



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 08:37 PM EST

PDB ID : 8G2C
Title : Crystal structure of the A2503-C2,C8-dimethylated *Thermus thermophilus* 70S ribosome in complex with tylosin, mRNA, aminoacylated A-site Phe-tRNA_{phe}, aminoacylated P-site fMet-tRNA_{met}, and deacylated E-site tRNA_{phe} at 2.65Å resolution
Authors : Aleksandrova, E.V.; Wu, K.J.Y.; Tresco, B.I.C.; Syroegin, E.A.; Killeavy, E.E.; Balasanyants, S.M.; Svetlov, M.S.; Gregory, S.T.; Atkinson, G.C.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2023-02-03
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)

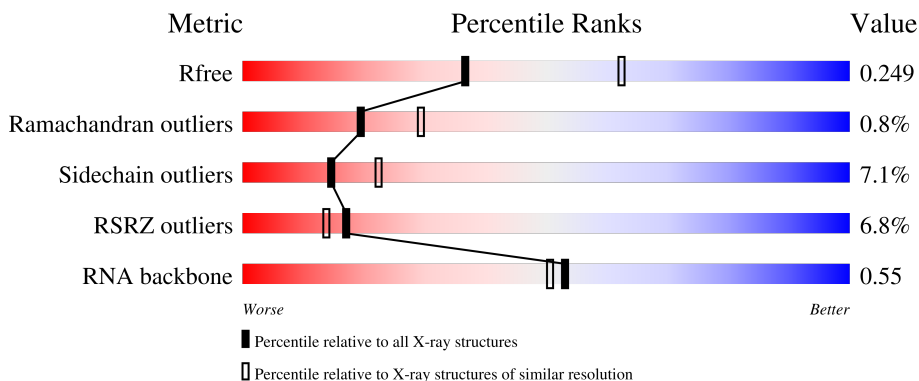
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)
RNA backbone	3102	1010 (2.96-2.36)



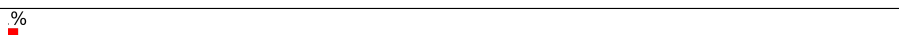
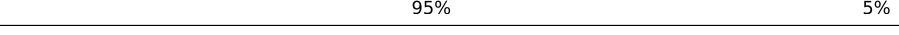
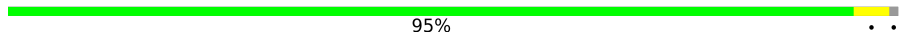

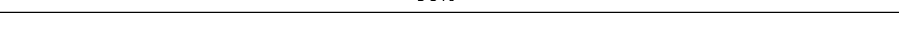



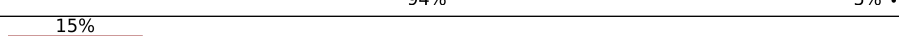

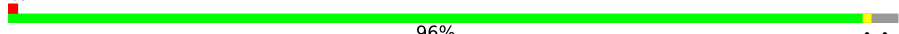
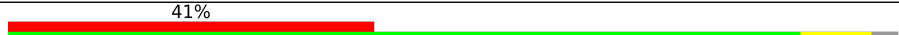
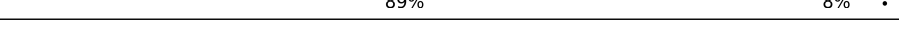



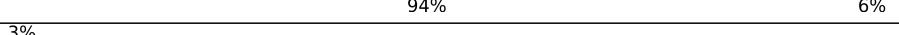
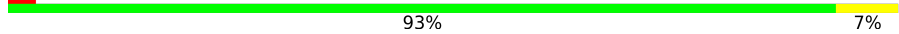

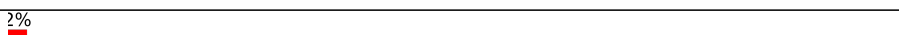
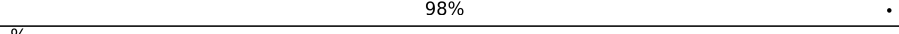
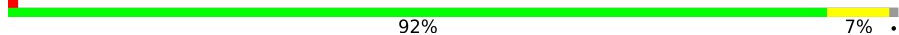

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	1A	2915	 5% 82% 16%
1	2A	2915	 3% 79% 17%
2	1B	121	 93% 7%

Continued on next page...

Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	2B	121	 72% 27%
3	1D	276	 2% 95%
3	2D	276	 95% 5%
4	1E	206	 95%
4	2E	206	 96%
5	1F	210	 90% 7%
5	2F	210	 2% 91% 5%
6	1G	182	 94% 5%
6	2G	182	 15% 90% 9%
7	1H	180	 96%
7	2H	180	 41% 89% 8%
8	1I	148	 86% 13%
8	2I	148	 5% 89% 10%
9	1N	140	 94% 6%
9	2N	140	 3% 93% 7%
10	1O	122	 98%
10	2O	122	 2% 98%
11	1P	150	 92% 7%
11	2P	150	 21% 89% 9%
12	1Q	141	 98%
12	2Q	141	 98%
13	1R	118	 96%
13	2R	118	 3% 97%
14	1S	112	 91% 7%
14	2S	112	 2% 87% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	1T	146	% 86% 10%
15	2T	146	6% 87% 10%
16	1U	118	96%
16	2U	118	% 94%
17	1V	101	94% 5%
17	2V	101	4% 95%
18	1W	113	% 95%
18	2W	113	93% 6%
19	1X	96	% 96%
19	2X	96	3% 96%
20	1Y	110	92% 5%
20	2Y	110	5% 90% 7%
21	1Z	206	2% 69% 5% 25%
21	2Z	206	9% 71% 7% 22%
22	10	85	98%
22	20	85	95%
23	11	98	2% 98%
23	21	98	6% 94% 5%
24	12	72	94%
24	22	72	94%
25	13	60	2% 88% 10%
25	23	60	8% 95%
26	14	71	8% 89% 6%
26	24	71	23% 83% 14%
27	15	60	2% 93% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	25	60	5% 95% ..
28	16	54	91% 7% .
28	26	54	6% 85% 13% .
29	17	49	2% 90% 8% .
29	27	49	8% 92% 6% .
30	18	65	92% 6% .
30	28	65	5% 91% 8% .
31	19	37	100%
31	29	37	11% 95% 5%
32	1a	1521	2% 82% 16% ..
32	2a	1521	4% 80% 18% ..
33	1b	256	11% 82% 8% 10%
33	2b	256	32% 82% 7% 10%
34	1c	239	81% 5% 14%
34	2c	239	33% 81% 5% 14%
35	1d	209	5% 92% 7%
35	2d	209	6% 92% 8%
36	1e	162	83% 9% 9%
36	2e	162	14% 82% 9% 9%
37	1f	101	5% 94% 5% .
37	2f	101	% 95% ..
38	1g	156	6% 88% 11% .
38	2g	156	22% 93% 6% .
39	1h	138	10% 96% ..
39	2h	138	9% 95% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	1i	128	6% 91% 7% ..
40	2i	128	55% 88% 12% .
41	1j	105	13% 84% 9% 8%
41	2j	105	44% 81% 10% 9%
42	1k	129	6% 81% 8% 12%
42	2k	129	% 84% 5% 12%
43	1l	132	88% 5% 8%
43	2l	132	2% 88% 5% 8%
44	1m	126	2% 88% 10% .
44	2m	126	22% 87% 9% ..
45	1n	61	92% 7% .
45	2n	61	70% 87% 11% .
46	1o	89	6% 97% ..
46	2o	89	93% 6% .
47	1p	88	85% 8% 7%
47	2p	88	3% 85% 8% 7%
48	1q	105	14% 90% . 6%
48	2q	105	6% 86% 9% 6%
49	1r	88	19% 75% . 23%
49	2r	88	% 73% .. 23%
50	1s	93	3% 85% . 11%
50	2s	93	40% 83% 5% . 11%
51	1t	106	14% 84% 5% . 9%
51	2t	106	25% 84% 7% 9%
52	1u	27	81% . 15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	5MU	1y	54	-	-	-	X
56	PSU	1y	55	-	-	-	X
56	PSU	2y	32	-	-	-	X
56	MIA	2y	37	-	-	-	X
56	G7M	2y	46	-	-	-	X
56	5MU	2y	54	-	-	-	X
57	MG	18	107	-	-	-	X
57	MG	1A	3016	-	-	-	X
57	MG	1A	3327	-	-	-	X
57	MG	1A	3388	-	-	-	X
57	MG	1A	3427	-	-	-	X
57	MG	1A	3434	-	-	-	X
57	MG	1A	3467	-	-	-	X
57	MG	1A	3909	-	-	-	X
57	MG	1F	315	-	-	-	X
57	MG	1U	210	-	-	-	X
57	MG	2A	3077	-	-	-	X
57	MG	2A	3177	-	-	-	X
57	MG	2A	3199	-	-	-	X
57	MG	2A	3203	-	-	-	X
57	MG	2A	3359	-	-	-	X
57	MG	2A	3395	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	2A	3548	-	-	-	X
57	MG	2A	3662	-	-	-	X
57	MG	2A	3675	-	-	-	X
57	MG	2D	306	-	-	-	X
57	MG	2a	1795	-	-	-	X
57	MG	2v	102	-	-	-	X

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 300115 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
			Total	C	N	O	P			
1	1A	2871	Total	C	N	O	P	0	0	0
			61853	27532	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60323	26849	11284	19390	2800			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a RNA chain called A-site Aminoacylated Phe-tRNA_{phe}.

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

- Molecule 55 is a RNA chain called P-site Aminoacylated fMet-tRNA_{met}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
55	1x	77	Total 1656	C 740	N 299	O 538	P 77	S 2	0	0	0
55	2x	77	Total 1656	C 740	N 299	O 538	P 77	S 2	0	0	0

- Molecule 56 is a RNA chain called E-site Deacylated tRNA_{phe}.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
56	1y	74	Total 1585	C 707	N 285	O 518	P 74	S 1	0	0	0
56	2y	73	Total 1565	C 698	N 283	O 510	P 73	S 1	0	0	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1099	Total 1099	Mg 1099	0	0
57	1B	34	Total 34	Mg 34	0	0
57	1D	12	Total 12	Mg 12	0	0
57	1E	10	Total 10	Mg 10	0	0
57	1F	15	Total 15	Mg 15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1H	1	Total 1	Mg 1	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	5	Total 5	Mg 5	0	0
57	1O	6	Total 6	Mg 6	0	0
57	1P	5	Total 5	Mg 5	0	0
57	1Q	7	Total 7	Mg 7	0	0
57	1R	6	Total 6	Mg 6	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	3	Total 3	Mg 3	0	0
57	1U	10	Total 10	Mg 10	0	0
57	1V	5	Total 5	Mg 5	0	0
57	1W	6	Total 6	Mg 6	0	0
57	1X	6	Total 6	Mg 6	0	0
57	1Y	2	Total 2	Mg 2	0	0
57	1Z	2	Total 2	Mg 2	0	0
57	10	10	Total 10	Mg 10	0	0
57	11	5	Total 5	Mg 5	0	0
57	12	3	Total 3	Mg 3	0	0
57	13	5	Total 5	Mg 5	0	0
57	14	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	15	6	Total Mg 6 6	0	0
57	16	1	Total Mg 1 1	0	0
57	17	5	Total Mg 5 5	0	0
57	18	7	Total Mg 7 7	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	214	Total Mg 214 214	0	0
57	1b	1	Total Mg 1 1	0	0
57	1e	2	Total Mg 2 2	0	0
57	1f	1	Total Mg 1 1	0	0
57	1h	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	1	Total Mg 1 1	0	0
57	1n	1	Total Mg 1 1	0	0
57	1p	1	Total Mg 1 1	0	0
57	1r	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	1w	5	Total Mg 5 5	0	0
57	1x	13	Total Mg 13 13	0	0
57	1y	1	Total Mg 1 1	0	0
57	2A	797	Total Mg 797 797	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2B	19	Total Mg 19 19	0	0
57	2D	8	Total Mg 8 8	0	0
57	2E	9	Total Mg 9 9	0	0
57	2F	8	Total Mg 8 8	0	0
57	2G	1	Total Mg 1 1	0	0
57	2N	1	Total Mg 1 1	0	0
57	2O	1	Total Mg 1 1	0	0
57	2P	2	Total Mg 2 2	0	0
57	2Q	4	Total Mg 4 4	0	0
57	2R	2	Total Mg 2 2	0	0
57	2T	2	Total Mg 2 2	0	0
57	2U	1	Total Mg 1 1	0	0
57	2V	2	Total Mg 2 2	0	0
57	2W	2	Total Mg 2 2	0	0
57	2X	2	Total Mg 2 2	0	0
57	2Y	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	2	Total Mg 2 2	0	0
57	23	2	Total Mg 2 2	0	0
57	25	4	Total Mg 4 4	0	0
57	27	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	28	5	Total 5	Mg 5	0	0
57	29	1	Total 1	Mg 1	0	0
57	2a	221	Total 221	Mg 221	0	0
57	2d	2	Total 2	Mg 2	0	0
57	2e	1	Total 1	Mg 1	0	0
57	2f	3	Total 3	Mg 3	0	0
57	2j	1	Total 1	Mg 1	0	0
57	2k	1	Total 1	Mg 1	0	0
57	2l	1	Total 1	Mg 1	0	0
57	2q	2	Total 2	Mg 2	0	0
57	2t	1	Total 1	Mg 1	0	0
57	2v	4	Total 4	Mg 4	0	0
57	2w	7	Total 7	Mg 7	0	0
57	2x	9	Total 9	Mg 9	0	0
57	2y	2	Total 2	Mg 2	0	0

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

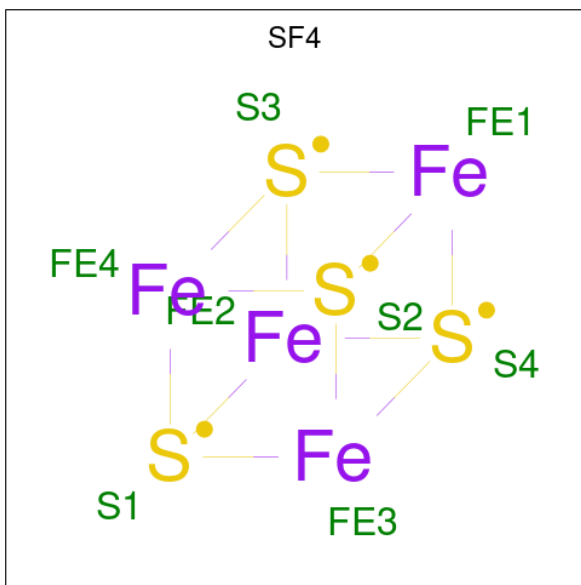
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1	Total 1	K 1	0	0

- Molecule 59 is TYLOSIN (three-letter code: TYK) (formula: C₄₆H₇₇NO₁₇) (labeled as "Ligand of Interest" by depositor).

