARG:NH1	2.40	0.54
1:1A:1066:A:H62	1:1A:1185:U:H3	1.55	0.54
1:2A:1906:A:H2'	1:2A:1907:C:O4'	2.08	0.54
1:2A:2304:C:H42	1:2A:2350:G:H1	1.55	0.54
1:2A:2815:G:H2'	1:2A:2816:G:H8	1.72	0.54
1:2A:26:G:N2	1:2A:536:G:H1'	2.23	0.54
16:2U:76:TYR:OH	16:2U:92:ARG:NH1	2.41	0.54
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.41	0.54
1:1A:1232:U:H4'	17:1V:79:VAL:HG22	1.89	0.54
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.27	0.54
9:2N:94:HIS:HB3	9:2N:97:ARG:HD3	1.90	0.54
15:2T:55:ASN:N	15:2T:59:THR:HG22	2.16	0.54
1:1A:2121:G:H1	1:1A:2210:U:H3	1.54	0.54
1:2A:2578:G:H2'	1:2A:2579:C:H6	1.73	0.54
6:2G:114:ILE:HB	6:2G:117:PHE:HB2	1.90	0.54
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.43	0.54
1:1A:1064:U:O2'	1:1A:1066:A:H2	1.91	0.54
1:1A:2210:U:H2'	1:1A:2211:G:C8	2.43	0.54
1:1A:2405:C:OP2	30:18:30:ARG:NH1	2.40	0.54
14:1S:23:ARG:NH2	14:1S:84:GLN:OE1	2.41	0.54
1:2A:1354:G:H4'	29:27:7:PRO:HB2	1.89	0.54
1:2A:681:G:H1	1:2A:696:C:N4	2.06	0.54
1:2A:895:A:H2	25:23:24:LYS:HB3	1.73	0.54
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.90	0.54
1:1A:1450:U:H2'	1:1A:1451:U:H6	1.73	0.54
1:1A:17:C:O2'	1:1A:576:U:OP1	2.20	0.54
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.08	0.54
19:2X:21:PHE:CZ	19:2X:92:LEU:HD12	2.43	0.54
1:1A:1409:G:P	23:11:3:LYS:HG3	2.49	0.53
29:17:5:TRP:NE1	29:17:7:PRO:HG3	2.23	0.53
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.90	0.53
13:1R:51:LEU:HD22	13:1R:66:VAL:HG22	1.89	0.53
15:1T:127:ALA:C	15:1T:129:ARG:H	2.12	0.53
1:2A:1942:G:H2'	1:2A:1943:G:H8	1.73	0.53
1:2A:2083:A:N7	1:2A:2514:A:N6	2.55	0.53
1:2A:483:G:O2'	1:2A:494:G:O6	2.16	0.53
15:2T:127:ALA:C	15:2T:129:ARG:H	2.11	0.53
1:1A:1220:G:H1'	1:1A:1221:A:C5'	2.37	0.53
1:1A:2404:A:OP2	59:1A:4183:HOH:O	2.18	0.53
3:1D:228:PRO:O	59:1D:401:HOH:O	2.18	0.53
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:405:G:N2	23:21:42:GLN:OE1	2.32	0.53
1:2A:1450:U:H2'	1:2A:1451:U:C6	2.43	0.53
1:2A:1768:G:H2'	1:2A:1769:A:C8	2.44	0.53
1:2A:2226:G:H3'	1:2A:2227:G:H8	1.74	0.53
1:2A:321:G:H5''	1:2A:322:A:OP1	2.08	0.53
1:2A:601:G:H2'	1:2A:602:C:C6	2.43	0.53
1:2A:663:U:H2'	1:2A:664:C:H6	1.72	0.53
1:2A:962:A:H5'	1:2A:963:A:OP2	2.08	0.53
18:2W:11:ARG:HD2	18:2W:82:LEU:HD12	1.89	0.53
29:17:24:THR:O	29:17:28:ARG:HG3	2.09	0.53
1:1A:1993:A:O2'	59:1A:4185:HOH:O	2.19	0.53
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.43	0.53
1:2A:1072:A:C2	1:2A:2499:A:H5'	2.44	0.53
1:2A:183:A:H5''	1:2A:184:A:O5'	2.06	0.53
7:2H:46:GLU:HB2	7:2H:49:VAL:HG12	1.90	0.53
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.90	0.53
24:12:32:LEU:HD13	24:12:36:ARG:HH11	1.73	0.53
2:1B:33:G:C2	2:1B:50:G:C2	2.97	0.53
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.09	0.53
16:1U:33:ARG:NH1	59:1U:5003:HOH:O	2.42	0.53
1:2A:332:G:N3	1:2A:352:G:O2'	2.41	0.53
3:2D:129:ASN:O	3:2D:193:VAL:HG12	2.07	0.53
11:2P:83:VAL:HG12	11:2P:112:LEU:HD21	1.91	0.53
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	1.90	0.53
59:1A:5041:HOH:O	13:1R:15:SER:HB3	2.07	0.53
2:1B:50:G:H5''	14:1S:61:ASN:HD22	1.73	0.53
15:1T:56:GLY:O	15:1T:59:THR:HG23	2.09	0.53
1:2A:909:A:H2'	1:2A:910:G:C8	2.44	0.53
1:2A:948:C:H2'	1:2A:949:C:C6	2.43	0.53
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.90	0.53
1:1A:1792:A:H2'	59:1A:6196:HOH:O	2.07	0.53
1:1A:2061:C:H2'	1:1A:2062:U:O4'	2.09	0.53
1:1A:2210:U:H2'	1:1A:2211:G:H8	1.72	0.53
1:1A:2307:U:OP2	14:1S:9:ARG:NH2	2.42	0.53
9:2N:36:GLY:HA2	9:2N:38:HIS:CE1	2.43	0.53
6:1G:109:VAL:HG13	26:14:33:VAL:HG11	1.90	0.53
1:1A:1158:U:H2'	1:1A:1159:G:C8	2.44	0.53
1:1A:1219:U:OP1	1:1A:1221:A:N6	2.42	0.53
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.43	0.53
26:24:24:THR:OG1	26:24:25:TYR:N	2.41	0.53
1:2A:2815:G:H2'	1:2A:2816:G:C8	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2302:U:OP1	1:1A:2391:C:O2'	2.22	0.53
4:1E:54:GLN:HB2	4:1E:76:ARG:HG3	1.91	0.53
1:2A:1638:G:H2'	1:2A:1639:G:H8	1.73	0.53
1:2A:2700:U:OP2	1:2A:2731:G:N2	2.39	0.53
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.91	0.53
1:1A:614:G:H2'	1:1A:615:G:C8	3.81	0.53
2:1B:66:A:H61	2:1B:108:U:H2'	1.74	0.53
1:1A:1992:A:OP2	3:1D:242:ARG:NH2	2.42	0.53
1:2A:1092:G:H1'	1:2A:1155:G:N2	2.24	0.53
1:1A:1066:A:H3'	1:1A:1066:A:C8	2.44	0.53
1:1A:2086:C:H2'	1:1A:2087:C:C6	2.44	0.53
1:1A:2878:G:H2'	1:1A:2879:C:O4'	2.09	0.53
3:1D:10:THR:OG1	3:1D:13:ARG:HB2	2.09	0.53
10:1O:35:VAL:HG21	10:1O:105:GLU:HG3	1.91	0.53
1:1A:2505:G:O2'	12:1Q:80:GLU:HA	2.09	0.53
21:1Z:180:VAL:HG13	21:1Z:183:LEU:HD12	1.90	0.53
1:2A:2115:G:H2'	1:2A:2116:C:H6	1.73	0.53
1:2A:2700:U:P	1:2A:2731:G:H22	2.32	0.53
1:1A:1218:A:H5'	1:1A:1221:A:H61	1.74	0.52
1:2A:830:A:H5'	1:2A:831:G:OP1	2.09	0.52
1:1A:1076:G:H21	31:19:36:GLN:HE22	1.57	0.52
1:1A:1826:U:H2'	1:1A:1827:C:C6	2.44	0.52
1:1A:2544:A:H2'	1:1A:2545:A:O4'	2.09	0.52
1:1A:448:A:OP2	59:1A:4135:HOH:O	2.19	0.52
1:2A:592:G:H2'	1:2A:2051:A:C5	2.44	0.52
1:2A:2117:U:H2'	1:2A:2118:C:C6	2.45	0.52
1:2A:656:A:H2'	1:2A:657:A:C8	2.44	0.52
1:1A:267:G:H5''	23:11:81:LYS:HE2	1.91	0.52
4:1E:54:GLN:HA	4:1E:54:GLN:HE21	1.75	0.52
25:23:6:VAL:HG22	25:23:56:VAL:HG12	1.92	0.52
1:2A:1109:C:N4	1:2A:1119:G:H1	2.00	0.52
1:2A:1373:G:H2'	1:2A:1375:C:C5	2.45	0.52
1:2A:670:A:H2'	1:2A:671:G:O4'	2.09	0.52
26:14:15:ILE:HD12	26:14:21:VAL:HG22	1.92	0.52
1:1A:1231:G:H5''	17:1V:81:TYR:CE1	2.44	0.52
1:1A:1416:G:H2'	1:1A:1417:U:H5	1.75	0.52
1:1A:903:C:H4'	22:10:23:VAL:HG21	1.91	0.52
15:1T:65:LYS:HE2	15:1T:67:SER:HB3	1.91	0.52
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.27	0.52
1:2A:1239:G:N2	1:2A:1240:C:C2	2.78	0.52
1:2A:405:G:O2'	1:2A:2243:U:OP1	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:775:G:C6	3:2D:208:LYS:HB2	2.44	0.52
1:2A:2848:G:H5'	13:2R:46:GLY:CA	2.36	0.52
1:1A:1869:G:C8	1:1A:1948:A:H1'	2.44	0.52
1:2A:1404:A:H2'	1:2A:1405:A:H5'	1.92	0.52
1:2A:2854:G:H2'	1:2A:2855:G:C8	2.45	0.52
1:2A:648:C:OP1	59:2A:3647:HOH:O	2.18	0.52
28:26:13:CYS:SG	28:26:47:THR:HG21	2.50	0.52
1:2A:2226:G:H5''	1:2A:2227:G:C8	2.45	0.52
1:2A:610:U:H2'	1:2A:611:C:C6	2.44	0.52
1:1A:1953:A:H2'	1:1A:1954:G:O4'	2.09	0.52
5:2F:197:ASP:O	5:2F:200:GLU:HB2	2.10	0.52
12:2Q:118:LEU:HD12	12:2Q:131:ILE:HG23	1.91	0.52
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.92	0.52
21:2Z:10:ARG:NH1	21:2Z:26:GLY:H	2.08	0.52
1:1A:1614:G:H5'	3:1D:60:ARG:HA	1.92	0.52
1:1A:877:G:O2'	11:1P:38:GLN:NE2	2.43	0.52
1:2A:1393:G:O6	1:2A:1394:A:N6	2.43	0.52
1:2A:554:G:N1	59:2A:3724:HOH:O	2.33	0.52
1:2A:724:C:H2'	1:2A:725:C:C6	2.45	0.52
1:2A:2601:A:O3'	3:2D:239:ARG:NH2	2.43	0.52
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.91	0.52
28:16:32:ASN:HB2	59:16:5009:HOH:O	2.10	0.52
1:1A:793:U:O2	1:1A:2035:A:H1'	2.09	0.52
1:2A:1093:A:N6	1:2A:1157:G:HO2'	2.06	0.52
1:2A:2026:A:H5''	1:2A:2027:C:OP2	2.09	0.52
1:2A:2284:A:H2'	1:2A:2285:A:H8	1.73	0.52
19:2X:21:PHE:HZ	19:2X:92:LEU:HD12	1.74	0.52
1:1A:224:C:H2'	1:1A:225:C:C6	2.45	0.52
1:1A:550:A:H2'	59:1A:4629:HOH:O	2.09	0.52
4:1E:29:GLY:HA3	59:1E:404:HOH:O	2.10	0.52
15:1T:55:ASN:N	15:1T:59:THR:HG22	2.18	0.52
1:2A:2411:G:H4'	28:26:18:ARG:HG2	1.92	0.52
1:2A:1573:A:OP2	59:2A:3649:HOH:O	2.19	0.52
1:2A:15:G:H2'	1:2A:16:G:H8	1.74	0.52
1:2A:1703:C:H2'	1:2A:1704:C:C6	2.45	0.52
1:2A:267:G:O2'	1:2A:268:G:H8	1.93	0.52
1:1A:1717:U:OP2	59:1A:4184:HOH:O	2.19	0.51
1:1A:1799:G:O2'	1:1A:1979:C:OP1	2.23	0.51
1:1A:404:C:O2'	59:1A:4147:HOH:O	2.13	0.51
1:2A:1102:A:H62	1:2A:1131:A:H2'	1.74	0.51
1:2A:1397:U:OP2	59:2A:3650:HOH:O	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:237:C:O2	30:28:12:LYS:NZ	2.32	0.51
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.43	0.51
16:2U:83:LEU:HG	16:2U:88:ILE:HB	1.91	0.51
1:1A:1734:U:O2	1:1A:1746:A:H5'	2.10	0.51
1:1A:77:G:H4'	1:1A:78:G:OP1	4.87	0.51
1:1A:894:G:H2'	1:1A:895:A:C8	2.46	0.51
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.45	0.51
2:2B:45:A:C8	6:2G:95:ARG:NH1	2.78	0.51
7:2H:40:GLU:OE2	7:2H:60:ARG:NH1	2.43	0.51
1:1A:1510:C:H2'	1:1A:1511:G:C8	2.46	0.51
1:1A:1512:G:H2'	1:1A:1593:C:H41	1.76	0.51
1:1A:2052:A:C6	1:1A:2509:C:H1'	2.45	0.51
7:1H:157:TYR:CE1	7:1H:172:LYS:HG3	2.46	0.51
9:1N:13:TRP:HB3	9:1N:135:PRO:HB3	1.90	0.51
29:27:24:THR:O	29:27:28:ARG:HG3	2.10	0.51
1:2A:26:G:O2'	1:2A:27:A:OP2	2.24	0.51
1:2A:671:G:O5'	1:2A:671:G:H8	1.93	0.51
1:2A:704:C:H2'	1:2A:705:C:C6	2.45	0.51
26:14:53:GLU:CB	26:14:54:GLY:HA2	2.40	0.51
31:19:27:CYS:SG	31:19:28:GLU:N	2.84	0.51
1:1A:468:A:H1'	1:1A:1245:C:O4'	2.10	0.51
1:1A:266:C:H3'	59:1A:4245:HOH:O	2.10	0.51
1:1A:2858:U:H4'	1:1A:2877:A:C2	2.45	0.51
1:1A:876:G:OP2	59:1A:4187:HOH:O	2.19	0.51
1:1A:1200:A:OP1	16:1U:55:ARG:HD3	2.10	0.51
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG13	1.93	0.51
1:2A:1346:A:H2	1:2A:1671:G:N3	2.08	0.51
1:2A:1967:U:H2'	1:2A:1968:C:C6	2.45	0.51
1:2A:2043:U:OP2	27:25:15:ARG:NH2	2.44	0.51
1:2A:2302:U:H2'	1:2A:2303:C:C6	2.46	0.51
1:1A:830:A:H5'	1:1A:831:G:OP1	2.10	0.51
7:1H:101:ARG:NH2	7:1H:122:THR:OG1	2.41	0.51
12:1Q:57:HIS:HD2	12:1Q:117:ALA:HB2	1.76	0.51
1:2A:2347:A:H61	22:20:43:THR:HG22	1.75	0.51
1:2A:843:C:OP1	5:2F:60:SER:OG	2.24	0.51
2:2B:24:G:N2	2:2B:27:C:N3	2.45	0.51
3:2D:242:ARG:N	3:2D:242:ARG:HD3	2.26	0.51
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.91	0.51
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.92	0.51
1:1A:1092:G:H1'	1:1A:1155:G:H22	1.76	0.51
20:1Y:92:ASN:CB	20:1Y:94:LYS:H	2.22	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:22:24:LEU:HG	24:22:28:LYS:HD3	1.93	0.51
1:2A:94:G:H4'	24:22:48:HIS:CD2	2.46	0.51
1:2A:1833:A:O2'	3:2D:259:THR:HG21	2.10	0.51
1:2A:350:G:N2	20:2Y:70:SER:OG	2.43	0.51
1:2A:555:C:OP1	1:2A:583:G:N1	2.43	0.51
1:2A:972:G:H2'	1:2A:973:G:O4'	2.10	0.51
2:2B:19:G:H1	2:2B:64:C:N4	2.09	0.51
1:1A:184:A:H62	11:1P:38:GLN:HE22	1.59	0.51
1:2A:2443:A:C6	1:2A:2444:A:C6	2.99	0.51
1:2A:1715:A:H5''	1:2A:2561:G:OP1	2.10	0.51
1:2A:754:C:H42	1:2A:769:G:H1	1.56	0.51
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.92	0.51
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.93	0.51
1:1A:1073:A:H61	1:1A:1170:G:H2'	1.76	0.51
1:1A:1924:G:OP1	3:1D:241:PRO:HB2	2.10	0.51
1:1A:1072:A:C2	1:1A:2499:A:H5'	2.45	0.51
1:1A:924:A:H2'	1:1A:925:G:C8	4.92	0.51
6:1G:143:GLU:O	26:14:28:LYS:NZ	2.34	0.51
1:2A:1073:A:N6	1:2A:1170:G:H2'	2.25	0.51
1:2A:1083:C:N4	1:2A:1162:G:H1	2.01	0.51
1:2A:1327:U:H2'	1:2A:1328:G:O4'	2.11	0.51
1:2A:1369:G:O6	59:2A:3638:HOH:O	2.16	0.51
1:2A:2309:A:H2'	1:2A:2310:G:O4'	2.10	0.51
1:2A:2359:U:O4	1:2A:2393:G:N1	2.44	0.51
1:2A:703:U:H2'	1:2A:704:C:C6	2.45	0.51
3:2D:126:GLN:HE21	3:2D:127:VAL:H	1.59	0.51
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.93	0.51
21:2Z:54:HIS:CG	21:2Z:101:PRO:HG3	2.46	0.51
1:1A:143:C:H5'	19:1X:2:LYS:HD2	1.92	0.51
1:1A:2828:G:OP1	59:1A:4186:HOH:O	2.19	0.51
3:1D:9:TYR:CZ	3:1D:13:ARG:HG2	2.46	0.51
11:1P:88:LEU:HD11	11:1P:114:ILE:HD12	1.91	0.51
1:2A:1424:A:H4'	1:2A:1425:G:OP2	2.09	0.51
31:19:26:ILE:H	31:19:26:ILE:HD13	1.75	0.51
1:1A:10:G:H2'	1:1A:11:U:H5''	1.92	0.51
1:1A:2033:G:OP1	18:1W:11:ARG:NH2	2.34	0.51
14:1S:15:ARG:NE	14:1S:88:ASP:OD2	2.37	0.51
1:2A:1070:G:N2	1:2A:1082:G:H1'	29.74	0.51
1:2A:1513:C:C5	1:2A:1592:C:H2'	2.46	0.51
1:2A:1942:G:H2'	1:2A:1943:G:C8	2.46	0.51
1:2A:2845:U:H2'	1:2A:2846:G:C8	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:900:G:H2'	1:2A:901:G:C8	2.40	0.51
5:2F:135:LYS:HG2	5:2F:137:LYS:HG2	1.93	0.51
1:2A:1711:A:H4'	10:2O:67:LYS:HB2	1.93	0.51
2:1B:25:A:OP1	59:1B:304:HOH:O	2.19	0.50
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.76	0.50
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.45	0.50
12:1Q:1:MET:SD	12:1Q:1:MET:N	2.69	0.50
1:2A:238:G:C6	1:2A:239:A:C6	2.99	0.50
1:2A:2416:G:H5'	11:2P:75:ILE:HD13	1.92	0.50
2:2B:72:G:O2'	2:2B:105:A:N6	2.44	0.50
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.94	0.50
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.43	0.50
1:1A:239:A:C5	1:1A:240:G:H1'	2.45	0.50
1:1A:1614:G:H4'	3:1D:59:LYS:HG2	1.93	0.50
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.94	0.50
28:26:21:TYR:CE1	28:26:38:LYS:HG2	2.46	0.50
11:2P:63:PRO:O	30:28:13:ARG:HB2	2.12	0.50
1:2A:1682:C:H2'	1:2A:1683:A:C8	2.46	0.50
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.11	0.50
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.44	0.50
11:1P:49:ARG:NH1	30:18:61:LEU:HD23	2.26	0.50
1:1A:141:G:H2'	1:1A:142:C:C6	2.47	0.50
1:1A:1694:C:OP1	59:1A:4156:HOH:O	2.19	0.50
1:1A:2862:C:H2'	1:1A:2863:G:C8	2.46	0.50
1:1A:26:G:N2	1:1A:536:G:H1'	2.26	0.50
20:1Y:13:VAL:HG12	20:1Y:74:PRO:HA	1.94	0.50
24:22:1:MET:SD	24:22:56:GLN:NE2	2.84	0.50
1:2A:1104:G:H3'	1:2A:1105:U:H6	1.74	0.50
1:2A:1826:U:H2'	1:2A:1827:C:C6	2.46	0.50
1:2A:346:G:O2'	1:2A:1249:U:N3	2.43	0.50
1:2A:757:G:O3'	3:2D:202:LYS:NZ	44.04	0.50
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.91	0.50
1:1A:1091:A:H3'	1:1A:1092:G:H5'	1.93	0.50
1:1A:2819:A:N6	1:1A:2899:G:O2'	2.45	0.50
1:1A:517:G:H2'	1:1A:518:G:O4'	2.11	0.50
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.45	0.50
7:1H:159:GLU:HG3	7:1H:169:VAL:HG11	1.93	0.50
1:2A:78:G:H1	1:2A:103:C:N4	2.09	0.50
1:2A:504:A:N3	1:2A:506:G:H5''	2.27	0.50
1:2A:898:G:H2'	1:2A:899:G:C8	2.46	0.50
5:2F:129:PHE:O	5:2F:132:VAL:HG13	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:60:ARG:NH2	21:2Z:181:GLU:OE2	2.31	0.50
1:1A:2283:U:H5''	1:1A:2284:A:OP1	2.12	0.50
1:1A:829:A:OP2	59:1A:4129:HOH:O	2.20	0.50
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.93	0.50
1:2A:211:A:O2'	1:2A:446:C:O2	2.29	0.50
1:2A:2805:G:N2	1:2A:2814:C:H1'	2.27	0.50
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.92	0.50
1:1A:680:C:H2'	1:1A:681:G:O4'	2.11	0.50
1:1A:703:U:H2'	1:1A:704:C:C6	2.47	0.50
8:1I:1:MET:N	8:1I:20:ASP:OD1	2.41	0.50
20:1Y:38:ILE:HD13	20:1Y:66:PRO:HA	1.94	0.50
1:2A:858:C:H2'	1:2A:859:U:H6	1.77	0.50
2:2B:24:G:H4'	2:2B:25:A:C8	2.47	0.50
6:2G:77:ILE:HG22	6:2G:80:PHE:H	1.77	0.50
1:1A:1626:A:H8	1:1A:1626:A:OP2	1.95	0.50
1:1A:2862:C:H2'	1:1A:2863:G:H8	1.75	0.50
1:1A:598:U:H2'	1:1A:599:G:C8	2.46	0.50
1:1A:989:A:H8	59:1A:5971:HOH:O	1.93	0.50
16:1U:36:ARG:HD2	16:1U:40:PHE:CZ	2.47	0.50
1:2A:1548:U:H2'	1:2A:1549:C:C6	2.47	0.50
1:2A:2205:G:H2'	1:2A:2206:C:C6	2.47	0.50
1:2A:2554:G:H2'	1:2A:2555:G:C8	2.46	0.50
1:2A:706:G:H5'	5:2F:99:TYR:CE2	2.47	0.50
15:2T:27:THR:HB	15:2T:89:VAL:HG22	1.94	0.50
19:2X:11:PRO:HB3	19:2X:92:LEU:HD21	1.92	0.50
25:13:29:ARG:HG3	25:13:30:ARG:HG3	1.93	0.50
1:1A:6:G:H2'	1:1A:7:A:O4'	2.12	0.50
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.94	0.50
14:1S:33:LYS:HB3	14:1S:34:HIS:CD2	2.47	0.50
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.94	0.50
26:24:59:PHE:HA	26:24:61:ARG:N	2.27	0.50
1:2A:1059:U:H2'	1:2A:1060:G:H8	1.77	0.50
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.76	0.50
1:2A:22:G:H2'	1:2A:23:G:C8	3.27	0.50
1:2A:29:G:H2'	1:2A:30:C:C6	2.46	0.50
1:2A:841:C:H2'	1:2A:842:C:H6	1.75	0.50
1:2A:948:C:H2'	1:2A:949:C:H6	1.77	0.50
3:2D:134:ARG:NH1	3:2D:188:GLU:OE2	2.44	0.50
17:2V:31:ALA:O	17:2V:61:VAL:HG12	2.10	0.50
1:1A:2563:U:C2	1:1A:2565:U:H5'	2.47	0.50
1:1A:885:U:H1'	1:1A:1235:G:H1'	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:108:GLY:HA3	21:1Z:116:VAL:HG13	1.93	0.50
26:24:26:SER:OG	26:24:27:THR:N	2.44	0.50
1:2A:2575:A:C2	1:2A:2658:U:H4'	2.47	0.50
1:2A:644:G:N3	1:2A:644:G:H5'	2.26	0.50
1:2A:661:A:H2'	11:2P:117:GLU:OE2	2.11	0.50
1:2A:751:A:H2'	1:2A:752:A:O4'	2.15	0.50
1:2A:821:G:N2	1:2A:840:G:H5'	2.26	0.50
5:2F:117:ARG:HH12	11:2P:1:MET:N	2.10	0.50
6:2G:11:TYR:O	6:2G:16:ARG:HG3	2.12	0.50
12:2Q:108:GLY:HA3	21:2Z:116:VAL:HG13	1.94	0.50
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.94	0.50
1:1A:2623:C:OP2	27:15:2:ALA:N	2.45	0.49
1:1A:171:C:H2'	1:1A:172:C:C6	3.30	0.49
1:1A:2044:G:H5'	1:1A:2628:C:H4'	1.94	0.49
1:1A:859:U:H2'	1:1A:860:C:C6	2.46	0.49
1:1A:928:G:N7	59:1A:4328:HOH:O	2.34	0.49
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.94	0.49
7:1H:144:VAL:O	7:1H:148:ILE:HG12	2.12	0.49
1:1A:1295:G:OP2	11:1P:21:ARG:NH1	2.43	0.49
1:2A:1262:C:H42	1:2A:1276:G:H1	1.60	0.49
1:2A:2641:G:H2'	1:2A:2642:G:H8	1.77	0.49
1:2A:779:G:N7	59:2A:3713:HOH:O	2.34	0.49
19:2X:36:LYS:HA	19:2X:39:ILE:HD12	1.92	0.49
26:14:58:ARG:O	26:14:60:GLN:N	2.45	0.49
1:1A:258:A:C6	1:1A:259:A:C6	3.83	0.49
1:1A:2901:G:N2	59:1A:4418:HOH:O	2.41	0.49
3:1D:164:GLN:NE2	3:1D:176:ARG:HH12	2.09	0.49
19:1X:31:HIS:CD2	19:1X:33:LYS:HB2	2.46	0.49
22:20:32:ARG:H	22:20:35:ASN:ND2	2.10	0.49
23:21:22:GLY:O	23:21:32:LYS:NZ	2.45	0.49
25:23:8:LEU:HD13	25:23:31:LEU:HD23	1.93	0.49
1:2A:2297:A:H4'	1:2A:2298:A:O4'	2.12	0.49
6:2G:73:ALA:HB3	6:2G:85:GLY:H	1.76	0.49
1:1A:2083:A:C2	1:1A:2514:A:N6	2.80	0.49
1:1A:675:G:OP1	30:18:19:SER:OG	2.24	0.49
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	1.95	0.49
1:2A:1406:G:H2'	1:2A:1407:C:C6	2.97	0.49
1:2A:2219:A:O2'	1:2A:2235:G:N2	2.45	0.49
1:2A:2568:G:H2'	1:2A:2569:C:C6	2.47	0.49
1:2A:766:C:H2'	1:2A:767:C:C6	2.47	0.49
9:2N:14:VAL:HG13	9:2N:138:LEU:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1416:G:H2'	1:1A:1417:U:C5	2.48	0.49
1:1A:207:G:OP2	59:1A:4189:HOH:O	2.20	0.49
12:1Q:21:THR:HG21	12:1Q:101:ARG:N	2.27	0.49
20:2Y:94:LYS:NZ	59:2Y:601:HOH:O	2.45	0.49
1:1A:1070:G:C4	1:1A:1179:C:H1'	2.48	0.49
1:1A:867:A:H2'	1:1A:990:G:H5''	1.94	0.49
5:1F:140:LEU:HD21	5:1F:170:LEU:HD11	1.93	0.49
21:1Z:24:LEU:HB2	21:1Z:41:LEU:HD23	1.94	0.49
1:2A:1225:C:H2'	1:2A:1226:A:H8	1.78	0.49
1:2A:1475:C:H2'	1:2A:1476:U:C6	2.47	0.49
1:2A:1643:C:H2'	1:2A:1644:C:H6	1.76	0.49
1:2A:1910:A:H2'	1:2A:1911:A:H8	1.76	0.49
1:2A:1920:G:N3	1:2A:1920:G:H2'	2.28	0.49
1:1A:1899:G:H2'	1:1A:1900:C:C6	2.47	0.49
1:1A:2107:U:H2'	1:1A:2108:G:C8	2.47	0.49
6:1G:73:ALA:HB3	6:1G:85:GLY:H	1.77	0.49
9:1N:61:ARG:HA	9:1N:61:ARG:HE	1.78	0.49
1:2A:8:U:H3	1:2A:2640:A:H2	1.59	0.49
1:1A:121:G:OP1	1:1A:1421:C:O2'	2.17	0.49
1:1A:161:G:H2'	1:1A:162:C:C6	2.48	0.49
1:1A:352:G:O6	20:1Y:19:LYS:N	2.37	0.49
1:1A:670:A:H2'	1:1A:671:G:O4'	2.13	0.49
4:1E:8:LYS:NZ	4:1E:188:VAL:O	2.45	0.49
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	1.95	0.49
1:2A:1102:A:N6	1:2A:1131:A:H2'	2.27	0.49
1:2A:531:A:H4'	1:2A:532:G:O5'	3.86	0.49
1:2A:863:C:O2'	1:2A:885:U:H5''	2.13	0.49
1:2A:910:G:C6	1:2A:911:C:N4	2.81	0.49
6:2G:64:THR:HB	6:2G:94:LEU:HD11	1.95	0.49
2:1B:76:G:O6	59:1B:303:HOH:O	2.18	0.49
13:1R:21:TYR:OH	13:1R:43:GLU:HG2	2.13	0.49
1:2A:1047:G:H2'	1:2A:1048:G:O4'	2.13	0.49
1:2A:2370:C:H2'	1:2A:2371:A:O4'	2.12	0.49
1:2A:993:C:N4	59:2A:3761:HOH:O	2.45	0.49
1:1A:2622:U:C4	27:15:3:LYS:HG2	2.48	0.49
1:1A:152:C:OP2	23:11:92:LYS:NZ	2.46	0.49
1:1A:2800:C:OP1	4:1E:61:ARG:NH2	2.45	0.49
6:1G:41:GLN:NE2	6:1G:153:ARG:HB3	2.27	0.49
12:1Q:22:LYS:N	59:1Q:5002:HOH:O	2.46	0.49
1:2A:1116:G:H1	1:2A:1124:C:N4	15.98	0.49
1:2A:1369:G:C2	1:2A:1376:A:C2	3.00	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1915:C:H2'	1:2A:1916:C:H6	1.76	0.49
1:2A:200:G:H2'	1:2A:201:A:O4'	2.13	0.49
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.28	0.49
1:1A:309:C:H2'	1:1A:310:C:C6	2.48	0.49
1:1A:69:A:N7	19:1X:31:HIS:HE1	2.10	0.49
19:1X:60:ARG:NH2	29:17:47:ARG:HH22	2.11	0.49
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.45	0.49
26:24:16:CYS:SG	26:24:17:GLY:N	2.86	0.49
1:2A:1231:G:H8	1:2A:1231:G:OP2	1.96	0.49
1:2A:1379:G:OP2	59:2A:3648:HOH:O	2.19	0.49
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.94	0.49
1:1A:1076:G:H5''	31:19:8:LYS:HE3	1.94	0.48
1:1A:1073:A:N6	1:1A:1170:G:H2'	2.27	0.48
8:1I:104:GLN:O	8:1I:106:GLY:N	2.45	0.48
1:2A:2088:G:O2'	1:2A:2090:G:H5''	2.13	0.48
1:2A:2646:C:O2'	4:2E:48:GLN:NE2	2.44	0.48
1:2A:353:A:HO2'	1:2A:354:A:H8	1.59	0.48
1:2A:494:G:N7	29:27:37:LYS:NZ	2.55	0.48
1:2A:786:U:H2'	1:2A:787:G:C8	2.48	0.48
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.49	0.48
5:2F:46:ARG:HH11	5:2F:46:ARG:HB3	3.58	0.48
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.13	0.48
1:1A:1410:A:O4'	23:11:41:ARG:NH2	2.46	0.48
1:1A:2254:U:H2'	1:1A:2255:U:C6	2.48	0.48
1:1A:2290:G:N7	22:10:14:ARG:NH1	2.61	0.48
1:1A:2578:G:H2'	1:1A:2579:C:C6	2.48	0.48
1:1A:211:A:O2'	1:1A:446:C:O2	2.26	0.48
1:1A:964:G:N2	1:1A:2280:A:OP2	2.46	0.48
1:2A:2375:C:OP1	22:20:55:ARG:NH1	2.45	0.48
1:2A:2386:G:N2	1:2A:2389:A:OP2	2.40	0.48
26:14:57:GLU:HA	26:14:58:ARG:HA	1.56	0.48
1:1A:2896:U:H2'	1:1A:2897:C:C6	2.48	0.48
1:1A:35:G:N3	1:1A:475:G:O2'	2.45	0.48
1:2A:1000:G:H2'	1:2A:1001:A:H2'	1.94	0.48
1:2A:149:C:H2'	1:2A:150:C:H6	2.06	0.48
1:2A:1856:G:H4'	3:2D:242:ARG:NH1	2.29	0.48
24:12:2:LYS:O	24:12:6:VAL:HG23	2.14	0.48
1:1A:1217:G:H22	1:1A:1221:A:P	2.37	0.48
1:1A:1659:A:OP1	1:1A:1662:C:N4	2.46	0.48
1:1A:2249:G:H2'	1:1A:2249:G:N3	2.28	0.48
1:1A:271:U:OP1	8:1I:50:ARG:NH2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:720:G:H1'	5:1F:74:ARG:HD3	1.96	0.48
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.12	0.48
23:21:19:GLN:HB3	23:21:35:THR:HG23	1.95	0.48
5:2F:7:TYR:O	5:2F:22:ALA:N	2.46	0.48
7:2H:42:ARG:HH11	7:2H:42:ARG:HB3	1.77	0.48
14:2S:35:ILE:HG12	14:2S:97:ARG:HH21	1.78	0.48
1:1A:2542:A:H5''	7:1H:157:TYR:CZ	2.47	0.48
1:1A:558:U:H2'	1:1A:559:C:C6	2.48	0.48
9:1N:73:THR:HG23	9:1N:82:LEU:HD11	1.96	0.48
1:1A:1056:G:OP1	16:1U:77:SER:OG	2.30	0.48
22:20:27:GLU:HB2	22:20:69:PHE:HD1	1.78	0.48
29:27:8:ASN:HB3	29:27:11:LYS:HB3	1.94	0.48
1:2A:1077:A:H2	1:2A:1167:G:H22	1.61	0.48
1:2A:1323:A:H2'	1:2A:1324:G:C8	2.48	0.48
1:2A:241:C:OP2	30:28:5:LYS:NZ	2.37	0.48
1:2A:235:G:H4'	1:2A:412:G:C5	2.49	0.48
1:2A:57:U:H2'	1:2A:58:G:H8	5.29	0.48
1:2A:967:U:H2'	1:2A:968:C:C6	2.49	0.48
6:2G:43:LEU:HB3	6:2G:44:GLY:H	1.47	0.48
16:2U:86:ALA:HB2	16:2U:116:ALA:HB2	1.95	0.48
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.48	0.48
30:18:6:THR:HB	30:18:8:LYS:HE2	1.95	0.48
1:1A:1224:C:H2'	1:1A:1225:C:C6	2.48	0.48
1:1A:141:G:H2'	1:1A:142:C:H6	1.79	0.48
1:1A:2601:A:H5''	3:1D:239:ARG:HG3	1.96	0.48
10:1O:16:ALA:HB2	10:1O:52:VAL:HG21	1.95	0.48
28:26:11:LEU:HB2	28:26:21:TYR:HB2	1.94	0.48
1:2A:1076:G:H21	31:29:36:GLN:HE22	1.61	0.48
1:2A:2328:C:N4	1:2A:2329:G:O6	2.47	0.48
1:2A:2574:U:O2	1:2A:2576:A:H8	1.97	0.48
1:2A:309:C:H2'	1:2A:310:C:C6	2.49	0.48
1:2A:440:C:O2'	1:2A:441:A:H5'	2.13	0.48
1:2A:1856:G:H4'	3:2D:242:ARG:CZ	2.44	0.48
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.77	0.48
6:2G:97:ASP:O	6:2G:101:ILE:HG13	2.13	0.48
21:2Z:5:LEU:HD13	21:2Z:47:VAL:HG21	1.95	0.48
1:1A:2873:G:OP1	15:1T:119:LYS:HD2	2.14	0.48
1:1A:307:U:H2'	1:1A:308:C:C6	2.49	0.48
1:2A:1403:G:O2'	1:2A:1404:A:H5''	2.12	0.48
1:2A:1480:G:H2'	1:2A:1481:G:O4'	2.14	0.48
1:2A:2477:C:H5''	31:29:6:SER:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:338:G:H2'	1:2A:339:C:C6	2.48	0.48
8:2I:72:LEU:HA	8:2I:75:LEU:HD22	1.96	0.48
1:1A:1735:A:N6	1:1A:1744:A:H2	2.05	0.48
1:1A:2863:G:H2'	1:1A:2864:C:C6	2.49	0.48
1:1A:825:U:P	1:1A:825:U:H6	3.48	0.48
1:1A:931:C:H3'	1:1A:932:C:H5''	1.96	0.48
1:2A:172:C:H2'	1:2A:173:U:C6	2.49	0.48
1:2A:1765:G:H8	1:2A:1769:A:H62	1.60	0.48
1:2A:2465:G:H1'	59:2A:3693:HOH:O	2.13	0.48
1:2A:2480:A:H2'	1:2A:2481:G:O4'	2.13	0.48
1:2A:26:G:HO2'	1:2A:27:A:P	2.34	0.48
1:2A:2801:C:O2	1:2A:2902:G:N2	2.46	0.48
6:2G:114:ILE:HD12	6:2G:117:PHE:CD2	2.48	0.48
10:2O:98:VAL:HG11	10:2O:114:ILE:HG23	1.95	0.48
1:2A:1297:G:N3	16:2U:33:ARG:HG2	2.28	0.48
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.95	0.48
1:1A:1548:U:H2'	1:1A:1549:C:C6	2.49	0.48
1:1A:955:A:N3	1:1A:2275:C:O2'	2.38	0.48
2:1B:65:C:H2'	59:1B:312:HOH:O	2.14	0.48
3:1D:37:LEU:HD13	3:1D:62:TYR:HB2	1.95	0.48
4:1E:9:VAL:HG13	4:1E:25:VAL:O	2.14	0.48
7:1H:11:VAL:HG13	7:1H:15:VAL:HG22	1.95	0.48
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.49	0.48
1:2A:84:C:H4'	1:2A:101:U:H1'	1.95	0.48
1:2A:2095:U:O4	59:2A:3651:HOH:O	2.19	0.48
1:2A:2691:C:OP2	4:2E:111:ARG:NH2	2.46	0.48
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.49	0.48
6:2G:173:LEU:HB3	6:2G:178:PHE:CG	2.48	0.48
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.47	0.48
1:1A:171:C:H2'	1:1A:172:C:H6	2.49	0.48
1:1A:1878:A:H2'	1:1A:1879:G:H8	1.79	0.48
1:1A:2095:U:H2'	1:1A:2096:U:C6	2.49	0.48
1:1A:955:A:N1	1:1A:2288:G:H1'	2.29	0.48
1:1A:2555:G:H1'	1:1A:2657:C:H4'	1.96	0.48
1:1A:439:C:O2	1:1A:475:G:N2	74.48	0.48
1:1A:8:U:N3	1:1A:2640:A:C2	2.82	0.48
11:1P:81:GLN:NE2	11:1P:105:LEU:O	2.47	0.48
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.95	0.48
1:2A:1529:G:C6	1:2A:1530:G:C5	3.02	0.48
1:2A:55:C:H2'	1:2A:56:G:O4'	2.14	0.48
2:2B:106:G:OP1	21:2Z:31:ARG:HG2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1475:C:H2'	1:1A:1476:U:H6	1.79	0.47
1:1A:2053:G:O2'	4:1E:145:LYS:HE3	2.14	0.47
1:1A:2554:G:H2'	1:1A:2555:G:C8	2.48	0.47
15:1T:11:GLU:OE1	15:1T:57:PHE:HB3	2.14	0.47
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.95	0.47
21:1Z:41:LEU:HD21	21:1Z:83:PRO:HG2	1.96	0.47
1:2A:1114:A:H4'	1:2A:1115:A:H5''	1.95	0.47
1:2A:1465:U:O2'	1:2A:1466:G:OP1	2.29	0.47
1:2A:2022:A:H2'	1:2A:2023:G:C8	2.49	0.47
4:2E:34:VAL:HG21	4:2E:78:LEU:HD11	1.96	0.47
15:2T:106:SER:O	15:2T:110:ILE:HG13	2.14	0.47
20:2Y:38:ILE:HD13	20:2Y:66:PRO:HA	1.95	0.47
1:1A:1402:U:H2'	1:1A:1403:G:O4'	2.15	0.47
1:1A:1409:G:OP2	23:11:3:LYS:HG3	2.14	0.47
1:1A:1457:A:H2'	1:1A:1458:G:C8	2.49	0.47
1:1A:1802:G:OP1	59:1A:4193:HOH:O	2.20	0.47
3:1D:37:LEU:HD22	3:1D:87:ASN:ND2	2.29	0.47
1:1A:346:G:C8	5:1F:171:PRO:HG3	2.49	0.47
8:1I:72:LEU:O	8:1I:74:ASN:N	2.47	0.47
14:1S:63:THR:OG1	14:1S:64:GLU:N	4.39	0.47
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.29	0.47
1:2A:127:C:H4'	1:2A:258:A:H1'	60.42	0.47
1:2A:2548:U:N3	1:2A:2549:C:C4	2.83	0.47
1:2A:2565:U:H2'	1:2A:2566:U:C6	2.48	0.47
4:2E:48:GLN:HA	4:2E:80:GLU:HA	1.96	0.47
1:2A:344:G:H5'	5:2F:134:GLY:O	2.14	0.47
6:2G:47:LYS:HB3	6:2G:48:GLU:H	1.39	0.47
13:2R:13:HIS:CE1	13:2R:16:HIS:HB2	2.48	0.47
1:1A:1845:A:H8	1:1A:1845:A:OP1	1.97	0.47
1:1A:2302:U:H2'	1:1A:2303:C:C6	2.49	0.47
1:1A:2458:G:O2'	1:1A:2511:U:OP2	2.28	0.47
1:1A:2583:A:N7	4:1E:144:ARG:HD2	2.29	0.47
1:1A:2640:A:O2'	1:1A:2641:G:OP2	2.24	0.47
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.46	0.47
11:1P:121:LYS:HG2	11:1P:122:PRO:HD2	1.96	0.47
25:23:9:VAL:HG12	25:23:32:GLN:HE22	1.79	0.47
30:28:54:GLU:O	30:28:58:ILE:HG13	2.15	0.47
1:2A:2218:U:H1'	1:2A:2219:A:C8	2.49	0.47
1:2A:898:G:H2'	1:2A:899:G:H8	1.77	0.47
6:2G:106:LEU:O	6:2G:111:LEU:HD22	2.14	0.47
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:323:A:P	20:2Y:86:ARG:HH21	2.38	0.47
1:1A:1552:A:O2'	1:1A:1553:A:H8	1.97	0.47
1:1A:2206:C:O2'	1:1A:2207:G:H5'	2.14	0.47
1:1A:1856:G:H4'	3:1D:242:ARG:CZ	2.44	0.47
14:1S:15:ARG:O	14:1S:19:LYS:HG3	2.14	0.47
1:2A:100:A:H5'	24:22:3:LEU:HD11	1.97	0.47
1:2A:1050:C:C2	1:2A:1188:A:C5	3.01	0.47
1:2A:1121:C:H3'	1:2A:1122:A:H8	1.78	0.47
1:2A:2670:G:N2	1:2A:2672:G:H3'	2.30	0.47
3:2D:16:MET:HG3	3:2D:206:LEU:O	2.14	0.47
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	1.96	0.47
1:1A:1827:C:H4'	3:1D:257:LEU:O	2.15	0.47
1:1A:2020:C:H4'	1:1A:2735:C:O2	2.15	0.47
1:1A:2086:C:H2'	1:1A:2087:C:H6	1.79	0.47
1:1A:1715:A:H5''	1:1A:2561:G:OP1	2.14	0.47
2:1B:28:C:H2'	2:1B:29:A:O4'	2.14	0.47
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.49	0.47
23:21:65:SER:OG	23:21:66:HIS:ND1	2.37	0.47
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.15	0.47
1:2A:1683:A:H4'	1:2A:2722:A:O2'	2.15	0.47
1:2A:2278:A:H5''	1:2A:2279:A:H5'	1.96	0.47
1:2A:2879:C:H2'	1:2A:2880:C:O4'	2.14	0.47
2:2B:3:C:H2'	2:2B:4:C:C6	2.49	0.47
8:2I:84:GLY:O	8:2I:86:THR:N	2.44	0.47
14:2S:10:ARG:HH21	14:2S:91:PRO:HB2	1.80	0.47
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.97	0.47
1:1A:1093:A:N1	1:1A:1157:G:O2'	2.45	0.47
1:1A:398:G:H8	23:11:65:SER:O	1.97	0.47
1:1A:935:C:O2'	1:1A:936:A:O4'	2.31	0.47
3:1D:142:VAL:HG23	3:1D:193:VAL:HA	1.97	0.47
4:1E:14:ILE:HG12	4:1E:21:VAL:HG13	1.96	0.47
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.94	0.47
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.68	0.47
1:2A:1095:A:H2'	1:2A:1096:G:C8	2.48	0.47
1:2A:1280:G:C6	1:2A:1281:G:N1	2.82	0.47
1:2A:2333:A:H2'	1:2A:2334:G:O4'	2.15	0.47
1:2A:2854:G:H2'	1:2A:2855:G:H8	1.80	0.47
1:2A:26:G:C2	1:2A:536:G:N3	2.81	0.47
1:2A:892:C:H4'	1:2A:893:U:O4'	2.15	0.47
1:2A:945:A:H2'	1:2A:946:A:O4'	2.15	0.47
6:2G:170:ARG:NH1	6:2G:174:GLU:OE1	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:161:G:H2'	1:1A:162:C:H6	1.80	0.47
1:1A:1813:A:OP1	59:1A:4102:HOH:O	2.20	0.47
1:1A:1984:U:H4'	1:1A:1985:G:OP1	2.15	0.47
1:1A:329:U:H2'	1:1A:330:G:O4'	2.14	0.47
1:1A:842:C:H2'	1:1A:843:C:C6	2.50	0.47
1:1A:1822:G:H5'	3:1D:205:VAL:HG13	1.97	0.47
7:1H:7:LEU:HG	7:1H:69:ARG:NH1	2.29	0.47
1:2A:1470:G:N2	1:2A:1619:G:N7	2.63	0.47
1:2A:2049:U:O4	59:2A:3642:HOH:O	2.16	0.47
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.34	0.47
1:1A:2298:A:N6	1:1A:2355:U:H3	2.05	0.47
1:1A:2575:A:C2	1:1A:2658:U:H4'	2.49	0.47
1:1A:663:U:H2'	1:1A:664:C:C6	2.50	0.47
1:1A:894:G:O6	1:1A:973:G:H2'	2.15	0.47
1:2A:2376:G:O6	30:28:39:LYS:HE3	2.15	0.47
1:2A:1673:G:H2'	1:2A:1674:U:C6	2.50	0.47
1:2A:1883:A:N1	1:2A:2108:G:H1'	2.29	0.47
1:2A:239:A:C5	1:2A:240:G:H1'	2.50	0.47
4:2E:101:ARG:NH1	4:2E:169:ASN:O	2.45	0.47
1:2A:2115:G:OP1	8:2I:22:LYS:HD2	2.14	0.47
13:2R:21:TYR:OH	13:2R:43:GLU:HG2	2.15	0.47
13:2R:59:ASP:N	13:2R:59:ASP:OD1	2.48	0.47
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.96	0.47
24:12:32:LEU:HD13	24:12:36:ARG:NH1	2.30	0.47
1:1A:2657:C:H2'	1:1A:2658:U:O4'	2.15	0.47
3:1D:21:PHE:HB3	3:1D:24:ILE:HD12	1.96	0.47
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.96	0.47
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.97	0.47
1:2A:1108:G:H2'	1:2A:1109:C:O4'	2.14	0.47
1:2A:113:C:H2'	1:2A:114:G:O4'	2.15	0.47
1:2A:1673:G:H2'	1:2A:1674:U:H6	1.80	0.47
1:2A:2805:G:H22	1:2A:2814:C:H1'	1.79	0.47
1:2A:330:G:H21	1:2A:353:A:H62	1.63	0.47
1:2A:448:A:H2'	1:2A:449:A:C8	2.50	0.47
1:2A:598:U:H2'	1:2A:599:G:C8	2.50	0.47
1:2A:732:G:N2	1:2A:834:A:H61	2.13	0.47
6:2G:3:LEU:HD12	26:24:25:TYR:CZ	2.50	0.47
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.42	0.47
1:2A:914:U:O2'	12:2Q:8:LYS:HE3	2.15	0.47
27:15:16:ARG:HG3	27:15:17:ASP:N	2.29	0.47
1:1A:1091:A:H3'	1:1A:1092:G:C5'	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:138:A:C8	1:1A:1453:C:O2'	2.66	0.47
1:1A:2330:G:N2	14:1S:3:ARG:HA	2.30	0.47
11:1P:112:LEU:HD13	11:1P:127:ALA:HB2	1.97	0.47
25:23:46:ASN:O	25:23:50:VAL:HG22	2.13	0.47
1:2A:2327:C:H2'	1:2A:2328:C:H6	1.80	0.47
1:2A:2495:G:C2	1:2A:2496:G:C8	3.03	0.47
1:2A:2573:U:H4'	10:2O:25:LEU:HD21	1.97	0.47
1:2A:25:G:C6	1:2A:26:G:N1	2.83	0.47
1:2A:2609:A:OP1	59:2A:3653:HOH:O	2.21	0.47
1:2A:325:C:H42	1:2A:338:G:H1	1.63	0.47
3:2D:72:LYS:HG3	3:2D:103:ARG:NH2	2.29	0.47
6:2G:13:GLU:HG3	6:2G:14:GLU:HG2	1.96	0.47
10:2O:20:MET:HE3	10:2O:44:LYS:HE3	1.97	0.47
17:2V:43:GLU:N	17:2V:43:GLU:OE2	2.47	0.47
21:2Z:108:PRO:HG3	21:2Z:141:VAL:HB	1.96	0.47
25:13:8:LEU:HD13	25:13:31:LEU:HD23	1.95	0.47
27:15:35:GLU:HG2	59:15:207:HOH:O	2.14	0.47
1:1A:1217:G:O2'	1:1A:1218:A:O5'	2.32	0.47
1:1A:264:U:H2'	1:1A:265:C:C6	2.50	0.47
1:1A:330:G:N2	1:1A:332:G:H3'	2.30	0.47
5:1F:18:ARG:HG2	5:1F:19:GLU:H	1.79	0.47
1:2A:141:G:H4'	19:2X:35:THR:HG21	1.96	0.47
1:2A:1389:G:O2'	1:2A:1430:G:H2'	2.14	0.47
1:2A:1552:A:H2'	1:2A:1553:A:O4'	2.15	0.47
1:2A:2239:G:C5	1:2A:2240:C:C4	3.03	0.47
1:2A:2328:C:HO2'	1:2A:2329:G:P	2.37	0.47
1:2A:2813:C:H2'	1:2A:2814:C:H6	1.79	0.47
1:2A:909:A:H2'	1:2A:910:G:H8	1.81	0.47
3:2D:71:ASP:HB3	3:2D:103:ARG:HH22	1.80	0.47
3:2D:124:PRO:O	3:2D:126:GLN:N	2.48	0.47
1:1A:2588:A:H5'	27:15:3:LYS:HD2	1.96	0.46
1:1A:1616:A:H2'	1:1A:1617:A:C8	2.50	0.46
1:1A:552:A:C2	1:1A:2064:C:H4'	2.51	0.46
1:1A:2095:U:OP2	59:1A:4194:HOH:O	2.21	0.46
1:1A:2207:G:H2'	1:1A:2208:G:O4'	2.15	0.46
1:1A:922:C:H2'	1:1A:923:U:O4'	2.14	0.46
2:1B:66:A:N6	2:1B:108:U:H2'	2.30	0.46
21:1Z:13:GLU:HB3	21:1Z:18:LEU:HD21	1.97	0.46
1:2A:2274:C:N4	22:20:15:ASP:OD1	2.48	0.46
1:2A:1302:C:H2'	1:2A:1303:C:O4'	2.68	0.46
1:2A:1457:A:H2'	1:2A:1458:G:H8	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2103:A:H5'	59:2A:3920:HOH:O	2.14	0.46
1:2A:2375:C:H2'	1:2A:2376:G:O4'	2.15	0.46
1:2A:792:A:H2'	1:2A:2623:C:H5''	1.97	0.46
1:2A:907:A:H2'	1:2A:908:G:O4'	2.15	0.46
3:2D:5:LYS:HG2	3:2D:17:THR:HG22	1.96	0.46
1:2A:810:A:H5'	3:2D:210:GLY:CA	2.45	0.46
4:2E:77:ILE:HD13	4:2E:77:ILE:HA	1.74	0.46
5:2F:140:LEU:HD21	5:2F:170:LEU:HD11	1.98	0.46
7:2H:9:ILE:HG12	7:2H:69:ARG:HD2	1.96	0.46
9:2N:34:LEU:O	9:2N:49:GLY:HA3	2.14	0.46
1:1A:1222:C:H2'	1:1A:1223:C:C6	2.50	0.46
1:1A:2734:G:H2'	1:1A:2735:C:C6	2.50	0.46
1:1A:288:G:C5	1:1A:289:G:H1'	5.75	0.46
1:2A:1039:C:O2'	1:2A:1041:A:OP1	2.28	0.46
1:2A:785:G:OP1	59:2A:3654:HOH:O	2.21	0.46
1:2A:982:G:N3	1:2A:982:G:H3'	4.26	0.46
9:2N:94:HIS:O	9:2N:97:ARG:HB2	2.15	0.46
14:2S:15:ARG:NE	14:2S:88:ASP:OD2	2.29	0.46
1:2A:324:G:OP2	20:2Y:84:ARG:NH2	2.48	0.46
24:12:22:GLU:HG2	24:12:64:LEU:HD11	1.96	0.46
1:1A:552:A:O2'	1:1A:553:A:H5'	2.15	0.46
6:1G:126:ASP:HB2	6:1G:130:ASN:HB2	1.96	0.46
8:1I:48:GLU:HG2	8:1I:52:ARG:HH22	1.81	0.46
20:1Y:68:HIS:ND1	20:1Y:70:SER:HB3	2.29	0.46
1:2A:1017:A:OP2	59:2A:3626:HOH:O	2.20	0.46
1:2A:1050:C:H2'	1:2A:1051:C:H6	1.79	0.46
1:2A:1423:A:O2'	1:2A:1425:G:N7	2.39	0.46
1:2A:1897:A:H2'	1:2A:1898:A:C8	2.51	0.46
1:2A:2785:C:OP1	4:2E:166:THR:OG1	2.28	0.46
1:2A:303:C:H2'	1:2A:304:G:O4'	2.15	0.46