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	1975	Total O 1975 1975	0	0
62	1B	59	Total O 59 59	0	0
62	1D	25	Total O 25 25	0	0
62	1E	25	Total O 25 25	0	0
62	1F	13	Total O 13 13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1G	2	Total 2	O 2	0	0
62	1H	2	Total 2	O 2	0	0
62	1N	5	Total 5	O 5	0	0
62	1O	4	Total 4	O 4	0	0
62	1P	23	Total 23	O 23	0	0
62	1Q	6	Total 6	O 6	0	0
62	1R	9	Total 9	O 9	0	0
62	1S	2	Total 2	O 2	0	0
62	1T	7	Total 7	O 7	0	0
62	1U	11	Total 11	O 11	0	0
62	1V	8	Total 8	O 8	0	0
62	1W	7	Total 7	O 7	0	0
62	1X	6	Total 6	O 6	0	0
62	1Y	3	Total 3	O 3	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	10	Total 10	O 10	0	0
62	11	6	Total 6	O 6	0	0
62	12	3	Total 3	O 3	0	0
62	13	3	Total 3	O 3	0	0
62	14	1	Total 1	O 1	0	0
62	15	6	Total 6	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	16	2	Total O 2 2	0	0
62	17	10	Total O 10 10	0	0
62	18	12	Total O 12 12	0	0
62	1a	377	Total O 377 377	0	0
62	1b	1	Total O 1 1	0	0
62	1e	2	Total O 2 2	0	0
62	1f	2	Total O 2 2	0	0
62	1l	6	Total O 6 6	0	0
62	1m	1	Total O 1 1	0	0
62	1o	1	Total O 1 1	0	0
62	1p	1	Total O 1 1	0	0
62	1q	2	Total O 2 2	0	0
62	1u	1	Total O 1 1	0	0
62	1v	5	Total O 5 5	0	0
62	1w	12	Total O 12 12	0	0
62	1x	15	Total O 15 15	0	0
62	1y	1	Total O 1 1	0	0
62	2A	1136	Total O 1136 1136	0	0
62	2B	22	Total O 22 22	0	0
62	2D	21	Total O 21 21	0	0
62	2E	16	Total O 16 16	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2F	13	Total 13	O 13	0	0
62	2O	2	Total 2	O 2	0	0
62	2P	5	Total 5	O 5	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	2	Total 2	O 2	0	0
62	2T	7	Total 7	O 7	0	0
62	2U	4	Total 4	O 4	0	0
62	2W	3	Total 3	O 3	0	0
62	2X	2	Total 2	O 2	0	0
62	2Z	1	Total 1	O 1	0	0
62	20	4	Total 4	O 4	0	0
62	21	7	Total 7	O 7	0	0
62	23	2	Total 2	O 2	0	0
62	25	1	Total 1	O 1	0	0
62	26	2	Total 2	O 2	0	0
62	27	4	Total 4	O 4	0	0
62	28	4	Total 4	O 4	0	0
62	29	1	Total 1	O 1	0	0
62	2a	254	Total 254	O 254	0	0
62	2c	1	Total 1	O 1	0	0
62	2d	1	Total 1	O 1	0	0

Continued on next page...

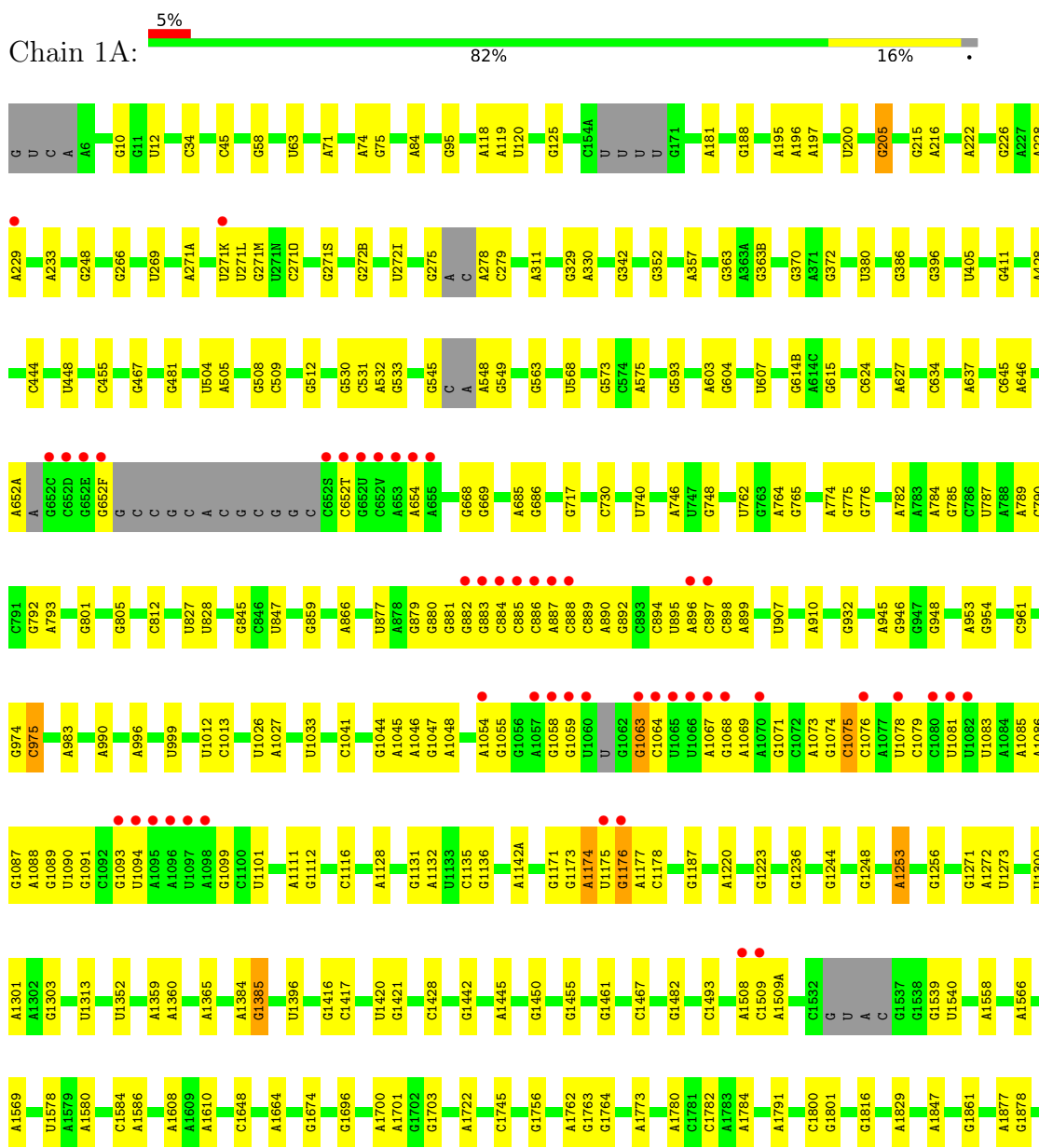
Continued from previous page...

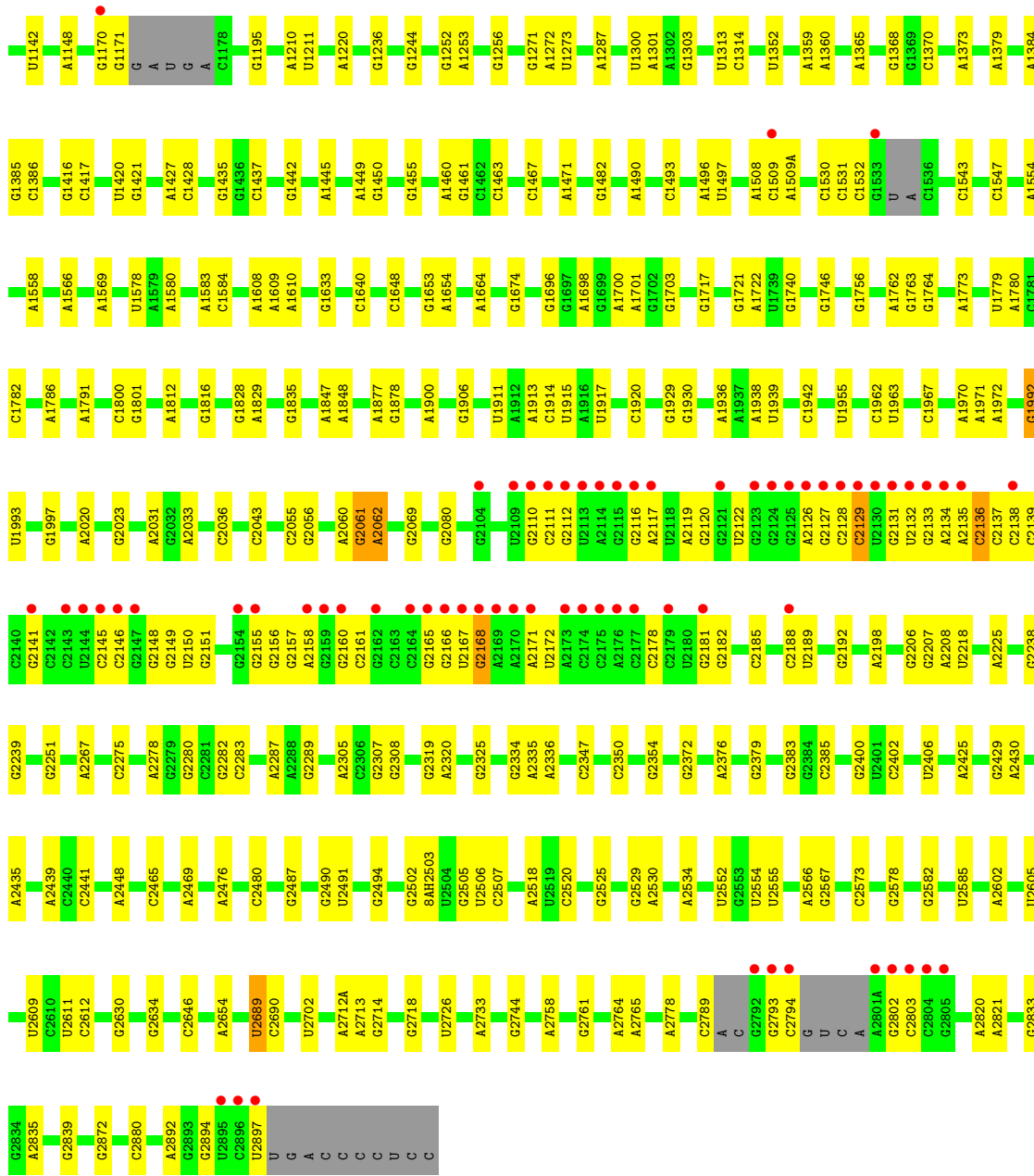
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2e	1	Total 1	O 1	0	0
62	2j	4	Total 4	O 4	0	0
62	2l	4	Total 4	O 4	0	0
62	2n	1	Total 1	O 1	0	0
62	2o	1	Total 1	O 1	0	0
62	2p	1	Total 1	O 1	0	0
62	2q	2	Total 2	O 2	0	0
62	2t	2	Total 2	O 2	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	3	Total 3	O 3	0	0
62	2x	10	Total 10	O 10	0	0
62	2y	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: 23S Ribosomal RNA

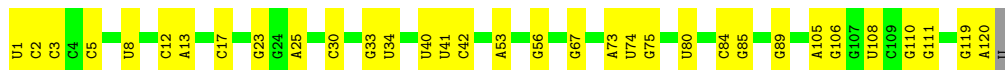




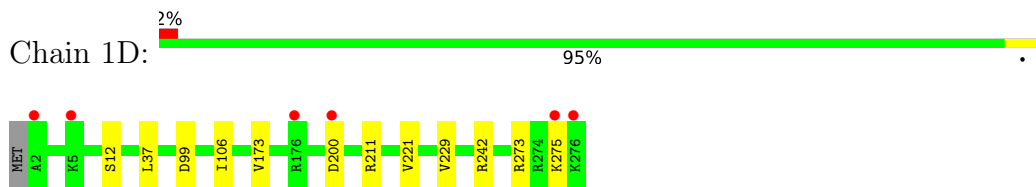
• Molecule 2: 5S Ribosomal RNA



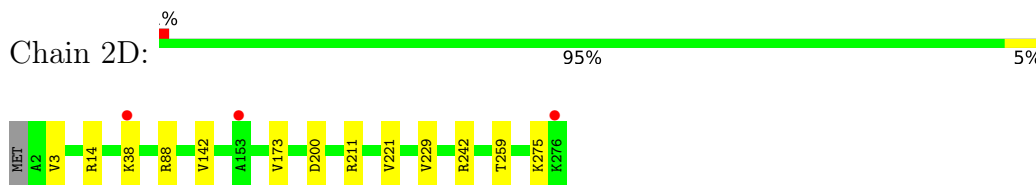
• Molecule 2: 5S Ribosomal RNA



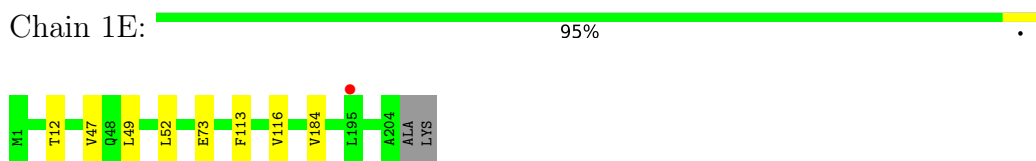
- Molecule 3: 50S ribosomal protein L2



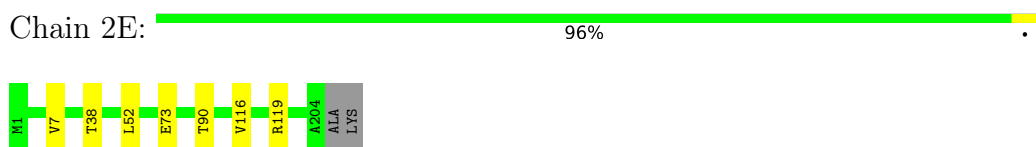
- Molecule 3: 50S ribosomal protein L2



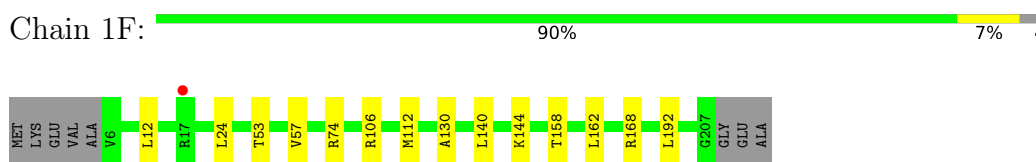
- Molecule 4: 50S ribosomal protein L3



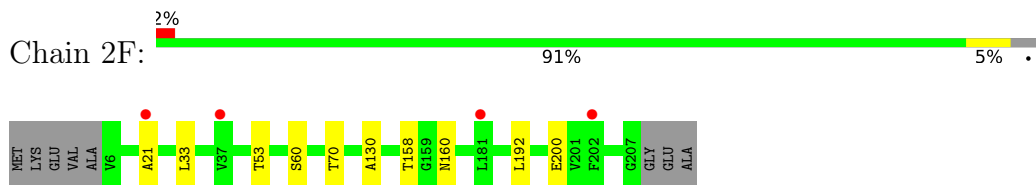
- Molecule 4: 50S ribosomal protein L3



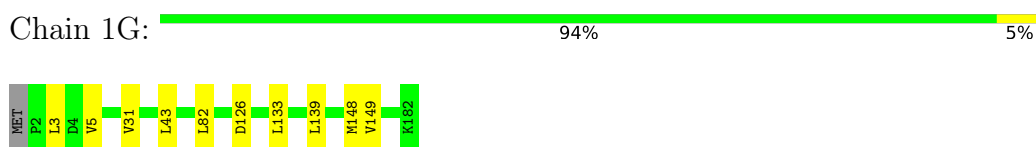
- Molecule 5: 50S ribosomal protein L4



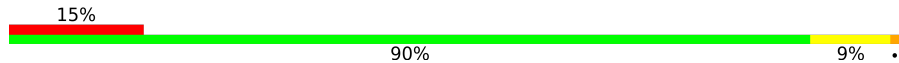
- Molecule 5: 50S ribosomal protein L4

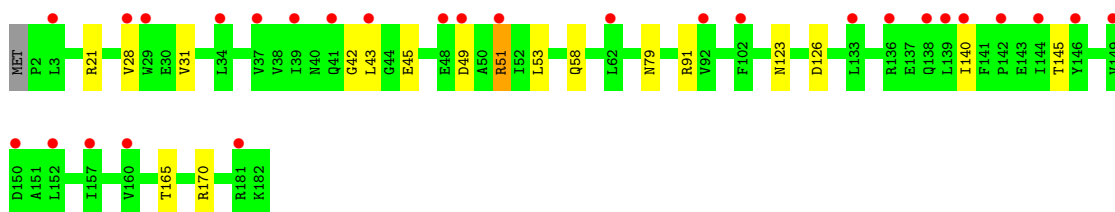


- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5

Chain 2G:  15% 90% 9% ..




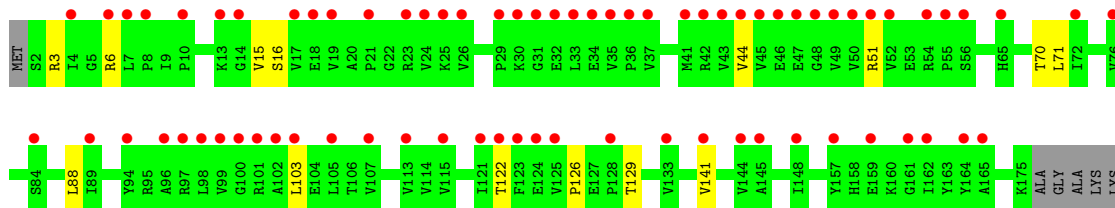
- Molecule 7: 50S ribosomal protein L6

Chain 1H:  1% 96% ..




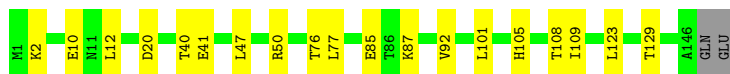
- Molecule 7: 50S ribosomal protein L6

Chain 2H:  41% 89% 8% .




- Molecule 8: 50S ribosomal protein L9

Chain 1I:  86% 13% .



- Molecule 8: 50S ribosomal protein L9

Chain 2I:  5% 89% 10% .

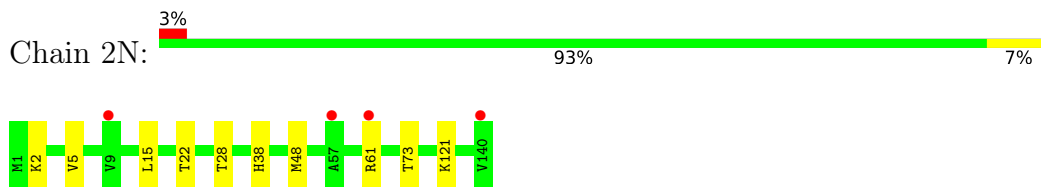


- Molecule 9: 50S ribosomal protein L13

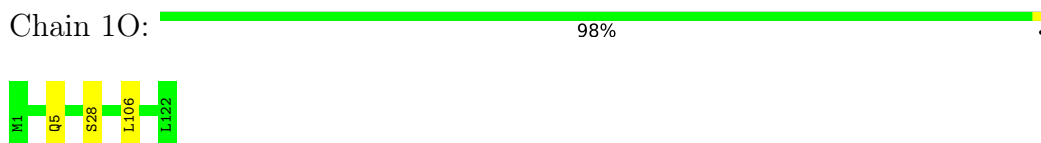
Chain 1N:  94% 6%



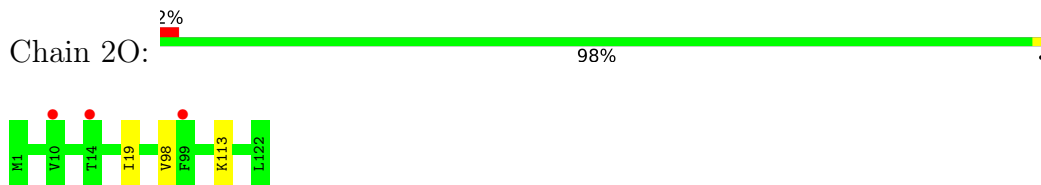
- Molecule 9: 50S ribosomal protein L13



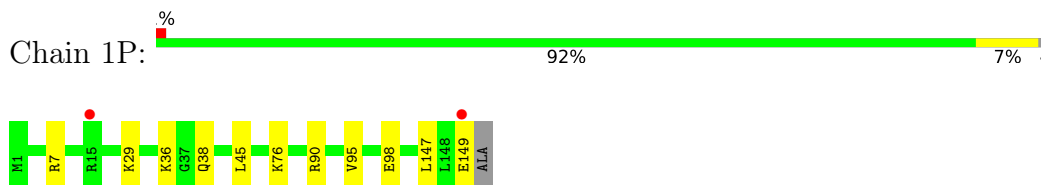
- Molecule 10: 50S ribosomal protein L14



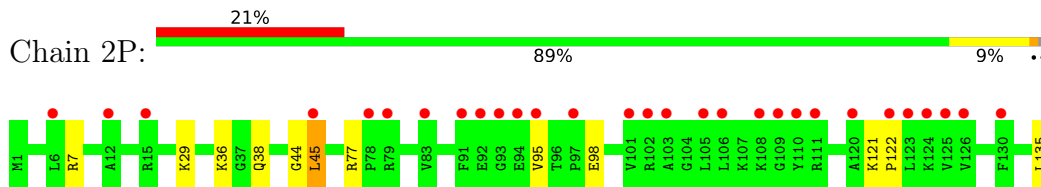
- Molecule 10: 50S ribosomal protein L14



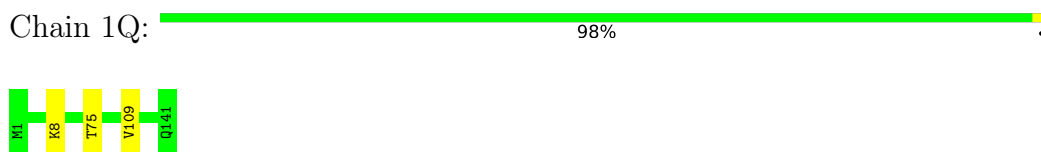
- Molecule 11: 50S ribosomal protein L15



- Molecule 11: 50S ribosomal protein L15



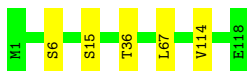
- Molecule 12: 50S ribosomal protein L16



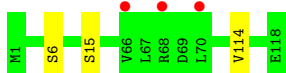
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



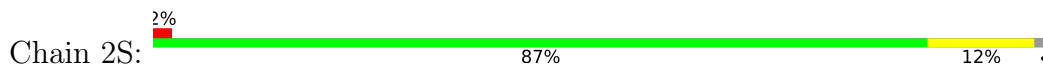
- Molecule 13: 50S ribosomal protein L17



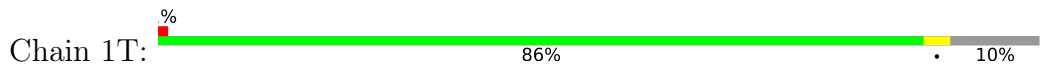
- Molecule 14: 50S ribosomal protein L18



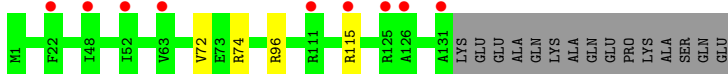
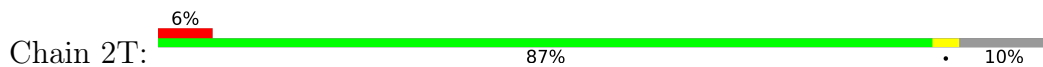
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

Chain 1U:  96%



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  94%



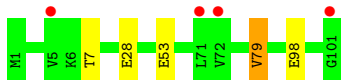
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  94%



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  95%



- Molecule 18: 50S ribosomal protein L22

Chain 1W:  95%



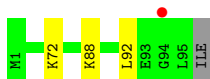
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  93%

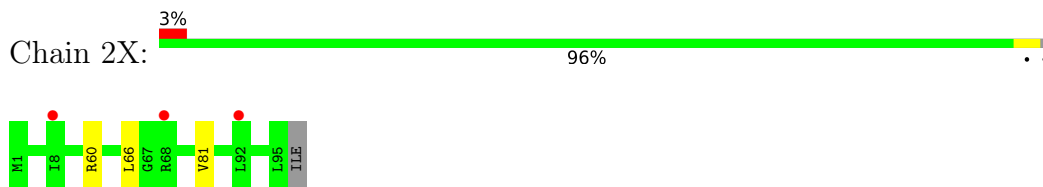


- Molecule 19: 50S ribosomal protein L23

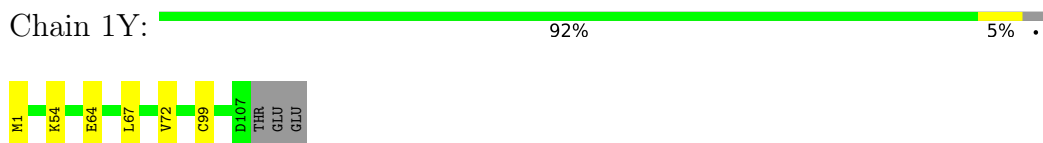
Chain 1X:  96%



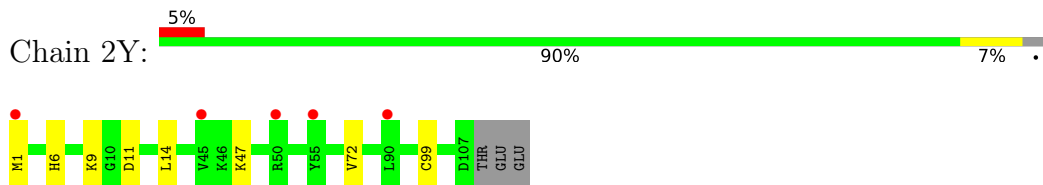
• Molecule 19: 50S ribosomal protein L23