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.47	0.46
5:2F:57:VAL:HG13	5:2F:59:TYR:H	1.80	0.46
14:2S:11:LYS:O	14:2S:15:ARG:HG3	2.15	0.46
14:2S:43:GLU:N	14:2S:43:GLU:OE2	5.19	0.46
15:2T:23:ARG:HG3	15:2T:120:ARG:NH1	2.31	0.46
15:2T:64:ARG:HB2	15:2T:73:GLU:HG2	1.98	0.46
23:11:85:LEU:HB3	23:11:89:GLU:HB2	1.97	0.46
1:1A:2078:A:N7	59:1A:4335:HOH:O	2.35	0.46
1:1A:2543:G:O2'	1:1A:2668:A:N1	2.47	0.46
1:1A:301:A:HO2'	1:1A:302:C:P	2.39	0.46
1:1A:402:C:OP1	59:1A:4196:HOH:O	2.21	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:839:A:OP2	1:1A:2092:A:O2'	2.32	0.46
1:1A:1830:C:OP2	3:1D:183:ARG:NH2	2.49	0.46
5:1F:129:PHE:CD1	5:1F:163:VAL:HG21	2.50	0.46
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	1.96	0.46
1:2A:1067:G:C6	1:2A:1184:C:N3	2.83	0.46
1:2A:138:A:C8	1:2A:1453:C:O2'	2.68	0.46
1:2A:2298:A:C5	1:2A:2300:G:C5	3.04	0.46
2:2B:49:C:H2'	2:2B:50:G:C8	2.51	0.46
6:2G:48:GLU:O	6:2G:51:ARG:HG3	2.15	0.46
10:2O:63:VAL:HG11	10:2O:85:VAL:HG23	1.98	0.46
14:2S:67:ARG:HG2	14:2S:71:ARG:CZ	2.45	0.46
1:2A:594:A:OP2	17:2V:78:LYS:HE2	2.16	0.46
1:1A:2710:C:H2'	1:1A:2711:C:O4'	2.15	0.46
1:1A:767:C:H2'	1:1A:768:A:C8	2.51	0.46
1:1A:820:A:H2'	1:1A:820:A:N3	2.30	0.46
6:1G:138:GLN:HE22	6:1G:153:ARG:NH2	2.13	0.46
30:28:63:PRO:HG2	30:28:64:TYR:CD2	2.50	0.46
1:2A:1118:A:H3'	1:2A:1119:G:C8	2.51	0.46
1:2A:1685:U:C2'	1:2A:1686:C:H5''	2.45	0.46
1:2A:2224:U:H1'	3:2D:151:LYS:HE2	1.97	0.46
1:2A:9:G:H1'	1:2A:2811:A:H62	1.81	0.46
1:2A:2898:C:H2'	1:2A:2899:G:O4'	2.15	0.46
1:2A:2901:G:H5''	1:2A:2902:G:O4'	2.16	0.46
1:2A:853:U:OP2	11:2P:41:ARG:NH2	2.45	0.46
1:2A:998:G:H5''	12:2Q:13:GLN:HB3	1.97	0.46
6:2G:33:ARG:N	6:2G:33:ARG:HD3	2.30	0.46
7:2H:169:VAL:HG12	7:2H:171:LEU:HD21	1.96	0.46
22:10:27:GLU:HB2	22:10:69:PHE:HD1	1.80	0.46
1:1A:2723:U:OP1	1:1A:2726:G:H4'	2.16	0.46
3:1D:175:LEU:HD12	3:1D:185:VAL:HG21	1.96	0.46
8:1I:56:LYS:O	8:1I:60:GLU:HB3	2.15	0.46
12:1Q:42:ILE:HD13	12:1Q:97:VAL:HB	1.96	0.46
18:1W:18:ARG:NH1	18:1W:76:VAL:O	2.49	0.46
23:21:3:LYS:H	23:21:61:ARG:NH1	2.14	0.46
1:2A:1399:A:H2'	1:2A:1400:G:O4'	2.15	0.46
1:2A:2484:U:O2	1:2A:2484:U:H2'	2.16	0.46
1:2A:2568:G:H2'	1:2A:2569:C:H6	1.81	0.46
1:2A:901:G:H2'	1:2A:902:C:C6	2.50	0.46
2:2B:5:C:OP1	2:2B:61:G:O2'	2.22	0.46
1:1A:825:U:H6	1:1A:825:U:OP2	3.63	0.46
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:152:ALA:O	21:1Z:155:LEU:HB2	2.16	0.46
1:2A:1102:A:O2'	1:2A:1103:G:OP1	2.28	0.46
1:2A:1305:G:C6	1:2A:1306:C:C4	3.03	0.46
1:2A:1846:G:H3'	3:2D:62:TYR:CE1	2.51	0.46
1:2A:488:G:N2	1:2A:491:A:OP2	2.48	0.46
1:2A:2583:A:N7	4:2E:144:ARG:HD2	2.31	0.46
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.64	0.46
1:1A:1311:G:O5'	18:1W:15:ARG:NH2	2.48	0.46
1:1A:1512:G:H2'	1:1A:1593:C:N4	2.31	0.46
1:1A:1828:U:H5'	3:1D:259:THR:CG2	2.38	0.46
3:1D:183:ARG:HG3	3:1D:270:ILE:HG12	1.98	0.46
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.65	0.46
59:1A:4363:HOH:O	12:1Q:75:THR:HG23	2.15	0.46
26:24:57:GLU:HA	26:24:58:ARG:HA	1.63	0.46
26:24:68:ARG:HH21	26:24:68:ARG:HB3	1.80	0.46
1:2A:1937:A:H2'	1:2A:1938:U:O4'	2.16	0.46
1:2A:2354:C:O2'	1:2A:2384:G:H4'	2.16	0.46
1:2A:2757:C:C4	1:2A:2758:U:C4	3.04	0.46
1:2A:40:C:H2'	1:2A:41:G:H8	1.81	0.46
1:2A:468:A:H5"	1:2A:469:C:OP1	2.16	0.46
1:2A:874:U:H4'	1:2A:877:G:N1	2.31	0.46
3:2D:2:ALA:O	3:2D:3:VAL:HB	2.16	0.46
11:2P:44:GLY:CA	11:2P:45:LEU:HB2	2.45	0.46
1:1A:1716:C:O2	4:1E:129:HIS:NE2	2.42	0.46
1:1A:604:G:H2'	1:1A:605:G:C8	2.51	0.46
16:1U:76:TYR:CE1	16:1U:80:ILE:HG13	2.51	0.46
19:1X:57:LEU:CD1	19:1X:78:LYS:HB2	2.46	0.46
23:21:50:ARG:HD2	23:21:57:GLU:OE1	2.16	0.46
26:24:58:ARG:HB3	26:24:59:PHE:HD1	1.81	0.46
1:2A:1132:G:C6	1:2A:1134:G:C4	3.04	0.46
1:2A:1508:C:H4'	1:2A:2714:C:H5'	1.98	0.46
1:2A:480:C:N3	1:2A:497:A:H2'	2.31	0.46
4:2E:163:GLU:HG2	4:2E:164:ARG:N	2.31	0.46
7:2H:2:SER:O	7:2H:3:ARG:HG2	2.16	0.46
11:2P:121:LYS:HB3	11:2P:121:LYS:HE2	1.78	0.46
1:1A:1939:A:O2'	1:1A:1941:C:N4	2.48	0.46
1:1A:1313:A:C2	1:1A:2034:A:C4	3.04	0.46
1:1A:539:A:H1'	1:1A:603:C:H1'	1.98	0.46
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.17	0.46
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.31	0.46
9:1N:131:GLN:H	9:1N:131:GLN:CD	2.20	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.69	0.46
1:2A:1176:G:C2	1:2A:1177:A:C4	3.04	0.46
1:2A:2713:U:H4'	1:2A:2714:C:OP1	2.16	0.46
1:2A:678:A:H61	1:2A:701:A:H1'	1.81	0.46
2:2B:98:G:H2'	2:2B:99:G:O4'	2.15	0.46
6:2G:33:ARG:O	6:2G:161:THR:HG23	2.16	0.46
7:2H:9:ILE:N	7:2H:50:VAL:O	2.27	0.46
20:2Y:48:ALA:HB2	20:2Y:60:PHE:CE2	2.51	0.46
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	1.97	0.46
1:1A:1158:U:H2'	1:1A:1159:G:H8	1.80	0.45
1:1A:1217:G:N2	1:1A:1221:A:OP2	2.48	0.45
1:1A:1317:A:H3'	1:1A:1318:U:H5''	1.97	0.45
1:1A:2540:G:H5''	1:1A:2541:A:H5''	1.98	0.45
1:1A:288:G:N7	1:1A:289:G:H1'	6.71	0.45
1:1A:907:A:H2'	1:1A:908:G:O4'	2.17	0.45
5:1F:107:LYS:HE3	5:1F:205:ARG:O	2.14	0.45
6:1G:106:LEU:HD12	6:1G:110:ALA:HB3	1.98	0.45
13:1R:55:ALA:HB2	13:1R:79:LEU:HD13	1.96	0.45
16:1U:86:ALA:O	17:1V:49:THR:HG23	2.16	0.45
1:2A:1225:C:H2'	1:2A:1226:A:C8	2.51	0.45
1:2A:748:G:C2	1:2A:777:C:C2	3.05	0.45
1:2A:955:A:O2'	1:2A:957:C:OP2	9.26	0.45
7:2H:121:ILE:HD11	7:2H:140:LYS:HG2	1.98	0.45
14:2S:10:ARG:HG2	14:2S:13:ARG:HH21	1.82	0.45
4:2E:12:THR:HG22	15:2T:58:ASN:OD1	2.16	0.45
20:2Y:5:MET:HE1	20:2Y:32:PRO:HA	1.98	0.45
26:14:63:TYR:N	26:14:63:TYR:CD1	2.83	0.45
1:1A:1633:C:H2'	1:1A:1634:C:H6	1.80	0.45
1:1A:904:U:O2	1:1A:2279:A:H2'	2.16	0.45
1:1A:2584:C:H3'	59:1A:4454:HOH:O	2.15	0.45
1:1A:288:G:N3	59:1A:4192:HOH:O	2.36	0.45
1:1A:2890:C:H2'	1:1A:2891:A:O4'	2.16	0.45
4:1E:18:ASP:HB3	15:1T:82:LEU:HD21	1.96	0.45
1:2A:1067:G:C5	1:2A:1184:C:C4	3.05	0.45
1:2A:1404:A:N1	1:2A:1417:U:O4	2.49	0.45
1:2A:2059:G:H2'	1:2A:2060:C:O4'	2.16	0.45
1:2A:2674:G:H3'	1:2A:2675:G:H8	1.80	0.45
1:2A:820:A:H2'	1:2A:820:A:N3	2.31	0.45
1:2A:902:C:HO2'	1:2A:903:C:P	2.38	0.45
5:2F:20:LEU:HD22	5:2F:20:LEU:HA	1.73	0.45
12:2Q:52:VAL:HG13	21:2Z:183:LEU:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.51	0.45
22:10:10:THR:HA	59:10:207:HOH:O	2.16	0.45
1:1A:330:G:H21	1:1A:353:A:H62	1.64	0.45
1:1A:334:A:C6	1:1A:351:U:C4	3.04	0.45
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.98	0.45
4:1E:143:ASN:HD22	4:1E:147:PRO:CD	2.29	0.45
11:1P:76:LYS:HE2	11:1P:76:LYS:HB3	1.51	0.45
1:2A:468:A:H1'	1:2A:1245:C:O4'	2.16	0.45
1:2A:2640:A:H1'	1:2A:2641:G:H5''	1.98	0.45
1:2A:775:G:O5'	3:2D:208:LYS:NZ	2.49	0.45
31:19:32:HIS:O	31:19:34:GLN:HG3	2.17	0.45
1:1A:1587:G:H5''	1:1A:1588:A:OP2	2.17	0.45
3:1D:68:LYS:HD2	3:1D:70:TRP:CZ2	2.51	0.45
4:1E:119:ARG:HG2	4:1E:160:TYR:CG	2.52	0.45
4:1E:48:GLN:OE1	4:1E:66:HIS:NE2	2.41	0.45
5:1F:37:VAL:HG21	11:1P:6:LEU:HD11	1.98	0.45
7:1H:13:LYS:HB3	7:1H:13:LYS:HE2	1.82	0.45
10:1O:35:VAL:HG21	10:1O:69:ILE:HD12	1.98	0.45
13:1R:55:ALA:HB1	13:1R:84:ALA:HB2	1.98	0.45
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.51	0.45
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.50	0.45
1:2A:1243:U:H2'	1:2A:1244:C:C6	2.51	0.45
1:2A:1603:C:OP2	1:2A:1604:A:O2'	2.30	0.45
1:2A:1739:U:H4'	1:2A:1740:C:OP2	2.17	0.45
1:2A:1887:G:C6	1:2A:1888:G:C6	3.04	0.45
1:2A:2223:C:H42	1:2A:2232:G:H1	1.65	0.45
1:2A:378:G:H2'	1:2A:379:G:C8	2.51	0.45
10:2O:68:GLU:OE2	10:2O:78:ARG:NH1	2.49	0.45
16:2U:97:ASP:OD1	16:2U:101:ARG:NH1	2.42	0.45
21:2Z:132:ASN:O	21:2Z:134:PRO:HD3	2.16	0.45
1:1A:1312:U:OP1	59:1A:4198:HOH:O	2.21	0.45
1:1A:2879:C:H2'	1:1A:2880:C:O4'	2.17	0.45
14:1S:48:LEU:HD23	14:1S:82:ILE:HD11	1.98	0.45
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.17	0.45
1:2A:504:A:HO2'	1:2A:506:G:H8	1.62	0.45
1:2A:619:U:H2'	1:2A:620:G:C8	2.51	0.45
1:2A:668:A:H5''	1:2A:669:C:OP1	2.16	0.45
26:14:40:HIS:O	26:14:43:TYR:N	2.50	0.45
1:1A:2393:G:H21	30:18:42:ARG:NH2	2.14	0.45
1:1A:346:G:H1'	1:1A:1249:U:O2	2.17	0.45
1:1A:435:C:OP1	59:1A:4197:HOH:O	2.21	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:114:ILE:HB	6:1G:117:PHE:HB2	1.99	0.45
6:2G:142:PRO:HB3	26:24:14:ILE:HD11	1.99	0.45
1:2A:1765:G:H8	1:2A:1769:A:N6	2.14	0.45
1:2A:2091:G:H2'	1:2A:2092:A:C8	2.50	0.45
1:2A:2331:A:H2'	1:2A:2331:A:N3	2.32	0.45
1:2A:2488:C:O2	31:29:4:ARG:NH2	2.36	0.45
1:2A:2590:C:H2'	1:2A:2591:U:O4'	2.17	0.45
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.82	0.45
13:2R:67:LEU:HD23	13:2R:76:VAL:HG21	1.98	0.45
1:1A:1783:G:N7	59:1A:4348:HOH:O	2.36	0.45
1:1A:2802:A:N3	1:1A:2802:A:H2'	2.31	0.45
1:1A:468:A:H3'	5:1F:45:ARG:HH21	1.81	0.45
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.37	0.45
7:1H:7:LEU:HA	7:1H:8:PRO:HD3	1.82	0.45
1:1A:872:U:H4'	11:1P:55:ARG:HB2	1.98	0.45
14:1S:6:ALA:O	14:1S:10:ARG:HB2	2.17	0.45
16:1U:85:LYS:HD3	16:1U:116:ALA:O	2.17	0.45
16:1U:34:LYS:HE2	16:1U:34:LYS:HA	1.98	0.45
1:2A:184:A:N3	1:2A:184:A:H2'	2.31	0.45
1:2A:2657:C:H2'	1:2A:2658:U:O4'	2.17	0.45
1:2A:440:C:H2'	1:2A:441:A:C8	2.52	0.45
1:2A:180:C:O2'	1:2A:848:A:N3	2.48	0.45
1:2A:979:C:H2'	1:2A:980:C:C6	2.52	0.45
2:2B:11:C:H3'	2:2B:12:C:C6	2.52	0.45
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.99	0.45
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.51	0.45
23:11:67:ILE:N	23:11:68:PRO:HD2	2.31	0.45
1:1A:1804:C:O5'	1:1A:1804:C:H6	2.00	0.45
1:1A:236:G:OP1	59:1A:4199:HOH:O	2.21	0.45
2:1B:45:A:OP2	6:1G:96:ARG:NH2	2.47	0.45
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.49	0.45
21:1Z:110:GLY:HA3	21:1Z:174:VAL:HG11	1.98	0.45
1:2A:1041:A:C2	1:2A:1042:G:C8	3.05	0.45
1:2A:1902:C:H2'	1:2A:1903:C:H6	1.82	0.45
1:2A:1789:A:H4'	1:2A:2727:C:O4'	2.17	0.45
1:2A:530:G:O3'	1:2A:531:A:H8	2.00	0.45
1:2A:857:U:H2'	11:2P:21:ARG:HA	1.99	0.45
10:2O:71:ARG:O	10:2O:74:GLY:N	2.44	0.45
14:2S:62:LYS:O	14:2S:65:VAL:HB	2.17	0.45
29:17:30:VAL:O	29:17:34:ARG:HG3	2.16	0.45
1:1A:1155:G:N2	1:1A:1156:A:H2	2.04	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:33:C:H5''	1:1A:34:G:OP2	2.16	0.45
5:1F:168:ARG:HG2	5:1F:175:THR:HG21	1.99	0.45
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.51	0.45
1:1A:2478:C:H4'	12:1Q:123:HIS:CD2	2.51	0.45
20:1Y:20:TYR:O	20:1Y:23:ARG:HB2	2.17	0.45
1:2A:2626:U:C2	27:25:7:PRO:HA	2.52	0.45
1:2A:1472:A:H4'	1:2A:1473:C:O4'	2.16	0.45
1:2A:2294:C:C2	1:2A:2400:G:C2	3.05	0.45
1:2A:2451:C:H5'	59:2A:3759:HOH:O	2.15	0.45
1:2A:2586:C:H2'	1:2A:2589:G:O6	2.17	0.45
1:2A:2659:C:H2'	1:2A:2660:U:C6	2.51	0.45
1:2A:2784:C:H2'	1:2A:2785:C:C6	2.52	0.45
4:2E:15:PHE:CD2	15:2T:81:PRO:HD3	2.51	0.45
13:2R:37:THR:OG1	13:2R:40:LYS:HG3	2.17	0.45
1:2A:1038:G:OP1	16:2U:50:ARG:NH2	2.50	0.45
1:1A:307:U:H2'	1:1A:308:C:H6	1.81	0.45
1:1A:846:A:OP1	1:1A:846:A:H8	2.00	0.45
6:1G:128:ARG:HB2	6:1G:128:ARG:HE	1.65	0.45
1:2A:1332:A:H5''	1:2A:1333:U:OP2	2.16	0.45
1:2A:2427:C:H2'	1:2A:2428:C:H6	1.82	0.45
1:2A:2704:A:H2'	1:2A:2705:G:C8	2.50	0.45
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.17	0.45
4:2E:1:MET:HE3	4:2E:199:ARG:HD2	1.98	0.45
1:2A:2649:G:OP1	4:2E:82:ARG:NH2	2.50	0.45
1:2A:2327:C:O2'	6:2G:128:ARG:NH2	2.50	0.45
6:2G:120:LEU:HB3	6:2G:131:TYR:OH	2.17	0.45
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.17	0.45
1:1A:1821:A:H3'	1:1A:1822:G:H8	1.82	0.44
1:1A:1873:C:H5'	3:1D:253:GLN:NE2	2.32	0.44
1:1A:2400:G:H5''	1:1A:2401:U:O4'	2.17	0.44
1:1A:266:C:O2	1:1A:277:G:N2	2.50	0.44
1:1A:286:G:N7	1:1A:447:U:H2'	2.32	0.44
1:1A:359:C:HO2'	20:1Y:35:TYR:HH	1.61	0.44
1:2A:1703:C:H2'	1:2A:1704:C:H6	1.82	0.44
1:2A:2080:A:O2'	5:2F:69:HIS:HD2	2.01	0.44
1:2A:2427:C:H2'	1:2A:2428:C:C6	2.52	0.44
1:2A:2526:C:H2'	1:2A:2527:G:H8	1.83	0.44
1:2A:629:U:OP1	5:2F:102:PRO:HA	2.16	0.44
7:2H:4:ILE:O	7:2H:69:ARG:HG2	2.17	0.44
9:2N:111:PRO:HA	9:2N:114:ARG:NH1	2.32	0.44
1:2A:909:A:OP2	12:2Q:22:LYS:HD2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.17	0.44
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.99	0.44
3:1D:168:ARG:H	3:1D:168:ARG:CD	4.51	0.44
1:1A:1833:A:H4'	3:1D:259:THR:HG23	1.98	0.44
4:1E:31:CYS:HA	4:1E:32:PRO:HD2	1.81	0.44
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.17	0.44
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.18	0.44
12:1Q:84:GLY:O	12:1Q:85:LYS:HB2	2.18	0.44
13:1R:38:VAL:HB	13:1R:39:PRO:HD3	1.99	0.44
21:1Z:40:ASP:HB3	21:1Z:43:GLU:HB2	1.99	0.44
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.98	0.44
1:2A:1154:C:H2'	1:2A:1155:G:H8	3.98	0.44
1:2A:1333:U:O4	13:2R:106:GLY:HA3	2.17	0.44
1:2A:2311:G:N1	1:2A:2328:C:N3	2.65	0.44
1:2A:621:G:H2'	1:2A:622:G:C8	3.39	0.44
1:2A:966:G:C6	1:2A:967:U:C4	3.05	0.44
1:2A:982:G:OP2	30:28:52:LYS:NZ	2.39	0.44
2:2B:1:U:H2'	2:2B:2:C:C5	2.52	0.44
4:2E:143:ASN:HD22	4:2E:147:PRO:CD	2.31	0.44
15:2T:98:LYS:N	15:2T:98:LYS:HD2	2.33	0.44
31:19:16:VAL:HG22	31:19:25:VAL:HG22	1.99	0.44
1:1A:1633:C:H2'	1:1A:1634:C:C6	2.51	0.44
1:1A:237:C:C2	1:1A:282:G:C2	58.53	0.44
5:1F:33:LEU:HA	5:1F:33:LEU:HD12	1.89	0.44
22:20:24:LYS:O	22:20:25:ARG:HD3	2.18	0.44
1:2A:1025:A:N3	1:2A:2058:G:O2'	2.44	0.44
1:2A:1056:G:C5	1:2A:1058:C:C4	3.05	0.44
1:2A:1702:C:H2'	1:2A:1703:C:H6	1.82	0.44
1:2A:2830:A:H2'	1:2A:2831:G:H8	1.81	0.44
1:2A:330:G:H2'	1:2A:332:G:OP2	2.17	0.44
1:2A:661:A:H4'	1:2A:662:G:O5'	2.18	0.44
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.98	0.44
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.38	0.44
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.60	0.44
1:1A:1565:U:H2'	1:1A:1566:G:O4'	2.17	0.44
1:1A:1816:A:H1'	1:1A:1959:A:N6	2.32	0.44
1:1A:195:A:H2'	1:1A:196:C:O4'	2.17	0.44
1:1A:2346:A:C8	1:1A:2348:G:C5	3.06	0.44
1:1A:26:G:C2	1:1A:536:G:N3	2.85	0.44
1:1A:830:A:C6	3:1D:229:VAL:HG11	2.53	0.44
1:1A:2316:A:H5''	6:1G:134:GLY:HA3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.98	0.44
10:1O:98:VAL:HG13	10:1O:117:LEU:HB3	2.00	0.44
14:1S:34:HIS:ND1	14:1S:53:SER:OG	2.46	0.44
26:24:40:HIS:HB3	26:24:43:TYR:HB2	2.00	0.44
1:2A:131:C:O4'	11:2P:1:MET:HG2	97.02	0.44
1:2A:1887:G:C6	1:2A:1888:G:N1	2.86	0.44
1:2A:222:C:H2'	1:2A:223:U:C6	2.53	0.44
1:2A:2830:A:C2	1:2A:2831:G:C4	3.05	0.44
1:2A:309:C:H2'	1:2A:310:C:H6	1.82	0.44
1:2A:464:G:H2'	1:2A:465:G:H8	1.83	0.44
1:2A:567:C:H5''	1:2A:568:G:OP2	2.18	0.44
1:2A:648:C:O2'	1:2A:703:U:H5''	2.17	0.44
2:2B:19:G:H2'	2:2B:20:C:O4'	2.17	0.44
2:2B:95:C:H2'	2:2B:96:U:C6	2.53	0.44
4:2E:111:ARG:HA	13:2R:1:MET:SD	2.58	0.44
4:2E:119:ARG:HD2	4:2E:120:TRP:CE2	2.52	0.44
4:2E:59:VAL:HG12	4:2E:64:LYS:HG3	1.97	0.44
14:2S:67:ARG:O	14:2S:71:ARG:HG3	2.18	0.44
19:2X:31:HIS:CD2	19:2X:33:LYS:HB2	2.53	0.44
20:2Y:23:ARG:HG2	20:2Y:42:VAL:HG22	1.99	0.44
26:14:14:ILE:HG13	26:14:22:ILE:HB	2.00	0.44
28:16:14:THR:OG1	28:16:48:VAL:HG13	2.17	0.44
1:1A:1337:U:H2'	1:1A:1338:C:C6	2.53	0.44
1:1A:1531:A:H2'	1:1A:1532:G:C8	2.52	0.44
1:1A:219:C:H2'	1:1A:220:G:O4'	2.18	0.44
1:1A:2211:G:H2'	1:1A:2212:G:O4'	2.17	0.44
1:1A:800:C:H2'	1:1A:801:C:H6	1.82	0.44
2:1B:89:G:H2'	2:1B:90:A:C8	2.53	0.44
6:1G:67:LYS:HD3	26:14:5:ILE:HB	2.00	0.44
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.98	0.44
13:1R:59:ASP:N	13:1R:59:ASP:OD1	2.50	0.44
14:1S:24:LEU:HB2	14:1S:85:VAL:HG23	1.99	0.44
20:1Y:5:MET:HG2	20:1Y:30:VAL:HG11	2.00	0.44
26:24:59:PHE:N	26:24:60:GLN:HB2	2.33	0.44
1:2A:2488:C:N4	31:29:10:ILE:HG23	2.32	0.44
1:2A:1404:A:H5'	1:2A:1404:A:N3	2.32	0.44
1:2A:875:A:N7	1:2A:2259:C:H5'	2.33	0.44
1:2A:412:G:OP1	59:2A:3652:HOH:O	2.21	0.44
1:2A:60:C:N3	1:2A:90:G:N2	2.49	0.44
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.35	0.44
21:2Z:54:HIS:ND1	21:2Z:101:PRO:HG3	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1729:C:H2'	1:1A:1730:C:C6	2.52	0.44
1:1A:2218:U:H1'	1:1A:2219:A:C8	2.53	0.44
1:1A:2330:G:N2	14:1S:3:ARG:HG2	2.32	0.44
1:1A:2347:A:H61	22:10:43:THR:HG22	1.82	0.44
1:1A:933:A:H1'	1:1A:935:C:OP2	2.18	0.44
3:1D:146:GLU:HB2	3:1D:189:CYS:HB3	1.99	0.44
1:1A:810:A:H2	3:1D:219:PRO:HG3	1.82	0.44
25:23:8:LEU:O	25:23:32:GLN:N	2.44	0.44
2:1B:12:C:H2'	22:10:73:GLY:HA3	2.00	0.44
26:14:15:ILE:HB	26:14:32:TYR:CD2	2.53	0.44
1:1A:1649:C:H5'	59:1A:5078:HOH:O	2.18	0.44
1:1A:1849:A:H5''	3:1D:161:THR:HG21	2.00	0.44
1:1A:2227:G:O2'	1:1A:2228:A:OP1	2.31	0.44
1:1A:2785:C:H2'	1:1A:2786:C:H6	1.83	0.44
1:1A:296:C:H2'	1:1A:297:G:C8	2.48	0.44
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.18	0.44
11:1P:107:LYS:O	11:1P:110:TYR:HB2	2.18	0.44
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.83	0.44
1:1A:956:A:H2'	12:1Q:9:TYR:OH	2.17	0.44
1:2A:2376:G:OP1	22:20:55:ARG:HG2	2.18	0.44
24:22:65:ASN:O	24:22:69:ARG:HG3	2.18	0.44
1:2A:1224:C:H2'	1:2A:1225:C:O4'	2.46	0.44
1:2A:1493:G:N2	1:2A:1510:C:O2	2.36	0.44
1:2A:1556:A:H2'	1:2A:1557:G:H8	1.83	0.44
1:2A:213:A:N6	1:2A:214:G:C2	2.86	0.44
1:2A:2508:A:H8	1:2A:2508:A:OP2	2.00	0.44
1:2A:2861:G:H2'	1:2A:2862:C:O4'	2.18	0.44
1:2A:2891:A:OP1	13:2R:96:ARG:NE	2.50	0.44
3:2D:171:ASP:O	3:2D:187:GLY:N	2.50	0.44
3:2D:275:LYS:HA	3:2D:275:LYS:HD2	1.69	0.44
5:2F:161:GLU:O	5:2F:165:ARG:HB2	2.18	0.44
6:2G:29:TRP:HE3	6:2G:33:ARG:HH21	1.66	0.44
14:2S:61:ASN:O	14:2S:65:VAL:HG23	2.17	0.44
1:2A:1426:G:C8	15:2T:118:ARG:HG2	88.36	0.44
1:1A:1524:G:O2'	1:1A:1604:A:N1	2.49	0.44
1:1A:2341:G:H2'	1:1A:2342:G:O4'	2.18	0.44
1:1A:322:A:N1	1:1A:345:A:O2'	2.39	0.44
7:1H:101:ARG:HA	7:1H:101:ARG:HD2	1.74	0.44
1:1A:661:A:H8	11:1P:117:GLU:HG3	1.83	0.44
2:1B:7:G:H5'	14:1S:29:PHE:CE2	2.53	0.44
16:1U:48:ALA:O	16:1U:51:LYS:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:29:17:ILE:HB	31:29:26:ILE:HD11	2.00	0.44
1:2A:2881:G:O2'	1:2A:2882:A:H5'	2.18	0.44
1:2A:33:C:H5''	1:2A:34:G:OP2	2.18	0.44
1:2A:902:C:H2'	1:2A:903:C:C6	2.53	0.44
4:2E:52:LEU:O	4:2E:76:ARG:N	2.39	0.44
7:2H:127:GLU:C	7:2H:129:THR:H	2.21	0.44
7:2H:126:PRO:HD2	7:2H:130:ARG:O	2.18	0.44
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	2.00	0.44
1:2A:2651:G:OP1	9:2N:97:ARG:NH2	2.51	0.44
13:2R:38:VAL:HB	13:2R:39:PRO:HD3	2.00	0.44
17:2V:81:TYR:C	17:2V:82:ARG:HD2	2.37	0.44
18:2W:75:TYR:CZ	18:2W:104:THR:HG21	2.53	0.44
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.75	0.44
6:1G:174:GLU:HG2	6:1G:180:PHE:CE2	2.52	0.44
14:1S:11:LYS:O	14:1S:15:ARG:HG3	2.18	0.44
1:2A:75:C:N4	1:2A:106:G:H1	2.15	0.44
1:2A:1814:A:OP2	59:2A:3601:HOH:O	2.20	0.44
1:2A:2458:G:N2	1:2A:2461:A:OP2	2.50	0.44
1:2A:2639:C:H1'	1:2A:2793:A:H2'	1.99	0.44
1:2A:668:A:H2'	1:2A:670:A:C2	2.53	0.44
1:2A:2314:G:O2'	6:2G:132:ASN:HB2	2.17	0.44
1:2A:580:G:H5'	9:2N:112:LEU:HD23	1.99	0.44
9:2N:96:GLU:HB2	9:2N:122:VAL:HG12	2.00	0.44
11:2P:21:ARG:HA	11:2P:21:ARG:HD3	1.84	0.44
1:1A:1424:A:H4'	1:1A:1425:G:OP2	2.17	0.43
1:1A:1878:A:H2'	1:1A:1879:G:C8	2.52	0.43
1:1A:2753:A:H2'	1:1A:2754:C:O4'	2.18	0.43
1:1A:2855:G:H2'	1:1A:2856:U:O4'	2.18	0.43
1:1A:1075:G:OP2	12:1Q:128:LYS:NZ	2.51	0.43
16:1U:108:GLU:OE2	16:1U:112:ARG:NH1	2.51	0.43
1:1A:141:G:H1'	19:1X:37:THR:HG21	2.00	0.43
12:1Q:60:ARG:NH1	21:1Z:180:VAL:HG23	2.33	0.43
1:2A:1209:G:H2'	1:2A:1210:U:C6	2.53	0.43
1:2A:1266:C:C2	1:2A:1274:G:C2	3.05	0.43
1:2A:216:A:H2'	1:2A:217:A:H5'	2.00	0.43
1:2A:2256:U:O2'	1:2A:2447:G:OP2	2.25	0.43
1:2A:77:G:H2'	1:2A:78:G:H8	1.83	0.43
1:2A:877:G:O2'	11:2P:38:GLN:NE2	2.51	0.43
3:2D:107:ALA:HA	3:2D:108:PRO:HD3	1.79	0.43
13:2R:21:TYR:CZ	13:2R:43:GLU:HG2	2.52	0.43
1:1A:1536:G:O2'	3:1D:101:GLU:HB2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:319:C:H2'	1:1A:320:C:H6	1.82	0.43
1:1A:510:C:H2'	1:1A:511:C:C6	2.54	0.43
2:1B:79:C:H2'	2:1B:80:U:O4'	2.18	0.43
3:1D:54:ARG:O	3:1D:218:ARG:HD3	2.18	0.43
4:1E:52:LEU:O	4:1E:75:VAL:HG22	2.18	0.43
1:1A:623:C:OP1	5:1F:108:LYS:HE2	2.18	0.43
8:1I:38:LEU:HB2	8:1I:40:THR:HG23	1.99	0.43
1:2A:1015:C:H2'	1:2A:1016:G:O4'	2.18	0.43
1:2A:1288:G:H2'	1:2A:1289:G:O4'	2.17	0.43
1:2A:2251:C:H2'	1:2A:2252:A:C8	2.50	0.43
1:2A:241:C:H2'	1:2A:242:G:O4'	2.17	0.43
1:2A:2438:C:H5"	1:2A:2439:G:OP1	2.17	0.43
1:2A:507:A:H1'	1:2A:522:G:N2	2.33	0.43
1:2A:830:A:C5	3:2D:229:VAL:HG21	2.53	0.43
2:2B:40:U:C2	2:2B:43:C:OP2	2.71	0.43
3:2D:3:VAL:HG13	3:2D:17:THR:HB	2.00	0.43
14:2S:94:TYR:CE1	14:2S:99:LYS:HG3	2.52	0.43
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	2.00	0.43
1:1A:900:G:N3	1:1A:1381:A:H2	126.63	0.43
1:1A:1833:A:H2'	1:1A:1834:C:O4'	2.18	0.43
1:1A:2712:C:H2'	1:1A:2713:U:H2'	1.99	0.43
1:1A:2820:G:N2	1:1A:2899:G:H1'	2.33	0.43
1:1A:283:G:C2	1:1A:284:U:O4	2.71	0.43
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.99	0.43
5:1F:32:LEU:HB3	5:1F:112:MET:HE1	1.99	0.43
16:1U:8:VAL:HG22	16:1U:11:ARG:NH2	2.33	0.43
1:2A:1039:C:OP2	16:2U:54:LYS:NZ	2.40	0.43
1:2A:1314:A:H2'	1:2A:1315:C:C6	2.52	0.43
1:2A:2030:G:OP1	18:2W:41:LYS:NZ	2.26	0.43
1:2A:2063:A:OP1	59:2A:3655:HOH:O	2.21	0.43
1:2A:2419:U:H2'	1:2A:2420:G:H8	1.83	0.43
1:2A:2685:G:H2'	1:2A:2686:A:C8	2.53	0.43
1:2A:2706:C:H2'	1:2A:2707:U:C6	2.53	0.43
1:2A:2857:G:O2'	1:2A:2876:G:N1	2.39	0.43
7:2H:55:PRO:HB2	7:2H:56:SER:H	1.65	0.43
11:2P:114:ILE:HG13	11:2P:125:VAL:HG21	2.00	0.43
11:2P:39:LYS:HA	11:2P:45:LEU:HG	1.99	0.43
21:2Z:92:SER:O	21:2Z:94:GLU:N	2.42	0.43
30:18:62:LEU:HB3	30:18:65:GLU:HG3	2.00	0.43
1:1A:1055:A:N3	1:1A:1198:C:H1'	2.34	0.43
1:1A:2221:C:O2	1:1A:2237:C:N4	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:21:THR:HG23	12:1Q:99:PRO:O	2.18	0.43
21:1Z:108:PRO:HB2	21:1Z:111:VAL:HG23	1.99	0.43
24:22:32:LEU:HD12	24:22:57:ILE:HD12	2.01	0.43
1:2A:1176:G:N2	1:2A:1177:A:N3	2.67	0.43
1:2A:2027:C:O5'	1:2A:2027:C:H6	2.01	0.43
1:2A:2241:G:H1'	23:21:45:ASN:OD1	2.18	0.43
1:2A:2381:G:C6	1:2A:2382:G:C6	3.06	0.43
1:2A:2302:U:O2'	1:2A:2385:C:O2	2.33	0.43
1:2A:38:C:O2	5:2F:46:ARG:NH2	2.49	0.43
1:2A:897:U:H5'	25:23:49:LYS:HD2	2.00	0.43
2:2B:73:A:C4	2:2B:105:A:C2	3.06	0.43
2:2B:21:G:C2	2:2B:63:G:C2	3.07	0.43
2:2B:28:C:H5''	14:2S:31:SER:OG	2.18	0.43
1:2A:2590:C:H4'	4:2E:134:ILE:HG12	2.00	0.43
14:2S:63:THR:OG1	14:2S:64:GLU:N	3.26	0.43
1:1A:2123:U:H2'	1:1A:2124:C:C6	2.54	0.43
1:1A:2331:A:N3	1:1A:2331:A:H2'	2.33	0.43
1:1A:438:A:H8	1:1A:438:A:O5'	2.02	0.43
1:1A:515:G:H2'	1:1A:516:A:C8	2.54	0.43
4:1E:12:THR:HG22	4:1E:13:ARG:N	2.34	0.43
14:1S:3:ARG:HD3	14:1S:3:ARG:C	2.39	0.43
19:1X:57:LEU:HD12	19:1X:78:LYS:HB2	2.00	0.43
23:21:40:ARG:C	23:21:40:ARG:HD3	2.39	0.43
1:2A:322:A:N1	1:2A:345:A:O2'	2.40	0.43
1:2A:37:A:H2'	1:2A:38:C:C6	2.54	0.43
2:2B:6:C:H2'	2:2B:7:G:O4'	2.18	0.43
3:2D:166:GLN:HB2	3:2D:174:ILE:HG22	2.01	0.43
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.54	0.43
8:2I:29:TYR:HD2	8:2I:30:LEU:HD23	1.83	0.43
27:15:16:ARG:O	27:15:20:ARG:HG3	2.18	0.43
1:1A:2224:U:O2'	1:1A:2225:C:H5'	2.18	0.43
1:1A:2339:A:H2'	1:1A:2340:G:H8	1.76	0.43
1:1A:2574:U:H1'	1:1A:2577:A:N6	2.33	0.43
1:1A:2671:A:H2'	1:1A:2672:G:O4'	2.19	0.43
1:1A:62:A:O3'	19:1X:71:GLY:HA3	2.18	0.43
1:1A:661:A:H4'	1:1A:662:G:O5'	2.19	0.43
13:1R:38:VAL:HG22	13:1R:112:ALA:HB2	2.00	0.43
27:25:33:CYS:HA	27:25:34:PRO:HD3	1.89	0.43
1:2A:1248:A:N6	1:2A:1285:U:H2'	2.33	0.43
1:2A:1854:G:OP1	3:2D:52:ARG:NH1	2.48	0.43
1:2A:2020:C:H4'	1:2A:2735:C:O2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2421:G:C2	1:2A:2422:A:H1'	2.53	0.43
1:2A:2429:A:C6	1:2A:2430:U:C4	3.06	0.43
1:2A:54:A:H2'	1:2A:55:C:O4'	2.19	0.43
6:2G:41:GLN:NE2	6:2G:153:ARG:HB3	2.31	0.43
8:2I:61:ARG:HD3	8:2I:61:ARG:HA	1.76	0.43
14:2S:31:SER:N	14:2S:34:HIS:O	2.45	0.43
18:2W:14:PRO:HG2	18:2W:78:GLU:CG	2.48	0.43
1:1A:1700:A:C1'	1:1A:2832:A:H5'	2.49	0.43
1:1A:492:G:O2'	1:1A:842:C:O2'	2.28	0.43
3:1D:70:TRP:HB3	3:1D:190:TYR:CE1	2.54	0.43
1:1A:1247:G:H5'	11:1P:3:LEU:HD22	2.01	0.43
21:1Z:102:LEU:HD13	21:1Z:123:ASP:HA	2.01	0.43
1:2A:1003:A:C6	1:2A:1004:A:C6	3.07	0.43
1:2A:1041:A:C6	1:2A:1205:G:N1	2.87	0.43
1:2A:2397:C:H2'	1:2A:2398:U:C6	2.53	0.43
1:2A:2793:A:H5''	1:2A:2794:G:H5'	2.00	0.43
1:2A:417:G:H2'	1:2A:418:C:O4'	2.19	0.43
1:2A:423:G:N7	59:2A:3739:HOH:O	2.37	0.43
1:2A:503:A:C6	1:2A:505:A:C6	3.07	0.43
3:2D:132:PRO:HG3	3:2D:190:TYR:CE1	2.53	0.43
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	2.00	0.43
5:2F:167:ALA:O	5:2F:170:LEU:HB2	2.19	0.43
20:2Y:68:HIS:ND1	20:2Y:70:SER:HB3	2.34	0.43
21:2Z:157:LEU:HD11	21:2Z:163:LEU:HD13	2.01	0.43
1:1A:1311:G:O4'	18:1W:15:ARG:NH2	2.51	0.43
1:1A:1857:C:OP2	3:1D:222:ARG:NH1	2.52	0.43
4:1E:170:LEU:HB3	4:1E:184:VAL:HG22	2.01	0.43
4:1E:2:LYS:HA	4:1E:84:PHE:CG	2.54	0.43
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.54	0.43
12:1Q:75:THR:HG21	12:1Q:87:LYS:NZ	2.33	0.43
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD21	2.01	0.43
1:2A:1276:G:H2'	1:2A:1277:G:C8	2.69	0.43
1:2A:2212:G:H2'	1:2A:2213:G:O4'	2.19	0.43
1:2A:2225:C:H1'	1:2A:2231:G:N2	2.34	0.43
1:2A:2388:A:H2'	1:2A:2389:A:C8	2.53	0.43
1:2A:915:G:C2	1:2A:954:A:C2	3.07	0.43
2:2B:38:C:O2	2:2B:48:A:H1'	2.19	0.43
1:2A:612:A:OP1	5:2F:95:ARG:NH1	2.52	0.43
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.19	0.43
11:2P:100:LEU:HD22	11:2P:105:LEU:HD12	2.00	0.43
1:1A:1311:G:O2'	1:1A:2033:G:O6	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:263:G:H2'	1:1A:264:U:O4'	2.19	0.43
1:1A:28:U:H2'	1:1A:29:G:C8	2.53	0.43
1:1A:363:A:H2'	1:1A:364:G:O4'	2.19	0.43
4:1E:115:GLY:O	4:1E:119:ARG:HB2	2.19	0.43
15:1T:51:ARG:HD3	59:1T:302:HOH:O	2.18	0.43
23:21:86:SER:OG	23:21:89:GLU:HG3	2.19	0.43
24:22:3:LEU:HD23	24:22:3:LEU:HA	1.80	0.43
1:2A:1313:A:C2	1:2A:2034:A:C4	3.06	0.43
1:2A:344:G:OP1	5:2F:135:LYS:NZ	2.52	0.43
1:2A:673:G:C5	1:2A:674:C:C4	3.07	0.43
2:2B:33:G:C2	2:2B:50:G:C2	3.07	0.43
2:2B:40:U:N3	2:2B:43:C:OP2	2.52	0.43
4:2E:5:LEU:HD11	4:2E:79:ARG:HB2	2.01	0.43
6:2G:114:ILE:HD12	6:2G:117:PHE:HD2	1.83	0.43
11:2P:38:GLN:HG2	11:2P:45:LEU:H	1.83	0.43
1:1A:1632:A:H2'	1:1A:1633:C:C6	2.54	0.43
1:1A:52:G:O2'	29:17:35:ARG:HD3	2.19	0.43
1:1A:806:G:H2'	1:1A:807:A:O4'	2.19	0.43
7:1H:4:ILE:O	7:1H:69:ARG:HG2	2.18	0.43
8:1I:140:LEU:HD23	8:1I:140:LEU:HA	1.77	0.43
8:1I:38:LEU:O	8:1I:40:THR:N	2.46	0.43
8:1I:84:GLY:O	8:1I:86:THR:N	2.52	0.43
1:2A:1333:U:C2	1:2A:1372:C:O2	2.72	0.43
1:2A:1556:A:H2'	1:2A:1557:G:C8	2.54	0.43
1:2A:2091:G:C2	1:2A:2453:C:C2	3.06	0.43
1:2A:2589:G:H1'	59:2A:3961:HOH:O	2.19	0.43
1:2A:323:A:H1'	1:2A:342:C:H1'	2.01	0.43
1:2A:768:A:H2'	1:2A:769:G:C8	2.54	0.43
2:2B:79:C:H2'	2:2B:80:U:O4'	2.19	0.43
1:2A:1835:U:O2	3:2D:50:THR:HB	2.19	0.43
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	2.01	0.43
1:2A:2330:G:C2	14:2S:3:ARG:HA	2.54	0.43
20:2Y:76:CYS:HA	20:2Y:77:PRO:HD3	1.93	0.43
26:14:40:HIS:HB3	26:14:43:TYR:CD1	2.54	0.42
1:1A:1380:U:H2'	1:1A:1381:A:O4'	2.19	0.42
1:1A:1862:C:OP2	59:1A:4202:HOH:O	2.22	0.42
1:1A:214:G:H21	1:1A:216:A:H62	1.67	0.42
1:1A:216:A:H3'	1:1A:217:A:C5'	2.46	0.42
1:1A:2568:G:H2'	1:1A:2569:C:C6	2.54	0.42
1:1A:2731:G:OP2	59:1A:4201:HOH:O	2.21	0.42
3:1D:249:PRO:HD2	3:1D:250:TRP:CZ3	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:101:PRO:O	21:1Z:102:LEU:HD12	2.18	0.42
25:23:48:GLU:HA	25:23:51:ALA:HB2	2.00	0.42
11:2P:63:PRO:HG2	30:28:25:MET:HB2	2.01	0.42
1:2A:1402:U:H2'	1:2A:1403:G:O4'	2.19	0.42
1:2A:1543:C:O4'	1:2A:1623:C:H4'	2.19	0.42
1:2A:2263:G:H2'	1:2A:2264:G:O4'	2.19	0.42
1:2A:232:A:C2	1:2A:243:A:C4	3.07	0.42
1:2A:24:U:C4	1:2A:25:G:C6	3.07	0.42
1:2A:2878:G:H2'	1:2A:2879:C:O4'	2.19	0.42
1:2A:351:U:H4'	20:2Y:68:HIS:CG	2.54	0.42
1:2A:44:C:OP2	1:2A:203:G:H5'	2.19	0.42
1:2A:493:G:H2'	1:2A:494:G:O4'	2.19	0.42
1:2A:846:A:OP1	1:2A:846:A:H8	2.03	0.42
5:2F:24:LEU:HD21	5:2F:114:VAL:HG12	2.01	0.42
1:2A:719:C:H5''	5:2F:81:PRO:HD2	1.99	0.42
8:2I:129:THR:HA	8:2I:138:ILE:O	2.19	0.42
1:1A:1638:G:H2'	1:1A:1639:G:C8	2.54	0.42
1:1A:2059:G:H2'	1:1A:2060:C:O4'	2.19	0.42
1:1A:703:U:H2'	1:1A:704:C:H6	1.84	0.42
10:1O:64:ARG:NH1	10:1O:81:ASP:OD1	2.52	0.42
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.65	0.42
6:2G:108:ASN:HA	26:24:37:SER:HB2	2.00	0.42
1:2A:1147:C:H2'	1:2A:1148:A:C8	2.51	0.42
1:2A:1567:G:H3'	1:2A:1568:U:H6	1.83	0.42
1:2A:1569:G:N2	1:2A:1570:G:H1'	2.34	0.42
1:2A:17:C:H2'	1:2A:18:C:C6	2.52	0.42
1:2A:1813:A:H5'	1:2A:2619:G:H4'	2.01	0.42
1:2A:2327:C:H2'	1:2A:2328:C:C6	2.54	0.42
1:2A:325:C:P	20:2Y:73:ARG:HH12	2.42	0.42
1:2A:754:C:N4	1:2A:769:G:H1	2.17	0.42
1:2A:770:U:H2'	1:2A:771:G:O4'	2.19	0.42
1:2A:885:U:H1'	1:2A:1235:G:H1'	2.01	0.42
1:2A:956:A:H2'	12:2Q:9:TYR:OH	2.18	0.42
2:2B:95:C:H2'	2:2B:96:U:H6	1.84	0.42
22:10:38:VAL:HB	22:10:59:LEU:HB2	2.01	0.42
23:11:23:LYS:HB3	23:11:29:GLY:HA3	2.01	0.42
30:18:62:LEU:HB3	30:18:65:GLU:CG	2.49	0.42
1:1A:1809:U:H2'	59:1A:4240:HOH:O	2.19	0.42
1:1A:875:A:N7	1:1A:2259:C:H5'	2.34	0.42
4:1E:116:VAL:HG11	4:1E:138:PRO:HB3	2.00	0.42
8:1I:129:THR:HG22	8:1I:139:GLN:NE2	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:46:LYS:HB3	11:1P:46:LYS:HE3	1.78	0.42
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	2.00	0.42
1:2A:1051:C:C2	1:2A:1182:G:N2	2.87	0.42
1:2A:1409:G:OP2	23:21:3:LYS:HG3	2.19	0.42
1:2A:138:A:H8	1:2A:1453:C:HO2'	1.64	0.42
1:2A:860:C:O2'	1:2A:861:C:H5'	2.20	0.42
1:2A:90:G:H2'	1:2A:91:C:C6	2.55	0.42
2:2B:102:A:H8	2:2B:102:A:O5'	2.01	0.42
3:2D:274:ARG:HE	3:2D:274:ARG:HB3	1.67	0.42
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	2.01	0.42
5:2F:106:ARG:H	5:2F:106:ARG:HG2	1.46	0.42
5:2F:46:ARG:NH1	5:2F:46:ARG:HB3	3.62	0.42
11:2P:38:GLN:HG2	11:2P:45:LEU:N	2.34	0.42
12:2Q:32:TYR:CE1	12:2Q:133:ARG:HG3	2.54	0.42
14:2S:26:LEU:HD22	14:2S:87:PHE:CD1	2.54	0.42
25:13:18:ASP:OD1	25:13:18:ASP:N	2.48	0.42
1:1A:237:C:O2	1:1A:281:G:N2	64.39	0.42
3:1D:37:LEU:HD22	3:1D:87:ASN:HD21	1.84	0.42
6:1G:7:LEU:HD13	6:1G:100:TRP:CE3	2.51	0.42
1:2A:865:A:C4	1:2A:1233:A:C2	3.07	0.42
1:2A:1879:G:H2'	1:2A:1880:G:H8	1.85	0.42
1:2A:1953:A:H2'	1:2A:1954:G:O4'	2.19	0.42
1:2A:2485:C:H5''	1:2A:2486:C:OP2	2.19	0.42
1:2A:2588:A:O4'	27:25:3:LYS:HB2	2.19	0.42
1:2A:352:G:H8	1:2A:352:G:OP1	2.02	0.42
1:2A:630:A:H2'	1:2A:631:A:C8	2.54	0.42
3:2D:4:LYS:HG2	3:2D:18:VAL:HG22	2.00	0.42
7:2H:102:ALA:HB2	7:2H:116:GLU:OE2	2.19	0.42
8:2I:77:LEU:HG	8:2I:101:LEU:HD12	2.02	0.42
12:2Q:32:TYR:OH	12:2Q:111:GLU:OE1	2.32	0.42
21:2Z:108:PRO:HD3	21:2Z:141:VAL:HG23	2.02	0.42
1:1A:1320:A:O2'	1:1A:1691:G:N3	2.52	0.42
1:1A:2523:C:H2'	1:1A:2524:G:O4'	2.19	0.42
7:1H:83:TYR:CZ	7:1H:138:LYS:HD2	2.55	0.42
10:1O:7:TYR:CE1	10:1O:20:MET:HB2	2.54	0.42
11:1P:65:ARG:HG3	11:1P:66:GLY:N	2.33	0.42
21:1Z:145:GLU:O	21:1Z:148:ASP:N	2.36	0.42
1:2A:1409:G:P	23:21:3:LYS:HG3	2.60	0.42
25:23:30:ARG:H	25:23:33:GLN:NE2	2.18	0.42
11:2P:65:ARG:HG3	30:28:25:MET:HG3	2.01	0.42
1:2A:1717:U:O2'	1:2A:1719:U:H5	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2291:G:O6	22:20:14:ARG:HD3	2.20	0.42
1:2A:29:G:C5	1:2A:30:C:C4	3.07	0.42
1:2A:905:G:O2'	1:2A:961:G:O6	2.28	0.42
5:2F:160:ASN:HB3	5:2F:163:VAL:HB	2.00	0.42
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.19	0.42
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	2.01	0.42
9:2N:120:LEU:HD22	9:2N:122:VAL:HG23	2.00	0.42
9:2N:4:TYR:HB2	16:2U:101:ARG:NH1	2.35	0.42
14:2S:84:GLN:CA	14:2S:111:GLU:HB2	2.46	0.42
28:16:6:ARG:NE	28:16:24:GLU:OE1	2.25	0.42
1:1A:2031:G:O6	59:1A:4195:HOH:O	2.21	0.42
1:1A:274:C:H2'	1:1A:275:C:C6	2.54	0.42
1:1A:282:G:O6	59:1A:4166:HOH:O	2.16	0.42
1:1A:682:G:H1	1:1A:695:C:N4	2.08	0.42
1:1A:769:G:H2'	1:1A:770:U:O4'	2.20	0.42
6:1G:11:TYR:HB2	6:1G:176:LEU:HD21	2.01	0.42
2:1B:57:A:H1'	6:1G:29:TRP:HB2	2.01	0.42
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	2.02	0.42
1:2A:897:U:O2'	25:23:42:ALA:O	2.31	0.42
1:2A:1443:C:H2'	1:2A:1444:C:O4'	2.74	0.42
1:2A:1726:U:O2	1:2A:1793:G:H3'	2.20	0.42
1:2A:2347:A:H61	22:20:43:THR:CG2	2.33	0.42
1:2A:2752:A:H2'	1:2A:2753:A:C8	2.54	0.42
1:2A:2801:C:H3'	59:2A:4107:HOH:O	2.20	0.42
1:2A:2880:C:N4	59:2A:3823:HOH:O	2.52	0.42
1:2A:378:G:H2'	1:2A:379:G:H8	1.84	0.42
1:2A:541:C:OP1	27:25:16:ARG:NH2	2.52	0.42
3:2D:213:ARG:HA	3:2D:213:ARG:HD2	1.83	0.42
6:2G:146:TYR:O	6:2G:149:VAL:HG12	2.20	0.42
6:2G:47:LYS:HE2	6:2G:47:LYS:HB2	1.71	0.42
1:1A:1960:U:OP1	1:1A:2615:U:O2'	2.35	0.42
1:1A:2356:G:OP2	28:16:38:LYS:NZ	2.53	0.42
1:1A:838:G:H5''	1:1A:839:A:H5'	2.02	0.42
1:1A:963:A:N3	2:1B:80:U:O2'	2.46	0.42
12:1Q:12:GLN:OE1	12:1Q:73:PRO:HD2	2.20	0.42
15:1T:7:ILE:O	15:1T:11:GLU:HG3	2.20	0.42
1:2A:903:C:H4'	22:20:23:VAL:HG21	2.01	0.42
28:26:40:CYS:HA	28:26:41:PRO:HD3	1.85	0.42
1:2A:1070:G:H22	1:2A:1082:G:H1'	30.10	0.42
1:2A:1332:A:C5	1:2A:1333:U:C4	3.08	0.42
1:2A:1350:C:C2	1:2A:1669:G:C2	3.08	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2687:C:O2	1:2A:2744:G:N2	2.51	0.42
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	2.01	0.42
12:2Q:47:ILE:HD12	12:2Q:70:PRO:HG3	2.01	0.42
1:1A:1540:A:H2'	1:1A:1541:A:H8	1.81	0.42
1:1A:2735:C:OP1	13:1R:3:HIS:ND1	2.47	0.42
1:1A:2746:A:H2'	1:1A:2747:G:O4'	2.20	0.42
1:1A:462:C:H2'	1:1A:463:G:C8	2.54	0.42
7:1H:38:SER:HB3	7:1H:41:MET:HG2	2.01	0.42
7:1H:71:LEU:HD12	7:1H:71:LEU:HA	1.88	0.42
8:1I:44:LEU:HD12	8:1I:44:LEU:HA	1.91	0.42
1:1A:411:C:O2	11:1P:71:VAL:HG21	2.20	0.42
13:1R:28:LEU:HD12	13:1R:44:LEU:HD13	2.01	0.42
18:1W:84:ARG:HG3	18:1W:98:LYS:HD2	2.01	0.42
1:2A:1701:A:H4'	4:2E:115:GLY:N	2.35	0.42
1:2A:1847:G:H3'	3:2D:157:ARG:HH21	1.85	0.42
1:2A:2091:G:C4	1:2A:2092:A:C8	3.08	0.42
1:2A:250:A:H2'	1:2A:251:C:O4'	2.20	0.42
1:2A:2589:G:H2'	1:2A:2590:C:C6	2.55	0.42
1:2A:582:C:H2'	1:2A:583:G:O4'	2.20	0.42
1:2A:623:C:O2	1:2A:627:C:H4'	2.20	0.42
1:2A:753:G:H2'	1:2A:754:C:O4'	2.19	0.42
1:2A:925:G:N7	1:2A:926:G:C8	2.88	0.42
6:2G:16:ARG:NH2	6:2G:28:VAL:HG12	2.34	0.42
1:2A:2695:U:H1'	10:2O:70:LYS:HE3	2.01	0.42
20:2Y:90:LEU:HB3	20:2Y:92:ASN:H	1.85	0.42
1:1A:1343:C:N4	1:1A:1344:G:C6	2.88	0.42
1:1A:963:A:H5''	2:1B:98:G:O2'	2.20	0.42
5:1F:126:VAL:HG21	5:1F:129:PHE:CZ	2.54	0.42
1:1A:1176:G:H21	9:1N:73:THR:HG21	1.85	0.42
14:1S:87:PHE:HB2	14:1S:112:PHE:CD2	2.55	0.42
21:1Z:129:SER:HA	21:1Z:130:PRO:HD3	1.91	0.42
1:2A:2547:G:H2'	1:2A:2548:U:O4'	2.20	0.42
1:2A:2596:U:H4'	1:2A:2597:C:OP1	2.19	0.42
1:2A:861:C:C2	1:2A:1237:G:C2	3.08	0.42
1:2A:919:G:N2	1:2A:950:U:C2	2.88	0.42
3:2D:72:LYS:HG3	3:2D:103:ARG:HH22	1.85	0.42
7:2H:106:THR:O	7:2H:106:THR:OG1	2.37	0.42
8:2I:135:GLU:C	8:2I:137:PRO:HD3	2.40	0.42
1:2A:1184:C:OP1	9:2N:23:LEU:HB3	2.19	0.42
1:2A:437:G:C5	11:2P:72:PRO:HB3	2.55	0.42
12:2Q:12:GLN:HG2	12:2Q:73:PRO:HD2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:84:GLY:O	12:2Q:85:LYS:HB2	2.20	0.42
1:1A:1153:U:H6	1:1A:1154:C:C6	2.38	0.42
1:1A:1620:C:N4	59:1A:4136:HOH:O	2.53	0.42
1:1A:2093:G:O6	59:1A:4203:HOH:O	2.22	0.42
1:1A:503:A:N1	1:1A:524:G:H4'	2.35	0.42
1:1A:510:C:H2'	1:1A:511:C:H6	1.84	0.42
1:1A:610:U:H2'	1:1A:611:C:H6	1.82	0.42
3:1D:213:ARG:HA	3:1D:213:ARG:HD2	1.84	0.42
6:1G:56:ALA:HA	6:1G:153:ARG:NH2	2.35	0.42
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.55	0.42
18:1W:65:LEU:HD12	18:1W:68:ARG:NH2	2.35	0.42
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	2.02	0.42
29:27:22:MET:HA	29:27:28:ARG:HG2	2.00	0.42
1:2A:1118:A:H3'	1:2A:1119:G:H8	1.84	0.42
1:2A:1450:U:H2'	1:2A:1451:U:H6	1.85	0.42
1:2A:2273:U:H4'	1:2A:2339:A:C2	2.55	0.42
1:2A:2282:G:H2'	1:2A:2283:U:C6	2.55	0.42
1:2A:2698:U:H2'	1:2A:2699:U:O4'	2.20	0.42
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.53	0.42
13:2R:100:LEU:HA	13:2R:100:LEU:HD12	1.90	0.42
1:2A:2389:A:H4'	14:2S:23:ARG:HH11	1.84	0.42
18:2W:16:LYS:O	18:2W:19:LEU:HB2	2.20	0.42
1:1A:1043:C:P	16:1U:92:ARG:HH22	2.43	0.41
1:1A:1257:A:N3	1:1A:1283:G:O2'	2.42	0.41
1:1A:1301:G:O6	59:1A:4191:HOH:O	2.20	0.41
1:1A:1345:U:H4'	1:1A:1346:A:H5'	2.01	0.41
1:1A:2778:G:N3	1:1A:2778:G:H2'	2.34	0.41
1:1A:738:C:O2'	3:1D:38:LYS:NZ	2.53	0.41
1:1A:910:G:O2'	1:1A:911:C:H5'	2.20	0.41
5:1F:12:LEU:HG	5:1F:124:LEU:HD11	2.01	0.41
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.51	0.41
21:1Z:11:GLU:HB3	21:1Z:12:GLY:H	1.65	0.41
21:1Z:185:GLU:OE2	21:1Z:186:GLU:HG3	2.20	0.41
25:23:22:ALA:HB2	25:23:49:LYS:HD3	2.01	0.41
31:29:17:ILE:HA	31:29:17:ILE:HD12	1.76	0.41
1:2A:1090:A:H4'	1:2A:1091:A:H5''	2.02	0.41
1:2A:1200:A:H5''	16:2U:55:ARG:HD3	2.02	0.41
1:2A:1404:A:C6	1:2A:1417:U:O4	2.73	0.41
1:2A:1883:A:H2'	1:2A:1884:A:C8	2.55	0.41
1:2A:2549:C:H2'	1:2A:2550:C:H6	1.84	0.41
1:2A:398:G:H8	23:21:65:SER:O	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:766:C:H2'	1:2A:767:C:H6	1.84	0.41
4:2E:31:CYS:HA	4:2E:32:PRO:HD2	1.82	0.41
14:2S:25:ARG:NH1	14:2S:42:ASP:OD1	2.46	0.41
1:1A:228:G:H1'	1:1A:258:A:N1	39.86	0.41
1:1A:2643:A:O2'	1:1A:2820:G:O2'	2.20	0.41
1:1A:62:A:C5	19:1X:66:LEU:HD13	2.55	0.41
1:1A:909:A:H2'	1:1A:910:G:C8	2.55	0.41
11:1P:100:LEU:HA	11:1P:100:LEU:HD23	1.86	0.41
14:1S:4:LEU:HD12	14:1S:4:LEU:HA	1.69	0.41
1:2A:2429:A:C5	1:2A:2430:U:C4	3.07	0.41
1:2A:38:C:H2'	1:2A:39:C:C6	2.55	0.41
1:2A:621:G:H2'	1:2A:622:G:H8	2.71	0.41
1:2A:624:G:O2'	1:2A:701:A:N6	2.52	0.41
1:2A:6:G:H2'	1:2A:7:A:C8	2.55	0.41
1:2A:930:C:H3'	1:2A:931:C:C6	2.55	0.41
3:2D:65:ILE:HB	3:2D:67:PHE:CE2	2.56	0.41
6:2G:145:THR:HG23	6:2G:148:MET:SD	2.60	0.41
12:2Q:27:VAL:O	12:2Q:27:VAL:HG12	2.20	0.41
16:2U:83:LEU:O	16:2U:87:GLY:N	2.50	0.41
1:1A:2588:A:O4'	27:15:3:LYS:HB2	2.20	0.41
1:1A:810:A:H5'	3:1D:210:GLY:HA2	2.02	0.41
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.38	0.41
1:1A:2668:A:O3'	7:1H:160:LYS:NZ	2.53	0.41
8:1I:110:ASP:HA	8:1I:111:PRO:HD2	1.72	0.41
1:1A:1711:A:H4'	10:1O:67:LYS:HB2	2.02	0.41
12:1Q:18:LYS:HE3	12:1Q:18:LYS:HB2	1.91	0.41
18:1W:79:GLY:HA3	18:1W:100:THR:HG22	2.02	0.41
20:1Y:43:ASN:HD22	20:1Y:43:ASN:HA	1.51	0.41
20:1Y:54:LYS:CA	20:1Y:56:PRO:HD3	2.44	0.41
26:24:60:GLN:H	26:24:62:ARG:HE	1.68	0.41
1:2A:1052:C:H42	1:2A:1089:G:H1	56.61	0.41
1:2A:1713:G:H22	1:2A:2013:G:H5'	1.84	0.41
1:2A:604:G:H2'	1:2A:605:G:C8	2.55	0.41
10:2O:93:PRO:HG3	10:2O:113:LYS:HB3	2.01	0.41
15:2T:54:ARG:HA	15:2T:59:THR:HG22	2.03	0.41
17:2V:89:GLN:HA	17:2V:90:PRO:HD3	1.86	0.41
28:16:21:TYR:CE2	28:16:38:LYS:HG2	2.56	0.41
28:16:14:THR:OG1	28:16:48:VAL:O	2.27	0.41
1:1A:1066:A:C3'	1:1A:1066:A:C8	3.04	0.41
5:1F:192:LEU:HD22	5:1F:194:MET:HG3	2.01	0.41
7:1H:104:GLU:HG3	7:1H:114:VAL:HG22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1067:G:N7	9:1N:66:LYS:HE2	2.36	0.41
12:1Q:75:THR:HG22	59:1Q:5006:HOH:O	2.21	0.41
25:23:12:PRO:O	25:23:15:TYR:HB2	2.20	0.41
1:2A:1067:G:C6	1:2A:1184:C:C4	3.08	0.41
1:2A:1073:A:N6	1:2A:1171:A:OP1	2.54	0.41
1:2A:2062:U:H2'	1:2A:2063:A:C8	2.56	0.41
1:2A:2358:C:H2'	1:2A:2359:U:C6	2.55	0.41
1:2A:2547:G:H2'	1:2A:2548:U:H6	1.85	0.41
1:2A:320:C:H2'	1:2A:321:G:O4'	2.21	0.41
1:2A:517:G:H2'	1:2A:518:G:O4'	2.19	0.41
1:2A:579:U:H2'	1:2A:580:G:H8	1.85	0.41
3:2D:264:LYS:HA	3:2D:265:PRO:HD3	1.93	0.41
12:2Q:69:PHE:HA	12:2Q:70:PRO:HD3	1.66	0.41
26:14:48:ARG:O	26:14:50:VAL:N	2.53	0.41
11:1P:63:PRO:HG2	30:18:25:MET:HB2	2.02	0.41
1:1A:955:A:H2'	1:1A:956:A:H5''	4.47	0.41
3:1D:132:PRO:HA	3:1D:190:TYR:HA	2.03	0.41
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	2.02	0.41
6:1G:46:ALA:HB2	6:1G:53:LEU:HD12	2.01	0.41
17:1V:1:MET:HB2	17:1V:43:GLU:OE2	2.20	0.41
18:1W:20:VAL:HG11	18:1W:44:ALA:HA	2.02	0.41
20:1Y:92:ASN:HB2	20:1Y:94:LYS:N	2.26	0.41
1:2A:1044:U:H5''	1:2A:1199:G:O6	2.21	0.41
1:2A:1337:U:H2'	1:2A:1338:C:C6	2.56	0.41
1:2A:1585:G:H2'	1:2A:1586:U:O4'	2.20	0.41
1:2A:1808:U:H2'	1:2A:1814:A:N6	2.34	0.41
1:2A:183:A:OP1	11:2P:46:LYS:NZ	2.42	0.41
1:2A:2371:A:C2	1:2A:2372:A:H1'	2.55	0.41
1:2A:2763:G:C4	7:2H:2:SER:HA	2.56	0.41
1:2A:363:A:H2'	1:2A:364:G:O4'	2.20	0.41
1:2A:483:G:O2'	29:27:39:ARG:HD3	2.20	0.41
1:2A:514:G:N7	18:2W:49:LYS:NZ	2.68	0.41
1:2A:776:C:H3'	59:2A:3981:HOH:O	2.21	0.41
10:2O:71:ARG:NE	10:2O:105:GLU:OE2	2.54	0.41
13:2R:65:LEU:HD12	13:2R:65:LEU:HA	1.86	0.41
20:2Y:40:GLU:O	20:2Y:42:VAL:HG23	2.20	0.41
1:1A:2367:C:O3'	22:10:20:ARG:HD3	2.20	0.41
26:14:56:VAL:HG12	26:14:60:GLN:HE22	1.85	0.41
1:1A:136:G:N7	59:1A:4364:HOH:O	2.37	0.41
1:1A:149:C:O2	1:1A:163:G:N2	7.03	0.41
1:1A:2208:G:H5''	1:1A:2209:C:OP1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:106:ILE:O	3:1D:108:PRO:HD3	2.21	0.41
22:20:43:THR:OG1	22:20:46:LYS:HG2	2.21	0.41
29:27:30:VAL:O	29:27:34:ARG:HG3	2.21	0.41
30:28:52:LYS:O	30:28:56:GLU:HG3	2.21	0.41
1:2A:1114:A:C5	1:2A:1118:A:C5	3.09	0.41
1:2A:2214:G:H2'	1:2A:2215:G:C8	2.56	0.41
1:2A:2296:C:OP2	28:26:6:ARG:NH1	2.53	0.41
1:2A:2735:C:H4'	13:2R:1:MET:HG3	2.02	0.41
1:2A:784:G:C6	1:2A:785:G:C2	3.08	0.41
3:2D:53:PHE:CE1	3:2D:221:VAL:HG12	2.55	0.41
3:2D:43:ARG:HA	3:2D:48:ARG:O	2.21	0.41
6:2G:68:PRO:HB2	6:2G:90:LEU:HB3	2.02	0.41
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.20	0.41
19:2X:5:TYR:CE1	24:22:30:ARG:HB2	2.56	0.41
21:2Z:105:VAL:O	21:2Z:141:VAL:HG22	2.21	0.41
23:11:73:LEU:HA	23:11:73:LEU:HD23	1.86	0.41
1:1A:2096:U:OP2	1:1A:2249:G:O2'	2.36	0.41
1:1A:275:C:H2'	1:1A:276:G:O4'	2.21	0.41
1:1A:819:U:O2'	3:1D:48:ARG:HD3	2.21	0.41
3:1D:76:PRO:HB2	3:1D:116:GLN:HE21	1.86	0.41
4:1E:12:THR:HG21	15:1T:11:GLU:HG2	2.02	0.41
30:28:34:TRP:CE2	30:28:35:GLN:HB2	2.56	0.41
1:2A:230:G:C8	30:28:3:LYS:HG3	2.56	0.41
1:2A:1342:C:OP1	1:2A:2721:C:H4'	2.20	0.41
1:2A:1488:G:H1	1:2A:1594:C:H42	1.68	0.41
1:2A:1887:G:O2'	1:2A:1906:A:N6	2.43	0.41
1:2A:2115:G:N2	1:2A:2217:C:H1'	2.35	0.41
1:2A:2547:G:C5	1:2A:2548:U:C5	3.08	0.41
1:2A:2574:U:N3	1:2A:2577:A:OP2	2.34	0.41
1:2A:368:A:N3	1:2A:370:A:N6	2.67	0.41
1:2A:542:G:H2'	1:2A:543:U:H6	1.85	0.41
1:2A:619:U:H2'	1:2A:620:G:H8	1.86	0.41
7:2H:71:LEU:HD22	7:2H:71:LEU:HA	1.89	0.41
19:2X:12:VAL:HG22	19:2X:29:TRP:NE1	2.36	0.41
12:2Q:60:ARG:HA	21:2Z:178:GLU:O	2.20	0.41
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.50	0.41
22:10:82:ARG:HA	22:10:83:PRO:HD3	1.86	0.41
26:14:68:ARG:HD2	26:14:68:ARG:HA	1.88	0.41
1:1A:1153:U:H1'	1:1A:1154:C:O5'	2.20	0.41
1:1A:1709:C:O2'	1:1A:1710:A:O5'	2.38	0.41
1:1A:2342:G:O2'	1:1A:2347:A:N1	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2604:U:H2'	1:1A:2605:C:C6	2.55	0.41
1:1A:2651:G:OP1	9:1N:97:ARG:NH2	2.48	0.41
1:1A:551:C:C5	1:1A:2791:U:H2'	2.55	0.41
5:1F:14:PRO:HD2	5:1F:127:GLU:OE1	2.21	0.41
8:1I:72:LEU:C	8:1I:74:ASN:N	2.74	0.41
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	2.01	0.41
1:2A:2038:U:O2	27:25:10:LYS:HB2	2.20	0.41
1:2A:1205:G:C6	1:2A:1206:C:N3	2.89	0.41
1:2A:1349:C:H2'	1:2A:1350:C:C6	3.23	0.41
1:2A:141:G:C2	1:2A:142:C:C2	3.09	0.41
1:2A:173:U:H4'	1:2A:206:A:H4'	2.03	0.41
1:2A:2710:C:H2'	1:2A:2711:C:O4'	2.20	0.41
1:2A:1700:A:H1'	1:2A:2832:A:H5'	2.03	0.41
1:2A:496:A:H2'	1:2A:497:A:O4'	2.20	0.41
1:2A:780:A:O2'	1:2A:1681:G:H5'	2.20	0.41
2:2B:19:G:N2	2:2B:64:C:N3	2.61	0.41
8:2I:53:ALA:O	8:2I:57:ARG:HG2	2.21	0.41
14:2S:36:TYR:CD1	14:2S:36:TYR:N	2.89	0.41
1:2A:797:A:H5'	18:2W:90:ARG:HA	2.03	0.41
24:12:60:LEU:HA	24:12:60:LEU:HD23	1.87	0.41
28:16:11:LEU:HB3	28:16:49:HIS:HB3	2.01	0.41
1:1A:815:G:H5'	1:1A:1424:A:N6	2.35	0.41
1:1A:1575:G:H2'	1:1A:1576:C:C6	2.55	0.41
1:1A:1631:A:O5'	1:1A:1631:A:H8	2.03	0.41
1:1A:2046:C:H2'	1:1A:2047:C:C6	2.56	0.41
1:1A:2783:C:H2'	1:1A:2784:C:C6	2.55	0.41
1:1A:764:A:C5	1:1A:765:C:H1'	2.56	0.41
4:1E:144:ARG:HB3	4:1E:145:LYS:H	1.39	0.41
7:1H:124:GLU:HB2	7:1H:132:ARG:HB3	2.03	0.41
10:1O:10:VAL:HG13	10:1O:17:ARG:C	2.40	0.41
11:1P:39:LYS:HB2	11:1P:45:LEU:HD21	2.03	0.41
19:1X:1:MET:HE1	24:12:26:ARG:HH21	1.85	0.41
20:1Y:30:VAL:HG22	20:1Y:37:VAL:HG12	2.03	0.41
21:1Z:92:SER:O	21:1Z:94:GLU:N	2.40	0.41
19:2X:5:TYR:HD1	24:22:33:MET:SD	2.44	0.41
27:25:38:ALA:CB	27:25:48:GLU:HG3	2.50	0.41
28:26:6:ARG:NE	28:26:24:GLU:OE1	2.25	0.41
1:2A:1072:A:N6	1:2A:1171:A:C4	2.89	0.41
1:2A:1067:G:C5	1:2A:1184:C:N4	2.89	0.41
1:2A:2423:A:H2'	1:2A:2424:G:O4'	2.20	0.41
1:2A:455:A:OP1	1:2A:455:A:H8	4.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:791:G:C2'	1:2A:792:A:H5'	2.51	0.41
1:2A:346:G:C8	5:2F:171:PRO:HG3	2.56	0.41
1:2A:2829:A:C5	13:2R:4:LEU:HD11	2.56	0.41
19:2X:12:VAL:HG21	19:2X:27:THR:HG22	2.03	0.41
1:1A:1222:C:H2'	1:1A:1223:C:H6	1.85	0.41
1:1A:1685:U:O2'	1:1A:1686:C:H5'	2.21	0.41
1:1A:2587:G:H1'	59:1A:4867:HOH:O	2.19	0.41
1:1A:25:G:C6	1:1A:26:G:C6	3.08	0.41
11:1P:59:LEU:HD22	11:1P:59:LEU:O	2.21	0.41
20:1Y:6:HIS:H	20:1Y:6:HIS:HD2	1.63	0.41
21:1Z:33:LEU:HD12	21:1Z:35:ARG:HG2	2.03	0.41
26:24:60:GLN:N	26:24:62:ARG:HE	2.19	0.41
1:2A:1101:G:H5''	1:2A:1102:A:H5'	2.02	0.41
1:2A:2048:G:C6	1:2A:2049:U:C4	3.09	0.41
1:2A:2224:U:H2'	1:2A:2225:C:H6	1.86	0.41
1:2A:2829:A:O2'	1:2A:2830:A:OP1	2.35	0.41
1:2A:338:G:H2'	1:2A:339:C:H6	1.86	0.41
1:2A:66:G:H2'	1:2A:67:C:O4'	2.21	0.41
1:2A:979:C:H2'	1:2A:980:C:H6	1.85	0.41
3:2D:136:ILE:HA	3:2D:137:PRO:HD3	1.90	0.41
3:2D:6:PHE:HE1	3:2D:18:VAL:HG13	1.86	0.41
1:2A:622:G:H5'	5:2F:32:LEU:HD12	2.03	0.41
9:2N:103:VAL:O	9:2N:107:LEU:HG	2.20	0.41
14:2S:15:ARG:O	14:2S:19:LYS:HG3	2.21	0.41
1:1A:1245:C:H2'	1:1A:1246:C:H6	1.86	0.41
1:1A:1319:A:N3	1:1A:1342:C:H1'	2.36	0.41
1:1A:1854:G:OP1	3:1D:52:ARG:NH1	2.53	0.41
1:1A:200:G:H2'	1:1A:201:A:O4'	2.21	0.41
1:1A:2330:G:C2	14:1S:3:ARG:HA	2.55	0.41
1:1A:238:G:OP2	30:18:13:ARG:NH2	2.47	0.41
1:1A:268:G:H2'	1:1A:269:C:C6	2.56	0.41
1:1A:485:A:H2'	1:1A:486:C:O4'	2.21	0.41
1:1A:873:U:O2	1:1A:2257:G:H4'	2.21	0.41
1:1A:909:A:H2'	1:1A:910:G:H8	1.85	0.41
2:1B:29:A:C2	2:1B:30:C:C2	3.09	0.41
3:1D:108:PRO:HG3	3:1D:143:HIS:CE1	2.56	0.41
3:1D:68:LYS:O	3:1D:69:ARG:HB2	2.20	0.41
3:1D:71:ASP:CB	3:1D:103:ARG:HH22	2.34	0.41
9:1N:67:LEU:HD12	9:1N:67:LEU:HA	1.79	0.41
14:1S:67:ARG:O	14:1S:71:ARG:HG3	2.20	0.41
1:2A:1090:A:N1	1:2A:1155:G:O2'	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1433:G:H2'	1:2A:1434:G:H8	1.86	0.41
1:2A:16:G:C6	1:2A:17:C:N4	2.89	0.41
1:2A:1803:A:C5	1:2A:1859:A:H1'	2.56	0.41
1:2A:2046:C:H2'	1:2A:2047:C:C6	2.56	0.41
1:2A:593:A:N6	1:2A:2510:C:O3'	2.53	0.41
1:2A:251:C:H2'	1:2A:252:C:O4'	2.21	0.41
1:2A:398:G:O2'	1:2A:399:U:OP2	2.39	0.41
1:2A:521:A:H2'	1:2A:522:G:O4'	2.20	0.41
5:2F:155:LEU:HD11	5:2F:176:LEU:HD12	2.01	0.41
6:2G:123:ASN:C	6:2G:125:PHE:H	2.25	0.41
9:2N:72:TYR:N	9:2N:85:ILE:O	2.37	0.41
13:2R:74:LYS:HG2	13:2R:77:ARG:HH21	1.85	0.41
14:2S:27:SER:HA	14:2S:88:ASP:HB3	2.03	0.41
14:2S:33:LYS:HB3	14:2S:34:HIS:CD2	2.56	0.41
2:2B:8:U:O2'	14:2S:40:ILE:HD13	2.21	0.41
14:2S:5:THR:OG1	14:2S:8:GLU:HG3	2.20	0.41
19:2X:31:HIS:HA	19:2X:32:PRO:HD3	1.84	0.41
25:13:59:VAL:HG23	25:13:60:GLU:HG2	2.03	0.40
1:1A:115:A:C8	1:1A:116:A:C8	3.09	0.40
1:1A:1320:A:H4'	1:1A:1321:A:O5'	2.20	0.40
1:1A:154:C:H42	1:1A:159:G:H1	1.67	0.40
1:1A:1738:U:H2'	1:1A:1740:C:C5	2.56	0.40
1:1A:504:A:N3	1:1A:506:G:H5''	2.36	0.40
1:1A:767:C:H2'	1:1A:768:A:H8	1.86	0.40
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.20	0.40
6:1G:181:ARG:HG3	6:1G:182:LYS:H	1.86	0.40
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.56	0.40
12:1Q:2:LEU:HB2	59:1Q:5008:HOH:O	2.21	0.40
1:1A:1297:G:N3	16:1U:33:ARG:HG2	2.37	0.40
1:1A:793:U:O2'	18:1W:92:ARG:NH2	2.54	0.40
21:1Z:75:ASN:HB2	21:1Z:85:HIS:HB3	2.02	0.40
1:2A:1140:A:N7	1:2A:1141:A:C5	2.89	0.40
1:2A:1330:G:N2	1:2A:1374:U:OP1	2.50	0.40
1:2A:1381:A:H2'	1:2A:1382:G:H8	1.86	0.40
1:2A:1456:C:H2'	1:2A:1457:A:H8	1.85	0.40
1:2A:1466:G:H2'	1:2A:1467:G:H8	1.86	0.40
1:2A:2314:G:C2'	1:2A:2315:G:H5'	2.51	0.40
1:2A:500:U:H5''	1:2A:501:G:OP2	2.21	0.40
1:2A:651:A:C6	1:2A:661:A:C8	3.09	0.40
1:2A:821:G:C4	1:2A:840:G:C8	3.09	0.40
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:12:LEU:HD23	8:2I:12:LEU:HA	1.90	0.40
8:2I:9:LEU:HA	8:2I:9:LEU:HD13	1.97	0.40
10:2O:71:ARG:HA	10:2O:72:PRO:HD3	1.92	0.40
13:2R:66:VAL:HG11	13:2R:79:LEU:HD12	2.03	0.40
14:2S:110:LEU:HD12	14:2S:110:LEU:HA	1.79	0.40
1:2A:1659:A:N1	18:2W:93:ALA:HB2	2.36	0.40
1:2A:82:A:H5'	20:2Y:8:LYS:HG2	2.03	0.40
21:2Z:28:MET:HE3	21:2Z:59:LEU:HD12	2.03	0.40
1:1A:1067:G:C5	1:1A:1068:U:C4	6.53	0.40
1:1A:2100:U:H2'	1:1A:2101:G:O4'	2.21	0.40
1:1A:2319:G:O2'	1:1A:2321:A:N7	2.54	0.40
1:1A:710:C:H2'	1:1A:711:C:C6	2.56	0.40
8:1I:99:GLU:O	8:1I:103:ARG:HG2	2.21	0.40
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.76	0.40
1:2A:1406:G:H2'	1:2A:1407:C:H6	2.25	0.40
1:2A:1475:C:H2'	1:2A:1476:U:H6	1.86	0.40
1:2A:210:A:N6	1:2A:212:G:C2	2.89	0.40
1:2A:2239:G:C6	1:2A:2240:C:C4	3.09	0.40
1:2A:1684:C:H5''	1:2A:2721:C:O2'	2.21	0.40
11:2P:3:LEU:HA	11:2P:3:LEU:HD12	1.87	0.40
12:2Q:72:LYS:HA	12:2Q:73:PRO:HD3	1.79	0.40
14:2S:36:TYR:OH	14:2S:54:LEU:HD22	2.20	0.40
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.21	0.40
1:1A:1404:A:C2	1:1A:1417:U:O4	2.74	0.40
1:1A:1528:G:O6	1:1A:1552:A:N6	2.55	0.40
1:1A:1687:A:N6	1:1A:1688:G:C2	2.88	0.40
1:1A:1687:A:H2'	1:1A:1688:G:O4'	2.21	0.40
1:1A:2247:C:H2'	1:1A:2248:G:O4'	2.21	0.40
1:1A:1001:A:N1	1:1A:2469:G:H4'	2.37	0.40
1:1A:2626:U:H2'	1:1A:2627:C:H6	1.87	0.40
1:1A:2859:A:OP2	1:1A:2875:U:H5	2.04	0.40
10:1O:23:ARG:HG3	10:1O:24:VAL:N	2.36	0.40
14:1S:36:TYR:CD1	14:1S:36:TYR:N	2.89	0.40
19:1X:47:PHE:O	19:1X:49:VAL:HG13	2.21	0.40
26:24:15:ILE:HB	26:24:32:TYR:CD1	2.57	0.40
1:2A:484:U:H5''	29:27:40:TRP:CD2	2.57	0.40
1:2A:1050:C:O2	1:2A:1188:A:C6	2.75	0.40
1:2A:1824:U:H2'	1:2A:1825:C:C6	2.57	0.40
1:2A:1873:C:H2'	1:2A:1874:C:C6	2.57	0.40
1:2A:814:G:O2'	1:2A:1424:A:N6	2.55	0.40
1:2A:845:G:OP2	1:2A:845:G:H8	3.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:33:ARG:NH1	6:2G:33:ARG:HB2	2.31	0.40
6:2G:45:GLU:H	6:2G:45:GLU:HG2	1.42	0.40
8:2I:134:PRO:C	8:2I:136:VAL:H	2.25	0.40
1:2A:2219:A:OP1	8:2I:33:ARG:NH2	2.54	0.40
9:2N:39:ARG:HA	9:2N:40:PRO:HD3	1.93	0.40
13:2R:100:LEU:HB2	13:2R:111:LEU:O	2.21	0.40
1:1A:1868:C:H41	1:1A:1920:G:P	2.44	0.40
1:1A:214:G:N2	1:1A:216:A:H62	2.19	0.40
1:1A:224:C:H2'	1:1A:225:C:H6	1.87	0.40
1:1A:863:C:O2'	1:1A:885:U:H5''	2.21	0.40
1:1A:929:G:N2	1:1A:948:C:O2	26.76	0.40
8:1I:106:GLY:HA2	8:1I:107:VAL:O	2.21	0.40
11:1P:77:ARG:HB2	11:1P:78:PRO:HD2	2.02	0.40
14:1S:46:VAL:HG12	14:1S:48:LEU:HD12	2.02	0.40
25:23:24:LYS:HE2	25:23:24:LYS:HB2	1.89	0.40
1:2A:1087:G:C5	1:2A:1088:C:C4	3.10	0.40
1:2A:1734:U:H2'	1:2A:1744:A:N6	2.36	0.40
1:2A:215:A:C2	1:2A:2418:G:H1'	2.55	0.40
1:2A:2589:G:OP1	59:2A:3659:HOH:O	2.22	0.40
1:2A:611:C:H2'	1:2A:612:A:C8	2.57	0.40
1:2A:724:C:H2'	1:2A:725:C:H6	1.83	0.40
1:2A:843:C:H2'	1:2A:844:G:O4'	2.22	0.40
1:2A:905:G:N2	1:2A:962:A:OP2	2.52	0.40
2:2B:108:U:H2'	2:2B:109:C:H5''	2.03	0.40
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.54	0.40
6:2G:96:ARG:O	6:2G:99:MET:HB3	2.21	0.40
7:2H:139:GLN:HG3	7:2H:140:LYS:N	2.35	0.40
9:2N:15:LEU:HD12	9:2N:137:LYS:HG2	2.02	0.40
12:2Q:29:PHE:HB2	12:2Q:105:GLU:OE2	2.22	0.40
17:2V:62:LEU:HD21	17:2V:95:LEU:HB2	2.04	0.40
1:2A:23:G:O2'	18:2W:77:ASP:HB3	2.22	0.40
21:2Z:10:ARG:HH12	21:2Z:26:GLY:H	1.69	0.40
1:1A:2358:C:O2'	28:16:21:TYR:OH	2.29	0.40
1:1A:1219:U:HO2'	1:1A:1220:G:P	2.44	0.40
1:1A:1305:G:C6	1:1A:1306:C:C4	3.10	0.40
1:1A:1907:C:H6	1:1A:1907:C:O5'	2.04	0.40
1:1A:2723:U:O2'	1:1A:2725:A:H5'	2.21	0.40
1:1A:981:U:H2'	1:1A:982:G:O4'	2.21	0.40
8:1I:77:LEU:HG	8:1I:101:LEU:HG	2.03	0.40
1:1A:611:C:P	11:1P:16:ARG:HH12	2.44	0.40
21:1Z:108:PRO:HG3	21:1Z:141:VAL:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:22:9:GLN:OE1	24:22:56:GLN:HG2	2.22	0.40
1:2A:1861:G:H2'	1:2A:1862:C:C6	2.57	0.40
1:2A:2040:A:H4'	16:2U:34:LYS:HD2	2.04	0.40
1:2A:2238:A:OP1	3:2D:263:ARG:HD2	2.22	0.40
1:2A:2389:A:H2'	14:2S:21:THR:HG21	2.04	0.40
1:2A:2419:U:H2'	1:2A:2420:G:C8	2.56	0.40
1:2A:2421:G:N2	1:2A:2422:A:H1'	2.37	0.40
1:2A:647:G:C6	1:2A:648:C:C4	3.10	0.40
6:2G:148:MET:HG3	6:2G:148:MET:H	1.52	0.40
7:2H:8:PRO:O	7:2H:69:ARG:NH1	2.54	0.40
8:2I:50:ARG:HB3	8:2I:50:ARG:HE	1.68	0.40
10:2O:122:LEU:HD13	15:2T:72:VAL:HG11	2.03	0.40
19:2X:15:GLU:HG2	59:2X:8103:HOH:O	2.21	0.40
1:2A:325:C:OP2	20:2Y:73:ARG:NH1	2.54	0.40
21:2Z:70:LEU:HD23	21:2Z:70:LEU:HA	1.80	0.40
21:2Z:7:ALA:O	21:2Z:62:PRO:HD3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:27:TYR:OH	37:2f:15:ASP:OD2[2_655]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	253 (93%)	20 (7%)	0	100	100
3	2D	273/276 (99%)	252 (92%)	19 (7%)	2 (1%)	22	54
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	61
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	29	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	45
5	2F	201/210 (96%)	193 (96%)	6 (3%)	2 (1%)	15	45
6	1G	179/182 (98%)	161 (90%)	15 (8%)	3 (2%)	9	31
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	5	19
7	1H	172/180 (96%)	161 (94%)	9 (5%)	2 (1%)	13	40
7	2H	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	13	40
8	1I	144/148 (97%)	126 (88%)	14 (10%)	4 (3%)	5	19
8	2I	144/148 (97%)	124 (86%)	19 (13%)	1 (1%)	22	54
9	1N	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
9	2N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	22	54
10	1O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	51
10	2O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	19	51
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	54
11	2P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	11	36
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	22	54
13	1R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100	100
14	1S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	17	48
14	2S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	17	48
15	1T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	45
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	45
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	92 (99%)	0	1 (1%)	14	42
19	2X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	42
20	1Y	105/110 (96%)	93 (89%)	10 (10%)	2 (2%)	8	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	2Y	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
21	1Z	184/206 (89%)	169 (92%)	15 (8%)	0	100	100
21	2Z	184/206 (89%)	167 (91%)	15 (8%)	2 (1%)	14	42
22	10	73/85 (86%)	70 (96%)	2 (3%)	1 (1%)	11	36
22	20	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	90 (95%)	5 (5%)	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%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	50 (75%)	8 (12%)	9 (13%)	0	0
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	2
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	43 (94%)	1 (2%)	2 (4%)	2	10
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	190 (83%)	31 (14%)	8 (4%)	3	14
33	2b	229/256 (90%)	188 (82%)	32 (14%)	9 (4%)	3	12
34	1c	204/239 (85%)	178 (87%)	22 (11%)	4 (2%)	7	27
34	2c	204/239 (85%)	173 (85%)	29 (14%)	2 (1%)	15	45
35	1d	206/209 (99%)	188 (91%)	13 (6%)	5 (2%)	6	22
35	2d	206/209 (99%)	188 (91%)	15 (7%)	3 (2%)	10	34
36	1e	146/162 (90%)	126 (86%)	15 (10%)	5 (3%)	3	15
36	2e	146/162 (90%)	129 (88%)	13 (9%)	4 (3%)	5	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	132 (86%)	20 (13%)	1 (1%)	22	54
38	2g	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	12	37
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	3 (2%)	2 (2%)	10	34
40	1i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	19	51
40	2i	125/128 (98%)	110 (88%)	13 (10%)	2 (2%)	9	32
41	1j	95/105 (90%)	80 (84%)	8 (8%)	7 (7%)	1	2
41	2j	94/105 (90%)	79 (84%)	13 (14%)	2 (2%)	7	26
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	8	29
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	8	29
43	1l	120/132 (91%)	115 (96%)	4 (3%)	1 (1%)	19	51
43	2l	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
44	1m	116/126 (92%)	103 (89%)	9 (8%)	4 (3%)	3	15
44	2m	114/126 (90%)	101 (89%)	11 (10%)	2 (2%)	8	29
45	1n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	31
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	12	37
47	2p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	15	45
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	59 (89%)	5 (8%)	2 (3%)	4	17
49	2r	66/88 (75%)	60 (91%)	5 (8%)	1 (2%)	10	34
50	1s	82/93 (88%)	72 (88%)	10 (12%)	0	100	100
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
51	1t	94/106 (89%)	79 (84%)	12 (13%)	3 (3%)	4	16
51	2t	94/106 (89%)	82 (87%)	8 (8%)	4 (4%)	2	10
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
55	1z	10/15 (67%)	9 (90%)	1 (10%)	0	100	100
55	2z	11/15 (73%)	7 (64%)	3 (27%)	1 (9%)	1	1
All	All	11431/12158 (94%)	10499 (92%)	791 (7%)	141 (1%)	13	40

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	51	ARG
6	1G	126	ASP
7	1H	126	PRO
14	1S	60	GLY
19	1X	94	GLY
26	14	50	VAL
26	14	53	GLU
26	14	59	PHE
26	14	68	ARG
33	1b	17	PHE
33	1b	125	PRO
33	1b	128	GLU
34	1c	107	GLN
35	1d	32	ALA
36	1e	73	ASN
40	1i	54	ASP
41	1j	55	LYS
41	1j	56	HIS
43	1l	29	GLY
44	1m	4	ILE
45	1n	3	ARG
51	1t	95	ALA
3	2D	125	ILE
5	2F	130	ALA
6	2G	14	GLU
6	2G	47	LYS
6	2G	51	ARG
6	2G	81	LYS
7	2H	55	PRO
7	2H	126	PRO
8	2I	10	GLU
12	2Q	28	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	2V	79	VAL
19	2X	94	GLY
21	2Z	128	VAL
26	24	47	GLN
26	24	50	VAL
26	24	63	TYR
29	27	46	VAL
33	2b	17	PHE
33	2b	121	LEU
33	2b	124	SER
36	2e	37	ARG
36	2e	73	ASN
51	2t	95	ALA
51	2t	99	LEU
55	2z	10	PRO
6	1G	47	LYS
7	1H	92	ILE
8	1I	106	GLY
17	1V	79	VAL
22	10	13	GLY
26	14	45	GLY
26	14	49	PHE
33	1b	165	VAL
34	1c	127	ARG
42	1k	49	GLY
44	1m	5	ALA
51	1t	47	GLY
26	24	45	GLY
26	24	54	GLY
33	2b	20	GLU
33	2b	93	VAL
33	2b	126	GLU
33	2b	165	VAL
34	2c	66	VAL
35	2d	20	TYR
41	2j	78	ASN
4	1E	52	LEU
8	1I	73	GLU
10	1O	5	GLN
11	1P	122	PRO
26	14	48	ARG
33	1b	231	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	9	CYS
35	1d	136	PRO
38	1g	4	ARG
41	1j	78	ASN
44	1m	21	TYR
6	2G	126	ASP
9	2N	2	LYS
35	2d	136	PRO
40	2i	39	GLY
40	2i	54	ASP
44	2m	106	ASN
49	2r	36	ASN
20	1Y	54	LYS
36	1e	72	GLN
41	1j	32	ALA
48	1q	68	ARG
4	2E	52	LEU
5	2F	18	ARG
10	2O	5	GLN
33	2b	125	PRO
33	2b	151	GLY
35	2d	46	LYS
36	2e	69	VAL
44	2m	21	TYR
20	1Y	53	PRO
34	1c	66	VAL
36	1e	69	VAL
36	1e	98	THR
47	1p	16	HIS
51	1t	100	ILE
3	2D	3	VAL
11	2P	29	LYS
11	2P	122	PRO
14	2S	84	GLN
34	2c	108	ASN
38	2g	4	ARG
38	2g	54	THR
39	2h	73	ASP
39	2h	133	LEU
42	2k	49	GLY
51	2t	47	GLY
5	1F	18	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1I	105	HIS
8	1I	107	VAL
26	14	47	GLN
33	1b	22	LYS
34	1c	126	ARG
41	1j	51	ARG
44	1m	67	GLU
49	1r	25	THR
49	1r	36	ASN
21	2Z	135	GLU
29	27	45	ALA
41	2j	56	HIS
26	14	54	GLY
42	1k	105	VAL
33	1b	230	VAL
35	1d	8	VAL
41	1j	77	PRO
42	2k	105	VAL
51	2t	100	ILE
36	1e	85	GLY
33	1b	227	GLY
35	1d	5	ILE
41	1j	75	ILE
36	2e	96	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	196 (91%)	19 (9%)	10	30
3	2D	216/218 (99%)	190 (88%)	26 (12%)	5	15
4	1E	164/166 (99%)	149 (91%)	15 (9%)	9	28
4	2E	164/166 (99%)	147 (90%)	17 (10%)	7	21
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	146 (92%)	13 (8%)	11	32
6	1G	143/156 (92%)	129 (90%)	14 (10%)	8	24
6	2G	142/156 (91%)	125 (88%)	17 (12%)	5	15
7	1H	144/148 (97%)	133 (92%)	11 (8%)	13	36
7	2H	144/148 (97%)	132 (92%)	12 (8%)	11	32
8	1I	110/124 (89%)	93 (84%)	17 (16%)	2	8
8	2I	104/124 (84%)	95 (91%)	9 (9%)	10	30
9	1N	118/119 (99%)	106 (90%)	12 (10%)	7	22
9	2N	118/119 (99%)	107 (91%)	11 (9%)	9	27
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	75
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	75
11	1P	116/116 (100%)	103 (89%)	13 (11%)	6	18
11	2P	115/116 (99%)	102 (89%)	13 (11%)	6	18
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	14	39
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	18	46
13	1R	101/101 (100%)	86 (85%)	15 (15%)	3	9
13	2R	101/101 (100%)	85 (84%)	16 (16%)	2	8
14	1S	87/88 (99%)	79 (91%)	8 (9%)	9	27
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	16
15	1T	115/127 (91%)	108 (94%)	7 (6%)	18	48
15	2T	113/127 (89%)	111 (98%)	2 (2%)	59	85
16	1U	93/94 (99%)	87 (94%)	6 (6%)	17	45
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	54
17	1V	80/82 (98%)	70 (88%)	10 (12%)	4	14
17	2V	80/82 (98%)	73 (91%)	7 (9%)	10	30
18	1W	90/92 (98%)	84 (93%)	6 (7%)	16	43
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21	52
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	66
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	77
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	14	40
20	2Y	85/91 (93%)	81 (95%)	4 (5%)	26	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	159/179 (89%)	146 (92%)	13 (8%)	11	32
21	2Z	156/179 (87%)	144 (92%)	12 (8%)	13	35
22	10	60/67 (90%)	55 (92%)	5 (8%)	11	32
22	20	60/67 (90%)	56 (93%)	4 (7%)	16	43
23	11	80/83 (96%)	76 (95%)	4 (5%)	24	57
23	21	80/83 (96%)	76 (95%)	4 (5%)	24	57
24	12	65/67 (97%)	61 (94%)	4 (6%)	18	47
24	22	65/67 (97%)	60 (92%)	5 (8%)	13	35
25	13	51/52 (98%)	47 (92%)	4 (8%)	12	34
25	23	50/52 (96%)	46 (92%)	4 (8%)	12	33
26	14	60/63 (95%)	52 (87%)	8 (13%)	4	11
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	9
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	33
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	49
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	49
28	26	50/52 (96%)	47 (94%)	3 (6%)	19	49
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	15
29	27	41/42 (98%)	39 (95%)	2 (5%)	25	57
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	38
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	38
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	76
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	76
33	1b	177/220 (80%)	149 (84%)	28 (16%)	2	8
33	2b	158/220 (72%)	137 (87%)	21 (13%)	4	11
34	1c	127/188 (68%)	117 (92%)	10 (8%)	12	34
34	2c	108/188 (57%)	91 (84%)	17 (16%)	2	8
35	1d	161/181 (89%)	144 (89%)	17 (11%)	6	20
35	2d	164/181 (91%)	145 (88%)	19 (12%)	5	16
36	1e	113/123 (92%)	103 (91%)	10 (9%)	10	30
36	2e	106/123 (86%)	94 (89%)	12 (11%)	6	18
37	1f	83/90 (92%)	77 (93%)	6 (7%)	14	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	86/90 (96%)	83 (96%)	3 (4%)	36	70
38	1g	111/127 (87%)	101 (91%)	10 (9%)	9	29
38	2g	107/127 (84%)	98 (92%)	9 (8%)	11	31
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	25
39	2h	111/119 (93%)	99 (89%)	12 (11%)	6	20
40	1i	89/99 (90%)	78 (88%)	11 (12%)	4	14
40	2i	80/99 (81%)	66 (82%)	14 (18%)	2	6
41	1j	60/92 (65%)	55 (92%)	5 (8%)	11	32
41	2j	62/92 (67%)	53 (86%)	9 (14%)	3	9
42	1k	82/99 (83%)	77 (94%)	5 (6%)	18	48
42	2k	82/99 (83%)	77 (94%)	5 (6%)	18	48
43	1l	95/109 (87%)	90 (95%)	5 (5%)	22	54
43	2l	94/109 (86%)	90 (96%)	4 (4%)	29	62
44	1m	90/101 (89%)	80 (89%)	10 (11%)	6	19
44	2m	87/101 (86%)	77 (88%)	10 (12%)	5	17
45	1n	47/50 (94%)	42 (89%)	5 (11%)	6	20
45	2n	43/50 (86%)	36 (84%)	7 (16%)	2	7
46	1o	75/80 (94%)	67 (89%)	8 (11%)	6	20
46	2o	78/80 (98%)	69 (88%)	9 (12%)	5	17
47	1p	67/74 (90%)	56 (84%)	11 (16%)	2	7
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	12
48	1q	91/97 (94%)	85 (93%)	6 (7%)	16	44
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	81
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7	22
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	22
50	1s	65/80 (81%)	57 (88%)	8 (12%)	4	14
50	2s	67/80 (84%)	59 (88%)	8 (12%)	5	15
51	1t	66/82 (80%)	57 (86%)	9 (14%)	3	11
51	2t	71/82 (87%)	66 (93%)	5 (7%)	15	41
52	1u	16/22 (73%)	15 (94%)	1 (6%)	18	46
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	1z	12/15 (80%)	12 (100%)	0	100	100
55	2z	13/15 (87%)	13 (100%)	0	100	100
All	All	9160/10096 (91%)	8322 (91%)	838 (9%)	9	28

All (838) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	13	ARG
3	1D	54	ARG
3	1D	61	LEU
3	1D	69	ARG
3	1D	71	ASP
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	111	LEU
3	1D	142	VAL
3	1D	155	LEU
3	1D	193	VAL
3	1D	206	LEU
3	1D	211	ARG
3	1D	217	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
3	1D	260	ARG
4	1E	7	VAL
4	1E	21	VAL
4	1E	54	GLN
4	1E	75	VAL
4	1E	79	ARG
4	1E	82	ARG
4	1E	111	ARG
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	163	GLU
4	1E	175	VAL
4	1E	181	LEU
4	1E	184	VAL
4	1E	195	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	20	LEU
5	1F	33	LEU
5	1F	38	ARG
5	1F	57	VAL
5	1F	74	ARG
5	1F	106	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	162	LEU
5	1F	170	LEU
5	1F	183	VAL
5	1F	191	ARG
5	1F	192	LEU
5	1F	195	ASP
5	1F	197	ASP
5	1F	201	VAL
6	1G	3	LEU
6	1G	7	LEU
6	1G	43	LEU
6	1G	45	GLU
6	1G	82	LEU
6	1G	140	ILE
6	1G	143	GLU
6	1G	148	MET
6	1G	159	VAL
6	1G	161	THR
6	1G	162	THR
6	1G	165	THR
6	1G	170	ARG
6	1G	174	GLU
7	1H	3	ARG
7	1H	13	LYS
7	1H	33	LEU
7	1H	45	VAL
7	1H	59	ARG
7	1H	69	ARG
7	1H	71	LEU
7	1H	84	SER
7	1H	98	LEU
7	1H	101	ARG
7	1H	139	GLN
8	1I	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1I	10	GLU
8	1I	12	LEU
8	1I	42	SER
8	1I	47	LEU
8	1I	57	ARG
8	1I	60	GLU
8	1I	66	GLU
8	1I	68	LEU
8	1I	74	ASN
8	1I	75	LEU
8	1I	77	LEU
8	1I	101	LEU
8	1I	103	ARG
8	1I	109	ILE
8	1I	140	LEU
8	1I	142	VAL
9	1N	8	GLN
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	48	MET
9	1N	61	ARG
9	1N	67	LEU
9	1N	73	THR
9	1N	87	LEU
9	1N	120	LEU
9	1N	137	LYS
10	1O	18	LYS
10	1O	24	VAL
10	1O	105	GLU
11	1P	3	LEU
11	1P	55	ARG
11	1P	56	SER
11	1P	59	LEU
11	1P	70	GLN
11	1P	76	LYS
11	1P	98	GLU
11	1P	99	LEU
11	1P	106	LEU
11	1P	112	LEU
11	1P	125	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	1P	136	GLU
11	1P	148	LEU
12	1Q	1	MET
12	1Q	6	ARG
12	1Q	8	LYS
12	1Q	16	ARG
12	1Q	35	VAL
12	1Q	45	GLN
12	1Q	59	ARG
12	1Q	60	ARG
13	1R	6	SER
13	1R	18	LEU
13	1R	24	GLN
13	1R	28	LEU
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	67	LEU
13	1R	75	LEU
13	1R	79	LEU
13	1R	91	GLN
13	1R	100	LEU
13	1R	111	LEU
14	1S	3	ARG
14	1S	4	LEU
14	1S	20	ARG
14	1S	36	TYR
14	1S	49	VAL
14	1S	59	LYS
14	1S	61	ASN
14	1S	85	VAL
15	1T	49	VAL
15	1T	89	VAL
15	1T	93	ARG
15	1T	96	ARG
15	1T	108	ARG
15	1T	118	ARG
15	1T	128	GLU
16	1U	8	VAL
16	1U	36	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1U	74	LEU
16	1U	77	SER
16	1U	92	ARG
16	1U	104	GLN
17	1V	18	LEU
17	1V	35	LEU
17	1V	43	GLU
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	60	ASN
18	1W	67	ASP
18	1W	107	LEU
19	1X	52	VAL
19	1X	57	LEU
19	1X	88	LYS
20	1Y	1	MET
20	1Y	2	ARG
20	1Y	23	ARG
20	1Y	26	LYS
20	1Y	43	ASN
20	1Y	99	CYS
21	1Z	6	LYS
21	1Z	11	GLU
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	107	THR
21	1Z	129	SER
21	1Z	150	LEU
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	162	GLU
21	1Z	170	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	10	10	THR
22	10	20	ARG
22	10	43	THR
22	10	49	LYS
22	10	55	ARG
23	11	21	ARG
23	11	40	ARG
23	11	59	THR
23	11	95	LEU
24	12	32	LEU
24	12	34	GLU
24	12	53	LEU
24	12	70	GLN
25	13	8	LEU
25	13	23	LEU
25	13	54	VAL
25	13	60	GLU
26	14	14	ILE
26	14	34	GLU
26	14	37	SER
26	14	49	PHE
26	14	56	VAL
26	14	58	ARG
26	14	60	GLN
26	14	63	TYR
27	15	16	ARG
27	15	29	THR
27	15	40	LYS
27	15	58	LEU
28	16	6	ARG
28	16	14	THR
28	16	48	VAL
29	17	1	MET
29	17	9	ARG
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
30	18	46	ARG
31	19	26	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	8	LYS
33	1b	10	LEU
33	1b	11	LEU
33	1b	16	HIS
33	1b	17	PHE
33	1b	21	ARG
33	1b	67	THR
33	1b	76	GLN
33	1b	80	ILE
33	1b	84	GLU
33	1b	86	GLU
33	1b	93	VAL
33	1b	112	VAL
33	1b	116	GLU
33	1b	127	ILE
33	1b	144	ARG
33	1b	153	ARG
33	1b	156	LYS
33	1b	169	LYS
33	1b	170	GLU
33	1b	185	ILE
33	1b	187	LEU
33	1b	190	THR
33	1b	215	LEU
33	1b	219	VAL
33	1b	221	LEU
33	1b	226	ARG
33	1b	230	VAL
34	1c	15	THR
34	1c	17	ASP
34	1c	29	TYR
34	1c	46	GLU
34	1c	47	LEU
34	1c	49	SER
34	1c	52	LEU
34	1c	64	VAL
34	1c	115	LEU
34	1c	195	VAL
35	1d	5	ILE
35	1d	15	GLU
35	1d	28	SER
35	1d	31	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	45	GLN
35	1d	49	ARG
35	1d	66	ARG
35	1d	101	LEU