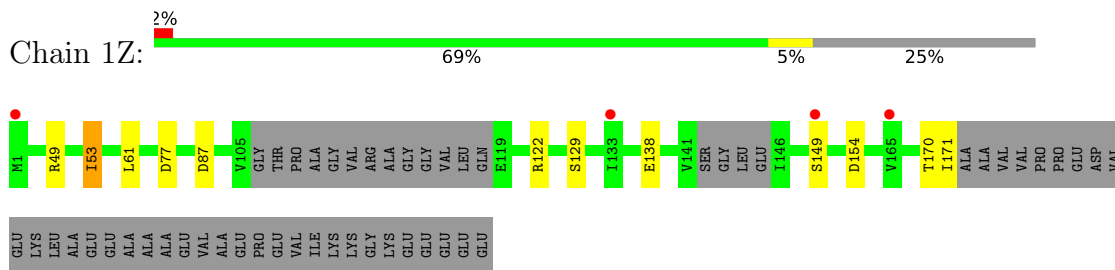
• Molecule 20: 50S ribosomal protein L24



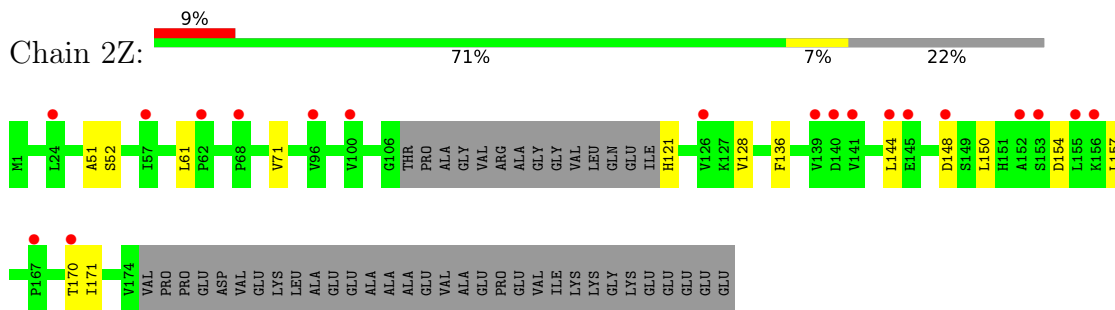
• Molecule 20: 50S ribosomal protein L24



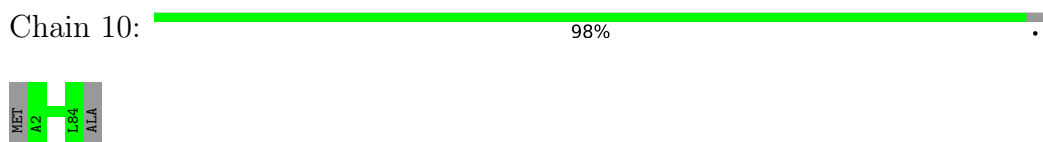
• Molecule 21: 50S ribosomal protein L25



• Molecule 21: 50S ribosomal protein L25



• Molecule 22: 50S ribosomal protein L27



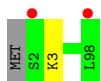
- Molecule 22: 50S ribosomal protein L27

Chain 20:  95%



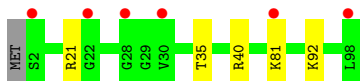
- Molecule 23: 50S ribosomal protein L28

Chain 11:  98%



- Molecule 23: 50S ribosomal protein L28

Chain 21:  94% 5%



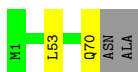
- Molecule 24: 50S ribosomal protein L29

Chain 12:  94%




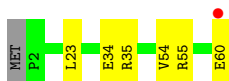
- Molecule 24: 50S ribosomal protein L29

Chain 22:  94%



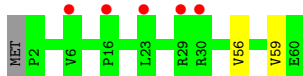
- Molecule 25: 50S ribosomal protein L30

Chain 13:  88% 10%

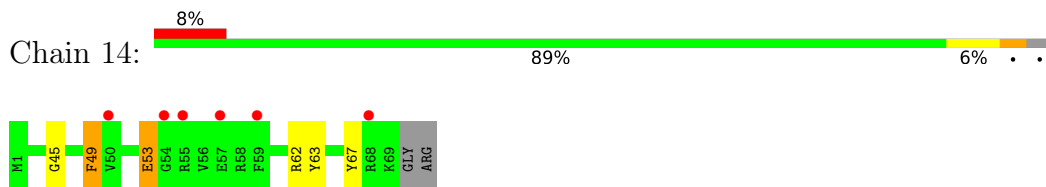


- Molecule 25: 50S ribosomal protein L30

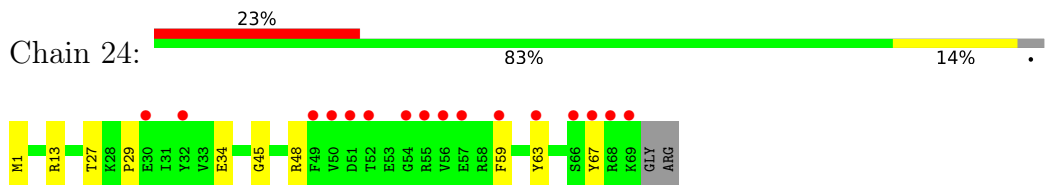
Chain 23:  95%



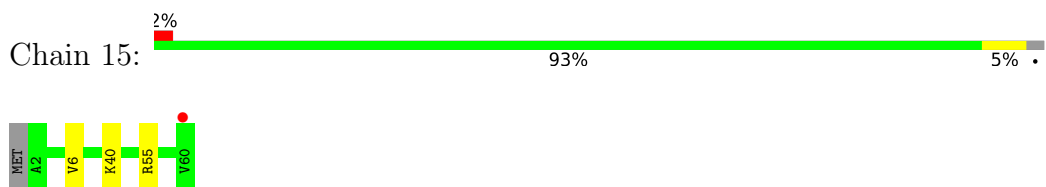
- Molecule 26: 50S ribosomal protein L31



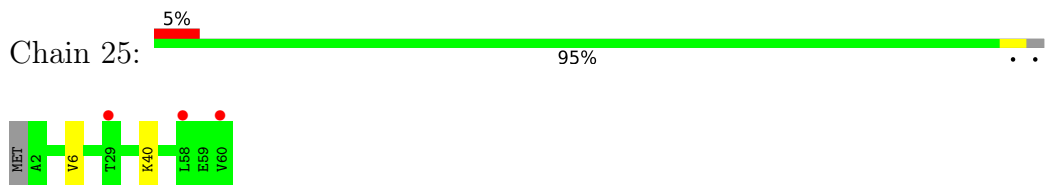
- Molecule 26: 50S ribosomal protein L31



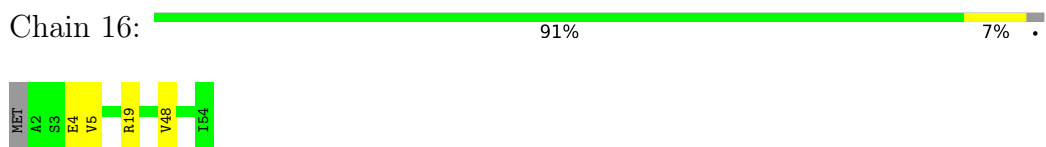
- Molecule 27: 50S ribosomal protein L32



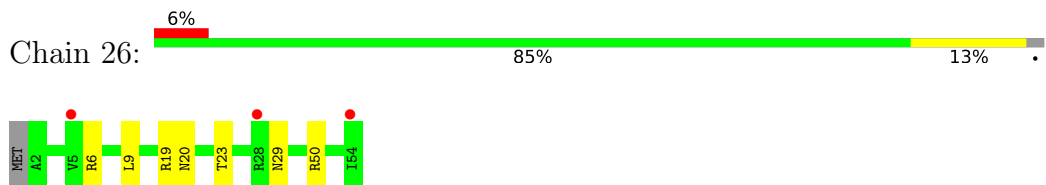
- Molecule 27: 50S ribosomal protein L32



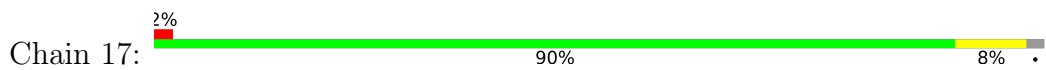
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

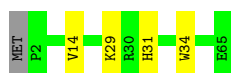




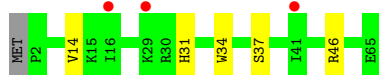
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

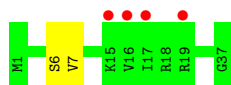


- Molecule 31: 50S ribosomal protein L36

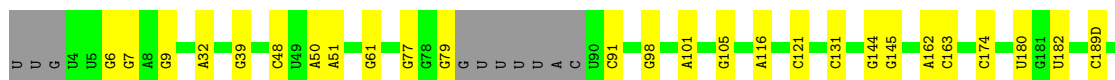
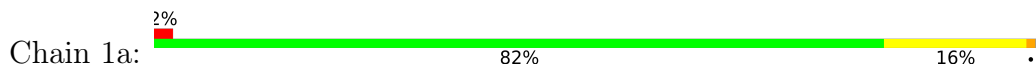


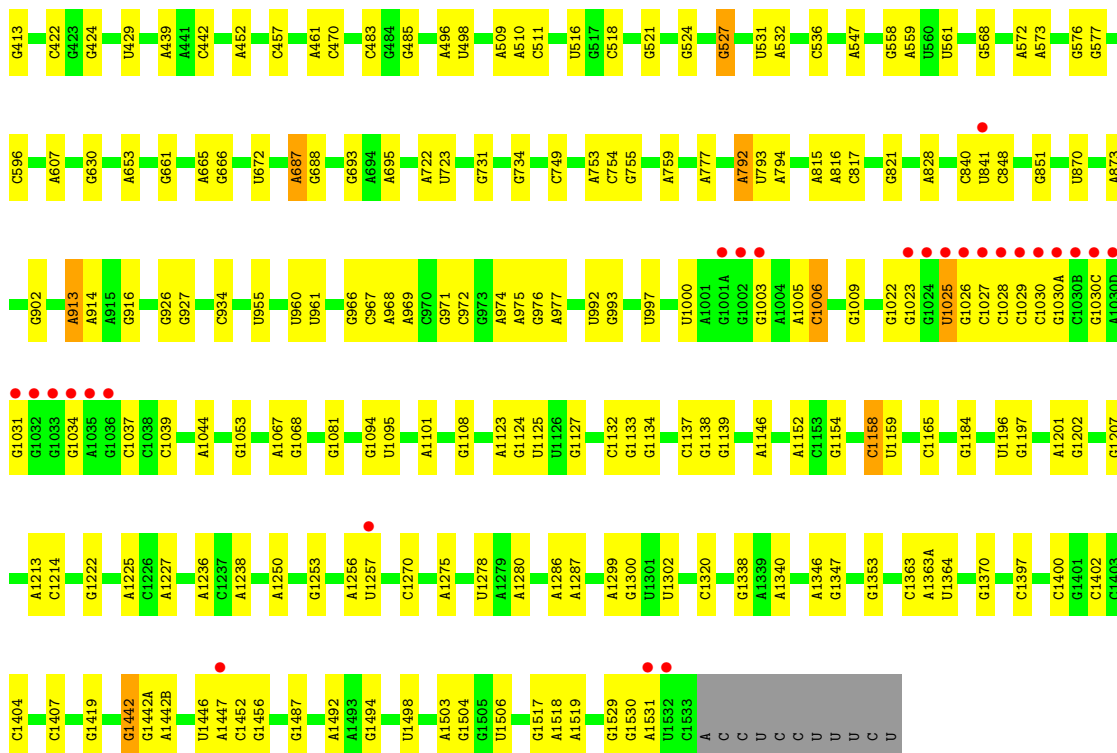
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

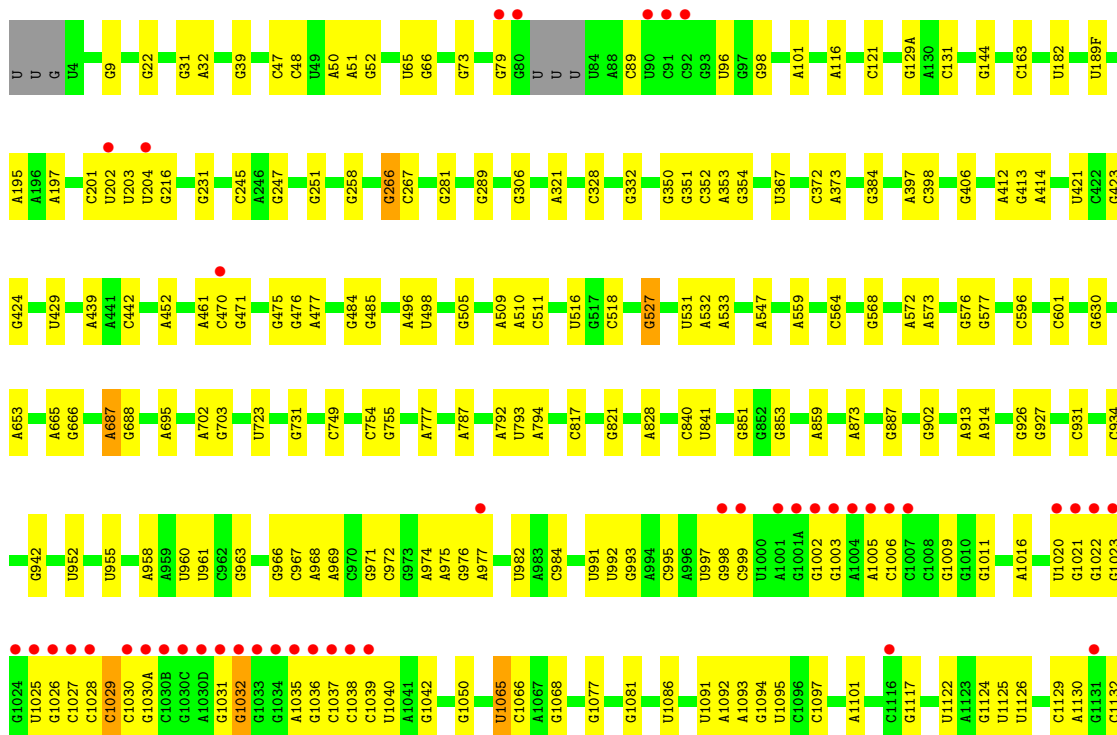
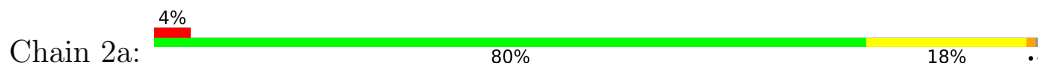


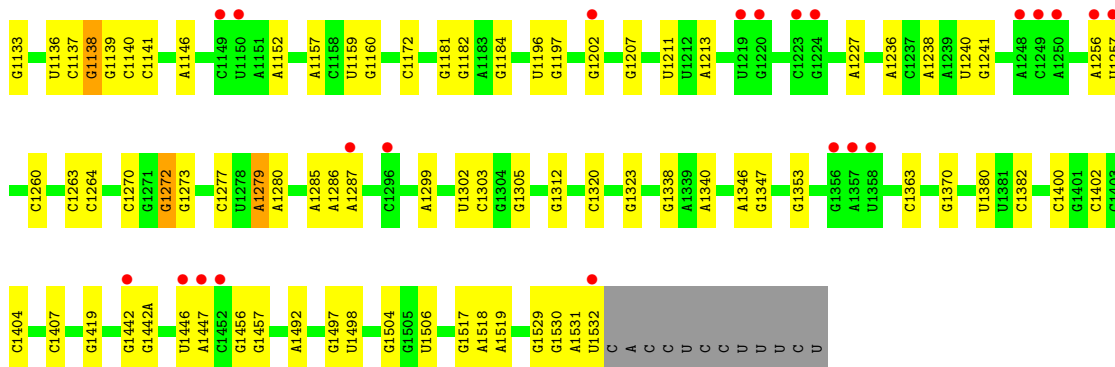
- Molecule 32: 16S Ribosomal RNA



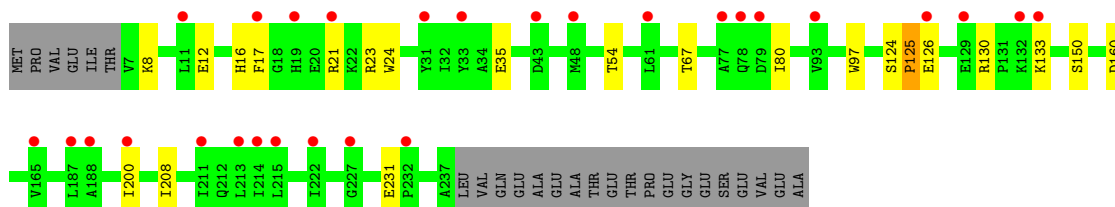
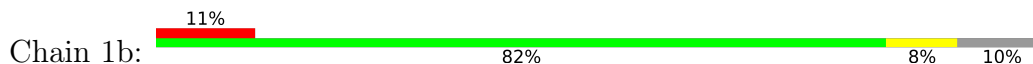


● Molecule 32: 16S Ribosomal RNA

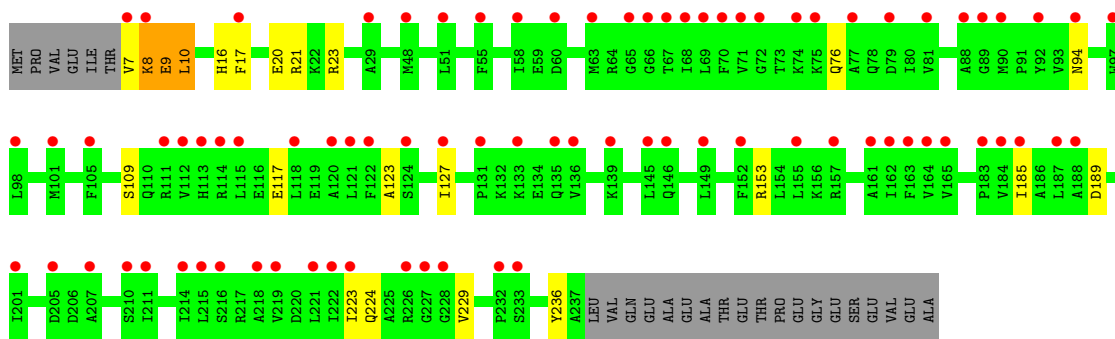
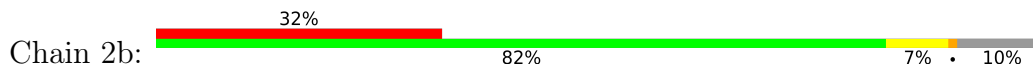




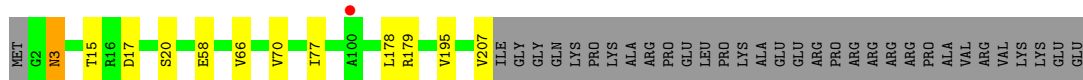
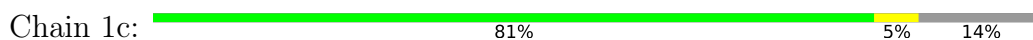
• Molecule 33: 30S ribosomal protein S2



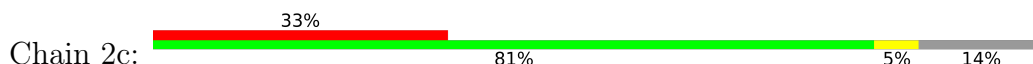
• Molecule 33: 30S ribosomal protein S2

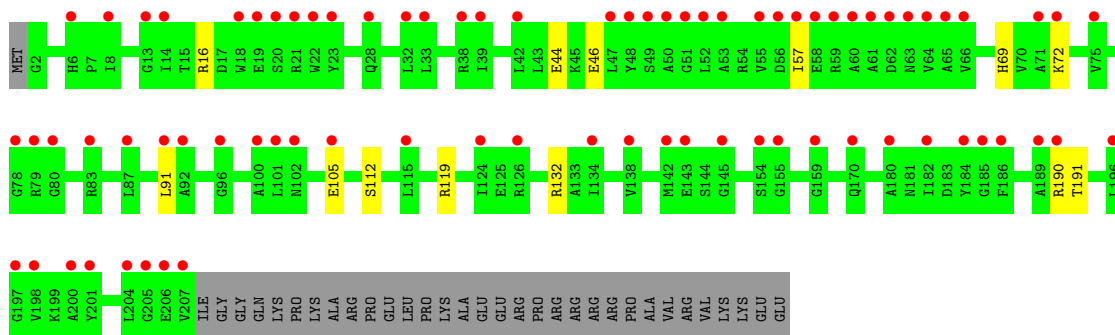


• Molecule 34: 30S ribosomal protein S3

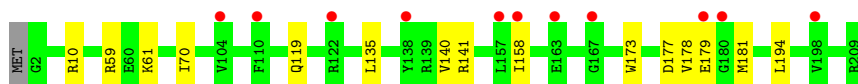


• Molecule 34: 30S ribosomal protein S3

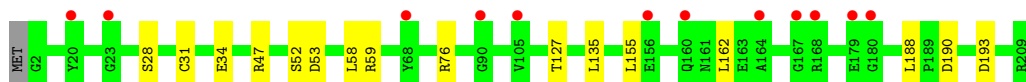




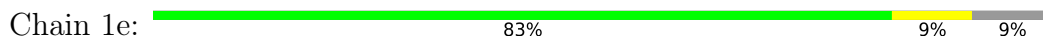
• Molecule 35: 30S ribosomal protein S4



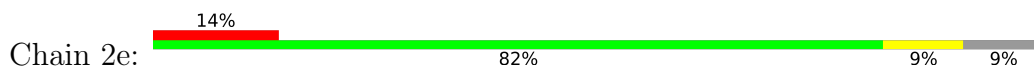
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5



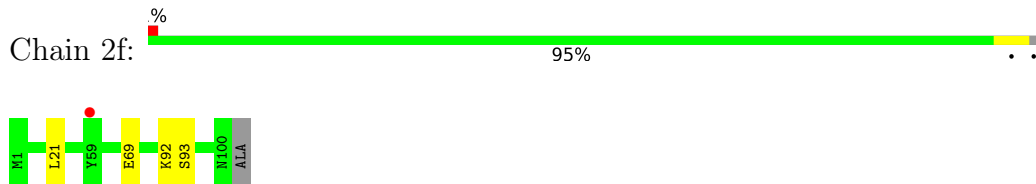
• Molecule 36: 30S ribosomal protein S5



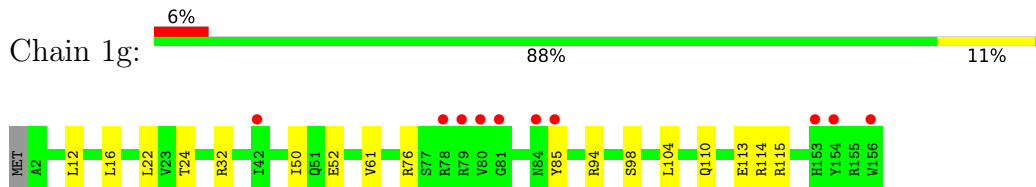
• Molecule 37: 30S ribosomal protein S6



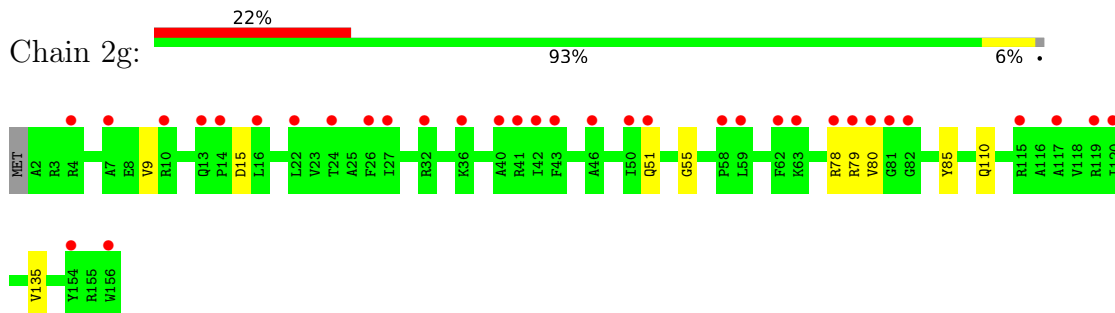
- Molecule 37: 30S ribosomal protein S6



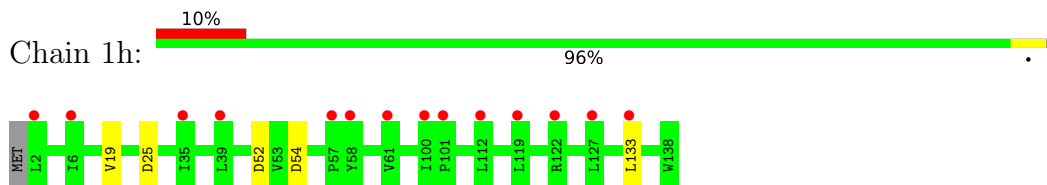
- Molecule 38: 30S ribosomal protein S7



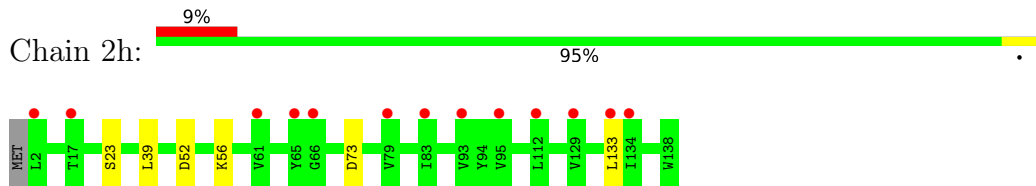
- Molecule 38: 30S ribosomal protein S7



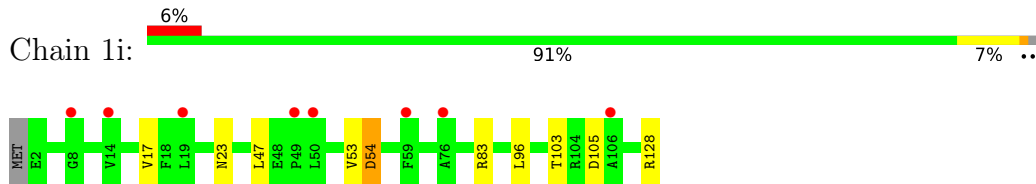
- Molecule 39: 30S ribosomal protein S8



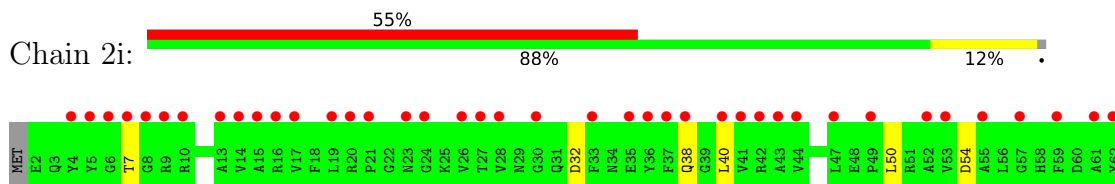
- Molecule 39: 30S ribosomal protein S8



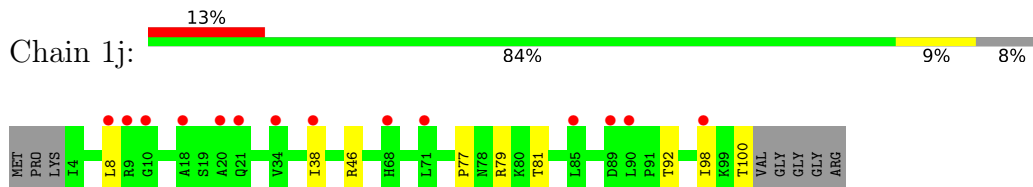
- Molecule 40: 30S ribosomal protein S9



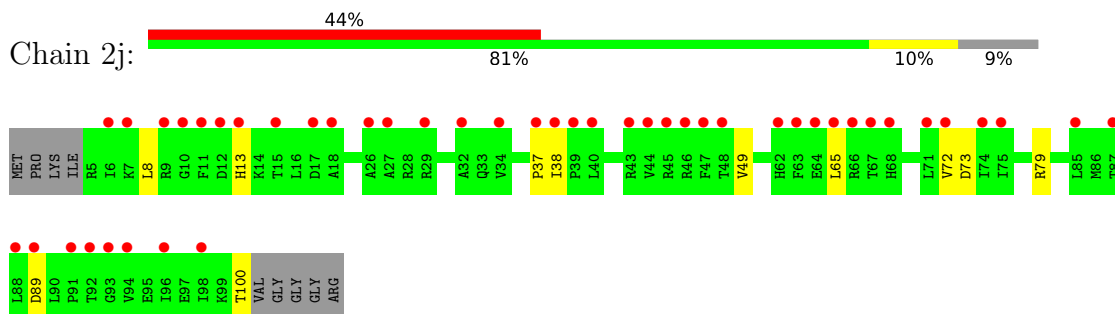
- Molecule 40: 30S ribosomal protein S9



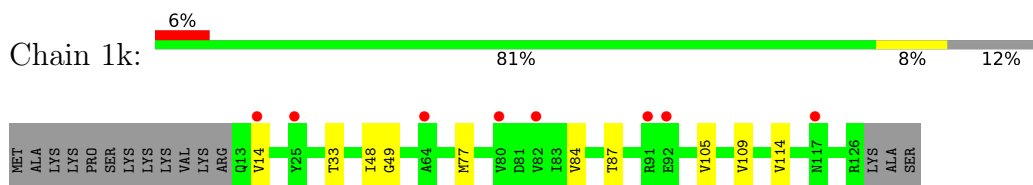
• Molecule 41: 30S ribosomal protein S10