35	1d	107	ARG
35	1d	150	GLU
35	1d	158	ILE
35	1d	162	LEU
35	1d	168	ARG
35	1d	181	MET
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
36	1e	31	LEU
36	1e	40	ARG
36	1e	41	VAL
36	1e	47	LYS
36	1e	51	VAL
36	1e	73	ASN
36	1e	78	HIS
36	1e	79	GLU
36	1e	91	LEU
36	1e	147	ASP
37	1f	46	ARG
37	1f	55	ASP
37	1f	65	VAL
37	1f	74	ASP
37	1f	75	LEU
37	1f	89	MET
38	1g	13	GLN
38	1g	15	ASP
38	1g	21	VAL
38	1g	22	LEU
38	1g	50	ILE
38	1g	56	GLN
38	1g	113	GLU
38	1g	114	ARG
38	1g	131	LYS
38	1g	138	LYS
39	1h	2	LEU
39	1h	21	LYS
39	1h	25	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	1h	52	ASP
39	1h	54	ASP
39	1h	60	ARG
39	1h	75	ARG
39	1h	78	GLN
39	1h	91	ARG
39	1h	98	LYS
39	1h	112	LEU
40	1i	23	ASN
40	1i	42	ARG
40	1i	50	LEU
40	1i	65	VAL
40	1i	75	ASP
40	1i	81	ILE
40	1i	92	TYR
40	1i	102	LEU
40	1i	113	LYS
40	1i	127	LYS
40	1i	128	ARG
41	1j	30	SER
41	1j	34	VAL
41	1j	43	ARG
41	1j	85	LEU
41	1j	92	THR
42	1k	14	VAL
42	1k	31	THR
42	1k	48	ILE
42	1k	84	VAL
42	1k	109	VAL
43	1l	27	LEU
43	1l	33	ARG
43	1l	41	ARG
43	1l	54	LYS
43	1l	67	THR
44	1m	3	ARG
44	1m	4	ILE
44	1m	19	LEU
44	1m	20	THR
44	1m	44	ARG
44	1m	49	THR
44	1m	56	LEU
44	1m	70	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	1m	102	ARG
44	1m	110	ARG
45	1n	6	LEU
45	1n	8	GLU
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
46	1o	3	ILE
46	1o	5	LYS
46	1o	17	ARG
46	1o	22	THR
46	1o	26	GLU
46	1o	38	ARG
46	1o	39	LEU
46	1o	71	GLN
47	1p	1	MET
47	1p	2	VAL
47	1p	5	ARG
47	1p	11	SER
47	1p	16	HIS
47	1p	19	ILE
47	1p	20	VAL
47	1p	25	ARG
47	1p	45	THR
47	1p	62	VAL
47	1p	67	THR
48	1q	68	ARG
48	1q	74	LEU
48	1q	78	GLU
48	1q	82	MET
48	1q	89	LEU
48	1q	98	LEU
49	1r	26	LEU
49	1r	32	ARG
49	1r	38	GLU
49	1r	54	ARG
49	1r	68	LYS
49	1r	76	LEU
50	1s	3	ARG
50	1s	5	LEU
50	1s	22	LEU
50	1s	28	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1s	37	ARG
50	1s	63	THR
50	1s	65	ASN
50	1s	81	ARG
51	1t	9	ASN
51	1t	10	LEU
51	1t	24	LEU
51	1t	30	LYS
51	1t	45	GLN
51	1t	60	GLU
51	1t	62	LEU
51	1t	86	ARG
51	1t	90	GLN
52	1u	15	ARG
3	2D	14	ARG
3	2D	38	LYS
3	2D	54	ARG
3	2D	61	LEU
3	2D	71	ASP
3	2D	94	LEU
3	2D	106	ILE
3	2D	111	LEU
3	2D	113	VAL
3	2D	134	ARG
3	2D	138	VAL
3	2D	141	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	183	ARG
3	2D	192	THR
3	2D	193	VAL
3	2D	211	ARG
3	2D	217	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	257	LEU
3	2D	260	ARG
3	2D	262	ARG
3	2D	274	ARG
3	2D	276	LYS
4	2E	7	VAL
4	2E	12	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	21	VAL
4	2E	24	THR
4	2E	49	LEU
4	2E	52	LEU
4	2E	75	VAL
4	2E	77	ILE
4	2E	82	ARG
4	2E	116	VAL
4	2E	119	ARG
4	2E	144	ARG
4	2E	163	GLU
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
4	2E	202	LYS
5	2F	20	LEU
5	2F	24	LEU
5	2F	27	GLU
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	106	ARG
5	2F	162	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	196	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	4	ASP
6	2G	28	VAL
6	2G	33	ARG
6	2G	43	LEU
6	2G	45	GLU
6	2G	60	LEU
6	2G	111	LEU
6	2G	113	ARG
6	2G	136	ARG
6	2G	140	ILE
6	2G	143	GLU
6	2G	145	THR
6	2G	148	MET
6	2G	159	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	162	THR
6	2G	170	ARG
6	2G	181	ARG
7	2H	3	ARG
7	2H	32	GLU
7	2H	33	LEU
7	2H	42	ARG
7	2H	49	VAL
7	2H	69	ARG
7	2H	71	LEU
7	2H	84	SER
7	2H	98	LEU
7	2H	106	THR
7	2H	139	GLN
7	2H	171	LEU
8	2I	43	ASN
8	2I	61	ARG
8	2I	75	LEU
8	2I	77	LEU
8	2I	101	LEU
8	2I	116	LEU
8	2I	121	LYS
8	2I	140	LEU
8	2I	142	VAL
9	2N	5	VAL
9	2N	33	LEU
9	2N	34	LEU
9	2N	46	VAL
9	2N	48	MET
9	2N	62	VAL
9	2N	73	THR
9	2N	87	LEU
9	2N	120	LEU
9	2N	137	LYS
9	2N	138	LEU
10	2O	24	VAL
10	2O	69	ILE
10	2O	94	ARG
11	2P	3	LEU
11	2P	45	LEU
11	2P	55	ARG
11	2P	56	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	2P	59	LEU
11	2P	65	ARG
11	2P	95	VAL
11	2P	96	THR
11	2P	102	ARG
11	2P	112	LEU
11	2P	121	LYS
11	2P	125	VAL
11	2P	148	LEU
12	2Q	1	MET
12	2Q	21	THR
12	2Q	35	VAL
12	2Q	45	GLN
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	110	THR
13	2R	1	MET
13	2R	6	SER
13	2R	18	LEU
13	2R	24	GLN
13	2R	28	LEU
13	2R	29	LEU
13	2R	44	LEU
13	2R	54	LEU
13	2R	65	LEU
13	2R	75	LEU
13	2R	79	LEU
13	2R	82	GLU
13	2R	86	ARG
13	2R	100	LEU
13	2R	102	GLU
13	2R	111	LEU
14	2S	14	VAL
14	2S	23	ARG
14	2S	36	TYR
14	2S	44	LYS
14	2S	58	LEU
14	2S	63	THR
14	2S	75	GLU
14	2S	80	LEU
14	2S	83	LYS
14	2S	85	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	2T	89	VAL
15	2T	96	ARG
16	2U	5	LYS
16	2U	36	ARG
16	2U	52	ARG
16	2U	74	LEU
16	2U	104	GLN
17	2V	18	LEU
17	2V	21	ARG
17	2V	35	LEU
17	2V	52	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	92	ARG
18	2W	107	LEU
19	2X	57	LEU
19	2X	92	LEU
20	2Y	43	ASN
20	2Y	44	ILE
20	2Y	90	LEU
20	2Y	99	CYS
21	2Z	18	LEU
21	2Z	33	LEU
21	2Z	61	LEU
21	2Z	73	GLN
21	2Z	86	VAL
21	2Z	107	THR
21	2Z	131	ARG
21	2Z	135	GLU
21	2Z	136	PHE
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
22	20	10	THR
22	20	20	ARG
22	20	55	ARG
22	20	82	ARG
23	21	21	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	21	35	THR
23	21	40	ARG
23	21	95	LEU
24	22	30	ARG
24	22	32	LEU
24	22	34	GLU
24	22	53	LEU
24	22	70	GLN
25	23	8	LEU
25	23	40	THR
25	23	54	VAL
25	23	56	VAL
26	24	1	MET
26	24	14	ILE
26	24	53	GLU
26	24	58	ARG
26	24	61	ARG
26	24	62	ARG
26	24	63	TYR
26	24	69	LYS
27	25	16	ARG
27	25	29	THR
27	25	40	LYS
28	26	6	ARG
28	26	14	THR
28	26	48	VAL
29	27	43	THR
29	27	46	VAL
30	28	30	ARG
30	28	31	HIS
30	28	34	TRP
30	28	37	SER
31	29	26	ILE
33	2b	8	LYS
33	2b	10	LEU
33	2b	24	TRP
33	2b	60	ASP
33	2b	63	MET
33	2b	67	THR
33	2b	90	MET
33	2b	93	VAL
33	2b	118	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	138	LEU
33	2b	152	PHE
33	2b	153	ARG
33	2b	154	LEU
33	2b	160	ASP
33	2b	165	VAL
33	2b	170	GLU
33	2b	179	LYS
33	2b	185	ILE
33	2b	187	LEU
33	2b	222	ILE
33	2b	224	GLN
34	2c	3	ASN
34	2c	5	ILE
34	2c	14	ILE
34	2c	15	THR
34	2c	17	ASP
34	2c	28	GLN
34	2c	29	TYR
34	2c	47	LEU
34	2c	52	LEU
34	2c	58	GLU
34	2c	64	VAL
34	2c	70	VAL
34	2c	125	GLU
34	2c	128	PHE
34	2c	131	ARG
34	2c	164	ARG
34	2c	178	LEU
35	2d	3	ARG
35	2d	5	ILE
35	2d	25	ARG
35	2d	26	CYS
35	2d	31	CYS
35	2d	34	GLU
35	2d	38	TYR
35	2d	47	ARG
35	2d	58	LEU
35	2d	66	ARG
35	2d	96	LEU
35	2d	101	LEU
35	2d	132	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	135	LEU
35	2d	145	GLU
35	2d	170	VAL
35	2d	187	ARG
35	2d	194	LEU
35	2d	201	GLN
36	2e	14	ARG
36	2e	27	ARG
36	2e	34	VAL
36	2e	41	VAL
36	2e	47	LYS
36	2e	50	GLU
36	2e	51	VAL
36	2e	71	LEU
36	2e	78	HIS
36	2e	91	LEU
36	2e	115	VAL
36	2e	147	ASP
37	2f	28	ARG
37	2f	65	VAL
37	2f	75	LEU
38	2g	45	ASP
38	2g	57	GLU
38	2g	63	LYS
38	2g	72	ARG
38	2g	97	GLN
38	2g	104	LEU
38	2g	113	GLU
38	2g	120	ILE
38	2g	154	TYR
39	2h	25	ASP
39	2h	51	VAL
39	2h	52	ASP
39	2h	60	ARG
39	2h	63	LEU
39	2h	78	GLN
39	2h	91	ARG
39	2h	111	ILE
39	2h	112	LEU
39	2h	115	SER
39	2h	120	THR
39	2h	125	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	2i	3	GLN
40	2i	23	ASN
40	2i	33	PHE
40	2i	38	GLN
40	2i	50	LEU
40	2i	65	VAL
40	2i	81	ILE
40	2i	89	ASN
40	2i	92	TYR
40	2i	102	LEU
40	2i	104	ARG
40	2i	107	ARG
40	2i	114	TYR
40	2i	124	GLN
41	2j	8	LEU
41	2j	16	LEU
41	2j	21	GLN
41	2j	25	GLU
41	2j	34	VAL
41	2j	48	THR
41	2j	68	HIS
41	2j	81	THR
41	2j	94	VAL
42	2k	14	VAL
42	2k	18	ARG
42	2k	70	LYS
42	2k	75	TYR
42	2k	126	ARG
43	2l	23	LYS
43	2l	33	ARG
43	2l	53	ARG
43	2l	55	VAL
44	2m	3	ARG
44	2m	40	ASN
44	2m	49	THR
44	2m	70	LEU
44	2m	81	LEU
44	2m	82	MET
44	2m	90	LEU
44	2m	102	ARG
44	2m	106	ASN
44	2m	110	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	2n	11	LYS
45	2n	17	LYS
45	2n	22	THR
45	2n	29	ARG
45	2n	33	VAL
45	2n	41	ARG
45	2n	53	LEU
46	2o	3	ILE
46	2o	5	LYS
46	2o	10	LYS
46	2o	22	THR
46	2o	24	SER
46	2o	26	GLU
46	2o	39	LEU
46	2o	41	GLU
46	2o	83	GLU
47	2p	1	MET
47	2p	2	VAL
47	2p	5	ARG
47	2p	16	HIS
47	2p	45	THR
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	72	ARG
48	2q	63	ARG
48	2q	74	LEU
49	2r	26	LEU
49	2r	32	ARG
49	2r	38	GLU
49	2r	68	LYS
49	2r	76	LEU
49	2r	82	THR
50	2s	3	ARG
50	2s	28	LYS
50	2s	34	TRP
50	2s	41	VAL
50	2s	48	THR
50	2s	63	THR
50	2s	65	ASN
50	2s	83	HIS
51	2t	10	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	2t	24	LEU
51	2t	62	LEU
51	2t	71	THR
51	2t	99	LEU
52	2u	15	ARG
52	2u	22	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	164	GLN
3	1D	253	GLN
4	1E	54	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	169	ASN
5	1F	203	GLN
5	1F	204	ASN
6	1G	40	ASN
8	1I	43	ASN
8	1I	105	HIS
8	1I	139	GLN
9	1N	8	GLN
9	1N	133	GLN
11	1P	38	GLN
11	1P	70	GLN
12	1Q	45	GLN
13	1R	24	GLN
13	1R	71	GLN
13	1R	91	GLN
14	1S	95	HIS
15	1T	123	GLN
16	1U	81	HIS
16	1U	94	ASN
16	1U	104	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	73	GLN
21	1Z	151	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	12	70	GLN
26	14	46	GLN
26	14	60	GLN
30	18	35	GLN
31	19	36	GLN
34	1c	170	GLN
35	1d	43	HIS
35	1d	123	HIS
35	1d	201	GLN
36	1e	141	GLN
37	1f	100	ASN
38	1g	11	GLN
38	1g	56	GLN
38	1g	86	GLN
40	1i	23	ASN
40	1i	73	GLN
40	1i	89	ASN
40	1i	117	HIS
40	1i	124	GLN
41	1j	56	HIS
42	1k	93	GLN
43	1l	78	GLN
43	1l	99	HIS
44	1m	92	HIS
46	1o	28	GLN
46	1o	62	GLN
47	1p	13	HIS
48	1q	16	GLN
48	1q	26	GLN
50	1s	47	HIS
50	1s	56	GLN
50	1s	65	ASN
50	1s	69	HIS
51	1t	9	ASN
51	1t	45	GLN
3	2D	126	GLN
3	2D	129	ASN
3	2D	164	GLN
3	2D	253	GLN
5	2F	69	HIS
5	2F	169	ASN
5	2F	203	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	40	ASN
6	2G	130	ASN
6	2G	132	ASN
8	2I	43	ASN
8	2I	105	HIS
11	2P	38	GLN
12	2Q	45	GLN
12	2Q	57	HIS
13	2R	24	GLN
13	2R	71	GLN
14	2S	68	GLN
14	2S	95	HIS
15	2T	123	GLN
16	2U	44	ASN
17	2V	64	HIS
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
20	2Y	43	ASN
21	2Z	55	HIS
21	2Z	73	GLN
22	20	50	ASN
25	23	32	GLN
25	23	33	GLN
28	26	32	ASN
31	29	36	GLN
33	2b	16	HIS
33	2b	19	HIS
33	2b	45	GLN
33	2b	78	GLN
33	2b	110	GLN
33	2b	224	GLN
34	2c	6	HIS
34	2c	28	GLN
34	2c	37	GLN
34	2c	102	ASN
34	2c	176	HIS
34	2c	181	ASN
35	2d	123	HIS
35	2d	160	GLN
36	2e	78	HIS
36	2e	141	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	2f	73	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	97	GLN
38	2g	110	GLN
38	2g	148	ASN
39	2h	15	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	73	GLN
40	2i	89	ASN
41	2j	13	HIS
41	2j	33	GLN
41	2j	56	HIS
41	2j	62	HIS
42	2k	93	GLN
42	2k	104	GLN
43	2l	75	HIS
43	2l	78	GLN
43	2l	99	HIS
44	2m	77	ASN
44	2m	92	HIS
46	2o	28	GLN
47	2p	16	HIS
50	2s	56	GLN
50	2s	69	HIS
50	2s	83	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2737/2915 (93%)	384 (14%)	19 (0%)
1	2A	2781/2915 (95%)	475 (17%)	25 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	22 (18%)	2 (1%)
32	1a	1472/1521 (96%)	256 (17%)	0
32	2a	1479/1521 (97%)	268 (18%)	0
53	1v	4/24 (16%)	1 (25%)	0
53	2v	4/24 (16%)	1 (25%)	0
54	1x	75/77 (97%)	18 (24%)	0
54	2x	75/77 (97%)	18 (24%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	8865/9316 (95%)	1452 (16%)	46 (0%)

All (1452) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	U
1	1A	33	C
1	1A	35	G
1	1A	44	C
1	1A	61	U
1	1A	62	A
1	1A	69	A
1	1A	72	A
1	1A	73	G
1	1A	82	A
1	1A	91	C
1	1A	115	A
1	1A	116	A
1	1A	117	U
1	1A	122	G
1	1A	128	G
1	1A	148	A
1	1A	170	A
1	1A	176	G
1	1A	184	A
1	1A	187	A
1	1A	193	G
1	1A	203	G
1	1A	204	A
1	1A	210	A
1	1A	211	A
1	1A	216	A
1	1A	217	A
1	1A	221	A
1	1A	236	G
1	1A	262	C
1	1A	268	G
1	1A	270	U
1	1A	271	U
1	1A	272	G
1	1A	273	U
1	1A	285	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	287	U
1	1A	288	G
1	1A	294	C
1	1A	295	U
1	1A	302	C
1	1A	334	A
1	1A	347	A
1	1A	352	G
1	1A	353	A
1	1A	365	G
1	1A	375	G
1	1A	386	G
1	1A	398	G
1	1A	406	U
1	1A	412	G
1	1A	422	G
1	1A	431	U
1	1A	433	G
1	1A	437	G
1	1A	438	A
1	1A	454	A
1	1A	467	G
1	1A	468	A
1	1A	469	C
1	1A	473	U
1	1A	476	C
1	1A	482	A
1	1A	495	A
1	1A	500	U
1	1A	506	G
1	1A	528	U
1	1A	529	A
1	1A	533	C
1	1A	554	G
1	1A	555	C
1	1A	556	A
1	1A	557	G
1	1A	572	G
1	1A	585	G
1	1A	595	G
1	1A	597	A
1	1A	608	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	614	G
1	1A	615	G
1	1A	625	A
1	1A	626	G
1	1A	629	U
1	1A	638	G
1	1A	640	G
1	1A	658	C
1	1A	661	A
1	1A	669	C
1	1A	670	A
1	1A	682	G
1	1A	696	C
1	1A	697	G
1	1A	715	G
1	1A	732	G
1	1A	744	C
1	1A	763	G
1	1A	776	C
1	1A	803	U
1	1A	821	G
1	1A	822	G
1	1A	828	A
1	1A	830	A
1	1A	831	G
1	1A	835	A
1	1A	836	C
1	1A	838	G
1	1A	848	A
1	1A	851	G
1	1A	858	C
1	1A	873	U
1	1A	874	U
1	1A	905	G
1	1A	912	A
1	1A	925	G
1	1A	931	C
1	1A	932	C
1	1A	933	A
1	1A	934	C
1	1A	935	C
1	1A	936	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	938	C
1	1A	941	A
1	1A	944	A
1	1A	955	A
1	1A	976	G
1	1A	985	A
1	1A	989	A
1	1A	990	G
1	1A	1002	U
1	1A	1003	A
1	1A	1005	C
1	1A	1008	C
1	1A	1018	G
1	1A	1019	C
1	1A	1028	A
1	1A	1041	A
1	1A	1057	U
1	1A	1058	C
1	1A	1067	G
1	1A	1071	U
1	1A	1078	U
1	1A	1086	C
1	1A	1090	A
1	1A	1091	A
1	1A	1092	G
1	1A	1150	U
1	1A	1153	U
1	1A	1154	C
1	1A	1156	A
1	1A	1157	G
1	1A	1173	A
1	1A	1174	A
1	1A	1175	U
1	1A	1179	C
1	1A	1180	G
1	1A	1183	G
1	1A	1215	G
1	1A	1217	G
1	1A	1218	A
1	1A	1219	U
1	1A	1220	G
1	1A	1221	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1264	A
1	1A	1286	A
1	1A	1298	A
1	1A	1301	G
1	1A	1316	G
1	1A	1317	A
1	1A	1318	U
1	1A	1321	A
1	1A	1345	U
1	1A	1346	A
1	1A	1348	G
1	1A	1360	C
1	1A	1366	A
1	1A	1397	U
1	1A	1404	A
1	1A	1405	A
1	1A	1410	A
1	1A	1429	A
1	1A	1430	G
1	1A	1440	A
1	1A	1461	G
1	1A	1462	C
1	1A	1465	U
1	1A	1466	G
1	1A	1467	G
1	1A	1472	A
1	1A	1473	C
1	1A	1482	C
1	1A	1490	A
1	1A	1495	A
1	1A	1496	G
1	1A	1501	G
1	1A	1505	G
1	1A	1507	G
1	1A	1508	C
1	1A	1513	C
1	1A	1524	G
1	1A	1528	G
1	1A	1553	A
1	1A	1554	C
1	1A	1555	A
1	1A	1570	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1578	C
1	1A	1588	A
1	1A	1604	A
1	1A	1612	A
1	1A	1615	A
1	1A	1624	U
1	1A	1626	A
1	1A	1627	G
1	1A	1630	C
1	1A	1631	A
1	1A	1653	A
1	1A	1654	A
1	1A	1655	A
1	1A	1694	C
1	1A	1700	A
1	1A	1704	C
1	1A	1710	A
1	1A	1720	G
1	1A	1746	A
1	1A	1747	A
1	1A	1766	A
1	1A	1767	U
1	1A	1776	G
1	1A	1793	G
1	1A	1794	G
1	1A	1799	G
1	1A	1803	A
1	1A	1804	C
1	1A	1810	A
1	1A	1812	C
1	1A	1821	A
1	1A	1830	C
1	1A	1831	G
1	1A	1846	G
1	1A	1858	G
1	1A	1859	A
1	1A	1869	G
1	1A	1877	A
1	1A	1899	G
1	1A	1910	A
1	1A	1921	A
1	1A	1927	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1933	A
1	1A	1934	A
1	1A	1936	U
1	1A	1940	A
1	1A	1948	A
1	1A	1950	G
1	1A	1951	G
1	1A	1958	A
1	1A	1959	A
1	1A	1976	U
1	1A	1984	U
1	1A	1986	C
1	1A	1988	C
1	1A	1991	A
1	1A	1992	A
1	1A	1993	A
1	1A	2013	G
1	1A	2014	U
1	1A	2018	G
1	1A	2041	A
1	1A	2044	G
1	1A	2052	A
1	1A	2053	G
1	1A	2054	A
1	1A	2064	C
1	1A	2074	G
1	1A	2076	C
1	1A	2077	G
1	1A	2081	A
1	1A	2082	G
1	1A	2083	A
1	1A	2090	G
1	1A	2114	G
1	1A	2205	G
1	1A	2206	C
1	1A	2207	G
1	1A	2209	C
1	1A	2212	G
1	1A	2216	C
1	1A	2219	A
1	1A	2226	G
1	1A	2227	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2228	A
1	1A	2229	U
1	1A	2236	A
1	1A	2249	G
1	1A	2250	G
1	1A	2279	A
1	1A	2280	A
1	1A	2284	A
1	1A	2286	C
1	1A	2290	G
1	1A	2291	G
1	1A	2294	C
1	1A	2298	A
1	1A	2316	A
1	1A	2319	G
1	1A	2331	A
1	1A	2332	G
1	1A	2336	G
1	1A	2338	A
1	1A	2345	G
1	1A	2346	A
1	1A	2347	A
1	1A	2354	C
1	1A	2358	C
1	1A	2361	C
1	1A	2394	G
1	1A	2396	C
1	1A	2417	U
1	1A	2421	G
1	1A	2433	A
1	1A	2435	C
1	1A	2436	A
1	1A	2440	G
1	1A	2441	A
1	1A	2446	A
1	1A	2449	U
1	1A	2450	A
1	1A	2452	C
1	1A	2459	A
1	1A	2460	U
1	1A	2479	G
1	1A	2485	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2487	A
1	1A	2489	A
1	1A	2513	G
1	1A	2516	G
1	1A	2517	U
1	1A	2529	A
1	1A	2531	C
1	1A	2540	G
1	1A	2565	U
1	1A	2566	U
1	1A	2577	A
1	1A	2578	G
1	1A	2584	C
1	1A	2593	G
1	1A	2613	A
1	1A	2620	U
1	1A	2621	C
1	1A	2622	U
1	1A	2623	C
1	1A	2640	A
1	1A	2641	G
1	1A	2643	A
1	1A	2649	G
1	1A	2665	A
1	1A	2700	U
1	1A	2701	C
1	1A	2702	C
1	1A	2713	U
1	1A	2714	C
1	1A	2724	A
1	1A	2725	A
1	1A	2726	G
1	1A	2738	U
1	1A	2745	A
1	1A	2769	A
1	1A	2770	A
1	1A	2776	A
1	1A	2777	A
1	1A	2778	G
1	1A	2790	A
1	1A	2802	A
1	1A	2812	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2827	G
1	1A	2829	A
1	1A	2830	A
1	1A	2844	A
1	1A	2845	U
1	1A	2881	G
1	1A	2882	A
1	1A	2889	C
1	1A	2900	A
1	1A	2902	G
1	1A	2903	U
2	1B	13	A
2	1B	24	G
2	1B	56	G
2	1B	65	C
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	6	U
32	1a	10	G
32	1a	33	A
32	1a	40	G
32	1a	41	C
32	1a	45	G
32	1a	48	C
32	1a	49	C
32	1a	51	A
32	1a	52	A
32	1a	62	G
32	1a	65	G
32	1a	66	U
32	1a	74	G
32	1a	76	G
32	1a	77	G
32	1a	78	G
32	1a	90	U
32	1a	91	G
32	1a	92	G
32	1a	95	A
32	1a	110	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	115	C
32	1a	126	C
32	1a	132	C
32	1a	139	G
32	1a	156	A
32	1a	161	G
32	1a	162	G
32	1a	168	U
32	1a	169	C
32	1a	178	G
32	1a	190	U
32	1a	202	A
32	1a	204	A
32	1a	211	U
32	1a	212	G
32	1a	218	U
32	1a	222	G
32	1a	243	G
32	1a	247	G
32	1a	254	G
32	1a	262	G
32	1a	263	C
32	1a	266	A
32	1a	277	G
32	1a	285	G
32	1a	317	A
32	1a	324	C
32	1a	325	A
32	1a	337	C
32	1a	338	C
32	1a	342	G
32	1a	343	G
32	1a	344	G
32	1a	347	G
32	1a	348	C
32	1a	349	A
32	1a	350	G
32	1a	351	C
32	1a	363	U
32	1a	368	C
32	1a	369	A
32	1a	380	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	393	A
32	1a	394	C
32	1a	402	G
32	1a	408	A
32	1a	409	G
32	1a	419	G
32	1a	420	G
32	1a	425	U
32	1a	435	A
32	1a	437	C
32	1a	441	G
32	1a	447	A
32	1a	448	A
32	1a	449	C
32	1a	455	A
32	1a	456	C
32	1a	457	G
32	1a	461	G
32	1a	470	G
32	1a	478	G
32	1a	481	A
32	1a	482	U
32	1a	489	G
32	1a	493	A
32	1a	494	A
32	1a	495	C
32	1a	496	U
32	1a	502	C
32	1a	508	G
32	1a	510	C
32	1a	511	G
32	1a	515	U
32	1a	516	A
32	1a	517	A
32	1a	529	C
32	1a	531	A
32	1a	543	A
32	1a	545	U
32	1a	547	A
32	1a	556	A
32	1a	557	A
32	1a	560	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	561	G
32	1a	576	G
32	1a	580	C
32	1a	599	C
32	1a	602	C
32	1a	614	G
32	1a	637	A
32	1a	645	G
32	1a	649	A
32	1a	671	A
32	1a	672	G
32	1a	677	G
32	1a	687	G
32	1a	707	U
32	1a	715	G
32	1a	718	G
32	1a	733	C
32	1a	737	A
32	1a	739	G
32	1a	743	A
32	1a	761	A
32	1a	777	U
32	1a	778	A
32	1a	799	A
32	1a	801	C
32	1a	805	G
32	1a	812	A
32	1a	813	G
32	1a	820	G
32	1a	824	C
32	1a	825	U
32	1a	826	C
32	1a	829	G
32	1a	837	A
32	1a	848	U
32	1a	850	A
32	1a	880	G
32	1a	892	A
32	1a	904	G
32	1a	905	G
32	1a	909	C
32	1a	912	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	913	A
32	1a	914	C
32	1a	938	U
32	1a	939	U
32	1a	946	A
32	1a	947	A
32	1a	949	G
32	1a	950	C
32	1a	952	A
32	1a	953	A
32	1a	954	G
32	1a	955	A
32	1a	960	U
32	1a	961	A
32	1a	970	U
32	1a	971	G
32	1a	972	A
32	1a	974	A
32	1a	982	G
32	1a	983	A
32	1a	984	A
32	1a	987	C
32	1a	988	G
32	1a	990	G
32	1a	992	G
32	1a	995	A
32	1a	1001	G
32	1a	1027	A
32	1a	1028	C
32	1a	1033	G
32	1a	1037	C
32	1a	1048	U
32	1a	1049	C
32	1a	1064	G
32	1a	1069	U
32	1a	1077	G
32	1a	1078	U
32	1a	1079	C
32	1a	1084	A
32	1a	1089	G
32	1a	1091	G
32	1a	1106	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1107	G
32	1a	1113	A
32	1a	1117	G
32	1a	1119	U
32	1a	1120	C
32	1a	1122	G
32	1a	1123	C
32	1a	1128	C
32	1a	1129	A
32	1a	1135	A
32	1a	1142	U
32	1a	1149	G
32	1a	1165	A
32	1a	1166	G
32	1a	1178	U
32	1a	1179	G
32	1a	1184	G
32	1a	1195	A
32	1a	1196	C
32	1a	1202	G
32	1a	1209	A
32	1a	1220	A
32	1a	1238	A
32	1a	1239	U
32	1a	1240	G
32	1a	1242	C
32	1a	1252	C
32	1a	1260	U
32	1a	1262	A
32	1a	1268	A
32	1a	1269	A
32	1a	1281	A
32	1a	1282	G
32	1a	1284	U
32	1a	1294	G
32	1a	1304	C
32	1a	1320	G
32	1a	1322	A
32	1a	1328	A
32	1a	1329	G
32	1a	1335	G
32	1a	1341	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1342	A
32	1a	1345	C
32	1a	1353	G
32	1a	1360	A
32	1a	1361	C
32	1a	1379	A
32	1a	1381	A
32	1a	1383	C
32	1a	1402	G
32	1a	1425	G
32	1a	1426	G
32	1a	1432	A
32	1a	1433	C
32	1a	1451	A
32	1a	1465	G
32	1a	1469	G
32	1a	1475	G
32	1a	1480	A
32	1a	1481	A
32	1a	1482	G
32	1a	1484	U
32	1a	1495	G
32	1a	1507	G
32	1a	1508	G
53	1v	15	A
54	1x	6	G
54	1x	9	G
54	1x	13	C
54	1x	17	C
54	1x	17(A)	U
54	1x	19	G
54	1x	20	U
54	1x	21	A
54	1x	31	G
54	1x	34	C
54	1x	37	A
54	1x	38	A
54	1x	42	G
54	1x	47	U
54	1x	56	C
54	1x	65	C
54	1x	70	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1x	76	A
1	2A	9	G
1	2A	11	U
1	2A	12	A
1	2A	14	G
1	2A	22	G
1	2A	33	C
1	2A	44	C
1	2A	59	G
1	2A	69	A
1	2A	72	A
1	2A	73	G
1	2A	77	G
1	2A	81	G
1	2A	82	A
1	2A	88	U
1	2A	91	C
1	2A	98	G
1	2A	99	G
1	2A	115	A
1	2A	116	A
1	2A	117	U
1	2A	122	G
1	2A	154	C
1	2A	155	U
1	2A	169	A
1	2A	184	A
1	2A	187	A
1	2A	193	G
1	2A	203	G
1	2A	204	A
1	2A	209	A
1	2A	210	A
1	2A	211	A
1	2A	216	A
1	2A	217	A
1	2A	218	U
1	2A	221	A
1	2A	236	G
1	2A	254	G
1	2A	268	G
1	2A	270	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	271	U
1	2A	272	G
1	2A	273	U
1	2A	274	C
1	2A	287	U
1	2A	288	G
1	2A	300	C
1	2A	301	A
1	2A	334	A
1	2A	345	A
1	2A	347	A
1	2A	350	G
1	2A	352	G
1	2A	353	A
1	2A	356	G
1	2A	357	C
1	2A	358	C
1	2A	361	G
1	2A	375	G
1	2A	385	U
1	2A	386	G
1	2A	388	G
1	2A	389	G
1	2A	405	G
1	2A	406	U
1	2A	412	G
1	2A	415	G
1	2A	422	G
1	2A	431	U
1	2A	433	G
1	2A	437	G
1	2A	438	A
1	2A	441	A
1	2A	448	A
1	2A	454	A
1	2A	468	A
1	2A	469	C
1	2A	479	A
1	2A	480	C
1	2A	481	C
1	2A	482	A
1	2A	495	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	500	U
1	2A	506	G
1	2A	509	C
1	2A	516	A
1	2A	520	G
1	2A	528	U
1	2A	529	A
1	2A	533	C
1	2A	552	A
1	2A	553	A
1	2A	554	G
1	2A	555	C
1	2A	556	A
1	2A	557	G
1	2A	568	G
1	2A	578	G
1	2A	585	G
1	2A	595	G
1	2A	597	A
1	2A	608	A
1	2A	625	A
1	2A	626	G
1	2A	629	U
1	2A	637	U
1	2A	638	G
1	2A	640	G
1	2A	651	A
1	2A	658	C
1	2A	661	A
1	2A	669	C
1	2A	670	A
1	2A	678	A
1	2A	679	G
1	2A	697	G
1	2A	698	C
1	2A	732	G
1	2A	772	G
1	2A	776	C
1	2A	811	G
1	2A	817	G
1	2A	821	G
1	2A	822	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	828	A
1	2A	830	A
1	2A	831	G
1	2A	836	C
1	2A	838	G
1	2A	840	G
1	2A	848	A
1	2A	851	G
1	2A	858	C
1	2A	865	A
1	2A	873	U
1	2A	898	G
1	2A	903	C
1	2A	905	G
1	2A	912	A
1	2A	913	C
1	2A	915	G
1	2A	921	G
1	2A	925	G
1	2A	926	G
1	2A	930	C
1	2A	932	C
1	2A	933	A
1	2A	934	C
1	2A	935	C
1	2A	936	A
1	2A	941	A
1	2A	945	A
1	2A	946	A
1	2A	955	A
1	2A	959	C
1	2A	962	A
1	2A	976	G
1	2A	977	A
1	2A	982	G
1	2A	985	A
1	2A	989	A
1	2A	990	G
1	2A	1001	A
1	2A	1003	A
1	2A	1005	C
1	2A	1017	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1018	G
1	2A	1019	C
1	2A	1025	A
1	2A	1028	A
1	2A	1041	A
1	2A	1050	C
1	2A	1057	U
1	2A	1058	C
1	2A	1062	G
1	2A	1065	A
1	2A	1066	A
1	2A	1067	G
1	2A	1070	G
1	2A	1072	A
1	2A	1078	U
1	2A	1082	G
1	2A	1083	C
1	2A	1084	G
1	2A	1087	G
1	2A	1088	C
1	2A	1091	A
1	2A	1092	G
1	2A	1093	A
1	2A	1103	G
1	2A	1105	U
1	2A	1106	U
1	2A	1107	G
1	2A	1108	G
1	2A	1109	C
1	2A	1110	U
1	2A	1115	A
1	2A	1118	A
1	2A	1120	C
1	2A	1121	C
1	2A	1126	U
1	2A	1127	U
1	2A	1128	U
1	2A	1131	A
1	2A	1133	A
1	2A	1140	A
1	2A	1142	U
1	2A	1143	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1146	U
1	2A	1156	A
1	2A	1157	G
1	2A	1158	U
1	2A	1159	G
1	2A	1161	C
1	2A	1167	G
1	2A	1175	U
1	2A	1179	C
1	2A	1180	G
1	2A	1183	G
1	2A	1187	A
1	2A	1216	G
1	2A	1240	C
1	2A	1256	G
1	2A	1285	U
1	2A	1289	G
1	2A	1298	A
1	2A	1301	G
1	2A	1307	A
1	2A	1316	G
1	2A	1317	A
1	2A	1318	U
1	2A	1332	A
1	2A	1345	U
1	2A	1346	A
1	2A	1350	C
1	2A	1359	C
1	2A	1364	G
1	2A	1374	U
1	2A	1397	U
1	2A	1404	A
1	2A	1405	A
1	2A	1410	A
1	2A	1413	G
1	2A	1415	C
1	2A	1425	G
1	2A	1429	A
1	2A	1430	G
1	2A	1431	C
1	2A	1447	C
1	2A	1448	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1461	G
1	2A	1462	C
1	2A	1465	U
1	2A	1466	G
1	2A	1472	A
1	2A	1473	C
1	2A	1490	A
1	2A	1495	A
1	2A	1496	G
1	2A	1501	G
1	2A	1506	A
1	2A	1513	C
1	2A	1517	A
1	2A	1528	G
1	2A	1534	U
1	2A	1535	A
1	2A	1538	C
1	2A	1542	U
1	2A	1554	C
1	2A	1555	A
1	2A	1579	G
1	2A	1583	G
1	2A	1589	C
1	2A	1590	A
1	2A	1593	C
1	2A	1601	G
1	2A	1604	A
1	2A	1605	G
1	2A	1612	A
1	2A	1615	A
1	2A	1624	U
1	2A	1626	A
1	2A	1630	C
1	2A	1631	A
1	2A	1639	G
1	2A	1652	C
1	2A	1653	A
1	2A	1654	A
1	2A	1655	A
1	2A	1661	A
1	2A	1686	C
1	2A	1694	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1700	A
1	2A	1710	A
1	2A	1720	G
1	2A	1746	A
1	2A	1747	A
1	2A	1765	G
1	2A	1766	A
1	2A	1768	G
1	2A	1771	C
1	2A	1786	G
1	2A	1788	G
1	2A	1792	A
1	2A	1793	G
1	2A	1794	G
1	2A	1799	G
1	2A	1803	A
1	2A	1810	A
1	2A	1812	C
1	2A	1821	A
1	2A	1830	C
1	2A	1831	G
1	2A	1846	G
1	2A	1858	G
1	2A	1877	A
1	2A	1889	A
1	2A	1891	G
1	2A	1898	A
1	2A	1899	G
1	2A	1921	A
1	2A	1924	G
1	2A	1925	G
1	2A	1927	G
1	2A	1934	A
1	2A	1935	C
1	2A	1948	A
1	2A	1950	G
1	2A	1951	G
1	2A	1952	U
1	2A	1959	A
1	2A	1976	U
1	2A	1984	U
1	2A	1988	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1991	A
1	2A	1992	A
1	2A	1993	A
1	2A	2014	U
1	2A	2018	G
1	2A	2026	A
1	2A	2041	A
1	2A	2044	G
1	2A	2051	A
1	2A	2052	A
1	2A	2054	A
1	2A	2060	C
1	2A	2064	C
1	2A	2067	G
1	2A	2076	C
1	2A	2077	G
1	2A	2081	A
1	2A	2082	G
1	2A	2083	A
1	2A	2090	G
1	2A	2120	U
1	2A	2207	G
1	2A	2209	C
1	2A	2213	G
1	2A	2217	C
1	2A	2219	A
1	2A	2226	G
1	2A	2227	G
1	2A	2228	A
1	2A	2236	A
1	2A	2249	G
1	2A	2278	A
1	2A	2280	A
1	2A	2286	C
1	2A	2290	G
1	2A	2294	C
1	2A	2298	A
1	2A	2300	G
1	2A	2316	A
1	2A	2318	G
1	2A	2319	G
1	2A	2322	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2323	U
1	2A	2328	C
1	2A	2329	G
1	2A	2330	G
1	2A	2331	A
1	2A	2333	A
1	2A	2336	G
1	2A	2345	G
1	2A	2346	A
1	2A	2347	A
1	2A	2354	C
1	2A	2358	C
1	2A	2361	C
1	2A	2387	A
1	2A	2394	G
1	2A	2396	C
1	2A	2399	A
1	2A	2402	G
1	2A	2417	U
1	2A	2421	G
1	2A	2433	A
1	2A	2434	U
1	2A	2436	A
1	2A	2439	G
1	2A	2440	G
1	2A	2441	A
1	2A	2445	A
1	2A	2446	A
1	2A	2450	A
1	2A	2452	C
1	2A	2456	G
1	2A	2459	A
1	2A	2460	U
1	2A	2476	C
1	2A	2479	G
1	2A	2480	A
1	2A	2485	C
1	2A	2487	A
1	2A	2489	A
1	2A	2497	G
1	2A	2513	G
1	2A	2516	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2517	U
1	2A	2529	A
1	2A	2531	C
1	2A	2540	G
1	2A	2565	U
1	2A	2577	A
1	2A	2578	G
1	2A	2584	C
1	2A	2613	A
1	2A	2620	U
1	2A	2622	U
1	2A	2623	C
1	2A	2640	A
1	2A	2641	G
1	2A	2650	A
1	2A	2665	A
1	2A	2674	G
1	2A	2693	U
1	2A	2700	U
1	2A	2701	C
1	2A	2702	C
1	2A	2713	U
1	2A	2714	C
1	2A	2724	A
1	2A	2725	A
1	2A	2726	G
1	2A	2738	U
1	2A	2745	A
1	2A	2763	G
1	2A	2764	C
1	2A	2769	A
1	2A	2776	A
1	2A	2777	A
1	2A	2778	G
1	2A	2790	A
1	2A	2801	C
1	2A	2805	G
1	2A	2812	G
1	2A	2817	U
1	2A	2827	G
1	2A	2829	A
1	2A	2830	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2842	G
1	2A	2843	G
1	2A	2844	A
1	2A	2848	G
1	2A	2881	G
1	2A	2882	A
1	2A	2885	G
1	2A	2889	C
1	2A	2895	G
1	2A	2900	A
1	2A	2902	G
1	2A	2903	U
1	2A	2904	C
1	2A	2905	U
2	2B	2	C
2	2B	7	G
2	2B	9	G
2	2B	13	A
2	2B	28	C
2	2B	30	C
2	2B	32	C
2	2B	33	G
2	2B	35	U
2	2B	43	C
2	2B	45	A
2	2B	46	A
2	2B	50	G
2	2B	52	A
2	2B	56	G
2	2B	64	C
2	2B	73	A
2	2B	85	G
2	2B	106	G
2	2B	110	G
2	2B	111	G
2	2B	120	A
32	2a	6	U
32	2a	7	G
32	2a	10	G
32	2a	11	A
32	2a	15	U
32	2a	16	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	23	G
32	2a	31	U
32	2a	33	A
32	2a	40	G
32	2a	43	G
32	2a	48	C
32	2a	49	C
32	2a	51	A
32	2a	52	A
32	2a	66	U
32	2a	67	G
32	2a	74	G
32	2a	79	G
32	2a	85	C
32	2a	91	G
32	2a	92	G
32	2a	110	A
32	2a	115	C
32	2a	124	G
32	2a	126	C
32	2a	138	A
32	2a	151	G
32	2a	158	C
32	2a	169	C
32	2a	177	U
32	2a	189	U
32	2a	190	U
32	2a	202	A
32	2a	204	A
32	2a	208	C
32	2a	210	U
32	2a	211	U
32	2a	212	G
32	2a	243	G
32	2a	247	G
32	2a	248	U
32	2a	254	G
32	2a	262	G
32	2a	263	C
32	2a	275	A
32	2a	277	G
32	2a	285	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	297	G
32	2a	310	C
32	2a	317	A
32	2a	324	C
32	2a	328	G
32	2a	340	A
32	2a	345	A
32	2a	346	G
32	2a	347	G
32	2a	348	C
32	2a	349	A
32	2a	350	G
32	2a	363	U
32	2a	368	C
32	2a	369	A
32	2a	380	G
32	2a	394	C
32	2a	402	G
32	2a	408	A
32	2a	417	U
32	2a	419	G
32	2a	425	U
32	2a	426	A
32	2a	435	A
32	2a	437	C
32	2a	447	A
32	2a	455	A
32	2a	456	C
32	2a	457	G
32	2a	463	A
32	2a	469	G
32	2a	470	G
32	2a	481	A
32	2a	482	U
32	2a	489	G
32	2a	493	A
32	2a	494	A
32	2a	495	C
32	2a	497	C
32	2a	502	C
32	2a	505	G
32	2a	511	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	515	U
32	2a	516	A
32	2a	517	A
32	2a	531	A
32	2a	543	A
32	2a	545	U
32	2a	546	C
32	2a	552	G
32	2a	556	A
32	2a	557	A
32	2a	560	G
32	2a	561	G
32	2a	580	C
32	2a	611	G
32	2a	614	G
32	2a	637	A
32	2a	645	G
32	2a	649	A
32	2a	650	G
32	2a	672	G
32	2a	677	G
32	2a	679	A
32	2a	696	A
32	2a	701	C
32	2a	704	C
32	2a	707	U
32	2a	708	G
32	2a	715	G
32	2a	733	C
32	2a	739	G
32	2a	744	G
32	2a	761	A
32	2a	776	A
32	2a	777	U
32	2a	778	A
32	2a	783	G
32	2a	800	A
32	2a	801	C
32	2a	812	A
32	2a	813	G
32	2a	822	G
32	2a	824	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	825	U
32	2a	826	C
32	2a	837	A
32	2a	845	G
32	2a	880	G
32	2a	892	A
32	2a	898	U
32	2a	904	G
32	2a	905	G
32	2a	909	C
32	2a	912	C
32	2a	913	A
32	2a	920	G
32	2a	938	U
32	2a	939	U
32	2a	946	A
32	2a	947	A
32	2a	949	G
32	2a	950	C
32	2a	952	A
32	2a	953	A
32	2a	954	G
32	2a	955	A
32	2a	956	A
32	2a	967	C
32	2a	970	U
32	2a	971	G
32	2a	973	C
32	2a	974	A
32	2a	977	C
32	2a	981	G
32	2a	983	A
32	2a	984	A
32	2a	985	C
32	2a	986	C
32	2a	988	G
32	2a	1001	G
32	2a	1002	G
32	2a	1027	A
32	2a	1028	C
32	2a	1033	G
32	2a	1036	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1037	C
32	2a	1038	A
32	2a	1039	U
32	2a	1047	G
32	2a	1048	U
32	2a	1049	C
32	2a	1064	G
32	2a	1077	G
32	2a	1078	U
32	2a	1084	A
32	2a	1091	G
32	2a	1096	C
32	2a	1101	C
32	2a	1105	U
32	2a	1109	U
32	2a	1112	C
32	2a	1113	A
32	2a	1116	G
32	2a	1118	U
32	2a	1119	U
32	2a	1120	C
32	2a	1121	G
32	2a	1122	G
32	2a	1129	A
32	2a	1130	C
32	2a	1140	A
32	2a	1142	U
32	2a	1165	A
32	2a	1168	G
32	2a	1171	C
32	2a	1172	G
32	2a	1178	U
32	2a	1184	G
32	2a	1193	U
32	2a	1194	U
32	2a	1196	C
32	2a	1210	C
32	2a	1220	A
32	2a	1222	U
32	2a	1223	G
32	2a	1235	G
32	2a	1239	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1240	G
32	2a	1242	C
32	2a	1243	A
32	2a	1244	C
32	2a	1251	A
32	2a	1255	G
32	2a	1262	A
32	2a	1263	U
32	2a	1264	C
32	2a	1268	A
32	2a	1269	A
32	2a	1281	A
32	2a	1285	C
32	2a	1287	G
32	2a	1300	A
32	2a	1304	C
32	2a	1305	G
32	2a	1308	C
32	2a	1320	G
32	2a	1328	A
32	2a	1329	G
32	2a	1332	A
32	2a	1341	C
32	2a	1342	A
32	2a	1345	C
32	2a	1347	U
32	2a	1353	G
32	2a	1364	U
32	2a	1380	C
32	2a	1381	A
32	2a	1402	G
32	2a	1425	G
32	2a	1426	G
32	2a	1427	A
32	2a	1431	U
32	2a	1432	A
32	2a	1433	C
32	2a	1434	G
32	2a	1467	G
32	2a	1475	G
32	2a	1477	A
32	2a	1480	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1481	A
32	2a	1482	G
32	2a	1484	U
32	2a	1495	G
32	2a	1497	A
32	2a	1498	G
32	2a	1507	G
32	2a	1508	G
32	2a	1509	A
32	2a	1510	U
53	2v	15	A
54	2x	6	G
54	2x	9	G
54	2x	13	C
54	2x	17	C
54	2x	17(A)	U
54	2x	19	G
54	2x	20	U
54	2x	21	A
54	2x	31	G
54	2x	34	C
54	2x	37	A
54	2x	38	A
54	2x	42	G
54	2x	47	U
54	2x	56	C
54	2x	65	C
54	2x	70	G
54	2x	76	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	183	A
1	1A	184	A
1	1A	301	A
1	1A	516	A
1	1A	873	U
1	1A	1153	U
1	1A	1218	A
1	1A	1220	G
1	1A	1285	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1320	A
1	1A	1425	G
1	1A	1465	U
1	1A	1653	A
1	1A	1709	C
1	1A	1792	A
1	1A	2013	G
1	1A	2417	U
1	1A	2700	U
1	1A	2768	U
1	2A	183	A
1	2A	184	A
1	2A	247	G
1	2A	357	C
1	2A	516	A
1	2A	810	A
1	2A	873	U
1	2A	902	C
1	2A	945	A
1	2A	1071	U
1	2A	1087	G
1	2A	1102	A
1	2A	1114	A
1	2A	1238	A
1	2A	1424	A
1	2A	1425	G
1	2A	1465	U
1	2A	1604	A
1	2A	1820	C
1	2A	1934	A
1	2A	2013	G
1	2A	2328	C
1	2A	2417	U
1	2A	2700	U
1	2A	2768	U
2	2B	42	C
2	2B	45	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
54	PSU	2x	55	54	17,21,22	1.52	2 (11%)	20,30,33	3.26	7 (35%)
54	4SU	2x	8	54	14,21,22	1.28	2 (14%)	15,30,33	2.67	2 (13%)
54	5MU	1x	54	54	15,22,23	1.11	1 (6%)	16,32,35	2.05	2 (12%)
54	4SU	1x	8	54	14,21,22	1.49	2 (14%)	15,30,33	2.63	2 (13%)
54	5MC	1x	32	54	15,22,23	1.27	1 (6%)	19,32,35	1.45	3 (15%)
54	5MU	2x	54	54	15,22,23	1.08	1 (6%)	16,32,35	1.90	2 (12%)
54	5MC	2x	32	54	15,22,23	1.31	1 (6%)	19,32,35	1.39	2 (10%)
54	PSU	1x	55	54	17,21,22	1.63	3 (17%)	20,30,33	3.34	6 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2x	55	54	-	2/7/25/26	0/2/2/2
54	4SU	2x	8	54	-	0/5/25/26	0/2/2/2
54	5MU	1x	54	54	-	0/5/25/26	0/2/2/2
54	4SU	1x	8	54	-	0/5/25/26	0/2/2/2
54	5MC	1x	32	54	-	0/5/25/26	0/2/2/2
54	5MU	2x	54	54	-	1/5/25/26	0/2/2/2
54	5MC	2x	32	54	-	1/5/25/26	0/2/2/2
54	PSU	1x	55	54	-	2/7/25/26	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	55	PSU	C5-C1'	-4.73	1.48	1.52
54	2x	32	5MC	C5-C4	4.71	1.48	1.41
54	1x	32	5MC	C5-C4	4.52	1.48	1.41
54	2x	55	PSU	C5-C1'	-3.78	1.49	1.52
54	1x	8	4SU	C2-N3	-3.77	1.30	1.38
54	2x	55	PSU	C4-C5	3.70	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1x	8	4SU	C4-S4	-3.65	1.60	1.67
54	1x	54	5MU	C4-C5	3.53	1.49	1.41
54	2x	54	5MU	C4-C5	3.52	1.49	1.41
54	2x	8	4SU	C4-S4	-3.49	1.61	1.67
54	1x	55	PSU	C4-C5	3.08	1.48	1.41
54	2x	8	4SU	C2-N3	-2.74	1.32	1.38
54	1x	55	PSU	O4'-C1'	-2.13	1.41	1.44

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1x	55	PSU	N1-C2-N3	-9.35	120.99	128.43
54	1x	8	4SU	C2-N3-C4	8.83	127.95	115.15
54	2x	8	4SU	C2-N3-C4	8.71	127.78	115.15
54	2x	55	PSU	N1-C2-N3	-8.63	121.57	128.43
54	1x	54	5MU	C4-N3-C2	7.54	121.51	115.14
54	1x	55	PSU	C4-N3-C2	7.28	121.29	115.14
54	2x	54	5MU	C4-N3-C2	7.02	121.07	115.14
54	2x	55	PSU	C4-N3-C2	6.91	120.97	115.14
54	1x	55	PSU	C5-C4-N3	-5.45	118.34	125.36
54	2x	55	PSU	C5-C4-N3	-5.44	118.35	125.36
54	2x	8	4SU	C5-C4-N3	-5.01	117.13	123.83
54	1x	8	4SU	C5-C4-N3	-4.76	117.46	123.83
54	2x	55	PSU	C5-C6-N1	-4.31	119.14	124.44
54	2x	55	PSU	C6-N1-C2	4.24	122.35	115.36
54	1x	55	PSU	C6-N1-C2	4.22	122.32	115.36
54	2x	32	5MC	C2-N3-C4	3.95	120.78	116.02
54	1x	55	PSU	C5-C6-N1	-3.89	119.66	124.44
54	1x	32	5MC	C2-N3-C4	3.60	120.36	116.02
54	1x	55	PSU	C5-C1'-C2'	-3.23	109.55	115.32
54	1x	32	5MC	N4-C4-N3	3.11	121.43	117.03
54	2x	55	PSU	C5-C1'-C2'	-2.90	110.15	115.32
54	2x	55	PSU	O4'-C1'-C5	2.44	113.71	109.93
54	2x	54	5MU	C5-C6-N1	-2.30	119.72	122.19
54	1x	32	5MC	C5-C6-N1	-2.20	119.82	122.19
54	1x	54	5MU	C5-C6-N1	-2.17	119.86	122.19
54	2x	32	5MC	N4-C4-N3	2.14	120.05	117.03

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	2x	32	5MC	C2'-C1'-N1-C6
54	1x	55	PSU	O4'-C4'-C5'-O5'
54	2x	55	PSU	O4'-C4'-C5'-O5'
54	1x	55	PSU	C3'-C4'-C5'-O5'
54	2x	55	PSU	C3'-C4'-C5'-O5'
54	2x	54	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2494 ligands modelled in this entry, 2492 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	2d	501	35	0,12,12	0.00	-	-		
58	SF4	1d	501	35	0,12,12	0.00	-	-		

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
58	SF4	2d	501	35	-	-	0/6/5/5
58	SF4	1d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	2746/2915 (94%)	0.04	26 (0%) 84 84	22, 41, 87, 114	0
1	2A	2790/2915 (95%)	-0.21	66 (2%) 59 56	25, 46, 93, 111	0
2	1B	120/121 (99%)	-0.07	0 100 100	36, 65, 80, 91	0
2	2B	120/121 (99%)	0.18	3 (2%) 57 55	41, 70, 83, 92	0
3	1D	275/276 (99%)	-0.28	0 100 100	23, 40, 57, 77	0
3	2D	275/276 (99%)	-0.30	3 (1%) 80 80	24, 43, 59, 78	0
4	1E	204/206 (99%)	-0.14	0 100 100	21, 43, 66, 81	0
4	2E	204/206 (99%)	-0.18	1 (0%) 91 91	23, 45, 67, 82	0
5	1F	203/210 (96%)	-0.09	0 100 100	22, 50, 75, 90	0
5	2F	203/210 (96%)	-0.21	2 (0%) 82 82	24, 54, 76, 93	0
6	1G	181/182 (99%)	-0.09	5 (2%) 53 49	50, 70, 83, 98	0
6	2G	181/182 (99%)	0.59	15 (8%) 11 8	54, 73, 85, 100	0
7	1H	174/180 (96%)	-0.05	1 (0%) 89 89	48, 64, 77, 82	0
7	2H	174/180 (96%)	0.98	27 (15%) 2 1	56, 69, 81, 83	0
8	1I	146/148 (98%)	0.19	0 100 100	45, 75, 84, 89	0
8	2I	146/148 (98%)	0.59	13 (8%) 9 7	47, 76, 85, 92	0
9	1N	140/140 (100%)	-0.13	0 100 100	27, 46, 66, 79	0
9	2N	140/140 (100%)	0.01	0 100 100	30, 50, 70, 81	0
10	1O	122/122 (100%)	-0.18	0 100 100	33, 45, 63, 70	0
10	2O	122/122 (100%)	-0.28	0 100 100	34, 47, 63, 73	0
11	1P	149/150 (99%)	-0.02	0 100 100	22, 52, 75, 86	0
11	2P	149/150 (99%)	0.37	11 (7%) 14 11	25, 56, 78, 89	0
12	1Q	141/141 (100%)	0.00	1 (0%) 87 87	31, 49, 63, 87	0
12	2Q	141/141 (100%)	-0.24	1 (0%) 87 87	35, 52, 66, 85	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%)	-0.38	0 100 100	19, 30, 47, 57	0
13	2R	118/118 (100%)	-0.14	0 100 100	35, 51, 65, 76	0
14	1S	110/112 (98%)	-0.24	0 100 100	33, 49, 65, 68	0
14	2S	110/112 (98%)	0.79	11 (10%) 7 5	65, 79, 88, 93	0
15	1T	131/146 (89%)	-0.29	0 100 100	29, 41, 70, 90	0
15	2T	131/146 (89%)	-0.22	0 100 100	47, 58, 78, 90	0
16	1U	116/118 (98%)	-0.49	0 100 100	19, 27, 44, 64	0
16	2U	116/118 (98%)	0.02	3 (2%) 56 52	37, 59, 77, 88	0
17	1V	101/101 (100%)	-0.17	0 100 100	27, 49, 65, 74	0
17	2V	101/101 (100%)	0.13	1 (0%) 82 82	30, 54, 71, 78	0
18	1W	112/113 (99%)	-0.25	0 100 100	23, 35, 55, 84	0
18	2W	112/113 (99%)	-0.27	0 100 100	26, 37, 57, 87	0
19	1X	95/96 (98%)	-0.09	0 100 100	31, 46, 66, 79	0
19	2X	95/96 (98%)	-0.02	3 (3%) 47 43	34, 49, 69, 78	0
20	1Y	107/110 (97%)	-0.09	1 (0%) 84 84	29, 47, 68, 85	0
20	2Y	107/110 (97%)	0.67	11 (10%) 6 5	55, 72, 83, 98	0
21	1Z	186/206 (90%)	-0.22	0 100 100	51, 68, 82, 92	0
21	2Z	186/206 (90%)	0.57	12 (6%) 18 14	55, 71, 84, 93	0
22	10	75/85 (88%)	-0.15	0 100 100	33, 45, 59, 66	0
22	20	75/85 (88%)	0.27	3 (4%) 38 33	37, 50, 64, 68	0
23	11	97/98 (98%)	-0.04	1 (1%) 82 82	28, 47, 71, 78	0
23	21	97/98 (98%)	-0.04	1 (1%) 82 82	30, 49, 73, 78	0
24	12	70/72 (97%)	-0.02	0 100 100	42, 58, 72, 80	0
24	22	70/72 (97%)	0.10	0 100 100	45, 61, 74, 79	0
25	13	59/60 (98%)	-0.09	0 100 100	32, 45, 65, 78	0
25	23	59/60 (98%)	0.47	5 (8%) 10 8	35, 50, 69, 80	0
26	14	69/71 (97%)	0.28	6 (8%) 10 7	52, 75, 99, 102	0
26	24	69/71 (97%)	0.93	7 (10%) 7 5	78, 93, 98, 103	0
27	15	59/60 (98%)	-0.41	0 100 100	15, 30, 45, 72	0
27	25	59/60 (98%)	-0.22	0 100 100	33, 50, 67, 72	0
28	16	53/54 (98%)	-0.26	0 100 100	38, 48, 59, 70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	-0.21	0 100 100	42, 51, 62, 72	0
29	17	48/49 (97%)	-0.07	1 (2%) 63 61	24, 31, 64, 81	0
29	27	48/49 (97%)	-0.01	3 (6%) 20 16	26, 34, 64, 82	0
30	18	64/65 (98%)	-0.09	0 100 100	30, 41, 49, 63	0
30	28	64/65 (98%)	-0.07	1 (1%) 72 71	33, 43, 52, 64	0
31	19	37/37 (100%)	0.25	0 100 100	38, 48, 70, 74	0
31	29	37/37 (100%)	0.24	2 (5%) 25 22	43, 53, 71, 77	0
32	1a	1477/1521 (97%)	0.05	35 (2%) 59 56	34, 72, 98, 114	0
32	2a	1483/1521 (97%)	0.12	41 (2%) 53 49	43, 78, 101, 115	0
33	1b	231/256 (90%)	0.62	26 (11%) 5 4	67, 86, 96, 115	0
33	2b	231/256 (90%)	0.77	28 (12%) 4 3	71, 88, 97, 106	0
34	1c	206/239 (86%)	0.49	15 (7%) 15 11	70, 84, 93, 99	0
34	2c	206/239 (86%)	0.83	24 (11%) 4 3	73, 85, 94, 96	0
35	1d	208/209 (99%)	0.21	5 (2%) 59 56	56, 77, 88, 100	0
35	2d	208/209 (99%)	0.15	3 (1%) 75 75	56, 73, 84, 92	0
36	1e	148/162 (91%)	-0.06	0 100 100	47, 67, 79, 87	0
36	2e	148/162 (91%)	-0.01	2 (1%) 75 75	56, 74, 84, 90	0
37	1f	100/101 (99%)	-0.19	0 100 100	55, 73, 84, 90	0
37	2f	100/101 (99%)	-0.11	2 (2%) 65 63	56, 74, 83, 87	0
38	1g	155/156 (99%)	0.48	12 (7%) 13 10	66, 79, 91, 98	0
38	2g	155/156 (99%)	0.87	19 (12%) 4 3	67, 81, 91, 97	0
39	1h	137/138 (99%)	0.05	1 (0%) 87 87	53, 69, 77, 82	0
39	2h	137/138 (99%)	0.35	5 (3%) 42 37	62, 75, 84, 91	0
40	1i	127/128 (99%)	0.77	11 (8%) 10 7	61, 87, 95, 97	0
40	2i	127/128 (99%)	1.43	31 (24%) 0 0	67, 88, 95, 102	0
41	1j	97/105 (92%)	0.93	12 (12%) 4 3	57, 87, 95, 98	0
41	2j	96/105 (91%)	1.35	23 (23%) 0 0	76, 91, 101, 102	0
42	1k	114/129 (88%)	0.03	1 (0%) 84 84	38, 67, 80, 94	0
42	2k	114/129 (88%)	0.36	5 (4%) 34 30	53, 76, 86, 92	0
43	1l	122/132 (92%)	-0.02	2 (1%) 72 71	49, 63, 76, 89	0
43	2l	122/132 (92%)	0.10	1 (0%) 86 86	56, 67, 76, 82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	118/126 (93%)	0.16	1 (0%) 86 86	58, 80, 87, 92	0
44	2m	116/126 (92%)	0.60	16 (13%) 2 2	70, 83, 89, 96	0
45	1n	60/61 (98%)	0.55	5 (8%) 11 8	60, 77, 86, 92	0
45	2n	60/61 (98%)	1.36	15 (25%) 0 0	77, 88, 94, 96	0
46	1o	88/89 (98%)	0.16	3 (3%) 45 40	50, 65, 82, 86	0
46	2o	88/89 (98%)	0.29	3 (3%) 45 40	60, 74, 87, 92	0
47	1p	82/88 (93%)	0.57	5 (6%) 21 17	62, 77, 88, 93	0
47	2p	82/88 (93%)	0.43	5 (6%) 21 17	59, 70, 79, 91	0
48	1q	99/105 (94%)	0.20	0 100 100	47, 68, 80, 83	0
48	2q	99/105 (94%)	0.25	2 (2%) 65 63	58, 72, 81, 85	0
49	1r	68/88 (77%)	0.48	4 (5%) 22 18	58, 68, 83, 87	0
49	2r	68/88 (77%)	0.84	10 (14%) 2 1	63, 74, 84, 88	0
50	1s	84/93 (90%)	0.69	7 (8%) 11 8	67, 81, 92, 98	0
50	2s	83/93 (89%)	1.65	31 (37%) 0 0	76, 91, 102, 105	0
51	1t	96/106 (90%)	0.42	1 (1%) 82 82	57, 75, 84, 90	0
51	2t	96/106 (90%)	0.30	2 (2%) 63 61	56, 73, 84, 87	0
52	1u	23/27 (85%)	0.74	2 (8%) 10 7	68, 77, 82, 85	0
52	2u	23/27 (85%)	1.80	9 (39%) 0 0	68, 80, 85, 88	0
53	1v	5/24 (20%)	0.36	0 100 100	50, 55, 86, 88	0
53	2v	5/24 (20%)	1.44	2 (40%) 0 0	73, 74, 89, 103	0
54	1x	72/77 (93%)	0.11	0 100 100	34, 68, 85, 99	0
54	2x	72/77 (93%)	0.35	1 (1%) 75 75	36, 71, 87, 101	0
55	1z	12/15 (80%)	0.12	0 100 100	29, 36, 72, 81	0
55	2z	13/15 (86%)	0.48	2 (15%) 2 1	31, 37, 84, 91	0
All	All	20521/21474 (95%)	0.10	677 (3%) 46 41	15, 62, 92, 115	0

All (677) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	1g	79	ARG	7.5
32	1a	980	G	7.5
32	2a	980	G	7.1
32	1a	981	G	6.9
33	1b	227	GLY	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	156	TRP	6.8
34	2c	155	GLY	6.6
32	2a	981	G	6.3
32	1a	979	A	6.0
38	2g	156	TRP	6.0
33	1b	228	GLY	5.9
1	2A	2812	G	5.9
32	2a	979	A	5.7
38	1g	78	ARG	5.5
41	1j	98	ILE	5.4
7	2H	111	HIS	5.4
40	2i	15	ALA	5.4
38	1g	80	VAL	5.3
52	2u	14	TRP	5.3
45	2n	25	VAL	5.3
7	2H	112	PRO	5.1
1	1A	1554	C	5.0
41	2j	85	LEU	5.0
20	2Y	1	MET	5.0
38	2g	78	ARG	4.9
34	2c	189	ALA	4.9
32	1a	982	G	4.8
1	1A	2815	G	4.8
12	1Q	59	ARG	4.7
40	2i	21	PRO	4.7
38	1g	81	GLY	4.6
41	2j	63	PHE	4.6
55	2z	13	PRO	4.5
26	24	68	ARG	4.5
32	2a	1509	A	4.5
40	2i	36	TYR	4.5
20	2Y	5	MET	4.5
38	2g	82	GLY	4.5
1	2A	2815	G	4.5
1	2A	2811	A	4.4
52	2u	13	ILE	4.4
50	2s	71	LEU	4.4
40	2i	5	TYR	4.3
7	2H	106	THR	4.3
49	2r	43	PHE	4.3
38	2g	154	TYR	4.3
38	2g	80	VAL	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	62	TYR	4.2
41	2j	5	ARG	4.2
32	1a	211	U	4.2
7	2H	115	VAL	4.2
1	2A	2805	G	4.2
32	1a	1023	U	4.2
33	2b	187	LEU	4.1
45	2n	49	HIS	4.1
50	2s	6	LYS	4.1
45	1n	2	ALA	4.0
32	1a	978	U	4.0
16	2U	88	ILE	4.0
29	17	48	LYS	4.0
6	2G	48	GLU	4.0
38	1g	77	SER	3.9
34	2c	8	ILE	3.9
40	2i	30	GLY	3.9
32	2a	1000	G	3.9
40	2i	7	THR	3.9
7	2H	103	LEU	3.9
32	2a	982	G	3.9
1	2A	217	A	3.9
38	2g	83	ALA	3.9
1	2A	2813	C	3.8
33	2b	118	LEU	3.8
20	1Y	1	MET	3.8
33	2b	101	MET	3.8
50	2s	8	GLY	3.8
41	1j	97	GLU	3.8
49	2r	66	LEU	3.8
40	2i	20	ARG	3.8
26	14	53	GLU	3.8
34	2c	2	GLY	3.8
50	2s	80	TYR	3.7
34	2c	180	ALA	3.7
19	2X	92	LEU	3.7
8	2I	11	ASN	3.7
6	2G	86	MET	3.7
40	2i	66	ARG	3.7
33	1b	232	PRO	3.7
1	2A	1149	C	3.7
35	2d	49	ARG	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	132	LYS	3.6
40	2i	68	GLY	3.6
33	2b	31	TYR	3.6
34	2c	186	PHE	3.6
32	2a	1510	U	3.6
50	2s	12	ASP	3.6
1	2A	1134	G	3.6
22	20	75	LEU	3.6
34	2c	66	VAL	3.6
41	1j	72	VAL	3.6
1	2A	1554	C	3.6
22	20	76	GLY	3.6
7	2H	95	ARG	3.6
50	2s	24	ALA	3.5
1	2A	1091	A	3.5
26	24	45	GLY	3.5
44	2m	94	ARG	3.5
8	2I	81	VAL	3.5
33	2b	131	PRO	3.5
53	2v	14	A	3.5
7	2H	2	SER	3.5
40	2i	9	ARG	3.5
1	1A	1098	C	3.5
7	2H	107	VAL	3.5
1	1A	2904	C	3.5
6	2G	27	ASN	3.4
19	2X	68	ARG	3.4
26	14	55	ARG	3.4
44	2m	95	GLY	3.4
32	2a	1239	U	3.4
40	2i	61	ALA	3.4
50	2s	34	TRP	3.4
41	1j	4	ILE	3.4
6	1G	51	ARG	3.4
8	2I	107	VAL	3.4
1	1A	2905	U	3.4
8	2I	46	ALA	3.4
8	2I	85	GLU	3.4
14	2S	58	LEU	3.4
40	1i	19	LEU	3.4
33	1b	29	ALA	3.4
32	2a	1024	A	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1120	C	3.4
1	1A	2814	C	3.4
6	2G	28	VAL	3.4
1	2A	2816	G	3.3
33	2b	37	ASN	3.3
6	2G	26	GLN	3.3
32	1a	209	U	3.3
33	2b	228	GLY	3.3
52	2u	6	ARG	3.3
1	2A	2904	C	3.3
50	2s	38	SER	3.3
32	2a	1025	G	3.3
34	1c	81	GLY	3.3
34	2c	179	ARG	3.3
1	2A	1132	G	3.3
26	24	49	PHE	3.2
7	2H	6	ARG	3.2
40	2i	115	GLY	3.2
41	2j	89	ASP	3.2
33	1b	122	PHE	3.2
47	1p	39	TYR	3.2
21	2Z	96	VAL	3.2
33	2b	188	ALA	3.2
41	2j	71	LEU	3.2
44	2m	102	ARG	3.2
1	2A	1130	A	3.2
34	1c	78	GLY	3.2
34	2c	190	ARG	3.2
52	2u	16	GLY	3.2
1	2A	2905	U	3.2
41	2j	40	LEU	3.2
49	2r	85	LEU	3.2
1	2A	2902	G	3.2
11	2P	118	GLY	3.2
32	2a	1026	C	3.2
32	1a	1024	A	3.2
6	2G	19	LEU	3.2
52	2u	17	THR	3.1
49	2r	31	LEU	3.1
50	2s	52	TYR	3.1
7	2H	101	ARG	3.1
33	1b	63	MET	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	2h	122	ARG	3.1
26	14	66	SER	3.1
41	2j	6	ILE	3.1
33	2b	165	VAL	3.1
50	2s	41	VAL	3.1
40	2i	16	ARG	3.1
34	2c	154	SER	3.1
41	2j	27	ALA	3.1
1	2A	678	A	3.1
1	1A	2205	G	3.1
47	1p	41	PRO	3.1
7	2H	114	VAL	3.1
17	2V	72	VAL	3.1
34	1c	206	GLU	3.1
41	1j	85	LEU	3.1
41	1j	90	LEU	3.0
1	1A	1220	G	3.0
1	2A	1089	G	3.0
32	1a	1002	G	3.0
41	2j	65	LEU	3.0
1	1A	2811	A	3.0
34	2c	57	ILE	3.0
52	2u	22	ARG	3.0
41	2j	74	ILE	3.0
50	2s	40	ILE	3.0
32	2a	1268	A	3.0
33	1b	33	TYR	3.0
1	2A	2806	C	3.0
32	2a	986	C	3.0
34	2c	124	ILE	3.0
40	2i	14	VAL	3.0
44	2m	7	VAL	3.0
1	2A	1128	U	3.0
31	29	37	GLY	3.0
38	2g	16	LEU	3.0
41	2j	8	LEU	3.0
34	2c	159	GLY	3.0
41	2j	10	GLY	3.0
50	2s	64	GLU	3.0
32	1a	825	U	3.0
1	2A	2804	G	3.0
41	1j	10	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	103	THR	3.0
21	2Z	125	LEU	2.9
11	2P	116	GLY	2.9
38	2g	79	ARG	2.9
1	1A	1149	C	2.9
45	2n	32	SER	2.9
32	2a	983	A	2.9
33	1b	16	HIS	2.9
32	2a	999	U	2.9
1	2A	2814	C	2.9
32	1a	72	C	2.9
34	1c	207	VAL	2.9
32	2a	1265	G	2.9
40	2i	76	ALA	2.9
1	1A	2813	C	2.9
26	14	52	THR	2.9
34	2c	167	TRP	2.9
34	1c	100	ALA	2.9
40	1i	15	ALA	2.9
38	1g	153	HIS	2.9
26	24	52	THR	2.9
38	2g	81	GLY	2.9
6	2G	17	PRO	2.9
32	1a	707	U	2.9
50	1s	56	GLN	2.9
50	2s	3	ARG	2.9
6	1G	49	ASP	2.9
33	2b	232	PRO	2.9
1	2A	1129	A	2.9
47	1p	19	ILE	2.9
7	2H	123	PHE	2.9
34	2c	77	ILE	2.9
50	2s	49	ILE	2.9
40	1i	8	GLY	2.9
5	2F	15	SER	2.8
47	2p	59	TRP	2.8
34	1c	64	VAL	2.8
1	1A	2804	G	2.8
32	1a	1000	G	2.8
32	2a	1002	G	2.8
42	2k	13	GLN	2.8
32	2a	1022	C	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1268	A	2.8
1	2A	2901	G	2.8
21	2Z	5	LEU	2.8
35	2d	183	GLY	2.8
1	2A	10	G	2.8
41	2j	26	ALA	2.8
49	2r	23	LYS	2.8
32	1a	1027	A	2.8
26	24	67	TYR	2.8
52	1u	18	TYR	2.8
1	2A	697	G	2.8
7	2H	97	ARG	2.8
16	2U	116	ALA	2.8
44	1m	2	ALA	2.8
41	1j	62	HIS	2.8
32	1a	977	C	2.8
44	2m	64	TRP	2.8
1	2A	1101	G	2.8
44	2m	78	ILE	2.8
52	2u	11	GLY	2.8
50	2s	79	THR	2.8
7	2H	102	ALA	2.8
32	1a	88	C	2.8
5	2F	14	PRO	2.8
7	2H	148	ILE	2.8
7	2H	44	VAL	2.8
6	2G	29	TRP	2.7
50	2s	43	GLU	2.7
34	2c	87	LEU	2.7
45	2n	2	ALA	2.7
54	2x	47	U	2.7
40	1i	102	LEU	2.7
26	14	57	GLU	2.7
20	2Y	55	TYR	2.7
39	2h	131	GLY	2.7
32	2a	978	U	2.7
40	2i	17	VAL	2.7
33	1b	123	ALA	2.7
33	1b	124	SER	2.7
14	2S	35	ILE	2.7
33	2b	197	VAL	2.7
11	2P	91	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	211	U	2.7
1	2A	669	C	2.7
32	2a	1184	G	2.7
33	1b	131	PRO	2.7
33	2b	123	ALA	2.7
1	2A	1106	U	2.7
1	1A	695	C	2.7
50	2s	20	LEU	2.7
32	2a	976	G	2.7
14	2S	34	HIS	2.7
33	2b	70	PHE	2.7
40	2i	88	TYR	2.7
8	2I	86	THR	2.7
7	2H	113	VAL	2.7
1	1A	2806	C	2.7
29	27	48	LYS	2.7
34	2c	147	LYS	2.7
19	2X	86	GLY	2.7
32	1a	77	G	2.7
45	2n	36	PHE	2.6
32	1a	983	A	2.6
7	2H	169	VAL	2.6
36	2e	22	GLY	2.6
44	2m	75	ALA	2.6
37	2f	97	PHE	2.6
45	2n	34	TYR	2.6
33	1b	132	LYS	2.6
45	1n	16	PHE	2.6
32	1a	1025	G	2.6
21	2Z	143	GLY	2.6
38	2g	132	GLY	2.6
50	2s	9	VAL	2.6
50	2s	53	ASN	2.6
33	1b	225	ALA	2.6
44	2m	42	ALA	2.6
1	1A	934	C	2.6
1	1A	2206	C	2.6
1	2A	934	C	2.6
33	1b	28	PHE	2.6
32	1a	1239	U	2.6
33	1b	31	TYR	2.6
34	1c	87	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2B	119	G	2.6
32	1a	984	A	2.6
38	2g	84	ASN	2.6
34	1c	39	ILE	2.6
40	2i	87	GLN	2.6
41	1j	71	LEU	2.6
45	2n	39	LEU	2.6
41	2j	49	VAL	2.6
50	1s	50	ALA	2.6
1	2A	1090	A	2.6
32	2a	984	A	2.6
32	2a	1023	U	2.6
26	14	54	GLY	2.6
43	2l	64	TYR	2.6
7	2H	93	GLY	2.6
34	1c	205	GLY	2.6
40	2i	8	GLY	2.6
40	2i	102	LEU	2.6
1	2A	2206	C	2.6
32	1a	1026	C	2.6
33	2b	218	ALA	2.6
11	2P	122	PRO	2.6
38	2g	54	THR	2.5
1	2A	9	G	2.5
7	2H	96	ALA	2.5
16	2U	117	GLN	2.5
47	2p	60	LEU	2.5
40	2i	95	LYS	2.5
41	2j	68	HIS	2.5
1	2A	1553	A	2.5
1	1A	2805	G	2.5
38	1g	84	ASN	2.5
46	1o	19	PRO	2.5
21	2Z	133	ILE	2.5
8	2I	77	LEU	2.5
21	2Z	175	VAL	2.5
14	2S	45	GLY	2.5
20	2Y	90	LEU	2.5
49	1r	31	LEU	2.5
32	1a	210	U	2.5
33	2b	152	PHE	2.5
7	1H	2	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	24	46	GLN	2.5
33	2b	201	ILE	2.5
41	2j	38	ILE	2.5
1	1A	2812	G	2.5
50	1s	61	TYR	2.5
25	23	59	VAL	2.5
33	2b	97	TRP	2.5
20	2Y	57	GLN	2.5
34	1c	193	TYR	2.5
38	2g	86	GLN	2.5
40	1i	36	TYR	2.5
32	2a	977	C	2.5
35	1d	175	SER	2.5
31	29	13	LYS	2.5
8	2l	14	ASP	2.5
47	1p	42	ARG	2.5
40	2i	27	THR	2.5
51	2t	41	ILE	2.5
33	2b	150	SER	2.5
40	1i	98	PRO	2.5
40	1i	6	GLY	2.5
1	2A	2125	G	2.5
11	2P	123	LEU	2.5
50	2s	35	SER	2.4
50	2s	76	PRO	2.4
32	2a	88	C	2.4
32	1a	999	U	2.4
49	2r	22	VAL	2.4
21	2Z	164	ALA	2.4
6	2G	137	GLU	2.4
1	2A	1104	G	2.4
7	2H	110	SER	2.4
40	2i	80	GLY	2.4
44	2m	92	HIS	2.4
1	2A	1150	U	2.4
14	2S	52	SER	2.4
22	20	69	PHE	2.4
35	1d	133	VAL	2.4
1	2A	1092	G	2.4
34	2c	160	ALA	2.4
25	23	60	GLU	2.4
50	2s	47	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	2P	85	LEU	2.4
55	2z	12	PRO	2.4
36	2e	148	VAL	2.4
7	2H	116	GLU	2.4
1	2A	5	A	2.4
1	2A	2817	U	2.4
33	2b	124	SER	2.4
52	1u	15	ARG	2.4
44	2m	40	ASN	2.4
50	2s	23	ASN	2.4
1	2A	1088	C	2.4
32	1a	208	C	2.4
32	1a	1022	C	2.4
32	1a	212	G	2.4
32	2a	1159	G	2.4
6	2G	25	TYR	2.4
50	1s	39	THR	2.4
4	2E	1	MET	2.4
1	2A	680	C	2.4
3	2D	270	ILE	2.4
11	2P	100	LEU	2.4
41	1j	6	ILE	2.4
46	2o	87	ILE	2.4
38	2g	113	GLU	2.4
6	1G	50	ALA	2.4
40	1i	46	ALA	2.4
32	2a	998	C	2.4
33	1b	136	VAL	2.4
1	2A	2330	G	2.4
14	2S	55	ALA	2.4
20	2Y	91	GLU	2.3
39	2h	128	GLY	2.3
45	2n	38	GLY	2.3
6	2G	49	ASP	2.3
33	1b	101	MET	2.3
1	1A	679	G	2.3
11	2P	88	LEU	2.3
32	2a	1207	A	2.3
35	1d	174	LEU	2.3
35	2d	146	ILE	2.3
38	1g	120	ILE	2.3
50	2s	16	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	1n	8	GLU	2.3
40	2i	37	PHE	2.3
21	2Z	50	GLN	2.3
34	1c	201	TYR	2.3
6	1G	78	SER	2.3
41	2j	98	ILE	2.3
47	2p	19	ILE	2.3
32	1a	985	C	2.3
52	2u	18	TYR	2.3
37	2f	89	MET	2.3
1	2A	1102	A	2.3
1	2A	1136	G	2.3
2	2B	118	G	2.3
6	1G	75	LYS	2.3
23	2l	29	GLY	2.3
32	1a	1121	G	2.3
46	1o	17	ARG	2.3
6	2G	2	PRO	2.3
43	1l	64	TYR	2.3
21	2Z	2	GLU	2.3
45	2n	8	GLU	2.3
34	2c	39	ILE	2.3
34	1c	158	GLY	2.3
50	1s	19	VAL	2.3
1	1A	682	G	2.3
32	2a	1001	G	2.3
32	2a	1021	C	2.3
45	2n	35	ARG	2.3
48	2q	10	VAL	2.3
32	2a	1114	G	2.3
32	2a	1147	G	2.3
33	2b	222	ILE	2.3
39	2h	127	LEU	2.3
47	2p	7	ALA	2.3
45	2n	29	ARG	2.3
50	1s	47	HIS	2.3
12	2Q	60	ARG	2.3
33	2b	83	MET	2.3
14	2S	46	VAL	2.3
7	2H	8	PRO	2.3
11	2P	1	MET	2.3
32	1a	73	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	37	PHE	2.3
1	2A	679	G	2.3
45	2n	18	VAL	2.2
50	2s	45	VAL	2.2
33	1b	222	ILE	2.2
34	2c	185	GLY	2.2
34	2c	194	GLY	2.2
42	2k	42	TRP	2.2
43	1l	28	LYS	2.2
39	1h	62	TYR	2.2
51	1t	55	ILE	2.2
11	2P	92	GLU	2.2
38	1g	56	GLN	2.2
49	2r	56	THR	2.2
33	1b	142	LEU	2.2
42	2k	90	GLY	2.2
40	2i	125	TYR	2.2
23	1l	2	SER	2.2
7	2H	128	PRO	2.2
21	2Z	155	LEU	2.2
34	2c	205	GLY	2.2
41	1j	96	ILE	2.2
49	2r	24	ALA	2.2
38	2g	18	TYR	2.2
1	1A	1097	C	2.2
1	2A	1125	C	2.2
14	2S	93	LYS	2.2
1	2A	1112	A	2.2
1	2A	1142	U	2.2
35	1d	23	GLY	2.2
40	2i	64	THR	2.2
20	2Y	48	ALA	2.2
1	2A	2121	G	2.2
7	2H	164	TYR	2.2
34	2c	197	GLY	2.2
50	2s	13	ASP	2.2
11	2P	90	ARG	2.2
30	28	21	LYS	2.2
33	1b	214	ILE	2.2
40	1i	106	ALA	2.2
40	2i	83	ARG	2.2
50	1s	40	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	94	TYR	2.2
33	2b	227	GLY	2.2
42	2k	96	ARG	2.2
50	2s	25	LYS	2.2
8	2I	19	VAL	2.2
34	2c	103	VAL	2.2
6	2G	72	ARG	2.2
1	1A	1150	U	2.2
1	2A	1071	U	2.2
1	2A	1127	U	2.2
8	2I	79	ILE	2.2
8	2I	100	ALA	2.2
38	2g	152	ALA	2.2
41	2j	18	ALA	2.2
14	2S	31	SER	2.2
45	2n	60	SER	2.2
49	1r	25	THR	2.2
39	2h	93	VAL	2.2
47	2p	39	TYR	2.2
20	2Y	2	ARG	2.2
33	1b	30	ARG	2.2
1	2A	33	C	2.2
1	2A	1135	U	2.2
32	2a	1266	C	2.2
33	2b	133	LYS	2.2
38	1g	82	GLY	2.1
38	2g	117	ALA	2.1
1	2A	6	G	2.1
45	1n	17	LYS	2.1
52	2u	24	ARG	2.1
38	1g	132	GLY	2.1
33	2b	121	LEU	2.1
41	2j	88	LEU	2.1
1	2A	1111	U	2.1
49	1r	24	ALA	2.1
41	1j	40	LEU	2.1
1	2A	1143	A	2.1
21	2Z	57	ILE	2.1
46	1o	6	GLU	2.1
41	2j	72	VAL	2.1
48	2q	8	GLY	2.1
41	2j	55	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	1p	38	TYR	2.1
32	2a	826	C	2.1
49	1r	52	PRO	2.1
44	2m	60	VAL	2.1
49	2r	21	LYS	2.1
14	2S	5	THR	2.1
44	2m	48	LEU	2.1
49	2r	46	GLU	2.1
33	1b	207	ALA	2.1
32	2a	1231	C	2.1
40	2i	65	VAL	2.1
38	2g	4	ARG	2.1
8	2I	72	LEU	2.1
20	2Y	89	PHE	2.1
45	1n	13	THR	2.1
51	2t	24	LEU	2.1
33	1b	195	ASP	2.1
2	2B	86	G	2.1
1	2A	1115	A	2.1
8	2I	92	VAL	2.1
32	2a	1432	A	2.1
21	2Z	65	GLN	2.1
1	1A	8	U	2.1
33	2b	161	ALA	2.1
20	2Y	58	GLY	2.1
25	23	47	VAL	2.1
32	2a	79	G	2.1
34	1c	98	ASN	2.1
6	2G	35	GLU	2.1
1	2A	300	C	2.1
1	2A	1110	U	2.1
1	2A	2903	U	2.1
29	27	47	ARG	2.1
29	27	46	VAL	2.1
33	2b	229	VAL	2.1
1	1A	2121	G	2.1
1	2A	1103	G	2.1
1	2A	2207	G	2.1
53	2v	18	G	2.1
1	2A	1131	A	2.0
14	2S	84	GLN	2.0
32	2a	985	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	4	SER	2.0
3	2D	273	ARG	2.0
32	1a	86	U	2.0
46	2o	86	GLY	2.0
50	2s	63	THR	2.0
6	2G	80	PHE	2.0
42	1k	13	GLN	2.0
1	2A	681	G	2.0
32	2a	1243	A	2.0
33	1b	41	ILE	2.0
3	2D	275	LYS	2.0
33	2b	105	PHE	2.0
33	1b	201	ILE	2.0
42	2k	43	SER	2.0
45	2n	11	LYS	2.0
1	2A	2124	C	2.0
40	2i	24	GLY	2.0
44	2m	6	GLY	2.0
44	2m	76	ALA	2.0
1	1A	1099	A	2.0
40	1i	7	THR	2.0
34	1c	79	ARG	2.0
40	2i	18	PHE	2.0
7	2H	105	LEU	2.0
50	2s	28	LYS	2.0
33	1b	19	HIS	2.0
41	2j	62	HIS	2.0
44	2m	38	GLY	2.0
46	2o	6	GLU	2.0
50	2s	31	ILE	2.0
35	1d	208	SER	2.0
1	1A	2204	C	2.0
32	1a	87	C	2.0
38	2g	85	TYR	2.0
32	2a	78	G	2.0
25	23	35	ARG	2.0
34	1c	179	ARG	2.0
40	1i	26	VAL	2.0
41	2j	34	VAL	2.0
25	23	26	LEU	2.0
26	24	8	LYS	2.0
20	2Y	43	ASN	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	2x	55	20/21	0.88	0.17	62,68,78,88	0
54	5MC	2x	32	21/22	0.91	0.25	68,80,88,91	0
54	5MU	2x	54	21/22	0.93	0.20	72,76,86,101	0
54	5MU	1x	54	21/22	0.94	0.17	50,67,76,78	0
54	5MC	1x	32	21/22	0.94	0.20	51,62,76,86	0
54	PSU	1x	55	20/21	0.94	0.18	57,65,79,80	0
54	4SU	2x	8	20/21	0.95	0.14	57,78,89,92	0
54	4SU	1x	8	20/21	0.96	0.17	47,65,79,80	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	1A	3298	1/1	0.35	0.29	81,81,81,81	0
56	MG	1A	3517	1/1	0.35	0.31	69,69,69,69	0
56	MG	1A	3901	1/1	0.36	0.59	86,86,86,86	0
56	MG	1F	304	1/1	0.41	0.57	73,73,73,73	0
56	MG	2A	3074	1/1	0.52	0.21	54,54,54,54	0
56	MG	2a	3006	1/1	0.54	0.14	77,77,77,77	0
56	MG	1a	1639	1/1	0.55	0.55	77,77,77,77	0
56	MG	2A	3093	1/1	0.55	0.55	57,57,57,57	0
56	MG	2G	3001	1/1	0.55	0.22	56,56,56,56	0
56	MG	1a	1756	1/1	0.58	0.49	58,58,58,58	0
56	MG	1A	3411	1/1	0.58	0.41	51,51,51,51	0
56	MG	1a	1645	1/1	0.59	0.40	78,78,78,78	0
56	MG	1A	4041	1/1	0.61	0.15	57,57,57,57	0
56	MG	14	502	1/1	0.61	0.25	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	3230	1/1	0.62	0.30	47,47,47,47	0
56	MG	1A	3548	1/1	0.62	0.17	72,72,72,72	0
56	MG	2a	3031	1/1	0.62	0.23	88,88,88,88	0
56	MG	1a	1802	1/1	0.63	0.27	68,68,68,68	0
56	MG	1A	4076	1/1	0.64	0.30	72,72,72,72	0
56	MG	1a	1757	1/1	0.64	0.42	69,69,69,69	0
56	MG	1A	3146	1/1	0.64	0.24	62,62,62,62	0
56	MG	2a	3153	1/1	0.65	0.17	92,92,92,92	0
56	MG	2a	3122	1/1	0.65	0.39	71,71,71,71	0
56	MG	1A	3544	1/1	0.66	0.39	61,61,61,61	0
56	MG	1A	3320	1/1	0.66	0.53	70,70,70,70	0
56	MG	1A	3369	1/1	0.66	0.39	67,67,67,67	0
57	ZN	24	501	1/1	0.67	0.07	133,133,133,133	0
56	MG	2a	3088	1/1	0.67	0.07	76,76,76,76	0
56	MG	2A	3124	1/1	0.67	0.35	65,65,65,65	0
56	MG	2a	3138	1/1	0.67	0.45	81,81,81,81	0
56	MG	2A	3194	1/1	0.68	0.25	56,56,56,56	0
56	MG	1A	3897	1/1	0.68	0.28	60,60,60,60	0
56	MG	2A	3197	1/1	0.68	0.15	63,63,63,63	0
56	MG	2a	3206	1/1	0.68	0.17	56,56,56,56	0
56	MG	2a	3053	1/1	0.68	0.16	99,99,99,99	0
56	MG	1A	3333	1/1	0.69	0.53	57,57,57,57	0
56	MG	1a	1851	1/1	0.69	0.12	56,56,56,56	0
56	MG	1A	3511	1/1	0.69	0.38	55,55,55,55	0
56	MG	2A	3243	1/1	0.69	0.13	69,69,69,69	0
56	MG	1A	3935	1/1	0.69	0.20	52,52,52,52	0
56	MG	2A	3171	1/1	0.69	0.32	49,49,49,49	0
56	MG	1A	3699	1/1	0.70	0.28	58,58,58,58	0
56	MG	2A	3065	1/1	0.70	0.17	55,55,55,55	0
56	MG	2A	3081	1/1	0.71	0.24	54,54,54,54	0
56	MG	2a	3150	1/1	0.71	0.28	76,76,76,76	0
56	MG	2A	3432	1/1	0.71	0.21	55,55,55,55	0
56	MG	1A	3502	1/1	0.72	0.15	70,70,70,70	0
56	MG	2A	3224	1/1	0.72	0.34	73,73,73,73	0
56	MG	1a	1823	1/1	0.72	0.26	71,71,71,71	0
56	MG	1A	3138	1/1	0.72	0.29	48,48,48,48	0
56	MG	1a	1619	1/1	0.72	0.15	75,75,75,75	0
56	MG	2a	3149	1/1	0.73	0.18	63,63,63,63	0
56	MG	1A	3016	1/1	0.73	0.16	56,56,56,56	0
56	MG	1A	3116	1/1	0.73	0.23	52,52,52,52	0
56	MG	2l	3002	1/1	0.73	0.27	68,68,68,68	0
56	MG	1Z	301	1/1	0.73	0.12	94,94,94,94	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	1T	206	1/1	0.73	0.43	76,76,76,76	0
56	MG	2a	3001	1/1	0.73	0.48	62,62,62,62	0
56	MG	1A	3237	1/1	0.73	0.15	58,58,58,58	0
56	MG	2a	3043	1/1	0.73	0.43	78,78,78,78	0
56	MG	2A	3104	1/1	0.73	0.17	59,59,59,59	0
56	MG	1a	1796	1/1	0.73	0.08	85,85,85,85	0
56	MG	1A	3326	1/1	0.73	0.17	62,62,62,62	0
56	MG	1A	3384	1/1	0.73	0.50	59,59,59,59	0
56	MG	1A	3218	1/1	0.74	0.30	58,58,58,58	0
56	MG	2Q	3005	1/1	0.74	0.31	54,54,54,54	0
56	MG	2A	3483	1/1	0.74	0.12	72,72,72,72	0
56	MG	2B	202	1/1	0.74	0.15	55,55,55,55	0
56	MG	1H	3002	1/1	0.74	0.25	62,62,62,62	0
56	MG	1a	1750	1/1	0.74	0.34	69,69,69,69	0
56	MG	11	102	1/1	0.74	0.24	65,65,65,65	0
56	MG	12	3001	1/1	0.74	0.44	57,57,57,57	0
56	MG	2a	3039	1/1	0.75	0.54	67,67,67,67	0
56	MG	2A	3184	1/1	0.75	0.28	45,45,45,45	0
56	MG	1A	4027	1/1	0.75	0.55	62,62,62,62	0
56	MG	1A	3012	1/1	0.75	0.23	66,66,66,66	0
56	MG	2a	3049	1/1	0.75	0.24	79,79,79,79	0
56	MG	2a	3068	1/1	0.75	0.37	56,56,56,56	0
56	MG	2A	3380	1/1	0.75	0.12	59,59,59,59	0
56	MG	1A	4058	1/1	0.75	0.33	48,48,48,48	0
56	MG	2A	3233	1/1	0.75	0.11	52,52,52,52	0
56	MG	1A	3478	1/1	0.76	0.31	49,49,49,49	0
56	MG	2a	3254	1/1	0.76	0.49	76,76,76,76	0
56	MG	1a	1615	1/1	0.76	0.32	66,66,66,66	0
56	MG	1A	3319	1/1	0.76	0.10	75,75,75,75	0
56	MG	1a	1699	1/1	0.76	0.20	58,58,58,58	0
56	MG	2a	3022	1/1	0.76	0.16	77,77,77,77	0
56	MG	1a	1752	1/1	0.76	0.17	61,61,61,61	0
56	MG	2A	3071	1/1	0.76	0.26	46,46,46,46	0
56	MG	1a	1786	1/1	0.77	0.19	49,49,49,49	0
56	MG	1A	3916	1/1	0.77	0.69	45,45,45,45	0
56	MG	2a	3054	1/1	0.77	0.08	96,96,96,96	0
56	MG	1A	3593	1/1	0.77	0.26	62,62,62,62	0
56	MG	1A	3318	1/1	0.77	0.17	65,65,65,65	0
56	MG	2a	3151	1/1	0.77	0.11	97,97,97,97	0
56	MG	1a	1628	1/1	0.77	0.29	57,57,57,57	0
56	MG	1T	202	1/1	0.77	0.27	51,51,51,51	0
56	MG	1A	3324	1/1	0.77	0.18	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	2a	3133	1/1	0.77	0.14	63,63,63,63	0
56	MG	2a	3044	1/1	0.77	0.12	71,71,71,71	0
56	MG	1A	3941	1/1	0.77	0.19	60,60,60,60	0
56	MG	1A	3007	1/1	0.78	0.63	73,73,73,73	0
56	MG	1B	205	1/1	0.78	0.16	56,56,56,56	0
56	MG	2A	3488	1/1	0.78	0.10	69,69,69,69	0
56	MG	2x	104	1/1	0.78	0.12	84,84,84,84	0
56	MG	2a	3191	1/1	0.78	0.35	88,88,88,88	0
56	MG	1A	3601	1/1	0.78	0.20	36,36,36,36	0
56	MG	2A	3114	1/1	0.78	0.26	50,50,50,50	0
56	MG	1A	3086	1/1	0.78	0.40	52,52,52,52	0
56	MG	2a	3130	1/1	0.78	0.26	50,50,50,50	0
56	MG	1a	1820	1/1	0.78	0.09	79,79,79,79	0
56	MG	1A	4054	1/1	0.78	0.43	69,69,69,69	0
56	MG	1A	3261	1/1	0.78	0.27	68,68,68,68	0
56	MG	2a	3164	1/1	0.78	0.10	80,80,80,80	0
56	MG	1A	3087	1/1	0.78	0.21	45,45,45,45	0
56	MG	1a	1816	1/1	0.78	0.24	76,76,76,76	0
56	MG	2a	3101	1/1	0.78	0.38	77,77,77,77	0
56	MG	2A	3261	1/1	0.78	0.13	43,43,43,43	0
56	MG	1X	3001	1/1	0.79	0.38	56,56,56,56	0
56	MG	2a	3051	1/1	0.79	0.20	91,91,91,91	0
56	MG	2a	3047	1/1	0.79	0.14	79,79,79,79	0
56	MG	2A	3035	1/1	0.79	0.13	54,54,54,54	0
56	MG	1A	3856	1/1	0.79	0.28	55,55,55,55	0
56	MG	2D	302	1/1	0.79	0.25	57,57,57,57	0
56	MG	2X	8001	1/1	0.79	0.16	45,45,45,45	0
56	MG	1a	1716	1/1	0.79	0.29	54,54,54,54	0
56	MG	2A	3206	1/1	0.79	0.26	50,50,50,50	0
56	MG	2a	3014	1/1	0.79	0.30	64,64,64,64	0
56	MG	1A	3804	1/1	0.79	0.11	66,66,66,66	0
56	MG	1A	3433	1/1	0.79	0.21	51,51,51,51	0
56	MG	1A	4016	1/1	0.79	0.21	77,77,77,77	0
56	MG	2A	3040	1/1	0.79	0.12	57,57,57,57	0
56	MG	1A	3094	1/1	0.80	0.34	54,54,54,54	0
56	MG	1a	1798	1/1	0.80	0.29	71,71,71,71	0
56	MG	1a	1686	1/1	0.80	0.12	62,62,62,62	0
56	MG	2A	3204	1/1	0.80	0.30	53,53,53,53	0
56	MG	1A	3289	1/1	0.80	0.18	61,61,61,61	0
56	MG	2q	201	1/1	0.80	0.13	58,58,58,58	0
56	MG	1a	1671	1/1	0.80	0.21	77,77,77,77	0
56	MG	1A	3335	1/1	0.80	0.75	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	1A	3471	1/1	0.80	0.23	55,55,55,55	0
56	MG	1a	1751	1/1	0.80	0.15	64,64,64,64	0
56	MG	2a	3005	1/1	0.80	0.36	72,72,72,72	0
56	MG	1a	1668	1/1	0.80	0.21	63,63,63,63	0
56	MG	2a	3072	1/1	0.80	0.21	65,65,65,65	0
56	MG	1a	1800	1/1	0.80	0.14	79,79,79,79	0
56	MG	1A	3242	1/1	0.80	0.42	67,67,67,67	0
56	MG	1A	3632	1/1	0.80	0.17	67,67,67,67	0
56	MG	2A	3252	1/1	0.80	0.15	43,43,43,43	0
56	MG	2t	201	1/1	0.80	0.26	58,58,58,58	0
56	MG	1A	3493	1/1	0.80	0.24	64,64,64,64	0
56	MG	2a	3017	1/1	0.80	0.26	61,61,61,61	0
56	MG	1A	3248	1/1	0.80	0.13	47,47,47,47	0
56	MG	1A	3847	1/1	0.81	0.16	55,55,55,55	0
56	MG	2e	3001	1/1	0.81	0.46	74,74,74,74	0
56	MG	1A	3383	1/1	0.81	0.17	67,67,67,67	0
56	MG	1A	3491	1/1	0.81	0.15	54,54,54,54	0
56	MG	1A	3524	1/1	0.81	0.15	68,68,68,68	0
56	MG	1A	3644	1/1	0.81	0.15	45,45,45,45	0
56	MG	2A	3256	1/1	0.81	0.14	43,43,43,43	0
56	MG	1A	3355	1/1	0.81	0.09	64,64,64,64	0
56	MG	1n	102	1/1	0.81	0.17	53,53,53,53	0
56	MG	1H	3003	1/1	0.81	0.30	65,65,65,65	0
56	MG	1A	3456	1/1	0.81	0.17	71,71,71,71	0
56	MG	1A	3027	1/1	0.81	0.37	47,47,47,47	0
56	MG	1a	1763	1/1	0.81	0.39	55,55,55,55	0
56	MG	1A	3494	1/1	0.81	0.57	68,68,68,68	0
56	MG	1A	3366	1/1	0.81	0.16	42,42,42,42	0
56	MG	1A	3019	1/1	0.81	0.45	46,46,46,46	0
56	MG	1B	210	1/1	0.81	0.24	56,56,56,56	0
56	MG	1E	304	1/1	0.81	0.29	65,65,65,65	0
56	MG	2A	3087	1/1	0.81	0.20	53,53,53,53	0
56	MG	1a	1825	1/1	0.81	0.31	73,73,73,73	0
56	MG	1A	3525	1/1	0.81	0.18	74,74,74,74	0
56	MG	2a	3230	1/1	0.81	0.11	67,67,67,67	0
56	MG	2A	3116	1/1	0.81	0.16	54,54,54,54	0
56	MG	1A	3828	1/1	0.81	0.12	49,49,49,49	0
56	MG	1A	3512	1/1	0.81	0.33	50,50,50,50	0
56	MG	10	106	1/1	0.81	0.19	54,54,54,54	0
56	MG	2A	3288	1/1	0.81	0.13	41,41,41,41	0
56	MG	1A	3011	1/1	0.81	0.23	47,47,47,47	0
56	MG	2A	3102	1/1	0.81	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	1A	4088	1/1	0.81	0.53	45,45,45,45	0
56	MG	1m	201	1/1	0.81	0.37	95,95,95,95	0
56	MG	1a	1700	1/1	0.81	0.28	60,60,60,60	0
56	MG	2x	106	1/1	0.81	0.20	82,82,82,82	0
56	MG	1A	3484	1/1	0.81	0.11	45,45,45,45	0
56	MG	1A	3123	1/1	0.82	0.25	49,49,49,49	0
56	MG	2a	3114	1/1	0.82	0.27	77,77,77,77	0
56	MG	2A	3131	1/1	0.82	0.11	56,56,56,56	0
56	MG	1a	1784	1/1	0.82	0.29	80,80,80,80	0
56	MG	2a	3226	1/1	0.82	0.08	77,77,77,77	0
56	MG	2A	3498	1/1	0.82	0.37	69,69,69,69	0
56	MG	1A	3404	1/1	0.82	0.34	54,54,54,54	0
56	MG	1A	3417	1/1	0.82	0.18	76,76,76,76	0
56	MG	2a	3175	1/1	0.82	0.15	66,66,66,66	0
56	MG	2A	3340	1/1	0.82	0.29	52,52,52,52	0
56	MG	2A	3467	1/1	0.82	0.22	47,47,47,47	0
56	MG	2A	3451	1/1	0.82	0.07	59,59,59,59	0
56	MG	1q	202	1/1	0.82	0.25	53,53,53,53	0
56	MG	1a	1636	1/1	0.82	0.72	53,53,53,53	0
56	MG	2a	3217	1/1	0.82	0.46	68,68,68,68	0
56	MG	1a	1653	1/1	0.82	0.18	56,56,56,56	0
57	ZN	2n	501	1/1	0.82	0.07	110,110,110,110	0
56	MG	1A	3448	1/1	0.82	0.19	56,56,56,56	0
56	MG	1A	3119	1/1	0.82	0.28	59,59,59,59	0
56	MG	1A	3759	1/1	0.82	0.10	68,68,68,68	0
56	MG	1B	212	1/1	0.82	0.38	59,59,59,59	0
56	MG	2a	3058	1/1	0.82	0.29	66,66,66,66	0
56	MG	2a	3173	1/1	0.82	0.13	43,43,43,43	0
56	MG	1a	1602	1/1	0.82	0.24	61,61,61,61	0
56	MG	1A	3174	1/1	0.82	0.13	47,47,47,47	0
56	MG	1a	1738	1/1	0.82	0.24	73,73,73,73	0
56	MG	2A	3186	1/1	0.82	0.22	59,59,59,59	0
56	MG	1a	1629	1/1	0.82	0.11	63,63,63,63	0
56	MG	2a	3137	1/1	0.82	0.17	62,62,62,62	0
56	MG	1A	3435	1/1	0.83	0.13	66,66,66,66	0
56	MG	2a	3202	1/1	0.83	0.15	52,52,52,52	0
56	MG	1a	1852	1/1	0.83	0.21	82,82,82,82	0
56	MG	2A	3246	1/1	0.83	0.14	55,55,55,55	0
56	MG	1A	3814	1/1	0.83	0.16	49,49,49,49	0
56	MG	1A	3969	1/1	0.83	0.18	77,77,77,77	0
56	MG	2a	3038	1/1	0.83	0.33	58,58,58,58	0
56	MG	2a	3033	1/1	0.83	0.52	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	3125	1/1	0.83	0.21	52,52,52,52	0
56	MG	2A	3028	1/1	0.83	0.20	53,53,53,53	0
56	MG	1A	3510	1/1	0.83	0.21	46,46,46,46	0
56	MG	1a	1806	1/1	0.83	0.20	51,51,51,51	0
56	MG	1a	1773	1/1	0.83	0.54	77,77,77,77	0
56	MG	1A	3387	1/1	0.83	0.18	54,54,54,54	0
56	MG	2A	3435	1/1	0.83	0.15	46,46,46,46	0
56	MG	2A	3205	1/1	0.83	0.20	43,43,43,43	0
56	MG	2A	3007	1/1	0.83	0.49	77,77,77,77	0
56	MG	1a	1649	1/1	0.83	0.21	59,59,59,59	0
56	MG	2A	3505	1/1	0.83	0.18	50,50,50,50	0
56	MG	1A	3390	1/1	0.83	0.13	52,52,52,52	0
56	MG	1a	1742	1/1	0.83	0.21	68,68,68,68	0
56	MG	1A	3402	1/1	0.83	0.44	60,60,60,60	0
56	MG	1A	3020	1/1	0.83	0.24	40,40,40,40	0
56	MG	1a	1640	1/1	0.83	0.22	78,78,78,78	0
56	MG	1A	3451	1/1	0.83	0.45	66,66,66,66	0
56	MG	2A	3392	1/1	0.83	0.17	55,55,55,55	0
56	MG	1A	3513	1/1	0.83	0.30	59,59,59,59	0
56	MG	2a	3055	1/1	0.83	0.21	81,81,81,81	0
56	MG	1A	3546	1/1	0.83	0.10	66,66,66,66	0
56	MG	2A	3476	1/1	0.83	0.33	66,66,66,66	0
56	MG	1A	3074	1/1	0.83	0.34	63,63,63,63	0
56	MG	1A	4083	1/1	0.83	0.24	65,65,65,65	0
56	MG	1x	108	1/1	0.83	0.23	49,49,49,49	0
56	MG	1A	3974	1/1	0.83	0.46	59,59,59,59	0
56	MG	2a	3229	1/1	0.83	0.21	57,57,57,57	0
56	MG	1A	3376	1/1	0.83	0.25	49,49,49,49	0
56	MG	2A	3436	1/1	0.83	0.15	44,44,44,44	0
56	MG	1A	3084	1/1	0.83	0.28	53,53,53,53	0
56	MG	1A	3540	1/1	0.83	0.47	48,48,48,48	0
56	MG	1A	3499	1/1	0.83	0.24	64,64,64,64	0
56	MG	1A	3162	1/1	0.84	0.40	38,38,38,38	0
56	MG	1a	1827	1/1	0.84	0.28	68,68,68,68	0
56	MG	2A	3062	1/1	0.84	0.25	46,46,46,46	0
56	MG	1A	3024	1/1	0.84	0.38	56,56,56,56	0
56	MG	2A	3443	1/1	0.84	0.15	63,63,63,63	0
56	MG	1A	3193	1/1	0.84	0.14	53,53,53,53	0
56	MG	1A	4044	1/1	0.84	0.36	44,44,44,44	0
56	MG	1r	3002	1/1	0.84	0.13	70,70,70,70	0
56	MG	1a	1791	1/1	0.84	0.17	82,82,82,82	0
56	MG	1A	3042	1/1	0.84	0.25	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	3274	1/1	0.84	0.22	37,37,37,37	0
56	MG	1A	3093	1/1	0.84	0.19	48,48,48,48	0
56	MG	1A	3914	1/1	0.84	0.21	41,41,41,41	0
56	MG	1A	4072	1/1	0.84	0.18	48,48,48,48	0
56	MG	2a	3076	1/1	0.84	0.47	65,65,65,65	0
56	MG	1a	1748	1/1	0.84	0.41	55,55,55,55	0
56	MG	1a	1792	1/1	0.84	0.17	92,92,92,92	0
56	MG	2A	3262	1/1	0.84	0.11	53,53,53,53	0
56	MG	1A	3194	1/1	0.84	0.19	39,39,39,39	0
56	MG	1A	3103	1/1	0.84	0.44	32,32,32,32	0
56	MG	2q	203	1/1	0.84	0.24	53,53,53,53	0
56	MG	2A	3445	1/1	0.84	0.26	74,74,74,74	0
56	MG	1A	3426	1/1	0.84	0.14	54,54,54,54	0
56	MG	18	3001	1/1	0.84	0.38	50,50,50,50	0
56	MG	1A	3439	1/1	0.84	0.17	50,50,50,50	0
56	MG	1A	3436	1/1	0.84	0.26	51,51,51,51	0
56	MG	1e	201	1/1	0.84	0.19	66,66,66,66	0
56	MG	1a	1809	1/1	0.84	0.25	54,54,54,54	0
56	MG	1A	3031	1/1	0.84	0.24	60,60,60,60	0
56	MG	1a	1908	1/1	0.84	0.07	53,53,53,53	0
56	MG	1A	3896	1/1	0.84	0.09	72,72,72,72	0
56	MG	1P	204	1/1	0.84	0.16	61,61,61,61	0
56	MG	2a	3147	1/1	0.85	0.25	68,68,68,68	0
56	MG	2a	3212	1/1	0.85	0.18	46,46,46,46	0
56	MG	1A	3090	1/1	0.85	0.23	47,47,47,47	0
56	MG	1A	3128	1/1	0.85	0.22	50,50,50,50	0
56	MG	2A	3433	1/1	0.85	0.26	43,43,43,43	0
56	MG	23	101	1/1	0.85	0.26	50,50,50,50	0
56	MG	2A	3314	1/1	0.85	0.11	43,43,43,43	0
56	MG	2A	3554	1/1	0.85	0.18	59,59,59,59	0
56	MG	1a	1696	1/1	0.85	0.12	48,48,48,48	0
56	MG	1a	1605	1/1	0.85	0.13	68,68,68,68	0
56	MG	2D	303	1/1	0.85	0.34	45,45,45,45	0