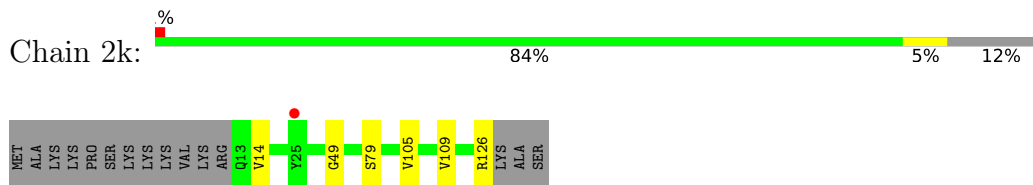
• Molecule 41: 30S ribosomal protein S10



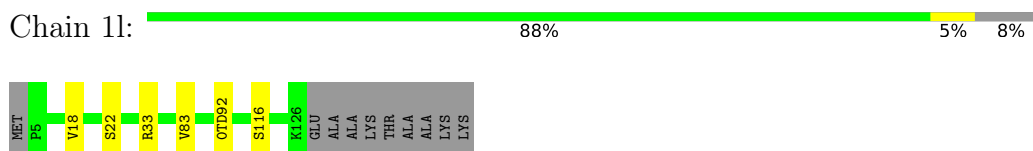
• Molecule 42: 30S ribosomal protein S11



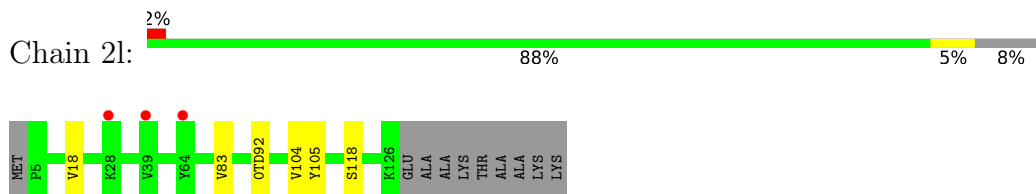
• Molecule 42: 30S ribosomal protein S11



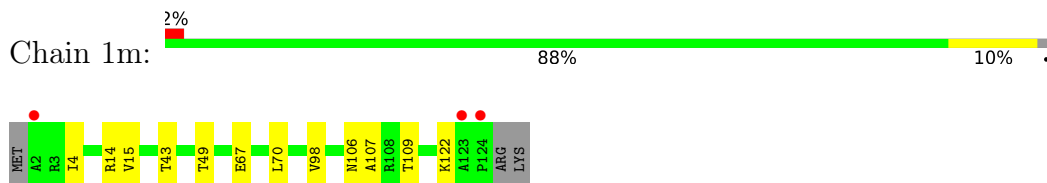
• Molecule 43: 30S ribosomal protein S12



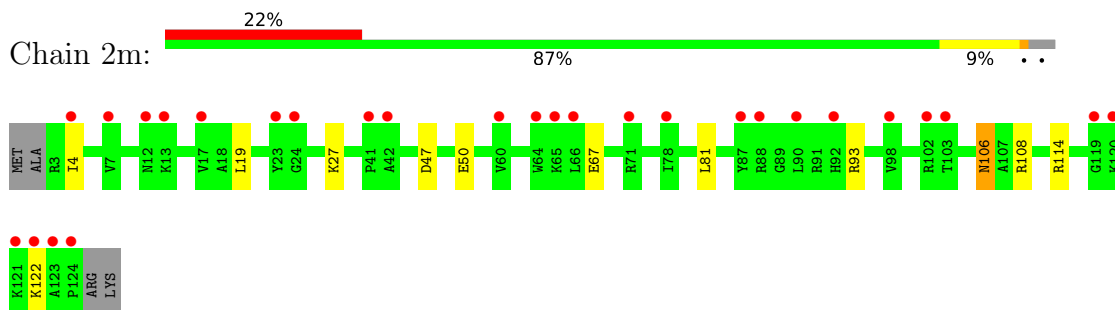
- Molecule 43: 30S ribosomal protein S12



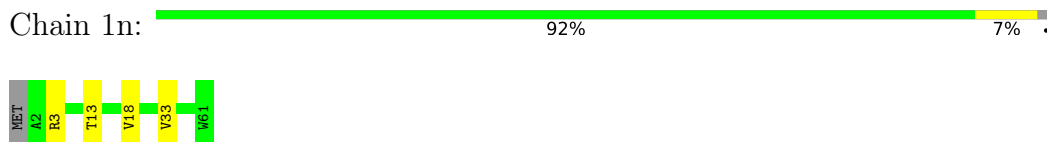
- Molecule 44: 30S ribosomal protein S13



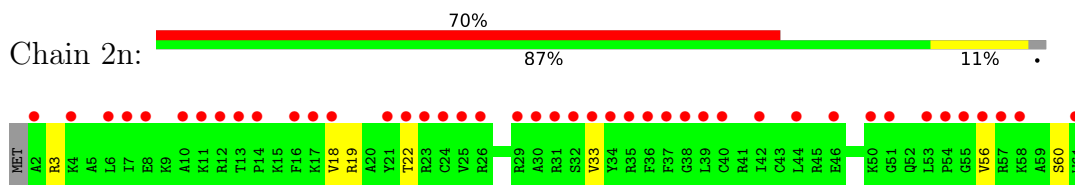
- Molecule 44: 30S ribosomal protein S13



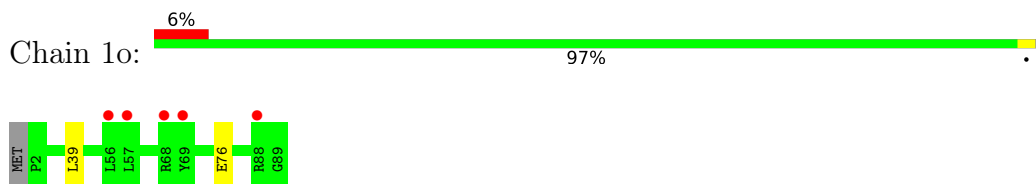
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15




- Molecule 46: 30S ribosomal protein S15

Chain 2o:  93% 6%




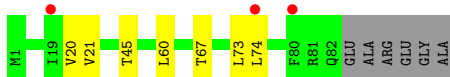
• Molecule 47: 30S ribosomal protein S16

Chain 1p:  85% 8% 7%




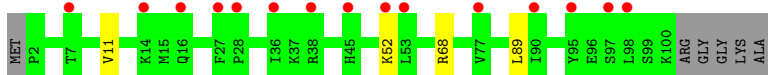
• Molecule 47: 30S ribosomal protein S16

Chain 2p:  3% 85% 8% 7%




• Molecule 48: 30S ribosomal protein S17

Chain 1q:  14% 90% 6%




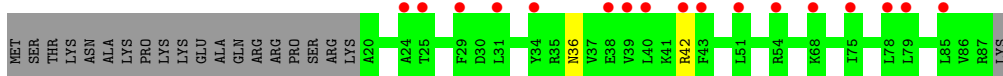
• Molecule 48: 30S ribosomal protein S17

Chain 2q:  6% 86% 9% 6%




• Molecule 49: 30S ribosomal protein S18

Chain 1r:  19% 75% 23%

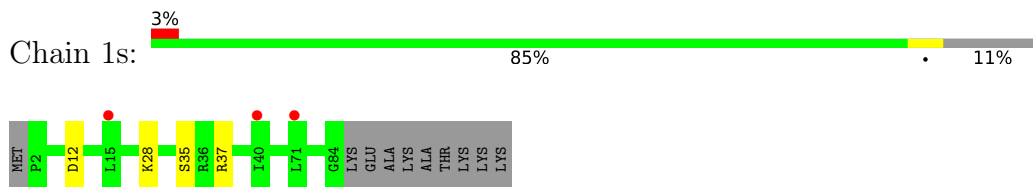


• Molecule 49: 30S ribosomal protein S18

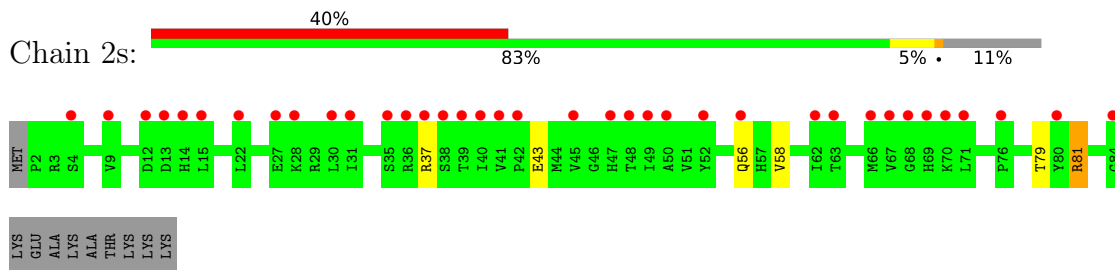
Chain 2r:  % 73% 23%



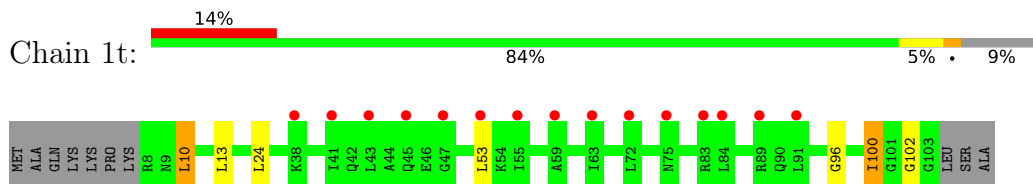
- Molecule 50: 30S ribosomal protein S19



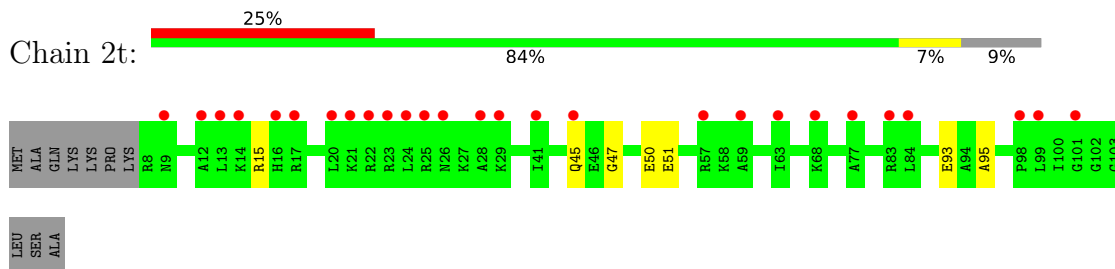
- Molecule 50: 30S ribosomal protein S19



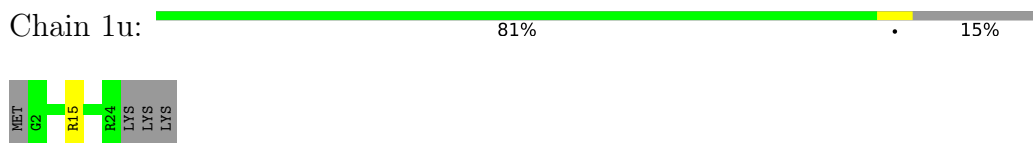
- Molecule 51: 30S ribosomal protein S20



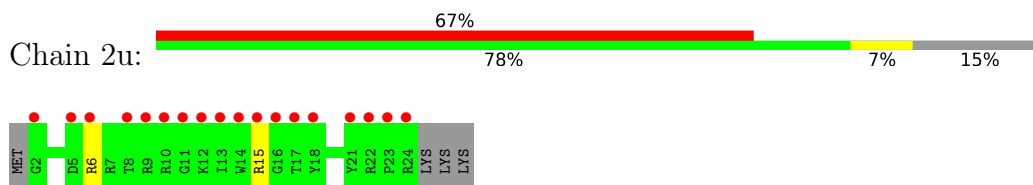
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