56	MG	1A	3873	1/1	0.85	0.20	41,41,41,41	0
56	MG	2a	3162	1/1	0.85	0.15	79,79,79,79	0
56	MG	1A	3014	1/1	0.85	0.10	55,55,55,55	0
56	MG	1A	3907	1/1	0.85	0.36	50,50,50,50	0
56	MG	1A	4038	1/1	0.85	0.13	54,54,54,54	0
56	MG	1A	3446	1/1	0.85	0.18	58,58,58,58	0
56	MG	2a	3019	1/1	0.85	0.31	72,72,72,72	0
56	MG	1A	3083	1/1	0.85	0.13	45,45,45,45	0
56	MG	1a	1764	1/1	0.85	0.16	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	2a	3145	1/1	0.85	0.12	95,95,95,95	0
56	MG	1a	1755	1/1	0.85	0.22	57,57,57,57	0
56	MG	1A	3509	1/1	0.85	0.29	68,68,68,68	0
56	MG	1A	3770	1/1	0.85	0.10	50,50,50,50	0
56	MG	2B	210	1/1	0.85	0.34	65,65,65,65	0
56	MG	1B	208	1/1	0.85	0.27	63,63,63,63	0
56	MG	1a	1899	1/1	0.85	0.47	64,64,64,64	0
56	MG	1A	3554	1/1	0.85	0.18	65,65,65,65	0
56	MG	1a	1903	1/1	0.85	0.24	56,56,56,56	0
56	MG	2B	204	1/1	0.85	0.37	65,65,65,65	0
56	MG	1A	3317	1/1	0.85	0.21	63,63,63,63	0
56	MG	1A	3101	1/1	0.85	0.18	50,50,50,50	0
56	MG	2a	3124	1/1	0.85	0.11	62,62,62,62	0
56	MG	1H	3004	1/1	0.85	0.24	66,66,66,66	0
56	MG	1A	4047	1/1	0.85	0.23	47,47,47,47	0
56	MG	1A	3306	1/1	0.85	0.66	69,69,69,69	0
56	MG	1a	1693	1/1	0.85	0.10	53,53,53,53	0
56	MG	2a	3193	1/1	0.85	0.16	65,65,65,65	0
56	MG	1B	227	1/1	0.85	0.30	69,69,69,69	0
56	MG	2a	3253	1/1	0.85	0.28	54,54,54,54	0
56	MG	1A	3056	1/1	0.85	0.15	59,59,59,59	0
56	MG	1A	3948	1/1	0.85	0.53	41,41,41,41	0
56	MG	2a	3020	1/1	0.85	0.47	44,44,44,44	0
56	MG	1a	1874	1/1	0.85	0.14	48,48,48,48	0
56	MG	1x	102	1/1	0.85	0.46	67,67,67,67	0
56	MG	2A	3308	1/1	0.85	0.29	53,53,53,53	0
56	MG	1A	3395	1/1	0.85	0.16	46,46,46,46	0
56	MG	2A	3196	1/1	0.85	0.17	47,47,47,47	0
56	MG	1A	3827	1/1	0.85	0.20	30,30,30,30	0
56	MG	1A	4036	1/1	0.85	0.19	54,54,54,54	0
56	MG	2a	3167	1/1	0.85	0.36	59,59,59,59	0
56	MG	2a	3070	1/1	0.85	0.22	66,66,66,66	0
56	MG	2A	3120	1/1	0.85	0.36	58,58,58,58	0
56	MG	2A	3437	1/1	0.85	0.13	69,69,69,69	0
56	MG	1A	4034	1/1	0.85	0.12	72,72,72,72	0
56	MG	1A	3408	1/1	0.85	0.35	58,58,58,58	0
56	MG	1A	3322	1/1	0.85	0.32	53,53,53,53	0
56	MG	1A	3348	1/1	0.85	0.30	52,52,52,52	0
56	MG	2A	3298	1/1	0.85	0.17	52,52,52,52	0
56	MG	2A	3557	1/1	0.85	0.16	54,54,54,54	0
56	MG	1a	1655	1/1	0.85	0.15	60,60,60,60	0
56	MG	2a	3121	1/1	0.85	0.11	88,88,88,88	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	3097	1/1	0.85	0.15	51,51,51,51	0
56	MG	1A	3287	1/1	0.85	0.30	38,38,38,38	0
56	MG	2A	3311	1/1	0.85	0.17	41,41,41,41	0
56	MG	1a	1818	1/1	0.85	0.17	81,81,81,81	0
56	MG	2a	3242	1/1	0.85	0.09	73,73,73,73	0
56	MG	2A	3076	1/1	0.85	0.22	56,56,56,56	0
56	MG	1A	3393	1/1	0.85	0.16	42,42,42,42	0
56	MG	2a	3094	1/1	0.85	0.32	55,55,55,55	0
56	MG	2d	502	1/1	0.86	0.49	61,61,61,61	0
56	MG	2a	3187	1/1	0.86	0.24	77,77,77,77	0
56	MG	1A	3316	1/1	0.86	0.29	51,51,51,51	0
56	MG	2A	3481	1/1	0.86	0.19	46,46,46,46	0
56	MG	2a	3064	1/1	0.86	0.27	79,79,79,79	0
56	MG	2a	3003	1/1	0.86	0.64	55,55,55,55	0
56	MG	2A	3151	1/1	0.86	0.40	54,54,54,54	0
56	MG	1a	1685	1/1	0.86	0.72	55,55,55,55	0
56	MG	1A	3488	1/1	0.86	0.18	43,43,43,43	0
56	MG	1a	1869	1/1	0.86	0.23	68,68,68,68	0
56	MG	2A	3146	1/1	0.86	0.17	35,35,35,35	0
56	MG	2A	3038	1/1	0.86	0.20	45,45,45,45	0
56	MG	1A	4035	1/1	0.86	0.18	46,46,46,46	0
56	MG	2A	3275	1/1	0.86	0.15	51,51,51,51	0
56	MG	2a	3111	1/1	0.86	0.37	60,60,60,60	0
56	MG	2a	3128	1/1	0.86	0.28	62,62,62,62	0
56	MG	1a	1687	1/1	0.86	0.12	42,42,42,42	0
56	MG	1A	3527	1/1	0.86	0.34	69,69,69,69	0
56	MG	2A	3364	1/1	0.86	0.17	44,44,44,44	0
56	MG	1B	230	1/1	0.86	0.23	67,67,67,67	0
56	MG	1A	3467	1/1	0.86	0.22	54,54,54,54	0
56	MG	2A	3012	1/1	0.86	0.08	71,71,71,71	0
56	MG	1E	302	1/1	0.86	0.41	41,41,41,41	0
56	MG	1A	4020	1/1	0.86	0.14	26,26,26,26	0
56	MG	1A	3428	1/1	0.86	0.16	43,43,43,43	0
56	MG	2A	3054	1/1	0.86	0.13	58,58,58,58	0
56	MG	2A	3044	1/1	0.86	0.22	51,51,51,51	0
56	MG	1a	1610	1/1	0.86	0.17	69,69,69,69	0
56	MG	1x	107	1/1	0.86	0.09	48,48,48,48	0
56	MG	1A	3026	1/1	0.86	0.27	47,47,47,47	0
56	MG	1A	3300	1/1	0.86	0.57	41,41,41,41	0
56	MG	1A	3327	1/1	0.86	0.15	44,44,44,44	0
56	MG	2a	3042	1/1	0.86	0.20	72,72,72,72	0
56	MG	1A	3940	1/1	0.86	0.21	65,65,65,65	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	3255	1/1	0.86	0.32	43,43,43,43	0
56	MG	2a	3036	1/1	0.86	0.16	59,59,59,59	0
56	MG	1a	1601	1/1	0.86	0.37	63,63,63,63	0
56	MG	1a	1616	1/1	0.86	0.22	55,55,55,55	0
56	MG	1A	3485	1/1	0.86	0.40	57,57,57,57	0
57	ZN	14	501	1/1	0.86	0.08	103,103,103,103	0
56	MG	1A	3238	1/1	0.86	0.38	52,52,52,52	0
56	MG	1a	1746	1/1	0.86	0.30	59,59,59,59	0
56	MG	2A	3223	1/1	0.86	0.12	70,70,70,70	0
56	MG	2a	3004	1/1	0.86	0.45	61,61,61,61	0
56	MG	2A	3353	1/1	0.86	0.27	41,41,41,41	0
56	MG	1A	3497	1/1	0.86	0.33	55,55,55,55	0
56	MG	1A	3336	1/1	0.86	0.18	58,58,58,58	0
56	MG	1A	3023	1/1	0.86	0.34	55,55,55,55	0
56	MG	2A	3015	1/1	0.86	0.12	57,57,57,57	0
56	MG	10	105	1/1	0.86	0.35	52,52,52,52	0
56	MG	2A	3172	1/1	0.86	0.29	63,63,63,63	0
56	MG	1A	3388	1/1	0.86	0.18	55,55,55,55	0
56	MG	1a	1720	1/1	0.86	0.29	45,45,45,45	0
56	MG	2A	3363	1/1	0.86	0.12	49,49,49,49	0
56	MG	1A	3430	1/1	0.86	0.36	41,41,41,41	0
56	MG	1A	3329	1/1	0.86	0.16	53,53,53,53	0
56	MG	1x	109	1/1	0.86	0.11	66,66,66,66	0
56	MG	1A	3356	1/1	0.86	0.16	63,63,63,63	0
56	MG	1A	3605	1/1	0.86	0.19	31,31,31,31	0
56	MG	1A	3357	1/1	0.86	0.13	54,54,54,54	0
56	MG	1A	3186	1/1	0.87	0.30	24,24,24,24	0
56	MG	1A	3567	1/1	0.87	0.11	40,40,40,40	0
56	MG	2A	3342	1/1	0.87	0.23	61,61,61,61	0
56	MG	2A	3192	1/1	0.87	0.40	43,43,43,43	0
56	MG	1A	3802	1/1	0.87	0.10	65,65,65,65	0
56	MG	2A	3011	1/1	0.87	0.16	48,48,48,48	0
56	MG	1A	3447	1/1	0.87	0.11	54,54,54,54	0
56	MG	1a	1641	1/1	0.87	0.25	47,47,47,47	0
56	MG	2A	3370	1/1	0.87	0.27	65,65,65,65	0
56	MG	1A	3826	1/1	0.87	0.16	17,17,17,17	0
56	MG	1A	3005	1/1	0.87	0.18	57,57,57,57	0
56	MG	2a	3117	1/1	0.87	0.38	66,66,66,66	0
56	MG	2A	3561	1/1	0.87	0.26	55,55,55,55	0
56	MG	2A	3543	1/1	0.87	0.30	49,49,49,49	0
56	MG	2A	3063	1/1	0.87	0.36	48,48,48,48	0
56	MG	2A	3244	1/1	0.87	0.29	85,85,85,85	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	3184	1/1	0.87	0.44	52,52,52,52	0
56	MG	1A	3100	1/1	0.87	0.19	51,51,51,51	0
56	MG	1o	101	1/1	0.87	0.31	81,81,81,81	0
56	MG	2A	3439	1/1	0.87	0.17	60,60,60,60	0
56	MG	1a	1783	1/1	0.87	0.31	73,73,73,73	0
56	MG	2A	3182	1/1	0.87	0.21	36,36,36,36	0
56	MG	2a	3197	1/1	0.87	0.13	78,78,78,78	0
56	MG	1A	3500	1/1	0.87	0.24	53,53,53,53	0
56	MG	2q	202	1/1	0.87	0.15	59,59,59,59	0
56	MG	1A	3331	1/1	0.87	0.35	62,62,62,62	0
56	MG	1a	1603	1/1	0.87	0.30	69,69,69,69	0
56	MG	2A	3348	1/1	0.87	0.17	60,60,60,60	0
56	MG	2A	3190	1/1	0.87	0.09	48,48,48,48	0
56	MG	2A	3220	1/1	0.87	0.17	72,72,72,72	0
56	MG	1a	1697	1/1	0.87	0.11	56,56,56,56	0
56	MG	2A	3559	1/1	0.87	0.36	56,56,56,56	0
56	MG	1a	1866	1/1	0.87	0.28	73,73,73,73	0
56	MG	1a	1761	1/1	0.87	0.20	65,65,65,65	0
56	MG	1a	1765	1/1	0.87	0.25	58,58,58,58	0
56	MG	1A	3876	1/1	0.87	0.17	33,33,33,33	0
56	MG	2A	3110	1/1	0.87	0.32	53,53,53,53	0
56	MG	2A	3365	1/1	0.87	0.08	41,41,41,41	0
56	MG	1A	3403	1/1	0.87	0.34	50,50,50,50	0
56	MG	1A	3501	1/1	0.87	0.15	51,51,51,51	0
56	MG	2A	3419	1/1	0.87	0.26	61,61,61,61	0
56	MG	1a	1622	1/1	0.87	0.20	49,49,49,49	0
56	MG	1f	3001	1/1	0.87	0.17	57,57,57,57	0
56	MG	2A	3504	1/1	0.87	0.20	42,42,42,42	0
56	MG	1A	3360	1/1	0.87	0.40	57,57,57,57	0
56	MG	1a	1719	1/1	0.87	0.60	68,68,68,68	0
56	MG	2A	3218	1/1	0.87	0.40	54,54,54,54	0
56	MG	2a	3198	1/1	0.87	0.18	65,65,65,65	0
56	MG	2A	3083	1/1	0.87	0.24	39,39,39,39	0
56	MG	2a	3159	1/1	0.87	0.22	58,58,58,58	0
56	MG	1a	1781	1/1	0.87	0.12	75,75,75,75	0
56	MG	2a	3030	1/1	0.87	0.24	51,51,51,51	0
56	MG	1A	3255	1/1	0.87	0.21	45,45,45,45	0
56	MG	2A	3094	1/1	0.87	0.22	43,43,43,43	0
56	MG	2a	3092	1/1	0.87	0.21	62,62,62,62	0
56	MG	1A	3458	1/1	0.88	0.07	48,48,48,48	0
56	MG	28	103	1/1	0.88	0.22	56,56,56,56	0
56	MG	2a	3214	1/1	0.88	0.12	73,73,73,73	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	3183	1/1	0.88	0.22	46,46,46,46	0
56	MG	2Z	301	1/1	0.88	0.08	70,70,70,70	0
56	MG	1A	3529	1/1	0.88	0.19	61,61,61,61	0
56	MG	1A	3838	1/1	0.88	0.25	64,64,64,64	0
56	MG	1a	1608	1/1	0.88	0.21	70,70,70,70	0
56	MG	1G	3001	1/1	0.88	0.10	50,50,50,50	0
56	MG	1a	1661	1/1	0.88	0.22	59,59,59,59	0
56	MG	1A	3728	1/1	0.88	0.32	62,62,62,62	0
56	MG	1A	3278	1/1	0.88	0.44	50,50,50,50	0
56	MG	1a	1669	1/1	0.88	0.19	37,37,37,37	0
56	MG	1a	1905	1/1	0.88	0.24	67,67,67,67	0
56	MG	1A	3993	1/1	0.88	0.10	34,34,34,34	0
56	MG	2a	3087	1/1	0.88	0.21	57,57,57,57	0
56	MG	1A	3180	1/1	0.88	0.08	34,34,34,34	0
56	MG	1A	3486	1/1	0.88	0.15	57,57,57,57	0
56	MG	1A	3029	1/1	0.88	0.34	71,71,71,71	0
56	MG	2a	3252	1/1	0.88	0.12	67,67,67,67	0
56	MG	2A	3208	1/1	0.88	0.22	48,48,48,48	0
56	MG	1Z	302	1/1	0.88	0.21	65,65,65,65	0
56	MG	1A	3104	1/1	0.88	0.25	52,52,52,52	0
56	MG	1A	3025	1/1	0.88	0.26	55,55,55,55	0
56	MG	1F	306	1/1	0.88	0.37	59,59,59,59	0
56	MG	1A	3150	1/1	0.88	0.45	44,44,44,44	0
56	MG	1D	302	1/1	0.88	0.32	52,52,52,52	0
56	MG	1A	3495	1/1	0.88	0.19	41,41,41,41	0
56	MG	2A	3442	1/1	0.88	0.10	66,66,66,66	0
56	MG	2A	3408	1/1	0.88	0.11	62,62,62,62	0
56	MG	1A	3076	1/1	0.88	0.17	51,51,51,51	0
56	MG	2A	3121	1/1	0.88	0.17	38,38,38,38	0
56	MG	1a	1726	1/1	0.88	0.08	68,68,68,68	0
56	MG	1a	1814	1/1	0.88	0.10	67,67,67,67	0
56	MG	1a	1754	1/1	0.88	0.38	51,51,51,51	0
56	MG	1a	1623	1/1	0.88	0.15	67,67,67,67	0
56	MG	1A	3479	1/1	0.88	0.23	59,59,59,59	0
56	MG	1A	3930	1/1	0.88	0.21	55,55,55,55	0
56	MG	1a	1829	1/1	0.88	0.22	45,45,45,45	0
56	MG	1A	3297	1/1	0.88	0.20	49,49,49,49	0
56	MG	1A	3276	1/1	0.88	0.15	51,51,51,51	0
56	MG	1A	3923	1/1	0.88	0.18	40,40,40,40	0
56	MG	2A	3107	1/1	0.88	0.23	49,49,49,49	0
56	MG	1A	3314	1/1	0.88	0.18	51,51,51,51	0
56	MG	2A	3238	1/1	0.88	0.20	30,30,30,30	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	4064	1/1	0.88	0.13	57,57,57,57	0
56	MG	2A	3470	1/1	0.88	0.08	64,64,64,64	0
56	MG	2A	3128	1/1	0.88	0.10	56,56,56,56	0
56	MG	1A	3983	1/1	0.88	0.27	31,31,31,31	0
56	MG	2A	3177	1/1	0.88	0.07	54,54,54,54	0
56	MG	20	8001	1/1	0.88	0.15	62,62,62,62	0
56	MG	1A	3351	1/1	0.88	0.14	46,46,46,46	0
56	MG	2A	3214	1/1	0.88	0.61	45,45,45,45	0
56	MG	2a	3163	1/1	0.88	0.46	94,94,94,94	0
56	MG	1A	3970	1/1	0.88	0.35	64,64,64,64	0
56	MG	2A	3306	1/1	0.88	0.15	32,32,32,32	0
56	MG	1A	3683	1/1	0.88	0.08	42,42,42,42	0
56	MG	2x	101	1/1	0.88	0.08	72,72,72,72	0
56	MG	1A	4026	1/1	0.88	0.43	63,63,63,63	0
56	MG	1B	214	1/1	0.88	0.23	56,56,56,56	0
56	MG	2d	503	1/1	0.88	0.13	62,62,62,62	0
56	MG	1a	1736	1/1	0.88	0.27	51,51,51,51	0
56	MG	2A	3318	1/1	0.88	0.13	43,43,43,43	0
56	MG	2A	3421	1/1	0.88	0.29	41,41,41,41	0
56	MG	2A	3161	1/1	0.88	0.08	38,38,38,38	0
56	MG	1a	1834	1/1	0.88	0.16	57,57,57,57	0
56	MG	1a	1611	1/1	0.88	0.22	46,46,46,46	0
56	MG	1A	3092	1/1	0.88	0.38	44,44,44,44	0
56	MG	2A	3055	1/1	0.88	0.29	35,35,35,35	0
56	MG	1N	3005	1/1	0.88	0.21	45,45,45,45	0
56	MG	1A	3453	1/1	0.88	0.29	72,72,72,72	0
56	MG	1a	1606	1/1	0.88	0.15	71,71,71,71	0
56	MG	1a	1692	1/1	0.88	0.21	64,64,64,64	0
56	MG	2A	3100	1/1	0.88	0.33	35,35,35,35	0
56	MG	2B	205	1/1	0.88	0.32	59,59,59,59	0
56	MG	1A	3129	1/1	0.88	0.22	42,42,42,42	0
56	MG	2A	3009	1/1	0.88	0.25	50,50,50,50	0
56	MG	1A	3723	1/1	0.88	0.11	29,29,29,29	0
56	MG	1A	3824	1/1	0.88	0.16	49,49,49,49	0
56	MG	2A	3181	1/1	0.88	0.09	48,48,48,48	0
56	MG	1A	3397	1/1	0.88	0.19	36,36,36,36	0
56	MG	1A	3063	1/1	0.88	0.14	57,57,57,57	0
56	MG	2A	3142	1/1	0.88	0.21	56,56,56,56	0
56	MG	1A	3373	1/1	0.88	0.18	44,44,44,44	0
56	MG	2A	3112	1/1	0.88	0.16	59,59,59,59	0
56	MG	1A	3666	1/1	0.88	0.20	25,25,25,25	0
56	MG	17	102	1/1	0.88	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	1878	1/1	0.89	0.42	67,67,67,67	0
56	MG	1A	3147	1/1	0.89	0.23	28,28,28,28	0
56	MG	1A	3835	1/1	0.89	0.13	47,47,47,47	0
56	MG	2a	3157	1/1	0.89	0.34	108,108,108,108	0
56	MG	1A	3989	1/1	0.89	0.53	31,31,31,31	0
56	MG	1A	3584	1/1	0.89	0.11	39,39,39,39	0
56	MG	1A	3396	1/1	0.89	0.10	55,55,55,55	0
56	MG	1A	3017	1/1	0.89	0.31	53,53,53,53	0
56	MG	1A	3115	1/1	0.89	0.13	56,56,56,56	0
56	MG	1a	1812	1/1	0.89	0.09	53,53,53,53	0
56	MG	1a	1880	1/1	0.89	0.20	69,69,69,69	0
56	MG	1k	201	1/1	0.89	0.19	49,49,49,49	0
56	MG	1A	3532	1/1	0.89	0.19	62,62,62,62	0
56	MG	1A	3032	1/1	0.89	0.37	44,44,44,44	0
56	MG	1A	3563	1/1	0.89	0.13	54,54,54,54	0
56	MG	1A	3711	1/1	0.89	0.14	61,61,61,61	0
56	MG	1A	3690	1/1	0.89	0.14	21,21,21,21	0
56	MG	2A	3449	1/1	0.89	0.22	57,57,57,57	0
56	MG	1A	3764	1/1	0.89	0.17	68,68,68,68	0
56	MG	2a	3115	1/1	0.89	0.20	50,50,50,50	0
56	MG	1A	3643	1/1	0.89	0.21	49,49,49,49	0
56	MG	1A	4025	1/1	0.89	0.31	80,80,80,80	0
56	MG	1A	3942	1/1	0.89	0.33	91,91,91,91	0
56	MG	1A	4029	1/1	0.89	0.14	42,42,42,42	0
56	MG	2a	3028	1/1	0.89	0.16	38,38,38,38	0
56	MG	2A	3239	1/1	0.89	0.30	59,59,59,59	0
56	MG	18	3002	1/1	0.89	0.21	58,58,58,58	0
56	MG	2A	3522	1/1	0.89	0.36	43,43,43,43	0
56	MG	1A	3350	1/1	0.89	0.38	60,60,60,60	0
56	MG	2a	3018	1/1	0.89	0.20	62,62,62,62	0
56	MG	1Q	206	1/1	0.89	0.22	53,53,53,53	0
56	MG	1A	3257	1/1	0.89	0.17	39,39,39,39	0
56	MG	2A	3550	1/1	0.89	0.12	39,39,39,39	0
56	MG	1a	1787	1/1	0.89	0.32	52,52,52,52	0
56	MG	1A	3337	1/1	0.89	0.20	44,44,44,44	0
56	MG	1A	3380	1/1	0.89	0.14	49,49,49,49	0
56	MG	1A	3678	1/1	0.89	0.12	39,39,39,39	0
56	MG	1a	1811	1/1	0.89	0.14	66,66,66,66	0
56	MG	1A	3979	1/1	0.89	0.20	55,55,55,55	0
56	MG	1A	3152	1/1	0.89	0.18	30,30,30,30	0
56	MG	1a	1767	1/1	0.89	0.13	71,71,71,71	0
56	MG	1A	4028	1/1	0.89	0.12	63,63,63,63	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	3121	1/1	0.89	0.23	72,72,72,72	0
56	MG	1A	4053	1/1	0.89	0.49	52,52,52,52	0
56	MG	1R	204	1/1	0.89	0.21	70,70,70,70	0
56	MG	1a	1644	1/1	0.89	0.20	75,75,75,75	0
56	MG	2A	3073	1/1	0.89	0.10	38,38,38,38	0
56	MG	2A	3253	1/1	0.89	0.23	59,59,59,59	0
56	MG	1A	3091	1/1	0.89	0.80	54,54,54,54	0
56	MG	2A	3021	1/1	0.89	0.48	58,58,58,58	0
56	MG	1A	3649	1/1	0.89	0.21	26,26,26,26	0
56	MG	2A	3359	1/1	0.89	0.15	57,57,57,57	0
56	MG	2A	3499	1/1	0.89	0.19	49,49,49,49	0
56	MG	1A	3908	1/1	0.89	0.16	51,51,51,51	0
56	MG	1A	3425	1/1	0.89	0.13	50,50,50,50	0
56	MG	2A	3082	1/1	0.89	0.13	57,57,57,57	0
56	MG	1A	3857	1/1	0.89	0.25	51,51,51,51	0
56	MG	2a	3141	1/1	0.89	0.08	70,70,70,70	0
56	MG	1A	3367	1/1	0.89	0.12	48,48,48,48	0
56	MG	2a	3235	1/1	0.89	0.18	73,73,73,73	0
56	MG	1A	3272	1/1	0.89	0.14	58,58,58,58	0
56	MG	1A	4063	1/1	0.89	0.18	47,47,47,47	0
56	MG	2A	3524	1/1	0.89	0.20	50,50,50,50	0
56	MG	1A	3504	1/1	0.89	0.20	62,62,62,62	0
56	MG	1A	3490	1/1	0.89	0.09	57,57,57,57	0
56	MG	1q	201	1/1	0.89	0.23	58,58,58,58	0
56	MG	1A	4006	1/1	0.89	0.32	35,35,35,35	0
56	MG	1a	1683	1/1	0.89	0.15	58,58,58,58	0
56	MG	1A	3173	1/1	0.89	0.19	40,40,40,40	0
56	MG	2a	3180	1/1	0.89	0.18	46,46,46,46	0
56	MG	1r	3003	1/1	0.89	0.16	49,49,49,49	0
56	MG	1W	3006	1/1	0.89	0.38	40,40,40,40	0
56	MG	1D	306	1/1	0.89	0.22	49,49,49,49	0
56	MG	2A	3478	1/1	0.89	0.19	50,50,50,50	0
56	MG	2A	3462	1/1	0.89	0.19	46,46,46,46	0
56	MG	2a	3182	1/1	0.89	0.16	78,78,78,78	0
56	MG	1A	3557	1/1	0.89	0.43	71,71,71,71	0
56	MG	1A	4077	1/1	0.89	0.20	47,47,47,47	0
56	MG	1A	3841	1/1	0.89	0.08	44,44,44,44	0
56	MG	1B	225	1/1	0.89	0.11	63,63,63,63	0
56	MG	2A	3270	1/1	0.89	0.09	59,59,59,59	0
56	MG	1A	3508	1/1	0.89	0.24	68,68,68,68	0
56	MG	2A	3401	1/1	0.89	0.29	70,70,70,70	0
56	MG	1A	3188	1/1	0.89	0.08	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	3494	1/1	0.89	0.24	38,38,38,38	0
56	MG	2A	3090	1/1	0.89	0.21	58,58,58,58	0
56	MG	1a	1855	1/1	0.89	0.27	48,48,48,48	0
56	MG	11	103	1/1	0.89	0.15	42,42,42,42	0
56	MG	2a	3165	1/1	0.89	0.49	74,74,74,74	0
56	MG	1A	3719	1/1	0.89	0.12	56,56,56,56	0
56	MG	1A	3143	1/1	0.89	0.20	34,34,34,34	0
56	MG	16	104	1/1	0.89	0.21	53,53,53,53	0
56	MG	1A	3263	1/1	0.89	0.22	42,42,42,42	0
56	MG	2A	3438	1/1	0.89	0.24	53,53,53,53	0
56	MG	1r	3001	1/1	0.89	0.23	61,61,61,61	0
56	MG	2a	3234	1/1	0.89	0.29	82,82,82,82	0
56	MG	2A	3251	1/1	0.89	0.20	49,49,49,49	0
56	MG	1A	3558	1/1	0.89	0.37	43,43,43,43	0
56	MG	1A	3265	1/1	0.89	0.24	27,27,27,27	0
56	MG	1A	3888	1/1	0.89	0.14	43,43,43,43	0
56	MG	1A	3749	1/1	0.89	0.26	43,43,43,43	0
56	MG	1O	3001	1/1	0.90	0.25	39,39,39,39	0
56	MG	2A	3057	1/1	0.90	0.20	52,52,52,52	0
56	MG	1a	1837	1/1	0.90	0.15	48,48,48,48	0
56	MG	2a	3095	1/1	0.90	0.09	41,41,41,41	0
56	MG	1N	3003	1/1	0.90	0.21	38,38,38,38	0
56	MG	1A	4049	1/1	0.90	0.25	49,49,49,49	0
56	MG	1A	3449	1/1	0.90	0.23	67,67,67,67	0
56	MG	1A	3585	1/1	0.90	0.20	14,14,14,14	0
56	MG	1A	3047	1/1	0.90	0.29	54,54,54,54	0
56	MG	1a	1621	1/1	0.90	0.28	57,57,57,57	0
56	MG	2A	3056	1/1	0.90	0.31	52,52,52,52	0
56	MG	1A	3406	1/1	0.90	0.23	49,49,49,49	0
56	MG	2A	3393	1/1	0.90	0.21	56,56,56,56	0
56	MG	2A	3549	1/1	0.90	0.17	49,49,49,49	0
56	MG	2A	3361	1/1	0.90	0.17	34,34,34,34	0
56	MG	1a	1703	1/1	0.90	0.19	52,52,52,52	0
56	MG	2A	3010	1/1	0.90	0.18	68,68,68,68	0
56	MG	1A	3281	1/1	0.90	0.07	62,62,62,62	0
56	MG	2a	3086	1/1	0.90	0.14	50,50,50,50	0
56	MG	1A	3868	1/1	0.90	0.19	84,84,84,84	0
56	MG	2A	3265	1/1	0.90	0.16	47,47,47,47	0
56	MG	2a	3023	1/1	0.90	0.21	66,66,66,66	0
56	MG	1a	1713	1/1	0.90	0.20	66,66,66,66	0
56	MG	2A	3123	1/1	0.90	0.25	57,57,57,57	0
56	MG	2a	3113	1/1	0.90	0.31	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	3301	1/1	0.90	0.20	64,64,64,64	0
56	MG	1A	3038	1/1	0.90	0.50	55,55,55,55	0
56	MG	2a	3178	1/1	0.90	0.21	55,55,55,55	0
56	MG	1a	1891	1/1	0.90	0.19	51,51,51,51	0
56	MG	1A	3464	1/1	0.90	0.16	57,57,57,57	0
56	MG	2a	3041	1/1	0.90	0.12	50,50,50,50	0
56	MG	1A	3296	1/1	0.90	0.22	49,49,49,49	0
56	MG	2A	3368	1/1	0.90	0.36	48,48,48,48	0
56	MG	1D	308	1/1	0.90	0.37	54,54,54,54	0
56	MG	1A	3535	1/1	0.90	0.31	59,59,59,59	0
56	MG	2B	206	1/1	0.90	0.21	37,37,37,37	0
56	MG	2A	3013	1/1	0.90	0.13	60,60,60,60	0
56	MG	1T	203	1/1	0.90	0.13	75,75,75,75	0
56	MG	2a	3223	1/1	0.90	0.17	77,77,77,77	0
56	MG	1a	1627	1/1	0.90	0.09	70,70,70,70	0
56	MG	1A	3575	1/1	0.90	0.33	57,57,57,57	0
56	MG	1A	3096	1/1	0.90	0.27	40,40,40,40	0
56	MG	1A	3311	1/1	0.90	0.22	44,44,44,44	0
56	MG	2A	3477	1/1	0.90	0.16	47,47,47,47	0
56	MG	2A	3195	1/1	0.90	0.19	47,47,47,47	0
56	MG	1G	3003	1/1	0.90	0.05	43,43,43,43	0
56	MG	2x	102	1/1	0.90	0.18	68,68,68,68	0
56	MG	1A	4086	1/1	0.90	0.16	63,63,63,63	0
56	MG	1A	3526	1/1	0.90	0.22	47,47,47,47	0
56	MG	2a	3142	1/1	0.90	0.47	80,80,80,80	0
56	MG	1A	3030	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3136	1/1	0.90	0.22	61,61,61,61	0
56	MG	1a	1730	1/1	0.90	0.27	44,44,44,44	0
56	MG	2A	3312	1/1	0.90	0.17	38,38,38,38	0
56	MG	1A	3477	1/1	0.90	0.37	40,40,40,40	0
56	MG	2A	3219	1/1	0.90	0.22	56,56,56,56	0
56	MG	1A	3358	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3825	1/1	0.90	0.32	45,45,45,45	0
56	MG	1A	3313	1/1	0.90	0.12	42,42,42,42	0
56	MG	2a	3119	1/1	0.90	0.10	69,69,69,69	0
56	MG	1A	3450	1/1	0.90	0.39	52,52,52,52	0
56	MG	1A	3399	1/1	0.90	0.37	45,45,45,45	0
56	MG	2A	3328	1/1	0.90	0.20	70,70,70,70	0
56	MG	1A	3647	1/1	0.90	0.18	19,19,19,19	0
56	MG	2a	3040	1/1	0.90	0.06	58,58,58,58	0
56	MG	1A	3670	1/1	0.90	0.26	37,37,37,37	0
56	MG	1A	3137	1/1	0.90	0.20	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	1b	3001	1/1	0.90	0.20	70,70,70,70	0
56	MG	1A	3955	1/1	0.90	0.12	21,21,21,21	0
56	MG	1A	4057	1/1	0.90	0.41	50,50,50,50	0
56	MG	1a	1673	1/1	0.90	0.42	46,46,46,46	0
56	MG	2a	3059	1/1	0.90	0.14	69,69,69,69	0
56	MG	1A	3345	1/1	0.90	0.22	63,63,63,63	0
56	MG	1A	3400	1/1	0.90	0.22	37,37,37,37	0
56	MG	1A	3072	1/1	0.90	0.24	46,46,46,46	0
56	MG	1A	3004	1/1	0.90	0.27	54,54,54,54	0
56	MG	1D	311	1/1	0.90	0.28	51,51,51,51	0
56	MG	1A	3095	1/1	0.90	0.22	46,46,46,46	0
56	MG	2a	3009	1/1	0.90	0.07	84,84,84,84	0
56	MG	1A	3398	1/1	0.90	0.19	46,46,46,46	0
56	MG	1A	3774	1/1	0.90	0.12	43,43,43,43	0
56	MG	1a	1744	1/1	0.90	0.63	58,58,58,58	0
56	MG	1A	3775	1/1	0.90	0.18	31,31,31,31	0
56	MG	2a	3104	1/1	0.90	0.30	54,54,54,54	0
56	MG	2A	3099	1/1	0.90	0.08	61,61,61,61	0
56	MG	1A	3899	1/1	0.90	0.19	77,77,77,77	0
56	MG	1A	3465	1/1	0.90	0.11	59,59,59,59	0
56	MG	2A	3263	1/1	0.90	0.09	42,42,42,42	0
56	MG	2a	3246	1/1	0.90	0.18	60,60,60,60	0
56	MG	1A	3689	1/1	0.91	0.08	65,65,65,65	0
56	MG	2A	3178	1/1	0.91	0.15	54,54,54,54	0
56	MG	1A	3120	1/1	0.91	0.28	59,59,59,59	0
56	MG	1A	4078	1/1	0.91	0.40	65,65,65,65	0
56	MG	1A	3832	1/1	0.91	0.16	34,34,34,34	0
56	MG	2A	3198	1/1	0.91	0.13	56,56,56,56	0
56	MG	2A	3207	1/1	0.91	0.35	49,49,49,49	0
56	MG	1V	202	1/1	0.91	0.18	28,28,28,28	0
56	MG	2a	3025	1/1	0.91	0.26	60,60,60,60	0
56	MG	1D	309	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3663	1/1	0.91	0.12	19,19,19,19	0
56	MG	2a	3224	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3410	1/1	0.91	0.13	52,52,52,52	0
56	MG	2A	3465	1/1	0.91	0.14	45,45,45,45	0
56	MG	1q	203	1/1	0.91	0.19	53,53,53,53	0
56	MG	1A	3514	1/1	0.91	0.29	59,59,59,59	0
56	MG	1a	1760	1/1	0.91	0.31	79,79,79,79	0
56	MG	1A	3075	1/1	0.91	0.17	46,46,46,46	0
56	MG	2a	3098	1/1	0.91	0.35	55,55,55,55	0
56	MG	2A	3025	1/1	0.91	0.37	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	1715	1/1	0.91	0.13	50,50,50,50	0
56	MG	2a	3210	1/1	0.91	0.20	78,78,78,78	0
56	MG	1A	3925	1/1	0.91	0.25	56,56,56,56	0
56	MG	1a	1718	1/1	0.91	0.13	75,75,75,75	0
56	MG	2A	3005	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3741	1/1	0.91	0.10	63,63,63,63	0
56	MG	1u	8001	1/1	0.91	0.16	53,53,53,53	0
56	MG	1A	3198	1/1	0.91	0.18	50,50,50,50	0
56	MG	2A	3346	1/1	0.91	0.06	69,69,69,69	0
56	MG	2a	3233	1/1	0.91	0.16	58,58,58,58	0
56	MG	2A	3240	1/1	0.91	0.18	34,34,34,34	0
56	MG	1A	3608	1/1	0.91	0.25	26,26,26,26	0
56	MG	2A	3418	1/1	0.91	0.25	52,52,52,52	0
56	MG	2x	107	1/1	0.91	0.11	78,78,78,78	0
56	MG	1R	205	1/1	0.91	0.24	28,28,28,28	0
56	MG	1A	3187	1/1	0.91	0.14	52,52,52,52	0
56	MG	2A	3422	1/1	0.91	0.13	73,73,73,73	0
56	MG	2a	3011	1/1	0.91	0.18	58,58,58,58	0
56	MG	1A	3236	1/1	0.91	0.12	58,58,58,58	0
56	MG	1A	3973	1/1	0.91	0.22	50,50,50,50	0
56	MG	1a	1747	1/1	0.91	0.24	64,64,64,64	0
56	MG	2A	3077	1/1	0.91	0.13	43,43,43,43	0
56	MG	1A	3659	1/1	0.91	0.16	17,17,17,17	0
56	MG	2A	3045	1/1	0.91	0.35	48,48,48,48	0
56	MG	2a	3225	1/1	0.91	0.19	59,59,59,59	0
56	MG	2A	3281	1/1	0.91	0.12	45,45,45,45	0
56	MG	2a	3194	1/1	0.91	0.38	44,44,44,44	0
56	MG	2a	3118	1/1	0.91	0.23	60,60,60,60	0
56	MG	1A	3161	1/1	0.91	0.36	47,47,47,47	0
56	MG	1A	3124	1/1	0.91	0.26	36,36,36,36	0
56	MG	1A	3949	1/1	0.91	0.23	35,35,35,35	0
56	MG	1A	3475	1/1	0.91	0.08	66,66,66,66	0
56	MG	1A	3860	1/1	0.91	0.20	38,38,38,38	0
56	MG	2O	202	1/1	0.91	0.12	37,37,37,37	0
56	MG	1A	3552	1/1	0.91	0.22	51,51,51,51	0
56	MG	1a	1647	1/1	0.91	0.28	53,53,53,53	0
56	MG	2A	3269	1/1	0.91	0.30	38,38,38,38	0
56	MG	2A	3512	1/1	0.91	0.23	38,38,38,38	0
56	MG	1A	3220	1/1	0.91	0.50	41,41,41,41	0
56	MG	1A	3641	1/1	0.91	0.12	52,52,52,52	0
56	MG	1A	3481	1/1	0.91	0.37	46,46,46,46	0
56	MG	1A	3107	1/1	0.91	0.58	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	3301	1/1	0.91	0.08	42,42,42,42	0
56	MG	2a	3052	1/1	0.91	0.09	81,81,81,81	0
56	MG	2A	3413	1/1	0.91	0.20	55,55,55,55	0
56	MG	1a	1659	1/1	0.91	0.26	52,52,52,52	0
56	MG	2A	3284	1/1	0.91	0.18	34,34,34,34	0
56	MG	1A	3550	1/1	0.91	0.20	68,68,68,68	0
56	MG	1a	1836	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	4075	1/1	0.91	0.30	61,61,61,61	0
56	MG	1a	1617	1/1	0.91	0.19	55,55,55,55	0
56	MG	1A	3133	1/1	0.91	0.38	48,48,48,48	0
56	MG	1A	3052	1/1	0.91	0.22	51,51,51,51	0
56	MG	2A	3531	1/1	0.91	0.28	52,52,52,52	0
56	MG	2A	3541	1/1	0.91	0.22	38,38,38,38	0
56	MG	2A	3072	1/1	0.91	0.24	29,29,29,29	0
56	MG	2a	3241	1/1	0.91	0.23	73,73,73,73	0
56	MG	1A	3290	1/1	0.91	0.18	30,30,30,30	0
56	MG	1a	1762	1/1	0.91	0.25	71,71,71,71	0
56	MG	1A	3533	1/1	0.91	0.09	56,56,56,56	0
56	MG	1a	1630	1/1	0.91	0.14	42,42,42,42	0
56	MG	2a	3179	1/1	0.91	0.07	58,58,58,58	0
56	MG	2A	3257	1/1	0.91	0.34	67,67,67,67	0
56	MG	2a	3211	1/1	0.91	0.35	55,55,55,55	0
56	MG	1A	3427	1/1	0.91	0.17	51,51,51,51	0
56	MG	1A	3657	1/1	0.91	0.13	34,34,34,34	0
56	MG	2A	3461	1/1	0.91	0.36	53,53,53,53	0
56	MG	2A	3085	1/1	0.91	0.16	38,38,38,38	0
56	MG	2a	3245	1/1	0.91	0.21	64,64,64,64	0
56	MG	2A	3050	1/1	0.91	0.41	55,55,55,55	0
56	MG	2A	3305	1/1	0.91	0.14	50,50,50,50	0
56	MG	1A	3048	1/1	0.91	0.20	51,51,51,51	0
56	MG	1a	1694	1/1	0.91	0.09	51,51,51,51	0
56	MG	1A	3382	1/1	0.91	0.08	53,53,53,53	0
56	MG	2A	3295	1/1	0.91	0.17	38,38,38,38	0
56	MG	1a	1604	1/1	0.91	0.27	60,60,60,60	0
56	MG	1A	3424	1/1	0.91	0.25	37,37,37,37	0
56	MG	1A	3117	1/1	0.91	0.10	62,62,62,62	0
56	MG	1x	101	1/1	0.91	0.22	64,64,64,64	0
56	MG	1E	307	1/1	0.91	0.33	57,57,57,57	0
56	MG	1A	3920	1/1	0.91	0.18	65,65,65,65	0
56	MG	2A	3135	1/1	0.91	0.10	43,43,43,43	0
56	MG	2A	3391	1/1	0.91	0.28	52,52,52,52	0
56	MG	1A	3057	1/1	0.91	0.06	47,47,47,47	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	4079	1/1	0.91	0.22	33,33,33,33	0
56	MG	10	103	1/1	0.91	0.23	62,62,62,62	0
56	MG	1a	1743	1/1	0.91	0.18	44,44,44,44	0
56	MG	1A	3140	1/1	0.91	0.22	36,36,36,36	0
56	MG	1A	3051	1/1	0.91	0.60	47,47,47,47	0
56	MG	1A	3008	1/1	0.91	0.22	51,51,51,51	0
56	MG	2a	3093	1/1	0.91	0.33	66,66,66,66	0
56	MG	1a	1888	1/1	0.91	0.20	60,60,60,60	0
56	MG	1a	1819	1/1	0.91	0.26	73,73,73,73	0
56	MG	1A	3252	1/1	0.91	0.18	56,56,56,56	0
56	MG	2A	3052	1/1	0.91	0.13	37,37,37,37	0
56	MG	25	502	1/1	0.91	0.53	54,54,54,54	0
56	MG	2A	3106	1/1	0.91	0.17	47,47,47,47	0
56	MG	1a	1741	1/1	0.91	0.13	48,48,48,48	0
56	MG	1a	1871	1/1	0.91	0.33	69,69,69,69	0
56	MG	1A	3279	1/1	0.91	0.25	41,41,41,41	0
56	MG	1a	1780	1/1	0.91	0.08	56,56,56,56	0
56	MG	1A	3639	1/1	0.91	0.28	47,47,47,47	0
56	MG	1A	3368	1/1	0.91	0.28	65,65,65,65	0
56	MG	2A	3485	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3522	1/1	0.91	0.07	50,50,50,50	0
56	MG	1B	223	1/1	0.91	0.14	65,65,65,65	0
56	MG	1A	3085	1/1	0.91	0.14	48,48,48,48	0
56	MG	1A	3614	1/1	0.91	0.28	57,57,57,57	0
56	MG	1A	3405	1/1	0.91	0.54	41,41,41,41	0
56	MG	1A	3041	1/1	0.91	0.22	51,51,51,51	0
56	MG	2a	3016	1/1	0.91	0.43	65,65,65,65	0
56	MG	1A	3015	1/1	0.91	0.29	51,51,51,51	0
56	MG	2A	3157	1/1	0.91	0.18	31,31,31,31	0
56	MG	1A	4000	1/1	0.91	0.11	69,69,69,69	0
56	MG	2a	3155	1/1	0.91	0.17	87,87,87,87	0
56	MG	1a	1777	1/1	0.91	0.18	54,54,54,54	0
56	MG	2A	3014	1/1	0.91	0.18	52,52,52,52	0
56	MG	1U	202	1/1	0.91	0.53	51,51,51,51	0
56	MG	2A	3030	1/1	0.91	0.37	64,64,64,64	0
56	MG	1A	3850	1/1	0.91	0.13	47,47,47,47	0
56	MG	2A	3276	1/1	0.91	0.09	60,60,60,60	0
56	MG	2A	3164	1/1	0.91	0.45	51,51,51,51	0
56	MG	1B	216	1/1	0.91	0.12	70,70,70,70	0
56	MG	1a	1877	1/1	0.91	0.25	52,52,52,52	0
56	MG	2A	3127	1/1	0.91	0.22	43,43,43,43	0
56	MG	2a	3010	1/1	0.91	0.20	44,44,44,44	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	3228	1/1	0.91	0.21	48,48,48,48	0
56	MG	2a	3255	1/1	0.91	0.09	57,57,57,57	0
56	MG	1a	1632	1/1	0.91	0.20	32,32,32,32	0
56	MG	1A	3219	1/1	0.91	0.21	56,56,56,56	0
56	MG	1A	3145	1/1	0.91	0.40	38,38,38,38	0
56	MG	2A	3160	1/1	0.91	0.13	49,49,49,49	0
56	MG	2a	3045	1/1	0.92	0.38	68,68,68,68	0
56	MG	1A	4062	1/1	0.92	0.27	49,49,49,49	0
56	MG	2Q	3002	1/1	0.92	0.18	55,55,55,55	0
56	MG	2A	3029	1/1	0.92	0.15	57,57,57,57	0
56	MG	2A	3034	1/1	0.92	0.17	44,44,44,44	0
56	MG	1A	3562	1/1	0.92	0.18	54,54,54,54	0
56	MG	1a	1909	1/1	0.92	0.11	71,71,71,71	0
56	MG	1A	3381	1/1	0.92	0.28	54,54,54,54	0
56	MG	1a	1797	1/1	0.92	0.21	73,73,73,73	0
56	MG	2A	3341	1/1	0.92	0.14	51,51,51,51	0
56	MG	1A	3118	1/1	0.92	0.18	47,47,47,47	0
56	MG	2a	3209	1/1	0.92	0.13	53,53,53,53	0
56	MG	1a	1739	1/1	0.92	0.06	70,70,70,70	0
56	MG	1A	3081	1/1	0.92	0.15	40,40,40,40	0
56	MG	2a	3061	1/1	0.92	0.22	71,71,71,71	0
56	MG	2N	8001	1/1	0.92	0.14	63,63,63,63	0
56	MG	1T	205	1/1	0.92	0.16	56,56,56,56	0
56	MG	2A	3431	1/1	0.92	0.16	50,50,50,50	0
56	MG	19	102	1/1	0.92	0.23	50,50,50,50	0
56	MG	2A	3210	1/1	0.92	0.35	31,31,31,31	0
56	MG	2A	3169	1/1	0.92	0.14	37,37,37,37	0
56	MG	1A	4066	1/1	0.92	0.30	35,35,35,35	0
56	MG	1A	3534	1/1	0.92	0.21	55,55,55,55	0
56	MG	15	104	1/1	0.92	0.25	53,53,53,53	0
56	MG	1P	201	1/1	0.92	0.16	49,49,49,49	0
56	MG	1A	3762	1/1	0.92	0.06	39,39,39,39	0
56	MG	1A	3386	1/1	0.92	0.24	68,68,68,68	0
56	MG	2A	3492	1/1	0.92	0.13	67,67,67,67	0
56	MG	1A	3209	1/1	0.92	0.38	39,39,39,39	0
56	MG	1e	202	1/1	0.92	0.09	65,65,65,65	0
56	MG	1A	3937	1/1	0.92	0.18	52,52,52,52	0
56	MG	1d	502	1/1	0.92	0.16	82,82,82,82	0
56	MG	2a	3203	1/1	0.92	0.13	58,58,58,58	0
56	MG	1A	3422	1/1	0.92	0.14	40,40,40,40	0
56	MG	1p	3002	1/1	0.92	0.14	77,77,77,77	0
56	MG	2a	3012	1/1	0.92	0.12	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3386	1/1	0.92	0.25	37,37,37,37	0
56	MG	1p	3001	1/1	0.92	0.26	52,52,52,52	0
56	MG	2A	3088	1/1	0.92	0.12	44,44,44,44	0
56	MG	2A	3510	1/1	0.92	0.28	61,61,61,61	0
56	MG	1A	3200	1/1	0.92	0.18	39,39,39,39	0
56	MG	1B	201	1/1	0.92	0.15	40,40,40,40	0
56	MG	1a	1817	1/1	0.92	0.15	54,54,54,54	0
56	MG	1A	3559	1/1	0.92	0.16	55,55,55,55	0
56	MG	1a	1789	1/1	0.92	0.29	60,60,60,60	0
56	MG	1U	205	1/1	0.92	0.48	41,41,41,41	0
56	MG	1A	3938	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	3286	1/1	0.92	0.12	40,40,40,40	0
56	MG	2A	3018	1/1	0.92	0.22	47,47,47,47	0
56	MG	2A	3144	1/1	0.92	0.34	41,41,41,41	0
56	MG	1A	3890	1/1	0.92	0.18	31,31,31,31	0
56	MG	1A	3061	1/1	0.92	0.17	51,51,51,51	0
56	MG	2a	3219	1/1	0.92	0.13	62,62,62,62	0
56	MG	1A	3034	1/1	0.92	0.14	49,49,49,49	0
56	MG	1E	310	1/1	0.92	0.35	49,49,49,49	0
56	MG	2A	3176	1/1	0.92	0.14	38,38,38,38	0
56	MG	2A	3247	1/1	0.92	0.12	59,59,59,59	0
56	MG	1a	1803	1/1	0.92	0.21	66,66,66,66	0
56	MG	2A	3339	1/1	0.92	0.32	63,63,63,63	0
56	MG	1l	202	1/1	0.92	0.09	58,58,58,58	0
56	MG	2A	3046	1/1	0.92	0.43	60,60,60,60	0
56	MG	1A	3158	1/1	0.92	0.20	32,32,32,32	0
56	MG	1A	3999	1/1	0.92	0.15	51,51,51,51	0
56	MG	2A	3372	1/1	0.92	0.11	33,33,33,33	0
56	MG	1A	3684	1/1	0.92	0.17	50,50,50,50	0
56	MG	1o	103	1/1	0.92	0.26	47,47,47,47	0
56	MG	1A	4061	1/1	0.92	0.23	61,61,61,61	0
56	MG	1B	213	1/1	0.92	0.09	50,50,50,50	0
56	MG	1a	1650	1/1	0.92	0.22	49,49,49,49	0
56	MG	1A	3304	1/1	0.92	0.23	45,45,45,45	0
56	MG	1A	3656	1/1	0.92	0.18	20,20,20,20	0
56	MG	1a	1733	1/1	0.92	0.58	52,52,52,52	0
56	MG	1a	1667	1/1	0.92	0.19	64,64,64,64	0
56	MG	1A	3765	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3848	1/1	0.92	0.18	45,45,45,45	0
56	MG	2a	3201	1/1	0.92	0.12	66,66,66,66	0
56	MG	1a	1656	1/1	0.92	0.24	84,84,84,84	0
56	MG	2Q	3001	1/1	0.92	0.41	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	1758	1/1	0.92	0.17	67,67,67,67	0
56	MG	2A	3235	1/1	0.92	0.21	57,57,57,57	0
56	MG	1A	3636	1/1	0.92	0.16	49,49,49,49	0
56	MG	2E	304	1/1	0.92	0.09	56,56,56,56	0
56	MG	1a	1904	1/1	0.92	0.20	76,76,76,76	0
56	MG	1A	3205	1/1	0.92	0.30	33,33,33,33	0
56	MG	2A	3409	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	4042	1/1	0.92	0.33	44,44,44,44	0
56	MG	2A	3553	1/1	0.92	0.23	41,41,41,41	0
56	MG	1a	1793	1/1	0.92	0.16	83,83,83,83	0
56	MG	1A	3772	1/1	0.92	0.28	43,43,43,43	0
56	MG	2A	3420	1/1	0.92	0.23	72,72,72,72	0
56	MG	2A	3064	1/1	0.92	0.45	56,56,56,56	0
56	MG	2a	3168	1/1	0.92	0.34	67,67,67,67	0
56	MG	1a	1684	1/1	0.92	0.11	57,57,57,57	0
56	MG	1a	1867	1/1	0.92	0.13	64,64,64,64	0
56	MG	1a	1717	1/1	0.92	0.18	47,47,47,47	0
56	MG	1A	3701	1/1	0.92	0.15	29,29,29,29	0
56	MG	2A	3188	1/1	0.92	0.33	41,41,41,41	0
56	MG	1a	1709	1/1	0.92	0.25	61,61,61,61	0
56	MG	2A	3343	1/1	0.92	0.08	55,55,55,55	0
56	MG	2a	3069	1/1	0.92	0.18	65,65,65,65	0
56	MG	1A	3354	1/1	0.92	0.07	84,84,84,84	0
56	MG	1A	3788	1/1	0.92	0.23	30,30,30,30	0
56	MG	1A	3996	1/1	0.92	0.07	37,37,37,37	0
56	MG	1P	202	1/1	0.92	0.26	59,59,59,59	0
56	MG	2a	3046	1/1	0.92	0.12	70,70,70,70	0
56	MG	1A	3452	1/1	0.92	0.16	50,50,50,50	0
56	MG	1A	3273	1/1	0.92	0.20	37,37,37,37	0
56	MG	1a	1886	1/1	0.92	0.09	56,56,56,56	0
56	MG	1a	1858	1/1	0.92	0.05	56,56,56,56	0
56	MG	2A	3316	1/1	0.92	0.10	55,55,55,55	0
56	MG	1a	1795	1/1	0.92	0.28	64,64,64,64	0
56	MG	1B	209	1/1	0.92	0.15	56,56,56,56	0
56	MG	1A	4019	1/1	0.92	0.22	39,39,39,39	0
56	MG	2A	3334	1/1	0.92	0.17	53,53,53,53	0
56	MG	1a	1815	1/1	0.92	0.17	73,73,73,73	0
56	MG	1A	3455	1/1	0.92	0.11	58,58,58,58	0
56	MG	2a	3056	1/1	0.92	0.17	58,58,58,58	0
56	MG	1A	3624	1/1	0.92	0.18	40,40,40,40	0
56	MG	1E	301	1/1	0.92	0.50	40,40,40,40	0
56	MG	2P	201	1/1	0.92	0.22	33,33,33,33	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	3998	1/1	0.92	0.22	59,59,59,59	0
56	MG	1A	3523	1/1	0.92	0.18	50,50,50,50	0
56	MG	2A	3496	1/1	0.92	0.12	35,35,35,35	0
56	MG	1A	3040	1/1	0.92	0.24	36,36,36,36	0
56	MG	2a	3026	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3279	1/1	0.92	0.13	51,51,51,51	0
56	MG	2A	3495	1/1	0.92	0.30	60,60,60,60	0
56	MG	1O	3003	1/1	0.92	0.12	60,60,60,60	0
56	MG	2A	3456	1/1	0.92	0.26	64,64,64,64	0
56	MG	2a	3215	1/1	0.92	0.12	53,53,53,53	0
56	MG	1A	3269	1/1	0.92	0.19	53,53,53,53	0
56	MG	1a	1727	1/1	0.92	0.17	56,56,56,56	0
56	MG	1A	3892	1/1	0.92	0.11	46,46,46,46	0
56	MG	2A	3041	1/1	0.92	0.15	41,41,41,41	0
56	MG	1A	3954	1/1	0.92	0.21	16,16,16,16	0
56	MG	1A	3151	1/1	0.92	0.15	45,45,45,45	0
56	MG	2a	3013	1/1	0.92	0.07	50,50,50,50	0
56	MG	1A	3616	1/1	0.92	0.25	29,29,29,29	0
56	MG	1A	3418	1/1	0.92	0.21	48,48,48,48	0
56	MG	1A	3579	1/1	0.92	0.29	41,41,41,41	0
56	MG	1A	3872	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3990	1/1	0.92	0.18	17,17,17,17	0
56	MG	1t	3001	1/1	0.92	0.43	53,53,53,53	0
56	MG	1A	3793	1/1	0.92	0.19	55,55,55,55	0
56	MG	2A	3019	1/1	0.92	0.16	48,48,48,48	0
56	MG	1A	3473	1/1	0.92	0.11	55,55,55,55	0
56	MG	1a	1749	1/1	0.92	0.15	64,64,64,64	0
56	MG	2l	3001	1/1	0.92	0.44	65,65,65,65	0
56	MG	2F	302	1/1	0.92	0.24	48,48,48,48	0
56	MG	1A	3122	1/1	0.92	0.28	56,56,56,56	0
56	MG	2A	3389	1/1	0.92	0.21	39,39,39,39	0
56	MG	1A	3648	1/1	0.92	0.18	26,26,26,26	0
56	MG	1A	3505	1/1	0.92	0.18	49,49,49,49	0
56	MG	2A	3547	1/1	0.92	0.24	52,52,52,52	0
56	MG	1a	1884	1/1	0.92	0.15	46,46,46,46	0
56	MG	1x	104	1/1	0.92	0.07	56,56,56,56	0
56	MG	2B	208	1/1	0.92	0.10	58,58,58,58	0
56	MG	2A	3166	1/1	0.92	0.12	32,32,32,32	0
56	MG	1a	1885	1/1	0.92	0.21	54,54,54,54	0
56	MG	1A	3414	1/1	0.92	0.21	50,50,50,50	0
56	MG	2a	3065	1/1	0.92	0.21	93,93,93,93	0
56	MG	1A	3053	1/1	0.92	0.25	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	1D	312	1/1	0.92	0.18	45,45,45,45	0
56	MG	2A	3289	1/1	0.92	0.18	37,37,37,37	0
56	MG	1A	3604	1/1	0.92	0.10	36,36,36,36	0
56	MG	1A	4010	1/1	0.92	0.26	37,37,37,37	0
56	MG	2A	3213	1/1	0.92	0.20	42,42,42,42	0
56	MG	1a	1853	1/1	0.92	0.12	70,70,70,70	0
56	MG	1a	1698	1/1	0.92	0.12	63,63,63,63	0
56	MG	1A	3582	1/1	0.92	0.20	25,25,25,25	0
56	MG	1A	3022	1/1	0.92	0.17	49,49,49,49	0
56	MG	2a	3100	1/1	0.93	0.33	80,80,80,80	0
56	MG	2A	3020	1/1	0.93	0.18	39,39,39,39	0
56	MG	1A	3303	1/1	0.93	0.24	50,50,50,50	0
56	MG	1A	3037	1/1	0.93	0.24	40,40,40,40	0
56	MG	1a	1680	1/1	0.93	0.14	55,55,55,55	0
56	MG	1F	303	1/1	0.93	0.45	32,32,32,32	0
56	MG	19	101	1/1	0.93	0.21	51,51,51,51	0
56	MG	2v	101	1/1	0.93	0.11	65,65,65,65	0
56	MG	1A	3862	1/1	0.93	0.21	45,45,45,45	0
56	MG	1A	3437	1/1	0.93	0.22	46,46,46,46	0
56	MG	1F	307	1/1	0.93	0.66	59,59,59,59	0
56	MG	1A	3361	1/1	0.93	0.28	45,45,45,45	0
56	MG	1B	202	1/1	0.93	0.26	63,63,63,63	0
56	MG	1A	3769	1/1	0.93	0.29	55,55,55,55	0
56	MG	1a	1843	1/1	0.93	0.19	55,55,55,55	0
56	MG	1A	3750	1/1	0.93	0.17	28,28,28,28	0
56	MG	2A	3335	1/1	0.93	0.20	35,35,35,35	0
56	MG	2A	3338	1/1	0.93	0.13	46,46,46,46	0
56	MG	2A	3271	1/1	0.93	0.14	50,50,50,50	0
56	MG	1A	3208	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3867	1/1	0.93	0.23	60,60,60,60	0
56	MG	1A	3836	1/1	0.93	0.13	25,25,25,25	0
56	MG	2A	3002	1/1	0.93	0.14	40,40,40,40	0
56	MG	1a	1769	1/1	0.93	0.11	63,63,63,63	0
56	MG	2a	3148	1/1	0.93	0.26	56,56,56,56	0
56	MG	1A	3686	1/1	0.93	0.17	28,28,28,28	0
56	MG	2a	3188	1/1	0.93	0.22	53,53,53,53	0
56	MG	1a	1794	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3506	1/1	0.93	0.10	51,51,51,51	0
56	MG	1a	1895	1/1	0.93	0.35	59,59,59,59	0
56	MG	1A	3886	1/1	0.93	0.09	42,42,42,42	0
56	MG	2A	3159	1/1	0.93	0.22	49,49,49,49	0
56	MG	1A	3555	1/1	0.93	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	2A	3486	1/1	0.93	0.20	42,42,42,42	0
56	MG	1a	1830	1/1	0.93	0.21	68,68,68,68	0
56	MG	1A	3992	1/1	0.93	0.09	36,36,36,36	0
56	MG	2a	3120	1/1	0.93	0.19	62,62,62,62	0
56	MG	1A	3516	1/1	0.93	0.48	52,52,52,52	0
56	MG	2a	3200	1/1	0.93	0.16	71,71,71,71	0
56	MG	2A	3474	1/1	0.93	0.13	51,51,51,51	0
56	MG	1o	102	1/1	0.93	0.16	72,72,72,72	0
56	MG	1A	3045	1/1	0.93	0.18	39,39,39,39	0
56	MG	1N	3002	1/1	0.93	0.29	48,48,48,48	0
56	MG	1A	3530	1/1	0.93	0.09	47,47,47,47	0
56	MG	1a	1759	1/1	0.93	0.61	66,66,66,66	0
56	MG	2A	3193	1/1	0.93	0.18	37,37,37,37	0
56	MG	2A	3084	1/1	0.93	0.19	26,26,26,26	0
56	MG	2A	3141	1/1	0.93	0.40	49,49,49,49	0
56	MG	1A	3330	1/1	0.93	0.27	39,39,39,39	0
56	MG	1A	3489	1/1	0.93	0.23	41,41,41,41	0
56	MG	1A	3595	1/1	0.93	0.12	66,66,66,66	0
56	MG	1A	3578	1/1	0.93	0.14	48,48,48,48	0
56	MG	1A	3197	1/1	0.93	0.12	23,23,23,23	0
56	MG	2a	3079	1/1	0.93	0.09	52,52,52,52	0
56	MG	2a	3161	1/1	0.93	0.20	63,63,63,63	0
56	MG	1A	3716	1/1	0.93	0.14	38,38,38,38	0
56	MG	2A	3356	1/1	0.93	0.14	38,38,38,38	0
56	MG	1A	3834	1/1	0.93	0.30	63,63,63,63	0
56	MG	1A	3334	1/1	0.93	0.19	73,73,73,73	0
56	MG	2A	3374	1/1	0.93	0.10	58,58,58,58	0
56	MG	2A	3092	1/1	0.93	0.23	48,48,48,48	0
56	MG	1A	3568	1/1	0.93	0.14	45,45,45,45	0
56	MG	1a	1872	1/1	0.93	0.13	57,57,57,57	0
56	MG	1A	3394	1/1	0.93	0.15	42,42,42,42	0
56	MG	2A	3277	1/1	0.93	0.14	44,44,44,44	0
56	MG	1a	1660	1/1	0.93	0.15	23,23,23,23	0
56	MG	1A	3885	1/1	0.93	0.20	54,54,54,54	0
56	MG	1A	3352	1/1	0.93	0.20	57,57,57,57	0
56	MG	2a	3249	1/1	0.93	0.26	36,36,36,36	0
56	MG	1a	1833	1/1	0.93	0.29	62,62,62,62	0
56	MG	1a	1690	1/1	0.93	0.10	57,57,57,57	0
56	MG	2A	3031	1/1	0.93	0.18	47,47,47,47	0
56	MG	2A	3366	1/1	0.93	0.22	50,50,50,50	0
56	MG	2A	3147	1/1	0.93	0.07	62,62,62,62	0
56	MG	1A	3229	1/1	0.93	0.14	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	3726	1/1	0.93	0.18	46,46,46,46	0
56	MG	2a	3160	1/1	0.93	0.17	61,61,61,61	0
56	MG	1A	3622	1/1	0.93	0.15	36,36,36,36	0
56	MG	2f	201	1/1	0.93	0.19	48,48,48,48	0
56	MG	1d	503	1/1	0.93	0.19	77,77,77,77	0
56	MG	2A	3447	1/1	0.93	0.24	43,43,43,43	0
56	MG	1A	3754	1/1	0.93	0.34	39,39,39,39	0
56	MG	1A	3136	1/1	0.93	0.09	35,35,35,35	0
56	MG	1A	3713	1/1	0.93	0.09	61,61,61,61	0
56	MG	1A	4030	1/1	0.93	0.16	43,43,43,43	0
56	MG	2a	3146	1/1	0.93	0.13	71,71,71,71	0
56	MG	1A	3849	1/1	0.93	0.14	52,52,52,52	0
56	MG	1A	4037	1/1	0.93	0.18	75,75,75,75	0
56	MG	1a	1813	1/1	0.93	0.12	75,75,75,75	0
56	MG	1A	3880	1/1	0.93	0.18	38,38,38,38	0
56	MG	1A	3006	1/1	0.93	0.24	54,54,54,54	0
56	MG	1A	3707	1/1	0.93	0.18	32,32,32,32	0
56	MG	1D	305	1/1	0.93	0.37	13,13,13,13	0
56	MG	1h	8002	1/1	0.93	0.45	80,80,80,80	0
56	MG	2a	3176	1/1	0.93	0.35	50,50,50,50	0
56	MG	2a	3082	1/1	0.93	0.22	54,54,54,54	0
56	MG	1R	202	1/1	0.93	0.51	55,55,55,55	0
56	MG	2a	3106	1/1	0.93	0.21	52,52,52,52	0
56	MG	1A	4048	1/1	0.93	0.11	48,48,48,48	0
56	MG	1A	3771	1/1	0.93	0.17	55,55,55,55	0
56	MG	1a	1664	1/1	0.93	0.30	62,62,62,62	0
56	MG	1a	1753	1/1	0.93	0.22	48,48,48,48	0
56	MG	1A	3349	1/1	0.93	0.19	35,35,35,35	0
56	MG	1A	3549	1/1	0.93	0.28	73,73,73,73	0
56	MG	1A	3768	1/1	0.93	0.18	8,8,8,8	0
56	MG	1A	3492	1/1	0.93	0.55	47,47,47,47	0
56	MG	2A	3489	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3199	1/1	0.93	0.23	21,21,21,21	0
56	MG	2A	3519	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3845	1/1	0.93	0.63	35,35,35,35	0
56	MG	1A	3858	1/1	0.93	0.24	53,53,53,53	0
56	MG	2A	3266	1/1	0.93	0.20	41,41,41,41	0
56	MG	1a	1778	1/1	0.93	0.09	48,48,48,48	0
56	MG	2a	3060	1/1	0.93	0.16	81,81,81,81	0
56	MG	1A	4018	1/1	0.93	0.17	45,45,45,45	0
56	MG	1A	3520	1/1	0.93	0.09	61,61,61,61	0
56	MG	1a	1807	1/1	0.93	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	2A	3448	1/1	0.93	0.12	62,62,62,62	0
56	MG	1A	3307	1/1	0.93	0.29	63,63,63,63	0
56	MG	1N	3001	1/1	0.93	0.21	44,44,44,44	0
56	MG	1N	3007	1/1	0.93	0.22	54,54,54,54	0
56	MG	1A	3855	1/1	0.93	0.14	48,48,48,48	0
56	MG	1A	3851	1/1	0.93	0.10	65,65,65,65	0
56	MG	2A	3544	1/1	0.93	0.16	48,48,48,48	0
56	MG	1A	3687	1/1	0.93	0.19	17,17,17,17	0
56	MG	1A	3556	1/1	0.93	0.27	58,58,58,58	0
56	MG	1A	3216	1/1	0.93	0.28	39,39,39,39	0
56	MG	1F	302	1/1	0.93	0.12	39,39,39,39	0
56	MG	2A	3003	1/1	0.93	0.13	43,43,43,43	0
56	MG	1B	221	1/1	0.93	0.14	30,30,30,30	0
56	MG	2F	303	1/1	0.93	0.10	52,52,52,52	0
56	MG	2I	3003	1/1	0.93	0.10	57,57,57,57	0
56	MG	2a	3154	1/1	0.93	0.19	71,71,71,71	0
56	MG	1A	3438	1/1	0.93	0.08	49,49,49,49	0
56	MG	1A	3779	1/1	0.93	0.13	35,35,35,35	0
56	MG	1a	1624	1/1	0.93	0.12	80,80,80,80	0
56	MG	1D	310	1/1	0.93	0.11	42,42,42,42	0
56	MG	2A	3133	1/1	0.93	0.11	35,35,35,35	0
56	MG	2A	3282	1/1	0.93	0.16	35,35,35,35	0
56	MG	1a	1782	1/1	0.93	0.09	73,73,73,73	0
56	MG	1A	3911	1/1	0.93	0.18	30,30,30,30	0
56	MG	2A	3501	1/1	0.93	0.20	37,37,37,37	0
56	MG	2I	3004	1/1	0.93	0.10	60,60,60,60	0
56	MG	1A	3883	1/1	0.93	0.13	36,36,36,36	0
56	MG	2a	3083	1/1	0.93	0.10	49,49,49,49	0
56	MG	2a	3171	1/1	0.93	0.29	46,46,46,46	0
56	MG	1A	3547	1/1	0.93	0.20	61,61,61,61	0
56	MG	2a	3135	1/1	0.93	0.20	73,73,73,73	0
56	MG	1A	3206	1/1	0.93	0.46	45,45,45,45	0
56	MG	1A	3139	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3963	1/1	0.93	0.13	27,27,27,27	0
56	MG	1A	3661	1/1	0.93	0.08	30,30,30,30	0
56	MG	1A	3050	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3172	1/1	0.93	0.22	31,31,31,31	0
56	MG	2a	3213	1/1	0.93	0.10	71,71,71,71	0
56	MG	2A	3317	1/1	0.93	0.26	36,36,36,36	0
56	MG	2a	3075	1/1	0.93	0.11	59,59,59,59	0
56	MG	2A	3473	1/1	0.93	0.17	41,41,41,41	0
56	MG	1A	4033	1/1	0.93	0.17	62,62,62,62	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	1U	203	1/1	0.93	0.16	29,29,29,29	0
56	MG	1A	3807	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	3697	1/1	0.93	0.11	41,41,41,41	0
56	MG	1A	3682	1/1	0.93	0.23	29,29,29,29	0
56	MG	1A	3282	1/1	0.93	0.22	54,54,54,54	0
56	MG	2A	3440	1/1	0.93	0.12	50,50,50,50	0
56	MG	2A	3241	1/1	0.93	0.15	56,56,56,56	0
56	MG	1A	3588	1/1	0.93	0.19	60,60,60,60	0
56	MG	1A	3178	1/1	0.93	0.12	37,37,37,37	0
56	MG	2A	3453	1/1	0.93	0.12	31,31,31,31	0
56	MG	1A	3049	1/1	0.93	0.10	37,37,37,37	0
56	MG	2a	3136	1/1	0.93	0.30	56,56,56,56	0
56	MG	2x	103	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3199	1/1	0.93	0.29	44,44,44,44	0
56	MG	1A	3650	1/1	0.93	0.12	28,28,28,28	0
56	MG	1A	3127	1/1	0.93	0.23	40,40,40,40	0
56	MG	2A	3352	1/1	0.93	0.19	38,38,38,38	0
56	MG	1A	3060	1/1	0.93	0.17	46,46,46,46	0
56	MG	1a	1810	1/1	0.93	0.18	59,59,59,59	0
56	MG	1A	3474	1/1	0.93	0.13	58,58,58,58	0
56	MG	1Q	209	1/1	0.93	0.21	59,59,59,59	0
56	MG	1A	3364	1/1	0.93	0.32	64,64,64,64	0
56	MG	1x	110	1/1	0.93	0.28	73,73,73,73	0
56	MG	2A	3189	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3270	1/1	0.93	0.31	41,41,41,41	0
56	MG	1A	3235	1/1	0.93	0.10	53,53,53,53	0
56	MG	1A	3618	1/1	0.93	0.09	68,68,68,68	0
56	MG	1A	3067	1/1	0.93	0.25	56,56,56,56	0
56	MG	1Q	204	1/1	0.93	0.21	45,45,45,45	0
56	MG	1A	3213	1/1	0.93	0.36	44,44,44,44	0
56	MG	10	104	1/1	0.93	0.10	47,47,47,47	0
56	MG	2A	3272	1/1	0.93	0.22	67,67,67,67	0
56	MG	2A	3471	1/1	0.93	0.23	63,63,63,63	0
56	MG	1A	3035	1/1	0.93	0.32	44,44,44,44	0
56	MG	1A	3780	1/1	0.93	0.19	26,26,26,26	0
56	MG	1a	1776	1/1	0.94	0.19	67,67,67,67	0
56	MG	2A	3217	1/1	0.94	0.15	41,41,41,41	0
56	MG	2A	3017	1/1	0.94	0.35	46,46,46,46	0
56	MG	2A	3327	1/1	0.94	0.14	44,44,44,44	0
56	MG	1A	3786	1/1	0.94	0.21	23,23,23,23	0
56	MG	2A	3497	1/1	0.94	0.16	46,46,46,46	0
56	MG	1a	1779	1/1	0.94	0.22	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	1A	3343	1/1	0.94	0.11	55,55,55,55	0
56	MG	1A	3787	1/1	0.94	0.18	26,26,26,26	0
56	MG	2A	3555	1/1	0.94	0.34	49,49,49,49	0
56	MG	2A	3376	1/1	0.94	0.17	19,19,19,19	0
56	MG	15	103	1/1	0.94	0.29	28,28,28,28	0
56	MG	1A	3805	1/1	0.94	0.16	49,49,49,49	0
56	MG	2A	3187	1/1	0.94	0.23	40,40,40,40	0
56	MG	1A	3141	1/1	0.94	0.24	39,39,39,39	0
56	MG	2A	3542	1/1	0.94	0.12	56,56,56,56	0
56	MG	1D	303	1/1	0.94	0.18	38,38,38,38	0
56	MG	2a	3099	1/1	0.94	0.30	41,41,41,41	0
56	MG	2A	3033	1/1	0.94	0.20	47,47,47,47	0
56	MG	2A	3228	1/1	0.94	0.11	44,44,44,44	0
56	MG	1B	226	1/1	0.94	0.16	71,71,71,71	0
56	MG	2a	3248	1/1	0.94	0.20	56,56,56,56	0
56	MG	2a	3158	1/1	0.94	0.22	65,65,65,65	0
56	MG	1A	3763	1/1	0.94	0.15	42,42,42,42	0
56	MG	2a	3032	1/1	0.94	0.27	59,59,59,59	0
56	MG	2l	3005	1/1	0.94	0.21	44,44,44,44	0
56	MG	1A	3853	1/1	0.94	0.11	35,35,35,35	0
56	MG	2A	3170	1/1	0.94	0.20	33,33,33,33	0
56	MG	2A	3304	1/1	0.94	0.09	66,66,66,66	0
56	MG	2A	3043	1/1	0.94	0.12	42,42,42,42	0
56	MG	2A	3539	1/1	0.94	0.17	57,57,57,57	0
56	MG	1A	3203	1/1	0.94	0.40	47,47,47,47	0
56	MG	1A	3274	1/1	0.94	0.22	47,47,47,47	0
56	MG	1A	3806	1/1	0.94	0.12	38,38,38,38	0
56	MG	2A	3452	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3071	1/1	0.94	0.47	37,37,37,37	0
56	MG	1A	3135	1/1	0.94	0.29	30,30,30,30	0
56	MG	2A	3515	1/1	0.94	0.14	55,55,55,55	0
56	MG	1A	3898	1/1	0.94	0.17	52,52,52,52	0
56	MG	2a	3207	1/1	0.94	0.08	59,59,59,59	0
56	MG	1B	229	1/1	0.94	0.12	36,36,36,36	0
56	MG	1l	101	1/1	0.94	0.20	50,50,50,50	0
56	MG	1W	3001	1/1	0.94	0.22	53,53,53,53	0
56	MG	1A	3044	1/1	0.94	0.35	60,60,60,60	0
56	MG	2a	3131	1/1	0.94	0.40	48,48,48,48	0
56	MG	1H	3001	1/1	0.94	0.26	35,35,35,35	0
56	MG	16	102	1/1	0.94	0.17	40,40,40,40	0
56	MG	2A	3066	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	3637	1/1	0.94	0.11	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	3228	1/1	0.94	0.26	58,58,58,58	0
56	MG	1A	3215	1/1	0.94	0.21	49,49,49,49	0
56	MG	1A	3312	1/1	0.94	0.18	41,41,41,41	0
56	MG	2a	3247	1/1	0.94	0.30	50,50,50,50	0
56	MG	1A	3758	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3922	1/1	0.94	0.18	25,25,25,25	0
56	MG	1A	3730	1/1	0.94	0.13	34,34,34,34	0
56	MG	2a	3222	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3013	1/1	0.94	0.24	43,43,43,43	0
56	MG	10	101	1/1	0.94	0.24	49,49,49,49	0
57	ZN	2Y	501	1/1	0.94	0.06	99,99,99,99	0
56	MG	2A	3047	1/1	0.94	0.18	37,37,37,37	0
56	MG	1a	1642	1/1	0.94	0.06	58,58,58,58	0
56	MG	1A	3183	1/1	0.94	0.31	28,28,28,28	0
56	MG	2A	3070	1/1	0.94	0.60	53,53,53,53	0
56	MG	1A	4002	1/1	0.94	0.12	65,65,65,65	0
56	MG	1A	3934	1/1	0.94	0.17	35,35,35,35	0
56	MG	1A	3009	1/1	0.94	0.38	42,42,42,42	0
56	MG	1A	3537	1/1	0.94	0.17	53,53,53,53	0
56	MG	2A	3129	1/1	0.94	0.19	33,33,33,33	0
56	MG	1A	3797	1/1	0.94	0.09	28,28,28,28	0
56	MG	1A	3419	1/1	0.94	0.39	52,52,52,52	0
56	MG	2A	3491	1/1	0.94	0.19	46,46,46,46	0
56	MG	1A	3362	1/1	0.94	0.20	49,49,49,49	0
56	MG	1A	3541	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3413	1/1	0.94	0.15	60,60,60,60	0
56	MG	2r	3001	1/1	0.94	0.15	55,55,55,55	0
56	MG	1a	1822	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3635	1/1	0.94	0.11	50,50,50,50	0
56	MG	1A	3258	1/1	0.94	0.20	63,63,63,63	0
56	MG	1A	3268	1/1	0.94	0.31	23,23,23,23	0
56	MG	2a	3097	1/1	0.94	0.29	55,55,55,55	0
56	MG	1a	1662	1/1	0.94	0.17	60,60,60,60	0
56	MG	2a	3186	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	4023	1/1	0.94	0.17	52,52,52,52	0
56	MG	1A	4070	1/1	0.94	0.24	47,47,47,47	0
56	MG	1A	3812	1/1	0.94	0.07	48,48,48,48	0
56	MG	2A	3537	1/1	0.94	0.26	47,47,47,47	0
56	MG	1A	3332	1/1	0.94	0.29	35,35,35,35	0
56	MG	1A	3070	1/1	0.94	0.45	48,48,48,48	0
56	MG	1A	3952	1/1	0.94	0.14	40,40,40,40	0
56	MG	1A	3308	1/1	0.94	0.40	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	3487	1/1	0.94	0.10	40,40,40,40	0
56	MG	1W	3004	1/1	0.94	0.17	40,40,40,40	0
56	MG	2A	3061	1/1	0.94	0.12	29,29,29,29	0
56	MG	1A	3590	1/1	0.94	0.18	51,51,51,51	0
56	MG	1A	3539	1/1	0.94	0.11	45,45,45,45	0
56	MG	1a	1729	1/1	0.94	0.17	75,75,75,75	0
56	MG	1A	3033	1/1	0.94	0.14	50,50,50,50	0
56	MG	1D	301	1/1	0.94	0.19	32,32,32,32	0
56	MG	1A	3909	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	4024	1/1	0.94	0.21	39,39,39,39	0
56	MG	2A	3404	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3253	1/1	0.94	0.23	32,32,32,32	0
56	MG	1A	4011	1/1	0.94	0.18	68,68,68,68	0
56	MG	2A	3032	1/1	0.94	0.08	62,62,62,62	0
56	MG	1A	3097	1/1	0.94	0.25	49,49,49,49	0
56	MG	2a	3074	1/1	0.94	0.36	47,47,47,47	0
56	MG	2a	3181	1/1	0.94	0.15	58,58,58,58	0
56	MG	1A	3561	1/1	0.94	0.09	72,72,72,72	0
56	MG	1A	3149	1/1	0.94	0.39	32,32,32,32	0
56	MG	1A	3305	1/1	0.94	0.12	50,50,50,50	0
56	MG	1A	3374	1/1	0.94	0.27	26,26,26,26	0
56	MG	1A	3859	1/1	0.94	0.13	52,52,52,52	0
56	MG	1a	1646	1/1	0.94	0.30	80,80,80,80	0
56	MG	2A	3345	1/1	0.94	0.10	60,60,60,60	0
56	MG	1a	1740	1/1	0.94	0.20	63,63,63,63	0
56	MG	1A	3878	1/1	0.94	0.15	37,37,37,37	0
56	MG	2a	3126	1/1	0.94	0.23	60,60,60,60	0
56	MG	1A	3371	1/1	0.94	0.18	46,46,46,46	0
56	MG	1A	3553	1/1	0.94	0.32	63,63,63,63	0
56	MG	1A	4032	1/1	0.94	0.13	38,38,38,38	0
56	MG	1a	1775	1/1	0.94	0.18	65,65,65,65	0
56	MG	2A	3513	1/1	0.94	0.31	26,26,26,26	0
56	MG	1a	1821	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3216	1/1	0.94	0.45	44,44,44,44	0
56	MG	1A	3619	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3110	1/1	0.94	0.26	65,65,65,65	0
56	MG	1B	203	1/1	0.94	0.12	39,39,39,39	0
56	MG	1B	207	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3103	1/1	0.94	0.11	46,46,46,46	0
56	MG	1a	1828	1/1	0.94	0.15	70,70,70,70	0
56	MG	1A	3444	1/1	0.94	0.23	57,57,57,57	0
56	MG	1A	3420	1/1	0.94	0.16	54,54,54,54	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	3077	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	4009	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3906	1/1	0.94	0.12	53,53,53,53	0
56	MG	1a	1848	1/1	0.94	0.23	77,77,77,77	0
56	MG	2z	8001	1/1	0.94	0.25	69,69,69,69	0
56	MG	2a	3090	1/1	0.94	0.37	47,47,47,47	0
56	MG	2a	3195	1/1	0.94	0.17	48,48,48,48	0
56	MG	1a	1695	1/1	0.94	0.24	53,53,53,53	0
56	MG	1A	3729	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	4003	1/1	0.94	0.21	44,44,44,44	0
56	MG	2Q	3004	1/1	0.94	0.28	41,41,41,41	0
56	MG	1A	3058	1/1	0.94	0.26	45,45,45,45	0
56	MG	1a	1870	1/1	0.94	0.17	75,75,75,75	0
56	MG	1A	3748	1/1	0.94	0.21	13,13,13,13	0
56	MG	1a	1887	1/1	0.94	0.26	47,47,47,47	0
56	MG	1A	3665	1/1	0.94	0.24	24,24,24,24	0
56	MG	2A	3250	1/1	0.94	0.26	30,30,30,30	0
56	MG	1A	3913	1/1	0.94	0.08	28,28,28,28	0
56	MG	1A	3144	1/1	0.94	0.34	48,48,48,48	0
57	ZN	1n	101	1/1	0.94	0.10	83,83,83,83	0
56	MG	2A	3048	1/1	0.94	0.14	45,45,45,45	0
56	MG	1A	3249	1/1	0.94	0.10	20,20,20,20	0
56	MG	2A	3149	1/1	0.94	0.24	63,63,63,63	0
56	MG	2a	3227	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3831	1/1	0.94	0.13	18,18,18,18	0
56	MG	2A	3027	1/1	0.94	0.07	56,56,56,56	0
56	MG	2A	3080	1/1	0.94	0.23	59,59,59,59	0
56	MG	1a	1768	1/1	0.94	0.25	56,56,56,56	0
56	MG	1a	1799	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3800	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	3629	1/1	0.94	0.15	33,33,33,33	0
56	MG	1A	3262	1/1	0.94	0.20	28,28,28,28	0
56	MG	1A	3712	1/1	0.94	0.24	56,56,56,56	0
56	MG	2A	3460	1/1	0.94	0.08	45,45,45,45	0
56	MG	2A	3016	1/1	0.94	0.29	51,51,51,51	0
56	MG	2A	3167	1/1	0.94	0.22	45,45,45,45	0
56	MG	2A	3425	1/1	0.94	0.09	48,48,48,48	0
56	MG	1A	3634	1/1	0.94	0.35	38,38,38,38	0
56	MG	1A	3708	1/1	0.94	0.16	59,59,59,59	0
56	MG	1a	1682	1/1	0.94	0.06	47,47,47,47	0
56	MG	1A	3919	1/1	0.94	0.10	51,51,51,51	0
56	MG	1a	1614	1/1	0.94	0.10	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	3042	1/1	0.94	0.25	46,46,46,46	0
56	MG	2A	3229	1/1	0.94	0.21	59,59,59,59	0
56	MG	2a	3116	1/1	0.94	0.13	45,45,45,45	0
56	MG	1a	1766	1/1	0.94	0.16	50,50,50,50	0
56	MG	1a	1893	1/1	0.94	0.37	69,69,69,69	0
56	MG	1A	3854	1/1	0.94	0.10	42,42,42,42	0
56	MG	2A	3525	1/1	0.94	0.39	36,36,36,36	0
56	MG	1a	1839	1/1	0.94	0.24	53,53,53,53	0
56	MG	2A	3132	1/1	0.94	0.11	45,45,45,45	0
56	MG	1a	1728	1/1	0.94	0.15	46,46,46,46	0
56	MG	1A	3217	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3752	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3794	1/1	0.94	0.18	19,19,19,19	0
56	MG	2a	3196	1/1	0.94	0.13	70,70,70,70	0
56	MG	1a	1654	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3429	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3111	1/1	0.94	0.20	36,36,36,36	0
56	MG	2A	3162	1/1	0.94	0.13	40,40,40,40	0
56	MG	2A	3320	1/1	0.94	0.22	53,53,53,53	0
56	MG	1x	106	1/1	0.94	0.07	42,42,42,42	0
56	MG	2A	3552	1/1	0.94	0.37	44,44,44,44	0
56	MG	1x	103	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	3646	1/1	0.94	0.18	65,65,65,65	0
56	MG	2D	305	1/1	0.94	0.30	29,29,29,29	0
56	MG	2a	3250	1/1	0.94	0.18	63,63,63,63	0
56	MG	2a	3127	1/1	0.94	0.21	50,50,50,50	0
56	MG	1A	3651	1/1	0.94	0.15	14,14,14,14	0
56	MG	1A	3747	1/1	0.94	0.36	50,50,50,50	0
56	MG	2F	301	1/1	0.94	0.18	49,49,49,49	0
56	MG	1A	4012	1/1	0.94	0.14	47,47,47,47	0
56	MG	1A	3734	1/1	0.94	0.19	46,46,46,46	0
56	MG	2A	3231	1/1	0.94	0.28	57,57,57,57	0
56	MG	1A	3621	1/1	0.94	0.18	40,40,40,40	0
56	MG	1A	3003	1/1	0.94	0.16	44,44,44,44	0
56	MG	1A	3259	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3370	1/1	0.94	0.12	49,49,49,49	0
56	MG	1a	1732	1/1	0.94	0.47	63,63,63,63	0
56	MG	1A	3519	1/1	0.94	0.18	48,48,48,48	0
56	MG	2A	3516	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3165	1/1	0.94	0.25	23,23,23,23	0
56	MG	13	101	1/1	0.94	0.21	47,47,47,47	0
56	MG	1A	3323	1/1	0.94	0.15	41,41,41,41	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	1801	1/1	0.94	0.12	65,65,65,65	0
56	MG	1a	1679	1/1	0.94	0.20	45,45,45,45	0
56	MG	2A	3259	1/1	0.94	0.13	39,39,39,39	0
56	MG	1A	3610	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	3829	1/1	0.94	0.13	18,18,18,18	0
56	MG	2A	3535	1/1	0.94	0.06	52,52,52,52	0
56	MG	1A	3679	1/1	0.94	0.12	38,38,38,38	0
56	MG	2A	3302	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3466	1/1	0.94	0.13	45,45,45,45	0
56	MG	2A	3479	1/1	0.94	0.25	47,47,47,47	0
56	MG	1A	3079	1/1	0.94	0.20	53,53,53,53	0
56	MG	1A	3302	1/1	0.94	0.22	59,59,59,59	0
56	MG	1A	3423	1/1	0.94	0.15	42,42,42,42	0
56	MG	1T	204	1/1	0.94	0.10	50,50,50,50	0
56	MG	2A	3200	1/1	0.94	0.20	50,50,50,50	0
56	MG	2B	201	1/1	0.94	0.18	57,57,57,57	0
56	MG	1A	3239	1/1	0.94	0.14	50,50,50,50	0
56	MG	1a	1638	1/1	0.94	0.18	52,52,52,52	0
56	MG	1A	3589	1/1	0.94	0.12	36,36,36,36	0
56	MG	2A	3526	1/1	0.94	0.09	50,50,50,50	0
56	MG	1A	3985	1/1	0.94	0.16	34,34,34,34	0
56	MG	2A	3234	1/1	0.94	0.11	65,65,65,65	0
56	MG	1A	3353	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3105	1/1	0.94	0.35	47,47,47,47	0
56	MG	2A	3296	1/1	0.94	0.29	57,57,57,57	0
56	MG	1A	3733	1/1	0.94	0.26	49,49,49,49	0
56	MG	1A	3718	1/1	0.94	0.15	36,36,36,36	0
56	MG	1A	3340	1/1	0.94	0.08	59,59,59,59	0
56	MG	1A	3207	1/1	0.94	0.25	42,42,42,42	0
56	MG	19	104	1/1	0.94	0.16	42,42,42,42	0
56	MG	1A	3077	1/1	0.94	0.26	48,48,48,48	0
56	MG	1A	3010	1/1	0.94	0.12	66,66,66,66	0
56	MG	1A	3833	1/1	0.94	0.11	50,50,50,50	0
56	MG	1a	1844	1/1	0.94	0.24	56,56,56,56	0
56	MG	1A	3080	1/1	0.94	0.07	53,53,53,53	0
56	MG	2a	3152	1/1	0.94	0.09	67,67,67,67	0
56	MG	1A	3372	1/1	0.95	0.12	50,50,50,50	0
56	MG	1a	1651	1/1	0.95	0.17	62,62,62,62	0
56	MG	2A	3387	1/1	0.95	0.26	38,38,38,38	0
56	MG	1A	3743	1/1	0.95	0.12	30,30,30,30	0
56	MG	2A	3137	1/1	0.95	0.17	33,33,33,33	0
56	MG	1A	3375	1/1	0.95	0.11	44,44,44,44	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	3389	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3884	1/1	0.95	0.15	58,58,58,58	0
56	MG	1A	3874	1/1	0.95	0.11	28,28,28,28	0
56	MG	1a	1689	1/1	0.95	0.15	48,48,48,48	0
56	MG	1A	3660	1/1	0.95	0.12	24,24,24,24	0
56	MG	1A	3782	1/1	0.95	0.13	19,19,19,19	0
56	MG	1A	4040	1/1	0.95	0.15	32,32,32,32	0
56	MG	2a	3073	1/1	0.95	0.10	63,63,63,63	0
56	MG	1a	1631	1/1	0.95	0.15	44,44,44,44	0
56	MG	2A	3457	1/1	0.95	0.28	46,46,46,46	0
56	MG	1A	4014	1/1	0.95	0.19	57,57,57,57	0
56	MG	1a	1846	1/1	0.95	0.10	25,25,25,25	0
56	MG	2a	3208	1/1	0.95	0.12	65,65,65,65	0
56	MG	1A	3902	1/1	0.95	0.15	42,42,42,42	0
56	MG	1A	3363	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	3757	1/1	0.95	0.12	49,49,49,49	0
56	MG	1A	3702	1/1	0.95	0.12	20,20,20,20	0
56	MG	1A	3157	1/1	0.95	0.22	43,43,43,43	0
56	MG	1A	3945	1/1	0.95	0.26	30,30,30,30	0
56	MG	2A	3521	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3174	1/1	0.95	0.17	56,56,56,56	0
56	MG	2A	3006	1/1	0.95	0.19	59,59,59,59	0
56	MG	1A	3966	1/1	0.95	0.17	19,19,19,19	0
56	MG	2a	3156	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3710	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3910	1/1	0.95	0.12	61,61,61,61	0
56	MG	1E	312	1/1	0.95	0.17	44,44,44,44	0
56	MG	1A	3761	1/1	0.95	0.19	67,67,67,67	0
56	MG	1A	3285	1/1	0.95	0.31	32,32,32,32	0
56	MG	1A	4039	1/1	0.95	0.08	56,56,56,56	0
56	MG	2A	3222	1/1	0.95	0.10	62,62,62,62	0
56	MG	2A	3109	1/1	0.95	0.26	54,54,54,54	0
56	MG	2A	3517	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	3672	1/1	0.95	0.23	29,29,29,29	0
56	MG	1a	1845	1/1	0.95	0.14	62,62,62,62	0
56	MG	2A	3115	1/1	0.95	0.16	41,41,41,41	0
56	MG	1A	3603	1/1	0.95	0.14	62,62,62,62	0
56	MG	1A	3720	1/1	0.95	0.17	45,45,45,45	0
56	MG	1a	1705	1/1	0.95	0.05	58,58,58,58	0
56	MG	1a	1670	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3284	1/1	0.95	0.11	52,52,52,52	0
56	MG	2a	3183	1/1	0.95	0.08	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	2A	3500	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3421	1/1	0.95	0.30	38,38,38,38	0
56	MG	1A	3685	1/1	0.95	0.18	16,16,16,16	0
56	MG	1a	1864	1/1	0.95	0.46	69,69,69,69	0
56	MG	1a	1805	1/1	0.95	0.14	61,61,61,61	0
56	MG	1U	206	1/1	0.95	0.38	38,38,38,38	0
56	MG	1A	4085	1/1	0.95	0.58	34,34,34,34	0
56	MG	1A	3247	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3240	1/1	0.95	0.16	32,32,32,32	0
56	MG	1A	3564	1/1	0.95	0.25	36,36,36,36	0
56	MG	1A	3654	1/1	0.95	0.12	44,44,44,44	0
56	MG	1Q	201	1/1	0.95	0.25	33,33,33,33	0
56	MG	2A	3536	1/1	0.95	0.14	42,42,42,42	0
56	MG	2D	301	1/1	0.95	0.11	49,49,49,49	0
56	MG	2A	3349	1/1	0.95	0.07	67,67,67,67	0
56	MG	1A	3587	1/1	0.95	0.25	42,42,42,42	0
56	MG	2A	3383	1/1	0.95	0.14	29,29,29,29	0
56	MG	1A	4068	1/1	0.95	0.24	39,39,39,39	0
56	MG	1a	1666	1/1	0.95	0.17	72,72,72,72	0
56	MG	1A	3976	1/1	0.95	0.21	42,42,42,42	0
56	MG	1P	205	1/1	0.95	0.18	53,53,53,53	0
56	MG	2A	3428	1/1	0.95	0.14	59,59,59,59	0
56	MG	2A	3278	1/1	0.95	0.27	43,43,43,43	0
56	MG	1A	3889	1/1	0.95	0.17	55,55,55,55	0
56	MG	1A	3059	1/1	0.95	0.27	32,32,32,32	0
56	MG	1A	3740	1/1	0.95	0.28	68,68,68,68	0
56	MG	1A	3598	1/1	0.95	0.17	30,30,30,30	0
56	MG	2A	3091	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	4082	1/1	0.95	0.11	66,66,66,66	0
56	MG	1A	3630	1/1	0.95	0.17	37,37,37,37	0
56	MG	1A	3470	1/1	0.95	0.11	51,51,51,51	0
56	MG	2A	3086	1/1	0.95	0.22	47,47,47,47	0
56	MG	1A	3445	1/1	0.95	0.12	46,46,46,46	0
56	MG	1a	1657	1/1	0.95	0.25	62,62,62,62	0
56	MG	2B	203	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3645	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	3566	1/1	0.95	0.22	34,34,34,34	0
56	MG	1A	3744	1/1	0.95	0.12	43,43,43,43	0
56	MG	2a	3232	1/1	0.95	0.12	54,54,54,54	0
56	MG	2A	3560	1/1	0.95	0.31	41,41,41,41	0
56	MG	1Y	502	1/1	0.95	0.12	40,40,40,40	0
56	MG	1A	3476	1/1	0.95	0.17	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	1a	1824	1/1	0.95	0.09	54,54,54,54	0
56	MG	1a	1675	1/1	0.95	0.09	42,42,42,42	0
56	MG	1a	1774	1/1	0.95	0.20	62,62,62,62	0
56	MG	1x	105	1/1	0.95	0.11	64,64,64,64	0
56	MG	1A	3164	1/1	0.95	0.14	40,40,40,40	0
56	MG	2A	3455	1/1	0.95	0.15	62,62,62,62	0
56	MG	1A	3234	1/1	0.95	0.05	46,46,46,46	0
56	MG	1A	3472	1/1	0.95	0.17	53,53,53,53	0
56	MG	1A	3066	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3565	1/1	0.95	0.31	41,41,41,41	0
56	MG	2a	3140	1/1	0.95	0.26	49,49,49,49	0
56	MG	1A	3776	1/1	0.95	0.18	31,31,31,31	0
56	MG	1A	3705	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3134	1/1	0.95	0.13	23,23,23,23	0
56	MG	2R	201	1/1	0.95	0.36	49,49,49,49	0
56	MG	1A	3416	1/1	0.95	0.12	66,66,66,66	0
56	MG	1A	3483	1/1	0.95	0.16	41,41,41,41	0
56	MG	2A	3101	1/1	0.95	0.07	56,56,56,56	0
56	MG	2a	3008	1/1	0.95	0.09	53,53,53,53	0
56	MG	2A	3377	1/1	0.95	0.15	33,33,33,33	0
56	MG	1a	1643	1/1	0.95	0.08	68,68,68,68	0
56	MG	1A	4013	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	3210	1/1	0.95	0.09	40,40,40,40	0
56	MG	2A	3371	1/1	0.95	0.12	52,52,52,52	0
56	MG	1A	3098	1/1	0.95	0.18	40,40,40,40	0
56	MG	1A	3971	1/1	0.95	0.12	27,27,27,27	0
56	MG	1A	3820	1/1	0.95	0.07	71,71,71,71	0
56	MG	2A	3490	1/1	0.95	0.17	66,66,66,66	0
56	MG	1a	1681	1/1	0.95	0.11	47,47,47,47	0
56	MG	2A	3119	1/1	0.95	0.27	35,35,35,35	0
56	MG	2A	3292	1/1	0.95	0.16	21,21,21,21	0
56	MG	1z	8001	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3947	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	3810	1/1	0.95	0.17	30,30,30,30	0
56	MG	2A	3236	1/1	0.95	0.08	60,60,60,60	0
56	MG	2Y	502	1/1	0.95	0.13	51,51,51,51	0
56	MG	1F	301	1/1	0.95	0.19	30,30,30,30	0
56	MG	1A	3001	1/1	0.95	0.24	31,31,31,31	0
56	MG	1a	1723	1/1	0.95	0.15	62,62,62,62	0
56	MG	1A	3745	1/1	0.95	0.09	57,57,57,57	0
56	MG	1A	3310	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	4017	1/1	0.95	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	2A	3209	1/1	0.95	0.43	54,54,54,54	0
56	MG	2A	3148	1/1	0.95	0.19	38,38,38,38	0
56	MG	1a	1625	1/1	0.95	0.12	34,34,34,34	0
56	MG	1E	306	1/1	0.95	0.34	57,57,57,57	0
56	MG	1A	3441	1/1	0.95	0.12	49,49,49,49	0
56	MG	1a	1652	1/1	0.95	0.20	60,60,60,60	0
56	MG	1A	3980	1/1	0.95	0.22	59,59,59,59	0
56	MG	2A	3285	1/1	0.95	0.12	33,33,33,33	0
56	MG	2A	3533	1/1	0.95	0.20	47,47,47,47	0
56	MG	1A	3995	1/1	0.95	0.31	54,54,54,54	0
56	MG	1A	4045	1/1	0.95	0.09	23,23,23,23	0
56	MG	1A	3339	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	4059	1/1	0.95	0.23	28,28,28,28	0
56	MG	2A	3163	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3819	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3440	1/1	0.95	0.15	39,39,39,39	0
56	MG	1a	1898	1/1	0.95	0.16	59,59,59,59	0
56	MG	1A	3658	1/1	0.95	0.13	13,13,13,13	0
56	MG	2A	3427	1/1	0.95	0.33	54,54,54,54	0
56	MG	2A	3191	1/1	0.95	0.16	37,37,37,37	0
56	MG	1A	3545	1/1	0.95	0.34	50,50,50,50	0
56	MG	2B	209	1/1	0.95	0.33	57,57,57,57	0
56	MG	2E	303	1/1	0.95	0.12	60,60,60,60	0
56	MG	2B	207	1/1	0.95	0.09	67,67,67,67	0
56	MG	2a	3220	1/1	0.95	0.25	85,85,85,85	0
56	MG	2A	3140	1/1	0.95	0.19	33,33,33,33	0
56	MG	1a	1875	1/1	0.95	0.05	58,58,58,58	0
56	MG	2A	3411	1/1	0.95	0.18	47,47,47,47	0
56	MG	1E	305	1/1	0.95	0.17	14,14,14,14	0
56	MG	1A	3168	1/1	0.95	0.19	35,35,35,35	0
56	MG	1A	3997	1/1	0.95	0.18	32,32,32,32	0
56	MG	2a	3170	1/1	0.95	0.22	72,72,72,72	0
56	MG	2a	3221	1/1	0.95	0.31	57,57,57,57	0
56	MG	1a	1626	1/1	0.95	0.52	68,68,68,68	0
56	MG	2a	3050	1/1	0.95	0.13	86,86,86,86	0
56	MG	1A	3944	1/1	0.95	0.38	39,39,39,39	0
56	MG	1A	3299	1/1	0.95	0.44	59,59,59,59	0
56	MG	2a	3066	1/1	0.95	0.38	64,64,64,64	0
56	MG	1A	3131	1/1	0.95	0.22	31,31,31,31	0
56	MG	1A	3244	1/1	0.95	0.16	35,35,35,35	0
56	MG	1a	1881	1/1	0.95	0.24	52,52,52,52	0
56	MG	1a	1894	1/1	0.95	0.29	63,63,63,63	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	2T	201	1/1	0.95	0.19	41,41,41,41	0
56	MG	2A	3098	1/1	0.95	0.17	41,41,41,41	0
56	MG	1A	3434	1/1	0.95	0.13	50,50,50,50	0
56	MG	1a	1879	1/1	0.95	0.09	52,52,52,52	0
56	MG	1E	308	1/1	0.95	0.38	35,35,35,35	0
56	MG	1A	3018	1/1	0.95	0.22	53,53,53,53	0
56	MG	1a	1607	1/1	0.95	0.11	60,60,60,60	0
56	MG	1a	1688	1/1	0.95	0.12	61,61,61,61	0
56	MG	1Q	205	1/1	0.95	0.15	40,40,40,40	0
56	MG	2A	3464	1/1	0.95	0.12	35,35,35,35	0
56	MG	1A	3148	1/1	0.95	0.29	51,51,51,51	0
56	MG	1A	3055	1/1	0.95	0.39	45,45,45,45	0
56	MG	2O	201	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3602	1/1	0.95	0.09	41,41,41,41	0
56	MG	1A	3068	1/1	0.95	0.25	45,45,45,45	0
56	MG	2A	3096	1/1	0.95	0.18	47,47,47,47	0
56	MG	2A	3303	1/1	0.95	0.20	30,30,30,30	0
56	MG	1A	3347	1/1	0.95	0.19	56,56,56,56	0
56	MG	2A	3138	1/1	0.95	0.23	47,47,47,47	0
56	MG	1A	3870	1/1	0.95	0.14	44,44,44,44	0
56	MG	1a	1672	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	3633	1/1	0.95	0.17	50,50,50,50	0
56	MG	2A	3508	1/1	0.95	0.20	42,42,42,42	0
56	MG	2a	3204	1/1	0.95	0.13	57,57,57,57	0
56	MG	2a	3134	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	3231	1/1	0.95	0.14	42,42,42,42	0
56	MG	2A	3405	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3891	1/1	0.95	0.26	68,68,68,68	0
57	ZN	26	501	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3245	1/1	0.95	0.20	18,18,18,18	0
56	MG	1A	4007	1/1	0.95	0.23	35,35,35,35	0
56	MG	1A	3864	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3599	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3830	1/1	0.95	0.09	34,34,34,34	0
56	MG	2A	3179	1/1	0.95	0.34	29,29,29,29	0
56	MG	2A	3024	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3341	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3606	1/1	0.95	0.21	28,28,28,28	0
56	MG	2A	3551	1/1	0.95	0.17	32,32,32,32	0
56	MG	2a	3169	1/1	0.95	0.18	67,67,67,67	0
56	MG	1A	3457	1/1	0.95	0.07	61,61,61,61	0
56	MG	2A	3168	1/1	0.95	0.19	33,33,33,33	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	3620	1/1	0.95	0.10	55,55,55,55	0
56	MG	2a	3243	1/1	0.95	0.26	74,74,74,74	0
56	MG	1a	1873	1/1	0.95	0.15	60,60,60,60	0
56	MG	2A	3130	1/1	0.95	0.22	49,49,49,49	0
56	MG	1A	3597	1/1	0.95	0.10	71,71,71,71	0
56	MG	1A	3073	1/1	0.95	0.15	46,46,46,46	0
56	MG	2A	3509	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3877	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3288	1/1	0.96	0.44	42,42,42,42	0
56	MG	1a	1785	1/1	0.96	0.13	60,60,60,60	0
56	MG	2a	3174	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3223	1/1	0.96	0.19	29,29,29,29	0
56	MG	1a	1831	1/1	0.96	0.12	84,84,84,84	0
56	MG	2a	3080	1/1	0.96	0.28	55,55,55,55	0
56	MG	1a	1842	1/1	0.96	0.37	48,48,48,48	0
56	MG	2A	3227	1/1	0.96	0.20	38,38,38,38	0
56	MG	1a	1706	1/1	0.96	0.20	52,52,52,52	0
56	MG	1A	3939	1/1	0.96	0.20	19,19,19,19	0
56	MG	1A	3521	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3638	1/1	0.96	0.20	38,38,38,38	0
56	MG	2A	3322	1/1	0.96	0.15	49,49,49,49	0
56	MG	2A	3468	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3191	1/1	0.96	0.12	28,28,28,28	0
56	MG	2A	3399	1/1	0.96	0.34	64,64,64,64	0
56	MG	1A	3021	1/1	0.96	0.24	56,56,56,56	0
56	MG	1A	3839	1/1	0.96	0.10	18,18,18,18	0
56	MG	1A	3392	1/1	0.96	0.14	33,33,33,33	0
56	MG	1A	3972	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3153	1/1	0.96	0.21	20,20,20,20	0
56	MG	1A	3280	1/1	0.96	0.06	43,43,43,43	0
56	MG	1a	1721	1/1	0.96	0.07	45,45,45,45	0
56	MG	2A	3309	1/1	0.96	0.17	37,37,37,37	0
56	MG	2A	3444	1/1	0.96	0.10	63,63,63,63	0