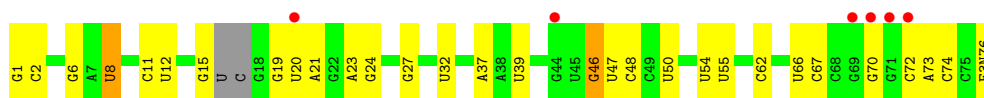
- Molecule 53: MF-mRNA



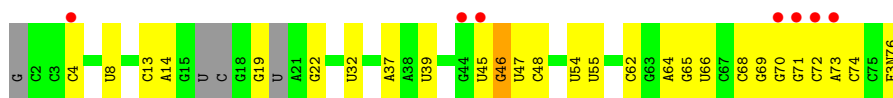
• Molecule 53: MF-mRNA



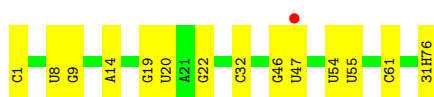
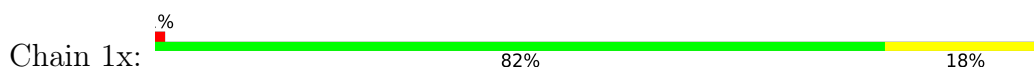
• Molecule 54: A-site Aminoacylated Phe-tRNAphe



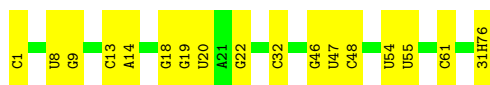
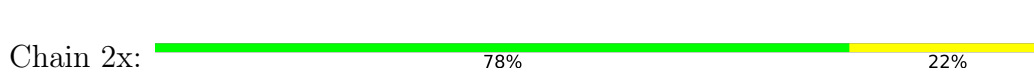
• Molecule 54: A-site Aminoacylated Phe-tRNAphe



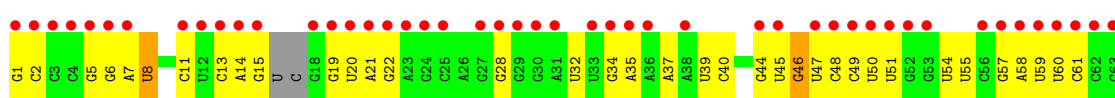
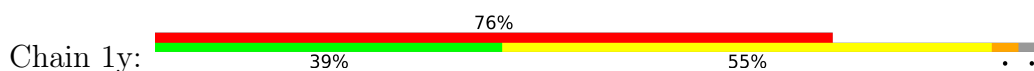
• Molecule 55: P-site Aminoacylated fMet-tRNAmet

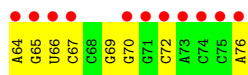


• Molecule 55: P-site Aminoacylated fMet-tRNAmet

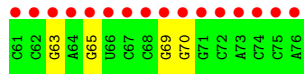
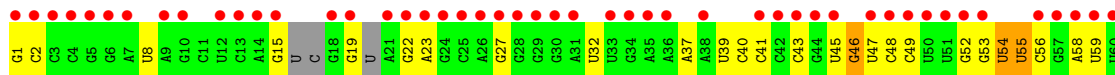
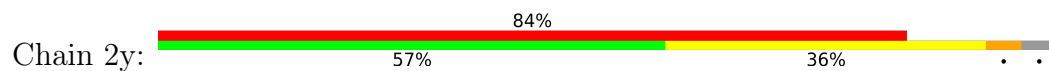


• Molecule 56: E-site Deacylated tRNAphe





- Molecule 56: E-site Deacylated tRNA^{phe}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.65Å 448.12Å 621.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	162.05 – 2.65 162.05 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (162.05-2.65) 98.7 (162.05-2.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.207 , 0.249 0.207 , 0.249	Depositor DCC
R_{free} test set	82773 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtrriage
Anisotropy	0.155	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	300115	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: 8AH, M2G, MG, 5MC, 2MU, F3N, K, 0TD, SF4, 31H, 4OC, ZN, OMG, TYK, MA6, PSU, MIA, 2MG, 5MU, G7M, UR3, OMC, 4SU

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	0.49	0/69010	0.93	57/107716 (0.1%)
1	2A	0.37	0/67294	0.84	25/105038 (0.0%)
2	1B	0.43	1/2882 (0.0%)	0.85	0/4494
2	2B	0.37	1/2879 (0.0%)	0.82	1/4487 (0.0%)
3	1D	0.36	0/2186	0.56	0/2944
3	2D	0.31	0/2186	0.51	0/2944
4	1E	0.33	0/1592	0.55	0/2149
4	2E	0.30	0/1592	0.50	0/2149
5	1F	0.32	0/1618	0.53	0/2191
5	2F	0.30	0/1614	0.50	0/2186
6	1G	0.31	0/1448	0.50	0/1957
6	2G	0.28	0/1453	0.47	0/1963
7	1H	0.32	0/1356	0.51	0/1834
7	2H	0.29	0/1356	0.47	0/1834
8	1I	0.29	0/1112	0.49	0/1514
8	2I	0.29	0/1079	0.50	0/1475
9	1N	0.33	0/1144	0.51	0/1543
9	2N	0.27	0/1144	0.45	0/1543
10	1O	0.34	0/943	0.53	0/1269
10	2O	0.30	0/943	0.54	0/1269
11	1P	0.31	0/1152	0.61	0/1533
11	2P	0.29	0/1152	0.53	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.32	0/982	0.52	0/1312
13	2R	0.26	0/982	0.49	0/1312
14	1S	0.31	0/883	0.49	0/1176
14	2S	0.29	0/880	0.47	0/1172
15	1T	0.32	0/1105	0.50	0/1477
15	2T	0.29	0/1097	0.49	0/1468
16	1U	0.35	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.43	0/1301
17	1V	0.32	0/782	0.54	0/1049
17	2V	0.29	0/782	0.49	0/1049
18	1W	0.34	0/897	0.51	0/1205
18	2W	0.30	0/897	0.47	0/1205
19	1X	0.38	0/764	0.58	0/1025
19	2X	0.30	0/764	0.53	0/1025
20	1Y	0.32	0/819	0.54	0/1095
20	2Y	0.31	0/819	0.50	0/1095
21	1Z	0.28	0/1267	0.49	0/1717
21	2Z	0.29	0/1299	0.50	0/1763
22	10	0.35	0/662	0.56	0/881
22	20	0.30	0/662	0.49	0/881
23	11	0.32	0/762	0.50	0/1014
23	21	0.31	0/762	0.47	0/1014
24	12	0.30	0/590	0.44	0/781
24	22	0.28	0/590	0.41	0/781
25	13	0.31	0/474	0.51	0/635
25	23	0.29	0/469	0.44	0/630
26	14	0.32	0/565	0.56	0/761
26	24	0.32	0/545	0.47	0/737
27	15	0.34	0/469	0.54	0/635
27	25	0.30	0/469	0.50	0/635
28	16	0.34	0/460	0.51	0/613
28	26	0.29	0/456	0.48	0/608
29	17	0.34	0/426	0.54	0/561
29	27	0.28	0/426	0.50	0/561
30	18	0.33	0/525	0.53	0/691
30	28	0.29	0/525	0.49	0/691
31	19	0.31	0/310	0.52	0/407
31	29	0.30	0/310	0.52	0/407
32	1a	0.36	0/35795	0.85	21/55864 (0.0%)
32	2a	0.34	3/35886 (0.0%)	0.87	36/56005 (0.1%)
33	1b	0.30	0/1881	0.48	0/2542
33	2b	0.30	0/1860	0.47	0/2518
34	1c	0.29	0/1572	0.46	0/2126
34	2c	0.29	0/1566	0.47	0/2119
35	1d	0.28	0/1685	0.44	0/2262
35	2d	0.28	0/1704	0.46	0/2284
36	1e	0.30	0/1145	0.50	0/1543
36	2e	0.30	0/1149	0.49	0/1548
37	1f	0.28	0/823	0.46	0/1115
37	2f	0.30	0/829	0.49	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.28	0/1250	0.44	0/1679
38	2g	0.29	0/1254	0.43	0/1683
39	1h	0.29	0/1108	0.48	0/1494
39	2h	0.29	0/1108	0.47	0/1494
40	1i	0.30	0/1002	0.50	0/1346
40	2i	0.30	0/997	0.48	0/1343
41	1j	0.28	0/722	0.50	0/982
41	2j	0.27	0/727	0.54	0/988
42	1k	0.28	0/844	0.47	0/1145
42	2k	0.29	0/848	0.47	0/1149
43	1l	0.34	0/937	0.54	0/1260
43	2l	0.27	0/937	0.50	0/1260
44	1m	0.28	0/969	0.49	0/1302
44	2m	0.29	0/961	0.51	0/1291
45	1n	0.32	0/501	0.48	0/664
45	2n	0.30	0/501	0.47	0/664
46	1o	0.27	0/739	0.44	0/985
46	2o	0.26	0/739	0.43	0/985
47	1p	0.27	0/697	0.47	0/939
47	2p	0.28	0/693	0.51	0/935
48	1q	0.28	0/836	0.48	0/1117
48	2q	0.27	0/836	0.46	0/1117
49	1r	0.27	0/560	0.51	0/746
49	2r	0.27	0/560	0.49	1/746 (0.1%)
50	1s	0.28	0/667	0.51	0/900
50	2s	0.32	0/661	0.56	0/893
51	1t	0.28	0/730	0.43	0/965
51	2t	0.26	0/729	0.41	0/965
52	1u	0.25	0/203	0.44	0/266
52	2u	0.28	0/203	0.47	0/266
53	1v	0.45	0/310	0.92	0/480
53	2v	0.38	0/310	0.84	0/480
54	1w	0.50	1/1581 (0.1%)	1.00	0/2458
54	2w	0.41	0/1531	0.98	0/2379
55	1x	0.59	5/1723 (0.3%)	1.11	20/2684 (0.7%)
55	2x	0.53	1/1723 (0.1%)	1.05	13/2684 (0.5%)
56	1y	0.56	1/1606 (0.1%)	1.11	5/2497 (0.2%)
56	2y	0.52	1/1583 (0.1%)	0.98	1/2459 (0.0%)
All	All	0.38	14/316632 (0.0%)	0.80	180/474029 (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
33	1b	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	1	C	OP3-P	-10.29	1.48	1.61
56	1y	1	G	OP3-P	-10.15	1.49	1.61
2	1B	1	U	OP3-P	-10.15	1.49	1.61
54	1w	1	G	OP3-P	-10.12	1.49	1.61
2	2B	1	U	OP3-P	-10.09	1.49	1.61
32	2a	1272	G	N1-C2	-10.07	1.29	1.37
55	2x	1	C	OP3-P	-9.95	1.49	1.61
56	2y	1	G	OP3-P	-9.92	1.49	1.61
32	2a	1272	G	C6-N1	-9.04	1.33	1.39
32	2a	1263	C	N3-C4	-6.34	1.29	1.33
55	1x	14	A	N7-C5	-5.41	1.36	1.39
55	1x	22	G	C8-N7	5.41	1.34	1.30
55	1x	22	G	N7-C5	5.39	1.42	1.39
55	1x	14	A	C8-N7	-5.22	1.27	1.31