56	MG	1A	3746	1/1	0.96	0.09	46,46,46,46	0
56	MG	1A	3816	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3798	1/1	0.96	0.14	19,19,19,19	0
56	MG	1A	3169	1/1	0.96	0.14	55,55,55,55	0
56	MG	2A	3381	1/1	0.96	0.28	41,41,41,41	0
56	MG	1A	3766	1/1	0.96	0.18	37,37,37,37	0
56	MG	1A	3653	1/1	0.96	0.22	48,48,48,48	0
56	MG	1A	3932	1/1	0.96	0.06	59,59,59,59	0
56	MG	2a	3190	1/1	0.96	0.11	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3046	1/1	0.96	0.20	45,45,45,45	0
56	MG	1A	3571	1/1	0.96	0.20	32,32,32,32	0
57	ZN	15	101	1/1	0.96	0.15	54,54,54,54	0
56	MG	1A	3171	1/1	0.96	0.29	51,51,51,51	0
56	MG	1A	3114	1/1	0.96	0.27	48,48,48,48	0
56	MG	2a	3216	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3879	1/1	0.96	0.11	49,49,49,49	0
56	MG	2a	3251	1/1	0.96	0.34	43,43,43,43	0
56	MG	2A	3532	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3460	1/1	0.96	0.25	52,52,52,52	0
56	MG	18	3003	1/1	0.96	0.22	35,35,35,35	0
56	MG	2A	3037	1/1	0.96	0.20	42,42,42,42	0
56	MG	2A	3378	1/1	0.96	0.13	41,41,41,41	0
56	MG	1A	3818	1/1	0.96	0.16	59,59,59,59	0
56	MG	1a	1620	1/1	0.96	0.18	54,54,54,54	0
56	MG	2A	3400	1/1	0.96	0.15	48,48,48,48	0
56	MG	2e	3002	1/1	0.96	0.10	64,64,64,64	0
56	MG	1a	1883	1/1	0.96	0.13	53,53,53,53	0
56	MG	1a	1722	1/1	0.96	0.19	47,47,47,47	0
56	MG	1R	203	1/1	0.96	0.15	35,35,35,35	0
56	MG	2A	3458	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3442	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3576	1/1	0.96	0.08	65,65,65,65	0
56	MG	1A	3986	1/1	0.96	0.21	49,49,49,49	0
56	MG	1A	3611	1/1	0.96	0.13	35,35,35,35	0
56	MG	1A	3987	1/1	0.96	0.19	58,58,58,58	0
56	MG	1a	1788	1/1	0.96	0.19	51,51,51,51	0
56	MG	1A	3727	1/1	0.96	0.16	49,49,49,49	0
56	MG	1a	1826	1/1	0.96	0.13	59,59,59,59	0
56	MG	1A	3159	1/1	0.96	0.21	36,36,36,36	0
56	MG	1A	3155	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3410	1/1	0.96	0.11	42,42,42,42	0
56	MG	1a	1859	1/1	0.96	0.23	59,59,59,59	0
56	MG	1A	3401	1/1	0.96	0.16	30,30,30,30	0
56	MG	1A	3918	1/1	0.96	0.12	61,61,61,61	0
56	MG	1A	3809	1/1	0.96	0.17	33,33,33,33	0
56	MG	2A	3221	1/1	0.96	0.20	39,39,39,39	0
56	MG	2a	3027	1/1	0.96	0.22	47,47,47,47	0
56	MG	2A	3324	1/1	0.96	0.05	43,43,43,43	0
56	MG	1A	3126	1/1	0.96	0.11	27,27,27,27	0
56	MG	2a	3063	1/1	0.96	0.32	85,85,85,85	0
56	MG	1a	1609	1/1	0.96	0.22	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	3540	1/1	0.96	0.23	46,46,46,46	0
56	MG	1A	3528	1/1	0.96	0.21	42,42,42,42	0
56	MG	1A	3542	1/1	0.96	0.38	63,63,63,63	0
56	MG	1A	3459	1/1	0.96	0.29	49,49,49,49	0
56	MG	1A	3431	1/1	0.96	0.13	43,43,43,43	0
56	MG	2A	3313	1/1	0.96	0.17	46,46,46,46	0
56	MG	1A	3160	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3881	1/1	0.96	0.07	64,64,64,64	0
56	MG	2A	3118	1/1	0.96	0.40	52,52,52,52	0
56	MG	1a	1856	1/1	0.96	0.11	41,41,41,41	0
56	MG	2a	3112	1/1	0.96	0.30	53,53,53,53	0
56	MG	1A	3054	1/1	0.96	0.29	53,53,53,53	0
56	MG	1A	3315	1/1	0.96	0.24	65,65,65,65	0
56	MG	2A	3511	1/1	0.96	0.21	40,40,40,40	0
56	MG	2a	3192	1/1	0.96	0.11	61,61,61,61	0
56	MG	1a	1804	1/1	0.96	0.24	37,37,37,37	0
56	MG	1A	3170	1/1	0.96	0.16	25,25,25,25	0
56	MG	1B	222	1/1	0.96	0.09	59,59,59,59	0
56	MG	2A	3407	1/1	0.96	0.22	46,46,46,46	0
56	MG	1A	3506	1/1	0.96	0.49	75,75,75,75	0
56	MG	1A	3692	1/1	0.96	0.19	18,18,18,18	0
56	MG	2A	3215	1/1	0.96	0.26	31,31,31,31	0
56	MG	1A	3751	1/1	0.96	0.10	74,74,74,74	0
56	MG	1A	3739	1/1	0.96	0.18	34,34,34,34	0
56	MG	1A	4022	1/1	0.96	0.15	43,43,43,43	0
56	MG	1A	3792	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3195	1/1	0.96	0.24	44,44,44,44	0
56	MG	1B	215	1/1	0.96	0.20	74,74,74,74	0
56	MG	1A	3106	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3865	1/1	0.96	0.19	72,72,72,72	0
56	MG	1a	1637	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	3767	1/1	0.96	0.26	33,33,33,33	0
56	MG	1a	1613	1/1	0.96	0.10	77,77,77,77	0
56	MG	2a	3125	1/1	0.96	0.18	33,33,33,33	0
56	MG	1a	1658	1/1	0.96	0.13	58,58,58,58	0
56	MG	1A	3230	1/1	0.96	0.19	35,35,35,35	0
56	MG	2A	3390	1/1	0.96	0.16	35,35,35,35	0
56	MG	1A	3099	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3921	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3179	1/1	0.96	0.40	22,22,22,22	0
56	MG	1A	3783	1/1	0.96	0.17	28,28,28,28	0
56	MG	1A	3538	1/1	0.96	0.15	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	1702	1/1	0.96	0.14	60,60,60,60	0
56	MG	1A	3454	1/1	0.96	0.22	64,64,64,64	0
56	MG	2A	3300	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3924	1/1	0.96	0.18	52,52,52,52	0
56	MG	1A	3675	1/1	0.96	0.27	42,42,42,42	0
56	MG	1A	3975	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3068	1/1	0.96	0.10	52,52,52,52	0
56	MG	1A	3737	1/1	0.96	0.19	18,18,18,18	0
56	MG	2A	3079	1/1	0.96	0.08	50,50,50,50	0
56	MG	2A	3089	1/1	0.96	0.32	36,36,36,36	0
56	MG	1a	1896	1/1	0.96	0.39	46,46,46,46	0
56	MG	1A	4074	1/1	0.96	0.20	47,47,47,47	0
56	MG	1A	3681	1/1	0.96	0.13	19,19,19,19	0
56	MG	1A	3931	1/1	0.96	0.09	32,32,32,32	0
56	MG	2A	3493	1/1	0.96	0.11	39,39,39,39	0
56	MG	1V	201	1/1	0.96	0.31	39,39,39,39	0
56	MG	2A	3484	1/1	0.96	0.29	47,47,47,47	0
56	MG	1N	3006	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3861	1/1	0.96	0.05	42,42,42,42	0
56	MG	1A	3735	1/1	0.96	0.14	63,63,63,63	0
56	MG	2A	3325	1/1	0.96	0.11	48,48,48,48	0
56	MG	1Q	208	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3466	1/1	0.96	0.04	55,55,55,55	0
56	MG	1A	3572	1/1	0.96	0.11	52,52,52,52	0
56	MG	2A	3514	1/1	0.96	0.11	71,71,71,71	0
56	MG	1A	3817	1/1	0.96	0.17	40,40,40,40	0
56	MG	1A	4065	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	3781	1/1	0.96	0.08	24,24,24,24	0
56	MG	1A	3936	1/1	0.96	0.33	33,33,33,33	0
56	MG	1A	3706	1/1	0.96	0.10	15,15,15,15	0
56	MG	1A	3415	1/1	0.96	0.12	39,39,39,39	0
56	MG	2E	302	1/1	0.96	0.27	36,36,36,36	0
56	MG	1A	3866	1/1	0.96	0.21	42,42,42,42	0
56	MG	2A	3173	1/1	0.96	0.15	27,27,27,27	0
56	MG	1a	1665	1/1	0.96	0.15	50,50,50,50	0
56	MG	1h	8001	1/1	0.96	0.09	60,60,60,60	0
56	MG	1A	3627	1/1	0.96	0.19	41,41,41,41	0
56	MG	1A	3613	1/1	0.96	0.18	41,41,41,41	0
56	MG	2A	3527	1/1	0.96	0.22	39,39,39,39	0
56	MG	1A	3163	1/1	0.96	0.10	32,32,32,32	0
56	MG	1a	1902	1/1	0.96	0.10	62,62,62,62	0
56	MG	1a	1854	1/1	0.96	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	1612	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3224	1/1	0.96	0.17	33,33,33,33	0
56	MG	2a	3034	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	3863	1/1	0.96	0.19	38,38,38,38	0
56	MG	2A	3530	1/1	0.96	0.26	43,43,43,43	0
56	MG	2a	3062	1/1	0.96	0.11	81,81,81,81	0
56	MG	1W	3003	1/1	0.96	0.21	33,33,33,33	0
56	MG	1a	1674	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	3843	1/1	0.96	0.17	53,53,53,53	0
56	MG	2A	3051	1/1	0.96	0.24	35,35,35,35	0
56	MG	1a	1711	1/1	0.96	0.13	62,62,62,62	0
56	MG	2A	3143	1/1	0.96	0.03	41,41,41,41	0
56	MG	1R	206	1/1	0.96	0.19	32,32,32,32	0
56	MG	2A	3416	1/1	0.96	0.11	36,36,36,36	0
56	MG	1a	1892	1/1	0.96	0.19	58,58,58,58	0
56	MG	1A	3667	1/1	0.96	0.21	14,14,14,14	0
56	MG	1A	3717	1/1	0.96	0.25	55,55,55,55	0
56	MG	1W	3002	1/1	0.96	0.17	35,35,35,35	0
56	MG	1A	3640	1/1	0.96	0.24	38,38,38,38	0
56	MG	1a	1704	1/1	0.96	0.19	48,48,48,48	0
56	MG	1A	3214	1/1	0.96	0.22	34,34,34,34	0
56	MG	1A	3102	1/1	0.96	0.28	49,49,49,49	0
56	MG	1a	1889	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3398	1/1	0.96	0.13	32,32,32,32	0
56	MG	2A	3426	1/1	0.96	0.12	46,46,46,46	0
56	MG	1A	4004	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3310	1/1	0.96	0.05	55,55,55,55	0
56	MG	1A	3204	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3799	1/1	0.96	0.14	20,20,20,20	0
56	MG	2A	3538	1/1	0.96	0.20	39,39,39,39	0
56	MG	1A	3961	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3556	1/1	0.96	0.16	55,55,55,55	0
56	MG	1A	3700	1/1	0.96	0.21	31,31,31,31	0
56	MG	1A	3777	1/1	0.96	0.16	30,30,30,30	0
56	MG	2A	3245	1/1	0.96	0.23	52,52,52,52	0
56	MG	2A	3291	1/1	0.96	0.19	37,37,37,37	0
56	MG	1N	3004	1/1	0.96	0.07	26,26,26,26	0
56	MG	1A	3551	1/1	0.96	0.14	55,55,55,55	0
56	MG	2E	301	1/1	0.96	0.40	36,36,36,36	0
56	MG	1A	4052	1/1	0.96	0.57	33,33,33,33	0
56	MG	2A	3424	1/1	0.96	0.11	63,63,63,63	0
56	MG	2a	3089	1/1	0.96	0.09	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	4081	1/1	0.96	0.25	42,42,42,42	0
56	MG	1a	1907	1/1	0.96	0.18	36,36,36,36	0
56	MG	2A	3026	1/1	0.96	0.41	49,49,49,49	0
56	MG	1A	3991	1/1	0.96	0.41	38,38,38,38	0
56	MG	1A	3695	1/1	0.96	0.10	13,13,13,13	0
56	MG	2A	3058	1/1	0.96	0.13	51,51,51,51	0
56	MG	1A	3293	1/1	0.96	0.20	11,11,11,11	0
56	MG	1A	3487	1/1	0.96	0.13	40,40,40,40	0
56	MG	1A	3673	1/1	0.96	0.09	25,25,25,25	0
56	MG	2a	3102	1/1	0.96	0.18	44,44,44,44	0
56	MG	1A	4073	1/1	0.96	0.42	48,48,48,48	0
56	MG	1a	1710	1/1	0.96	0.16	45,45,45,45	0
56	MG	2A	3384	1/1	0.96	0.15	39,39,39,39	0
56	MG	1A	3791	1/1	0.96	0.36	51,51,51,51	0
56	MG	1a	1745	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3822	1/1	0.96	0.21	21,21,21,21	0
56	MG	2A	3175	1/1	0.96	0.18	34,34,34,34	0
56	MG	1A	3773	1/1	0.96	0.31	48,48,48,48	0
56	MG	2A	3067	1/1	0.96	0.13	49,49,49,49	0
56	MG	1A	3275	1/1	0.96	0.29	41,41,41,41	0
56	MG	1A	3462	1/1	0.96	0.18	47,47,47,47	0
56	MG	15	102	1/1	0.96	0.17	52,52,52,52	0
56	MG	1a	1850	1/1	0.96	0.23	44,44,44,44	0
56	MG	1A	3953	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3241	1/1	0.96	0.20	23,23,23,23	0
56	MG	1B	206	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3988	1/1	0.96	0.37	39,39,39,39	0
56	MG	1A	3531	1/1	0.96	0.09	45,45,45,45	0
56	MG	2a	3084	1/1	0.96	0.20	50,50,50,50	0
56	MG	2A	3126	1/1	0.96	0.50	43,43,43,43	0
56	MG	1A	3904	1/1	0.96	0.20	17,17,17,17	0
56	MG	1A	3515	1/1	0.96	0.55	41,41,41,41	0
56	MG	1A	3480	1/1	0.96	0.17	54,54,54,54	0
56	MG	1A	3166	1/1	0.96	0.16	35,35,35,35	0
56	MG	1A	3957	1/1	0.96	0.26	34,34,34,34	0
56	MG	1A	3036	1/1	0.96	0.24	40,40,40,40	0
56	MG	1a	1841	1/1	0.96	0.20	52,52,52,52	0
56	MG	1A	3167	1/1	0.96	0.21	25,25,25,25	0
56	MG	2A	3158	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3784	1/1	0.96	0.19	20,20,20,20	0
56	MG	2A	3558	1/1	0.96	0.71	43,43,43,43	0
56	MG	2A	3388	1/1	0.96	0.12	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	3423	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3801	1/1	0.96	0.17	40,40,40,40	0
56	MG	1A	4031	1/1	0.96	0.24	66,66,66,66	0
56	MG	1A	3379	1/1	0.96	0.34	43,43,43,43	0
56	MG	2A	3344	1/1	0.96	0.27	59,59,59,59	0
56	MG	1a	1663	1/1	0.96	0.13	52,52,52,52	0
56	MG	2A	3402	1/1	0.96	0.28	44,44,44,44	0
56	MG	2A	3280	1/1	0.96	0.10	58,58,58,58	0
56	MG	2A	3117	1/1	0.96	0.31	46,46,46,46	0
56	MG	2A	3417	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3053	1/1	0.96	0.28	43,43,43,43	0
56	MG	2A	3264	1/1	0.96	0.23	29,29,29,29	0
56	MG	1A	3676	1/1	0.96	0.14	40,40,40,40	0
56	MG	1A	3250	1/1	0.96	0.14	22,22,22,22	0
56	MG	2a	3078	1/1	0.96	0.13	61,61,61,61	0
56	MG	1A	3202	1/1	0.96	0.47	50,50,50,50	0
56	MG	2A	3330	1/1	0.96	0.18	40,40,40,40	0
56	MG	2A	3060	1/1	0.97	0.27	40,40,40,40	0
56	MG	1A	3385	1/1	0.97	0.18	45,45,45,45	0
56	MG	2A	3319	1/1	0.97	0.27	51,51,51,51	0
56	MG	1A	3222	1/1	0.97	0.12	19,19,19,19	0
56	MG	2a	3218	1/1	0.97	0.19	67,67,67,67	0
56	MG	2A	3434	1/1	0.97	0.18	42,42,42,42	0
56	MG	1Q	202	1/1	0.97	0.28	32,32,32,32	0
56	MG	2a	3129	1/1	0.97	0.20	60,60,60,60	0
56	MG	1A	3409	1/1	0.97	0.14	42,42,42,42	0
56	MG	2A	3326	1/1	0.97	0.13	43,43,43,43	0
56	MG	1a	1861	1/1	0.97	0.12	51,51,51,51	0
56	MG	2A	3113	1/1	0.97	0.15	29,29,29,29	0
56	MG	2A	3122	1/1	0.97	0.18	51,51,51,51	0
56	MG	1A	3573	1/1	0.97	0.09	41,41,41,41	0
56	MG	2A	3232	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	4021	1/1	0.97	0.15	59,59,59,59	0
56	MG	2A	3412	1/1	0.97	0.23	54,54,54,54	0
56	MG	1A	3507	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	3900	1/1	0.97	0.23	39,39,39,39	0
56	MG	1E	303	1/1	0.97	0.09	31,31,31,31	0
56	MG	1P	203	1/1	0.97	0.33	28,28,28,28	0
56	MG	2F	304	1/1	0.97	0.15	41,41,41,41	0
56	MG	2a	3132	1/1	0.97	0.10	57,57,57,57	0
56	MG	1A	3377	1/1	0.97	0.31	24,24,24,24	0
56	MG	2A	3545	1/1	0.97	0.25	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	3199	1/1	0.97	0.48	64,64,64,64	0
56	MG	2A	3441	1/1	0.97	0.13	55,55,55,55	0
56	MG	1A	3291	1/1	0.97	0.38	41,41,41,41	0
56	MG	1a	1868	1/1	0.97	0.17	44,44,44,44	0
56	MG	1a	1865	1/1	0.97	0.26	51,51,51,51	0
56	MG	1A	4055	1/1	0.97	0.17	43,43,43,43	0
56	MG	1A	3926	1/1	0.97	0.16	51,51,51,51	0
56	MG	1a	1734	1/1	0.97	0.35	53,53,53,53	0
56	MG	1a	1840	1/1	0.97	0.15	27,27,27,27	0
56	MG	1A	3894	1/1	0.97	0.15	50,50,50,50	0
56	MG	1A	3112	1/1	0.97	0.49	51,51,51,51	0
56	MG	2A	3502	1/1	0.97	0.09	37,37,37,37	0
56	MG	2A	3307	1/1	0.97	0.15	60,60,60,60	0
56	MG	1A	3929	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3984	1/1	0.97	0.41	32,32,32,32	0
56	MG	2A	3299	1/1	0.97	0.15	64,64,64,64	0
56	MG	1A	3808	1/1	0.97	0.13	73,73,73,73	0
56	MG	2A	3367	1/1	0.97	0.24	54,54,54,54	0
56	MG	1A	3132	1/1	0.97	0.11	33,33,33,33	0
56	MG	1A	3295	1/1	0.97	0.19	42,42,42,42	0
56	MG	1A	3903	1/1	0.97	0.10	71,71,71,71	0
56	MG	1A	3813	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3674	1/1	0.97	0.17	24,24,24,24	0
56	MG	2a	3048	1/1	0.97	0.09	66,66,66,66	0
56	MG	1T	201	1/1	0.97	0.07	41,41,41,41	0
56	MG	1a	1735	1/1	0.97	0.12	45,45,45,45	0
56	MG	1a	1860	1/1	0.97	0.17	61,61,61,61	0
56	MG	1B	220	1/1	0.97	0.10	42,42,42,42	0
56	MG	2a	3096	1/1	0.97	0.14	55,55,55,55	0
56	MG	2a	3123	1/1	0.97	0.10	39,39,39,39	0
56	MG	2A	3078	1/1	0.97	0.07	48,48,48,48	0
56	MG	1a	1906	1/1	0.97	0.32	45,45,45,45	0
56	MG	1O	3002	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3260	1/1	0.97	0.24	31,31,31,31	0
56	MG	10	102	1/1	0.97	0.05	48,48,48,48	0
56	MG	1A	3753	1/1	0.97	0.11	34,34,34,34	0
56	MG	1A	3407	1/1	0.97	0.44	40,40,40,40	0
56	MG	1A	3328	1/1	0.97	0.09	27,27,27,27	0
56	MG	1a	1847	1/1	0.97	0.20	53,53,53,53	0
56	MG	1A	3821	1/1	0.97	0.17	21,21,21,21	0
56	MG	1A	4090	1/1	0.97	0.24	26,26,26,26	0
56	MG	1A	3227	1/1	0.97	0.20	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	1A	3790	1/1	0.97	0.20	19,19,19,19	0
56	MG	2a	3236	1/1	0.97	0.23	83,83,83,83	0
56	MG	2A	3290	1/1	0.97	0.13	36,36,36,36	0
56	MG	2A	3105	1/1	0.97	0.36	28,28,28,28	0
56	MG	1A	3721	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3369	1/1	0.97	0.17	56,56,56,56	0
56	MG	1A	3586	1/1	0.97	0.18	33,33,33,33	0
56	MG	2A	3023	1/1	0.97	0.16	45,45,45,45	0
56	MG	1A	3887	1/1	0.97	0.21	45,45,45,45	0
56	MG	1A	3626	1/1	0.97	0.18	45,45,45,45	0
56	MG	2A	3503	1/1	0.97	0.05	37,37,37,37	0
56	MG	2a	3139	1/1	0.97	0.17	53,53,53,53	0
56	MG	1A	3950	1/1	0.97	0.10	64,64,64,64	0
56	MG	2A	3528	1/1	0.97	0.17	46,46,46,46	0
56	MG	1A	3895	1/1	0.97	0.08	40,40,40,40	0
56	MG	1Q	203	1/1	0.97	0.15	41,41,41,41	0
56	MG	1B	217	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3731	1/1	0.97	0.11	45,45,45,45	0
56	MG	2a	3184	1/1	0.97	0.22	53,53,53,53	0
56	MG	2A	3125	1/1	0.97	0.18	52,52,52,52	0
56	MG	1A	4015	1/1	0.97	0.38	46,46,46,46	0
56	MG	1A	3177	1/1	0.97	0.30	33,33,33,33	0
56	MG	2A	3336	1/1	0.97	0.07	74,74,74,74	0
56	MG	1A	3181	1/1	0.97	0.15	38,38,38,38	0
56	MG	1U	204	1/1	0.97	0.24	40,40,40,40	0
56	MG	1A	3583	1/1	0.97	0.13	49,49,49,49	0
56	MG	2A	3249	1/1	0.97	0.17	56,56,56,56	0
56	MG	1A	4084	1/1	0.97	0.44	32,32,32,32	0
56	MG	1a	1771	1/1	0.97	0.08	48,48,48,48	0
56	MG	2A	3134	1/1	0.97	0.10	44,44,44,44	0
56	MG	1A	4087	1/1	0.97	0.44	42,42,42,42	0
56	MG	1A	3951	1/1	0.97	0.17	36,36,36,36	0
56	MG	2A	3036	1/1	0.97	0.26	30,30,30,30	0
56	MG	2a	3189	1/1	0.97	0.37	76,76,76,76	0
56	MG	1A	3325	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3840	1/1	0.97	0.18	59,59,59,59	0
56	MG	1A	3968	1/1	0.97	0.16	26,26,26,26	0
56	MG	1B	224	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3977	1/1	0.97	0.11	31,31,31,31	0
56	MG	2A	3294	1/1	0.97	0.32	50,50,50,50	0
56	MG	1A	3277	1/1	0.97	0.12	34,34,34,34	0
56	MG	1A	4060	1/1	0.97	0.13	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	3546	1/1	0.97	0.21	49,49,49,49	0
56	MG	1A	3959	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3344	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3109	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3089	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3709	1/1	0.97	0.26	38,38,38,38	0
56	MG	1A	3292	1/1	0.97	0.22	62,62,62,62	0
56	MG	1A	4071	1/1	0.97	0.33	44,44,44,44	0
56	MG	2A	3463	1/1	0.97	0.32	44,44,44,44	0
56	MG	28	101	1/1	0.97	0.21	45,45,45,45	0
56	MG	2A	3226	1/1	0.97	0.20	42,42,42,42	0
56	MG	2A	3446	1/1	0.97	0.07	55,55,55,55	0
56	MG	2A	3430	1/1	0.97	0.20	50,50,50,50	0
56	MG	2a	3244	1/1	0.97	0.13	64,64,64,64	0
56	MG	2a	3238	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3755	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3267	1/1	0.97	0.26	22,22,22,22	0
56	MG	1A	3256	1/1	0.97	0.72	44,44,44,44	0
56	MG	1A	3211	1/1	0.97	0.39	37,37,37,37	0
56	MG	2A	3469	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3837	1/1	0.97	0.12	26,26,26,26	0
56	MG	2A	3165	1/1	0.97	0.23	42,42,42,42	0
56	MG	2A	3357	1/1	0.97	0.31	52,52,52,52	0
56	MG	2A	3152	1/1	0.97	0.15	30,30,30,30	0
56	MG	1A	3232	1/1	0.97	0.12	44,44,44,44	0
56	MG	1A	3432	1/1	0.97	0.08	53,53,53,53	0
56	MG	2A	3414	1/1	0.97	0.26	50,50,50,50	0
56	MG	2A	3153	1/1	0.97	0.10	52,52,52,52	0
56	MG	1A	3875	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3309	1/1	0.97	0.18	59,59,59,59	0
56	MG	1A	3917	1/1	0.97	0.09	35,35,35,35	0
56	MG	1a	1701	1/1	0.97	0.16	63,63,63,63	0
56	MG	1a	1832	1/1	0.97	0.15	52,52,52,52	0
56	MG	1a	1900	1/1	0.97	0.22	47,47,47,47	0
56	MG	1Q	207	1/1	0.97	0.35	41,41,41,41	0
56	MG	2A	3075	1/1	0.97	0.30	48,48,48,48	0
56	MG	1A	3518	1/1	0.97	0.13	51,51,51,51	0
56	MG	2A	3406	1/1	0.97	0.20	55,55,55,55	0
56	MG	2A	3267	1/1	0.97	0.35	38,38,38,38	0
56	MG	1A	3815	1/1	0.97	0.16	20,20,20,20	0
56	MG	1A	3062	1/1	0.97	0.19	56,56,56,56	0
56	MG	1A	3342	1/1	0.97	0.16	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	3574	1/1	0.97	0.17	37,37,37,37	0
56	MG	1a	1737	1/1	0.97	0.46	48,48,48,48	0
56	MG	1a	1882	1/1	0.97	0.13	60,60,60,60	0
56	MG	2a	3205	1/1	0.97	0.29	57,57,57,57	0
56	MG	1A	3871	1/1	0.97	0.10	31,31,31,31	0
56	MG	1a	1901	1/1	0.97	0.10	47,47,47,47	0
56	MG	1e	203	1/1	0.97	0.28	84,84,84,84	0
56	MG	1A	3946	1/1	0.97	0.17	24,24,24,24	0
56	MG	2a	3067	1/1	0.97	0.46	57,57,57,57	0
56	MG	1A	3321	1/1	0.97	0.21	33,33,33,33	0
56	MG	1A	3912	1/1	0.97	0.14	56,56,56,56	0
56	MG	2A	3454	1/1	0.97	0.07	57,57,57,57	0
56	MG	2D	304	1/1	0.97	0.14	36,36,36,36	0
56	MG	1A	3994	1/1	0.97	0.11	23,23,23,23	0
56	MG	1A	3560	1/1	0.97	0.12	63,63,63,63	0
56	MG	1A	3581	1/1	0.97	0.43	54,54,54,54	0
56	MG	1A	3498	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	3543	1/1	0.97	0.14	46,46,46,46	0
56	MG	1A	3742	1/1	0.97	0.13	52,52,52,52	0
56	MG	1A	3111	1/1	0.97	0.34	35,35,35,35	0
56	MG	1a	1731	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3346	1/1	0.97	0.21	55,55,55,55	0
56	MG	1B	204	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	4080	1/1	0.97	0.65	36,36,36,36	0
56	MG	1a	1724	1/1	0.97	0.14	62,62,62,62	0
56	MG	1A	3243	1/1	0.97	0.17	38,38,38,38	0
56	MG	2A	3248	1/1	0.97	0.16	35,35,35,35	0
56	MG	1l	201	1/1	0.97	0.11	35,35,35,35	0
56	MG	1D	307	1/1	0.97	0.34	37,37,37,37	0
56	MG	1A	3669	1/1	0.97	0.11	17,17,17,17	0
56	MG	2A	3297	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	3496	1/1	0.97	0.27	42,42,42,42	0
56	MG	2a	3231	1/1	0.97	0.23	59,59,59,59	0
56	MG	1A	3233	1/1	0.97	0.24	36,36,36,36	0
56	MG	1A	3156	1/1	0.97	0.14	50,50,50,50	0
56	MG	2A	3203	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3196	1/1	0.97	0.30	37,37,37,37	0
56	MG	19	105	1/1	0.97	0.19	34,34,34,34	0
56	MG	2a	3144	1/1	0.97	0.14	66,66,66,66	0
56	MG	1A	3962	1/1	0.97	0.22	14,14,14,14	0
56	MG	1A	3664	1/1	0.97	0.16	19,19,19,19	0
56	MG	2A	3212	1/1	0.97	0.33	34,34,34,34	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	3396	1/1	0.97	0.28	49,49,49,49	0
56	MG	2A	3321	1/1	0.97	0.21	26,26,26,26	0
56	MG	1D	304	1/1	0.97	0.24	34,34,34,34	0
56	MG	2a	3015	1/1	0.97	0.16	62,62,62,62	0
56	MG	2A	3472	1/1	0.97	0.13	50,50,50,50	0
56	MG	1B	218	1/1	0.97	0.16	34,34,34,34	0
56	MG	1R	201	1/1	0.97	0.18	32,32,32,32	0
56	MG	1A	4046	1/1	0.97	0.33	45,45,45,45	0
56	MG	1F	305	1/1	0.97	0.20	40,40,40,40	0
56	MG	1a	1772	1/1	0.97	0.09	62,62,62,62	0
56	MG	1A	3190	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3391	1/1	0.97	0.11	51,51,51,51	0
56	MG	1A	3691	1/1	0.97	0.14	54,54,54,54	0
56	MG	2A	3523	1/1	0.97	0.31	34,34,34,34	0
56	MG	1A	3958	1/1	0.97	0.17	40,40,40,40	0
56	MG	1A	3221	1/1	0.97	0.26	28,28,28,28	0
56	MG	2A	3382	1/1	0.97	0.19	46,46,46,46	0
56	MG	1A	3964	1/1	0.97	0.08	50,50,50,50	0
56	MG	2A	3395	1/1	0.97	0.24	47,47,47,47	0
56	MG	1A	3623	1/1	0.97	0.17	45,45,45,45	0
56	MG	1A	4050	1/1	0.97	0.40	84,84,84,84	0
56	MG	2A	3518	1/1	0.97	0.15	32,32,32,32	0
56	MG	1A	3443	1/1	0.97	0.39	72,72,72,72	0
56	MG	2A	3362	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3652	1/1	0.97	0.22	24,24,24,24	0
56	MG	19	106	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3254	1/1	0.97	0.14	41,41,41,41	0
56	MG	1a	1849	1/1	0.97	0.05	38,38,38,38	0
56	MG	2a	3085	1/1	0.97	0.12	48,48,48,48	0
57	ZN	29	501	1/1	0.97	0.05	66,66,66,66	0
56	MG	2A	3069	1/1	0.97	0.28	42,42,42,42	0
56	MG	1a	1633	1/1	0.97	0.20	77,77,77,77	0
56	MG	1A	3591	1/1	0.97	0.19	32,32,32,32	0
56	MG	2a	3237	1/1	0.97	0.11	59,59,59,59	0
56	MG	1A	3927	1/1	0.97	0.23	66,66,66,66	0
56	MG	2a	3007	1/1	0.97	0.35	40,40,40,40	0
56	MG	2A	3329	1/1	0.97	0.23	55,55,55,55	0
56	MG	1A	3175	1/1	0.97	0.42	43,43,43,43	0
56	MG	1A	3725	1/1	0.97	0.12	18,18,18,18	0
56	MG	1A	3002	1/1	0.97	0.29	38,38,38,38	0
56	MG	2A	3001	1/1	0.97	0.18	35,35,35,35	0
56	MG	1A	3981	1/1	0.97	0.18	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	1a	1863	1/1	0.97	0.12	42,42,42,42	0
56	MG	1A	3069	1/1	0.97	0.14	39,39,39,39	0
56	MG	1a	1897	1/1	0.97	0.28	84,84,84,84	0
56	MG	2A	3355	1/1	0.97	0.25	45,45,45,45	0
56	MG	1A	3803	1/1	0.97	0.19	22,22,22,22	0
56	MG	2A	3049	1/1	0.97	0.15	56,56,56,56	0
56	MG	2A	3548	1/1	0.97	0.18	38,38,38,38	0
56	MG	2A	3529	1/1	0.97	0.33	53,53,53,53	0
56	MG	1A	3928	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3696	1/1	0.98	0.26	32,32,32,32	0
56	MG	2A	3008	1/1	0.98	0.15	51,51,51,51	0
56	MG	1A	4001	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3043	1/1	0.98	0.16	55,55,55,55	0
56	MG	1A	3596	1/1	0.98	0.19	44,44,44,44	0
56	MG	2A	3480	1/1	0.98	0.06	21,21,21,21	0
56	MG	2A	3415	1/1	0.98	0.20	57,57,57,57	0
56	MG	2a	3091	1/1	0.98	0.33	46,46,46,46	0
56	MG	2A	3287	1/1	0.98	0.20	33,33,33,33	0
56	MG	1A	3680	1/1	0.98	0.25	44,44,44,44	0
56	MG	1a	1838	1/1	0.98	0.28	39,39,39,39	0
56	MG	1a	1676	1/1	0.98	0.09	55,55,55,55	0
56	MG	2A	3254	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3612	1/1	0.98	0.20	23,23,23,23	0
56	MG	16	105	1/1	0.98	0.22	44,44,44,44	0
56	MG	1a	1857	1/1	0.98	0.09	71,71,71,71	0
56	MG	1A	3756	1/1	0.98	0.17	30,30,30,30	0
56	MG	1a	1725	1/1	0.98	0.36	51,51,51,51	0
56	MG	1A	3724	1/1	0.98	0.16	38,38,38,38	0
56	MG	1U	201	1/1	0.98	0.11	26,26,26,26	0
56	MG	1A	3694	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3811	1/1	0.98	0.20	28,28,28,28	0
56	MG	2A	3022	1/1	0.98	0.15	46,46,46,46	0
56	MG	2A	3268	1/1	0.98	0.09	44,44,44,44	0
56	MG	1A	4056	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3698	1/1	0.98	0.04	26,26,26,26	0
56	MG	1A	3463	1/1	0.98	0.11	39,39,39,39	0
56	MG	2A	3397	1/1	0.98	0.05	58,58,58,58	0
56	MG	1A	3201	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3704	1/1	0.98	0.11	45,45,45,45	0
56	MG	2A	3154	1/1	0.98	0.29	42,42,42,42	0
56	MG	28	102	1/1	0.98	0.25	50,50,50,50	0
56	MG	1A	3905	1/1	0.98	0.25	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	3103	1/1	0.98	0.12	48,48,48,48	0
56	MG	1A	3715	1/1	0.98	0.11	9,9,9,9	0
56	MG	1A	3359	1/1	0.98	0.09	37,37,37,37	0
56	MG	1A	3662	1/1	0.98	0.13	30,30,30,30	0
56	MG	1D	313	1/1	0.98	0.13	39,39,39,39	0
56	MG	2A	3202	1/1	0.98	0.27	38,38,38,38	0
56	MG	1A	3226	1/1	0.98	0.22	23,23,23,23	0
56	MG	1A	3176	1/1	0.98	0.08	30,30,30,30	0
56	MG	1A	3189	1/1	0.98	0.21	34,34,34,34	0
56	MG	2A	3360	1/1	0.98	0.25	43,43,43,43	0
56	MG	2A	3237	1/1	0.98	0.23	37,37,37,37	0
56	MG	1A	3960	1/1	0.98	0.15	28,28,28,28	0
56	MG	1A	3225	1/1	0.98	0.09	21,21,21,21	0
56	MG	1A	3628	1/1	0.98	0.10	43,43,43,43	0
56	MG	2A	3482	1/1	0.98	0.13	52,52,52,52	0
56	MG	2Q	3003	1/1	0.98	0.18	44,44,44,44	0
56	MG	1A	3852	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3580	1/1	0.98	0.21	36,36,36,36	0
56	MG	1A	3064	1/1	0.98	0.14	48,48,48,48	0
56	MG	2A	3059	1/1	0.98	0.13	37,37,37,37	0
56	MG	1A	4089	1/1	0.98	0.26	29,29,29,29	0
56	MG	1A	3039	1/1	0.98	0.29	71,71,71,71	0
56	MG	1a	1876	1/1	0.98	0.16	62,62,62,62	0
56	MG	1A	3246	1/1	0.98	0.13	23,23,23,23	0
56	MG	1A	3982	1/1	0.98	0.11	21,21,21,21	0
56	MG	1A	3844	1/1	0.98	0.12	18,18,18,18	0
56	MG	2A	3459	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3271	1/1	0.98	0.12	54,54,54,54	0
56	MG	1A	3264	1/1	0.98	0.32	27,27,27,27	0
56	MG	2a	3143	1/1	0.98	0.06	42,42,42,42	0
56	MG	2A	3258	1/1	0.98	0.37	62,62,62,62	0
56	MG	1a	1890	1/1	0.98	0.21	40,40,40,40	0
56	MG	2A	3373	1/1	0.98	0.15	48,48,48,48	0
56	MG	2A	3286	1/1	0.98	0.21	47,47,47,47	0
56	MG	1A	3967	1/1	0.98	0.27	57,57,57,57	0
56	MG	1A	4008	1/1	0.98	0.10	20,20,20,20	0
56	MG	1a	1678	1/1	0.98	0.32	51,51,51,51	0
56	MG	2a	3166	1/1	0.98	0.32	60,60,60,60	0
56	MG	1A	3693	1/1	0.98	0.12	25,25,25,25	0
56	MG	1a	1691	1/1	0.98	0.04	66,66,66,66	0
56	MG	2a	3071	1/1	0.98	0.23	72,72,72,72	0
56	MG	1B	219	1/1	0.98	0.25	62,62,62,62	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	1618	1/1	0.98	0.09	77,77,77,77	0
56	MG	2O	203	1/1	0.98	0.11	41,41,41,41	0
56	MG	1A	3338	1/1	0.98	0.07	52,52,52,52	0
56	MG	1A	3677	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3192	1/1	0.98	0.21	46,46,46,46	0
56	MG	2A	3095	1/1	0.98	0.25	46,46,46,46	0
56	MG	1a	1790	1/1	0.98	0.16	62,62,62,62	0
56	MG	2A	3333	1/1	0.98	0.15	35,35,35,35	0
56	MG	1P	206	1/1	0.98	0.20	42,42,42,42	0
56	MG	1a	1634	1/1	0.98	0.19	55,55,55,55	0
56	MG	2A	3211	1/1	0.98	0.40	33,33,33,33	0
56	MG	1A	3795	1/1	0.98	0.14	13,13,13,13	0
57	ZN	1Y	501	1/1	0.98	0.07	62,62,62,62	0
56	MG	2A	3242	1/1	0.98	0.26	22,22,22,22	0
56	MG	2a	3024	1/1	0.98	0.16	78,78,78,78	0
56	MG	2A	3394	1/1	0.98	0.09	54,54,54,54	0
56	MG	1A	3978	1/1	0.98	0.30	36,36,36,36	0
56	MG	1A	3078	1/1	0.98	0.10	61,61,61,61	0
56	MG	2A	3350	1/1	0.98	0.14	62,62,62,62	0
56	MG	2A	3260	1/1	0.98	0.29	39,39,39,39	0
56	MG	17	101	1/1	0.98	0.10	26,26,26,26	0
56	MG	1a	1714	1/1	0.98	0.17	57,57,57,57	0
56	MG	1A	3412	1/1	0.98	0.16	42,42,42,42	0
56	MG	2a	3029	1/1	0.98	0.14	66,66,66,66	0
56	MG	1A	3378	1/1	0.98	0.13	35,35,35,35	0
56	MG	1A	3846	1/1	0.98	0.08	66,66,66,66	0
56	MG	1B	211	1/1	0.98	0.14	39,39,39,39	0
56	MG	1a	1677	1/1	0.98	0.22	48,48,48,48	0
56	MG	2A	3358	1/1	0.98	0.07	60,60,60,60	0
56	MG	2A	3155	1/1	0.98	0.17	37,37,37,37	0
56	MG	1A	3671	1/1	0.98	0.20	27,27,27,27	0
56	MG	1A	3154	1/1	0.98	0.50	30,30,30,30	0
56	MG	1A	3570	1/1	0.98	0.13	46,46,46,46	0
56	MG	2a	3240	1/1	0.98	0.35	66,66,66,66	0
56	MG	1A	3577	1/1	0.98	0.20	30,30,30,30	0
56	MG	2A	3403	1/1	0.98	0.16	57,57,57,57	0
56	MG	2a	3057	1/1	0.98	0.27	70,70,70,70	0
56	MG	1A	3609	1/1	0.98	0.13	38,38,38,38	0
56	MG	2A	3273	1/1	0.98	0.13	53,53,53,53	0
56	MG	1E	309	1/1	0.98	0.04	54,54,54,54	0
56	MG	2A	3180	1/1	0.98	0.20	29,29,29,29	0
56	MG	1A	3823	1/1	0.98	0.22	17,17,17,17	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	0.98	0.33	65,65,65,65	0
56	MG	2A	3150	1/1	0.98	0.16	30,30,30,30	0
56	MG	2A	3331	1/1	0.98	0.18	45,45,45,45	0
56	MG	1G	3002	1/1	0.98	0.14	52,52,52,52	0
56	MG	2A	3347	1/1	0.98	0.06	56,56,56,56	0
56	MG	1A	3760	1/1	0.98	0.13	34,34,34,34	0
56	MG	1W	3005	1/1	0.98	0.22	42,42,42,42	0
56	MG	2x	105	1/1	0.98	0.14	52,52,52,52	0
56	MG	1A	3482	1/1	0.98	0.14	12,12,12,12	0
56	MG	1A	3108	1/1	0.98	0.11	52,52,52,52	0
56	MG	2A	3475	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3789	1/1	0.98	0.15	14,14,14,14	0
56	MG	1A	3461	1/1	0.98	0.23	48,48,48,48	0
56	MG	2A	3379	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3569	1/1	0.98	0.20	40,40,40,40	0
56	MG	2a	3035	1/1	0.98	0.12	59,59,59,59	0
56	MG	2A	3139	1/1	0.98	0.31	35,35,35,35	0
56	MG	1A	3536	1/1	0.98	0.13	48,48,48,48	0
56	MG	13	102	1/1	0.98	0.15	46,46,46,46	0
56	MG	1a	1635	1/1	0.98	0.26	56,56,56,56	0
56	MG	1A	3130	1/1	0.98	0.15	21,21,21,21	0
56	MG	16	101	1/1	0.98	0.22	55,55,55,55	0
56	MG	1A	3869	1/1	0.98	0.18	40,40,40,40	0
56	MG	2A	3039	1/1	0.98	0.17	38,38,38,38	0
56	MG	1A	3503	1/1	0.98	0.16	30,30,30,30	0
56	MG	1A	4005	1/1	0.98	0.09	42,42,42,42	0
56	MG	1F	308	1/1	0.98	0.14	36,36,36,36	0
56	MG	1A	3615	1/1	0.98	0.06	39,39,39,39	0
56	MG	2A	3354	1/1	0.98	0.08	48,48,48,48	0
56	MG	1a	1707	1/1	0.98	0.10	31,31,31,31	0
56	MG	1A	3028	1/1	0.98	0.20	50,50,50,50	0
56	MG	2a	3185	1/1	0.98	0.12	57,57,57,57	0
56	MG	1A	3631	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3365	1/1	0.98	0.08	30,30,30,30	0
56	MG	1A	3688	1/1	0.98	0.15	8,8,8,8	0
56	MG	1a	1712	1/1	0.98	0.04	40,40,40,40	0
56	MG	2a	3037	1/1	0.98	0.20	50,50,50,50	0
56	MG	2A	3225	1/1	0.98	0.43	58,58,58,58	0
56	MG	2A	3507	1/1	0.98	0.09	38,38,38,38	0
56	MG	1A	3842	1/1	0.98	0.07	54,54,54,54	0
56	MG	1A	4067	1/1	0.98	0.12	21,21,21,21	0
56	MG	1A	3212	1/1	0.98	0.32	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	3337	1/1	0.98	0.04	59,59,59,59	0
56	MG	2A	3385	1/1	0.98	0.09	61,61,61,61	0
56	MG	2a	3109	1/1	0.98	0.31	42,42,42,42	0
56	MG	1A	3185	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	3251	1/1	0.98	0.12	31,31,31,31	0
56	MG	1A	3778	1/1	0.98	0.19	19,19,19,19	0
56	MG	2A	3323	1/1	0.98	0.18	43,43,43,43	0
56	MG	1A	3893	1/1	0.98	0.13	51,51,51,51	0
56	MG	2A	3351	1/1	0.98	0.07	49,49,49,49	0
56	MG	2A	3375	1/1	0.98	0.14	46,46,46,46	0
56	MG	2A	3185	1/1	0.98	0.21	32,32,32,32	0
56	MG	1A	3714	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3915	1/1	0.98	0.14	52,52,52,52	0
56	MG	2A	3283	1/1	0.98	0.24	35,35,35,35	0
56	MG	1v	3001	1/1	0.99	0.13	41,41,41,41	0
56	MG	1A	3703	1/1	0.99	0.19	18,18,18,18	0
56	MG	1A	3933	1/1	0.99	0.10	46,46,46,46	0
56	MG	1A	3668	1/1	0.99	0.16	17,17,17,17	0
58	SF4	1d	501	8/8	0.99	0.13	64,72,77,86	0
56	MG	2a	3108	1/1	0.99	0.10	68,68,68,68	0
56	MG	1A	3266	1/1	0.99	0.16	18,18,18,18	0
56	MG	1A	3617	1/1	0.99	0.18	13,13,13,13	0
56	MG	1A	3607	1/1	0.99	0.23	26,26,26,26	0
56	MG	2A	3450	1/1	0.99	0.09	56,56,56,56	0
56	MG	1A	4051	1/1	0.99	0.21	15,15,15,15	0
56	MG	1A	3113	1/1	0.99	0.16	35,35,35,35	0
56	MG	2A	3108	1/1	0.99	0.05	52,52,52,52	0
56	MG	2A	3429	1/1	0.99	0.10	53,53,53,53	0
56	MG	1a	1835	1/1	0.99	0.20	51,51,51,51	0
56	MG	1A	3738	1/1	0.99	0.20	17,17,17,17	0
56	MG	2A	3156	1/1	0.99	0.24	23,23,23,23	0
56	MG	1A	3736	1/1	0.99	0.20	15,15,15,15	0
56	MG	2U	201	1/1	0.99	0.21	49,49,49,49	0
56	MG	2A	3520	1/1	0.99	0.10	37,37,37,37	0
56	MG	1A	3796	1/1	0.99	0.16	24,24,24,24	0
56	MG	2a	3002	1/1	0.99	0.15	58,58,58,58	0
56	MG	2A	3315	1/1	0.99	0.17	39,39,39,39	0
56	MG	1A	3943	1/1	0.99	0.15	44,44,44,44	0
57	ZN	16	103	1/1	0.99	0.16	45,45,45,45	0
56	MG	1A	3142	1/1	0.99	0.11	20,20,20,20	0
56	MG	2a	3172	1/1	0.99	0.08	42,42,42,42	0
56	MG	1E	311	1/1	0.99	0.12	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	2R	202	1/1	0.99	0.11	35,35,35,35	0
56	MG	1A	3642	1/1	0.99	0.26	38,38,38,38	0
58	SF4	2d	501	8/8	0.99	0.10	58,72,80,87	0
56	MG	2a	3110	1/1	0.99	0.10	55,55,55,55	0
56	MG	2A	3293	1/1	0.99	0.17	30,30,30,30	0
56	MG	1A	4043	1/1	0.99	0.10	26,26,26,26	0
56	MG	1A	3655	1/1	0.99	0.11	24,24,24,24	0
56	MG	1A	3468	1/1	0.99	0.05	39,39,39,39	0
56	MG	1A	3594	1/1	0.99	0.14	40,40,40,40	0
56	MG	1A	3600	1/1	0.99	0.10	56,56,56,56	0
56	MG	2a	3107	1/1	0.99	0.08	57,57,57,57	0
56	MG	1a	1862	1/1	0.99	0.13	35,35,35,35	0
56	MG	1A	3732	1/1	0.99	0.12	26,26,26,26	0
57	ZN	19	103	1/1	0.99	0.12	47,47,47,47	0
56	MG	1B	228	1/1	0.99	0.09	36,36,36,36	0
56	MG	1A	3182	1/1	0.99	0.27	32,32,32,32	0
56	MG	1A	3882	1/1	0.99	0.17	36,36,36,36	0
56	MG	1A	3965	1/1	0.99	0.14	36,36,36,36	0
56	MG	1A	3956	1/1	0.99	0.18	12,12,12,12	0
56	MG	1a	1808	1/1	0.99	0.14	33,33,33,33	0
56	MG	2A	3201	1/1	0.99	0.22	47,47,47,47	0
56	MG	1A	3722	1/1	0.99	0.08	49,49,49,49	0
56	MG	1A	3785	1/1	0.99	0.12	26,26,26,26	0
56	MG	1a	1708	1/1	0.99	0.14	67,67,67,67	0
56	MG	1A	4069	1/1	0.99	0.11	47,47,47,47	0
56	MG	1A	3592	1/1	0.99	0.13	25,25,25,25	0
56	MG	1A	3088	1/1	0.99	0.13	53,53,53,53	0
56	MG	1a	1770	1/1	0.99	0.14	70,70,70,70	0
56	MG	1A	3065	1/1	0.99	0.13	39,39,39,39	0
56	MG	2a	3021	1/1	0.99	0.18	58,58,58,58	0
56	MG	2a	3177	1/1	0.99	0.15	69,69,69,69	0
56	MG	1A	3082	1/1	0.99	0.06	33,33,33,33	0
56	MG	2a	3239	1/1	0.99	0.43	55,55,55,55	0
56	MG	2A	3534	1/1	0.99	0.16	39,39,39,39	0
56	MG	1a	1648	1/1	0.99	0.07	48,48,48,48	0
57	ZN	25	501	1/1	0.99	0.10	50,50,50,50	0
56	MG	1A	3294	1/1	0.99	0.19	55,55,55,55	0
56	MG	1A	3625	1/1	0.99	0.11	31,31,31,31	0
56	MG	1A	3283	1/1	0.99	0.24	43,43,43,43	0
56	MG	2A	3332	1/1	0.99	0.13	42,42,42,42	0
56	MG	1A	3469	1/1	0.99	0.34	33,33,33,33	0
56	MG	2a	3105	1/1	0.99	0.09	62,62,62,62	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	3145	1/1	0.99	0.16	25,25,25,25	0
56	MG	2A	3004	1/1	1.00	0.08	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.