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	27.29	135.27	118.90
32	2a	1272	G	N3-C2-N2	24.11	136.78	119.90
32	2a	1272	G	C5-C6-O6	22.16	141.89	128.60
32	2a	1272	G	N1-C2-N2	-18.59	99.47	116.20
32	2a	1272	G	C6-N1-C2	16.24	134.84	125.10
32	2a	1263	C	N3-C2-O2	-15.40	111.12	121.90
32	2a	1263	C	C2-N3-C4	15.22	127.51	119.90
32	2a	1272	G	N1-C6-O6	-12.50	112.40	119.90
32	2a	1263	C	C5-C6-N1	12.20	127.10	121.00
55	1x	46	G	C6-N1-C2	-12.06	117.86	125.10
32	2a	1272	G	C5-C6-N1	-11.67	105.66	111.50
1	2A	2136	C	N1-C2-O2	10.63	125.28	118.90
1	1A	1075	C	N1-C2-O2	10.41	125.14	118.90
1	1A	1075	C	C2-N3-C4	10.40	125.10	119.90
55	1x	22	G	C5-N7-C8	-10.04	99.28	104.30
1	1A	1063	G	C5-C6-O6	10.00	134.60	128.60
55	2x	46	G	C6-N1-C2	-9.93	119.14	125.10
32	2a	1263	C	C4-C5-C6	-9.87	112.46	117.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	14	A	C4-C5-C6	9.81	121.91	117.00
55	2x	14	A	C4-C5-C6	9.58	121.79	117.00
55	2x	14	A	C5-N7-C8	9.57	108.69	103.90
32	2a	1263	C	C2-N1-C1'	9.52	129.27	118.80
1	1A	1063	G	C6-N1-C2	8.59	130.26	125.10
55	1x	14	A	C5-N7-C8	8.57	108.19	103.90
32	2a	1263	C	C6-N1-C2	-8.35	116.96	120.30
1	1A	512	G	O4'-C1'-N9	8.32	114.86	108.20
2	2B	80	U	O4'-C1'-N1	8.30	114.84	108.20
1	1A	2682	U	O5'-P-OP2	-8.25	98.28	105.70
32	2a	1263	C	N1-C2-N3	-8.07	113.55	119.20
32	2a	1272	G	C2-N3-C4	-8.05	107.88	111.90
1	1A	948	G	O5'-P-OP1	-8.05	98.46	105.70
32	1a	1025	U	N1-C2-O2	7.76	128.23	122.80
1	1A	740	U	O5'-P-OP2	-7.64	98.82	105.70
32	2a	1263	C	N3-C4-N4	-7.60	112.68	118.00
55	1x	46	G	N3-C2-N2	-7.59	114.59	119.90
55	1x	46	G	C5-C6-N1	7.58	115.29	111.50
55	1x	14	A	C5-C6-N1	-7.40	114.00	117.70
55	2x	22	G	C5-N7-C8	-7.38	100.61	104.30
55	1x	22	G	C4-C5-C6	-7.38	114.38	118.80
1	1A	793	A	O5'-P-OP2	-7.37	99.06	105.70
32	2a	1263	C	C5-C4-N4	7.24	125.27	120.20
55	1x	22	G	N7-C8-N9	7.12	116.66	113.10
1	2A	2136	C	N3-C2-O2	-7.10	116.93	121.90
1	2A	2129	C	N1-C2-O2	6.96	123.08	118.90
1	1A	975	C	N1-C2-O2	-6.85	114.79	118.90
55	2x	14	A	C5-C6-N1	-6.83	114.28	117.70
1	2A	512	G	O4'-C1'-N9	6.83	113.66	108.20
1	1A	1992	G	P-O3'-C3'	6.78	127.84	119.70
1	1A	1063	G	N3-C2-N2	6.74	124.61	119.90
1	1A	1784	A	O5'-P-OP2	-6.66	99.71	105.70
32	2a	1029	C	N1-C2-O2	6.65	122.89	118.90
1	1A	1086	A	N1-C6-N6	-6.61	114.64	118.60
1	2A	2155	G	C6-N1-C2	6.60	129.06	125.10
32	1a	1034	G	C6-N1-C2	6.55	129.03	125.10
32	2a	1272	G	C8-N9-C1'	-6.54	118.49	127.00
1	1A	226	G	O4'-C1'-N9	6.47	113.38	108.20
1	1A	2689	U	P-O3'-C3'	6.46	127.45	119.70
1	1A	2593	U	N3-C4-O4	-6.43	114.90	119.40
1	1A	2629	A	P-O3'-C3'	6.41	127.39	119.70
32	1a	558	G	O5'-P-OP1	-6.37	99.97	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C4-N9-C1'	6.30	134.70	126.50
1	1A	2122	U	C5-C4-O4	6.30	129.68	125.90
1	2A	1313	U	C2-N1-C1'	6.28	125.24	117.70
56	1y	22	G	N1-C6-O6	6.25	123.65	119.90
55	1x	22	G	C5-C6-N1	6.24	114.62	111.50
32	1a	1067	A	P-O3'-C3'	6.23	127.17	119.70
55	1x	22	G	N1-C6-O6	-6.21	116.17	119.90
1	2A	2155	G	N3-C2-N2	6.11	124.18	119.90
55	2x	22	G	C4-C5-C6	-6.11	115.14	118.80
32	1a	754	C	C2-N1-C1'	6.08	125.49	118.80
32	2a	1263	C	C6-N1-C1'	-6.07	113.52	120.80
1	1A	1075	C	C5-C4-N4	6.05	124.44	120.20
1	2A	2062	A	N1-C6-N6	6.04	122.23	118.60
1	1A	845	G	O4'-C1'-N9	6.04	113.03	108.20
1	2A	141	A	C8-N9-C4	-6.03	103.39	105.80
55	1x	22	G	C8-N9-C1'	5.99	134.78	127.00
1	1A	624	C	O5'-P-OP1	-5.98	100.32	105.70
55	2x	46	G	N3-C2-N2	-5.93	115.75	119.90
32	2a	754	C	C2-N1-C1'	5.92	125.31	118.80
1	1A	2848	G	O4'-C1'-N9	5.91	112.93	108.20
56	2y	22	G	N1-C6-O6	5.88	123.43	119.90
32	2a	1279	A	OP1-P-O3'	5.87	118.12	105.20
1	2A	2155	G	C5-C6-O6	5.87	132.12	128.60
1	1A	2501	C	C2-N1-C1'	-5.84	112.37	118.80
55	1x	46	G	N9-C4-C5	5.77	107.71	105.40
1	1A	847	U	C2-N1-C1'	5.76	124.62	117.70
1	1A	1063	G	N1-C6-O6	-5.75	116.45	119.90
1	1A	1253	A	C5-N7-C8	5.75	106.78	103.90
1	1A	205	G	O5'-P-OP2	-5.74	100.53	105.70
32	2a	913	A	P-O3'-C3'	5.72	126.57	119.70
1	1A	1253	A	N7-C8-N9	-5.72	110.94	113.80
1	2A	2061	G	O5'-P-OP2	-5.71	100.56	105.70
55	1x	46	G	N1-C2-N3	5.69	127.31	123.90
1	2A	141	A	N7-C8-N9	5.66	116.63	113.80
32	2a	754	C	N1-C2-O2	5.65	122.29	118.90
55	2x	46	G	C5-C6-N1	5.65	114.33	111.50
32	1a	1442	G	N3-C4-C5	-5.65	125.78	128.60
32	2a	952	U	C5-C4-O4	5.65	129.29	125.90
32	2a	266	G	P-O3'-C3'	5.64	126.47	119.70
32	1a	1225	A	C5-C6-N6	5.63	128.21	123.70
55	1x	14	A	C4-N9-C1'	5.63	136.43	126.30
55	1x	14	A	C8-N9-C1'	-5.63	117.57	127.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1075	C	N3-C4-C5	-5.62	119.65	121.90
1	2A	847	U	C2-N1-C1'	5.62	124.45	117.70
1	1A	2134	A	P-O3'-C3'	5.61	126.44	119.70
32	2a	1279	A	P-O3'-C3'	5.61	126.43	119.70
1	1A	999	U	O5'-P-OP2	-5.59	100.67	105.70
32	1a	754	C	N1-C2-O2	5.57	122.25	118.90
1	1A	1174	A	P-O3'-C3'	5.54	126.35	119.70
1	1A	748	G	O4'-C1'-N9	5.53	112.62	108.20
1	1A	1174	A	OP1-P-O3'	5.52	117.35	105.20
32	1a	266	G	P-O3'-C3'	5.51	126.31	119.70
55	2x	46	G	N1-C2-N3	5.50	127.20	123.90
1	2A	1992	G	P-O3'-C3'	5.50	126.30	119.70
1	2A	801	G	O5'-P-OP2	-5.50	100.75	105.70
55	1x	22	G	C4-C5-N7	5.50	113.00	110.80
55	2x	46	G	C4-C5-N7	-5.48	108.61	110.80
1	1A	1075	C	N3-C2-O2	-5.45	118.08	121.90
56	1y	15	G	N3-C2-N2	5.44	123.71	119.90
32	1a	1006	C	N1-C2-O2	5.43	122.16	118.90
32	1a	913	A	P-O3'-C3'	5.42	126.21	119.70
55	1x	22	G	N3-C4-N9	-5.41	122.75	126.00
32	1a	955	U	C2-N3-C4	5.39	130.23	127.00
32	2a	1032	G	C6-N1-C2	5.38	128.33	125.10
32	1a	1158	C	C2-N1-C1'	5.36	124.69	118.80
1	1A	372	G	O4'-C1'-N9	5.35	112.48	108.20
1	1A	2825	C	C6-N1-C2	-5.35	118.16	120.30
55	1x	46	G	C4-C5-N7	-5.35	108.66	110.80
55	2x	14	A	C4-C5-N7	-5.35	108.03	110.70
1	1A	1187	G	N1-C6-O6	-5.33	116.70	119.90
56	1y	22	G	C4-C5-C6	5.33	122.00	118.80
55	1x	46	G	C5-C6-O6	-5.31	125.42	128.60
1	2A	2160	G	C4-N9-C1'	5.31	133.40	126.50
32	2a	79	G	C5-C6-O6	5.30	131.78	128.60
1	1A	1313	U	C2-N1-C1'	5.30	124.06	117.70
1	1A	2167	U	C2-N1-C1'	5.30	124.06	117.70
32	2a	1138	G	C4-N9-C1'	5.27	133.35	126.50
1	2A	1633	G	C8-N9-C4	-5.26	104.30	106.40
1	1A	1385	G	O4'-C1'-N9	5.26	112.41	108.20
32	2a	1029	C	N3-C2-O2	-5.25	118.22	121.90
1	1A	1253	A	C8-N9-C4	5.25	107.90	105.80
32	1a	1442	G	C2-N3-C4	5.24	114.52	111.90
32	1a	1034	G	C5-C6-O6	5.24	131.74	128.60
1	1A	2461	C	N3-C2-O2	-5.24	118.23	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2129	C	C2-N3-C4	5.23	122.52	119.90
1	2A	383	U	O4'-C1'-N1	5.23	112.38	108.20
1	1A	787	U	O5'-P-OP1	-5.22	101.00	105.70
1	1A	954	G	O5'-P-OP1	-5.22	101.00	105.70
1	1A	1223	G	N1-C6-O6	-5.20	116.78	119.90
1	1A	1131	G	O4'-C1'-N9	5.20	112.36	108.20
32	2a	1032	G	C5-C6-O6	5.18	131.71	128.60
32	2a	1065	U	P-O3'-C3'	5.18	125.91	119.70
1	1A	1176	G	OP1-P-O3'	5.16	116.56	105.20
1	1A	2036	C	O5'-P-OP1	-5.16	101.05	105.70
56	1y	50	U	C2-N3-C4	5.16	130.10	127.00
1	2A	2168	G	C4-N9-C1'	5.16	133.21	126.50
32	2a	955	U	C2-N3-C4	5.15	130.09	127.00
32	2a	687	A	P-O3'-C3'	5.15	125.88	119.70
55	2x	14	A	C8-N9-C1'	-5.12	118.48	127.70
1	1A	2685	G	N1-C6-O6	-5.12	116.83	119.90
1	2A	2160	G	C8-N9-C1'	-5.12	120.34	127.00
32	1a	1025	U	C2-N1-C1'	5.12	123.84	117.70
1	2A	1779	U	O4'-C1'-N1	5.11	112.28	108.20
1	1A	1063	G	C5-C6-N1	-5.10	108.95	111.50
32	1a	792	A	O4'-C1'-N9	5.08	112.27	108.20
1	1A	2461	C	N1-C2-O2	5.08	121.95	118.90
32	1a	687	A	P-O3'-C3'	5.08	125.80	119.70
1	2A	2689	U	P-O3'-C3'	5.08	125.79	119.70
1	2A	1698	A	O4'-C1'-N9	5.07	112.25	108.20
1	1A	668	G	OP2-P-O3'	5.06	116.33	105.20
32	1a	1531	A	N7-C8-N9	5.06	116.33	113.80
1	1A	801	G	O5'-P-OP2	-5.05	101.16	105.70
56	1y	64	A	C6-N1-C2	5.05	121.63	118.60
32	1a	1158	C	N1-C2-O2	5.04	121.92	118.90
55	2x	22	G	C8-N9-C1'	5.02	133.53	127.00
1	1A	1936	A	O4'-C1'-N9	5.01	112.21	108.20
32	1a	1225	A	C6-N1-C2	5.01	121.61	118.60
49	2r	31	LEU	CA-CB-CG	5.01	126.81	115.30
1	2A	2335	A	O4'-C1'-N9	5.00	112.20	108.20
1	1A	975	C	C2-N1-C1'	-5.00	113.30	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	125	PRO	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100	100
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	29	43
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	29	43
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	29	43
5	2F	200/210 (95%)	194 (97%)	4 (2%)	2 (1%)	15	23
6	1G	179/182 (98%)	168 (94%)	11 (6%)	0	100	100
6	2G	179/182 (98%)	159 (89%)	17 (10%)	3 (2%)	9	13
7	1H	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	25	37
8	1I	144/148 (97%)	124 (86%)	20 (14%)	0	100	100
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	11	16
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	22	33
10	1O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	19	29
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	7	10
11	2P	147/150 (98%)	130 (88%)	11 (8%)	6 (4%)	3	3
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	122 (88%)	17 (12%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	4 (4%)	2 (2%)	8	11
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	23
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	23
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	2 (2%)	1 (1%)	17	26
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	15	23
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	135 (91%)	12 (8%)	1 (1%)	22	33
21	2Z	156/206 (76%)	130 (83%)	22 (14%)	4 (3%)	5	7
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	21
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	12
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
26	24	67/71 (94%)	52 (78%)	12 (18%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	197 (86%)	27 (12%)	5 (2%)	6	9
33	2b	229/256 (90%)	194 (85%)	28 (12%)	7 (3%)	4	5
34	1c	204/239 (85%)	186 (91%)	17 (8%)	1 (0%)	29	43
34	2c	204/239 (85%)	180 (88%)	24 (12%)	0	100	100
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	29	43
35	2d	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
36	1e	146/162 (90%)	133 (91%)	11 (8%)	2 (1%)	11	16
36	2e	146/162 (90%)	137 (94%)	7 (5%)	2 (1%)	11	16
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
38	1g	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	22	33
38	2g	153/156 (98%)	133 (87%)	18 (12%)	2 (1%)	12	18
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	121 (90%)	13 (10%)	1 (1%)	22	33
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	29
40	2i	125/128 (98%)	104 (83%)	21 (17%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	7	10
41	2j	94/105 (90%)	82 (87%)	10 (11%)	2 (2%)	7	10
42	1k	112/129 (87%)	101 (90%)	8 (7%)	3 (3%)	5	6
42	2k	112/129 (87%)	101 (90%)	10 (9%)	1 (1%)	17	26
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	7 (6%)	1 (1%)	19	29
44	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	9	13
44	2m	120/126 (95%)	103 (86%)	15 (12%)	2 (2%)	9	13
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	2n	58/61 (95%)	52 (90%)	5 (9%)	1 (2%)	9	13
46	1o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
47	1p	80/88 (91%)	73 (91%)	7 (9%)	0	100	100
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	15	23
48	2q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	7	10
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	10	15
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	2s	81/93 (87%)	66 (82%)	14 (17%)	1 (1%)	13	19
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	3
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7	10
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11368/12128 (94%)	10509 (92%)	769 (7%)	90 (1%)	19	29

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	29	LYS
11	1P	36	LYS
21	1Z	53	ILE
26	14	45	GLY
26	14	62	ARG
33	1b	17	PHE
40	1i	54	ASP
44	1m	107	ALA
5	2F	130	ALA
8	2I	10	GLU
11	2P	29	LYS
11	2P	36	LYS
21	2Z	52	SER
33	2b	10	LEU
33	2b	17	PHE
33	2b	123	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	2g	80	VAL
41	2j	79	ARG
44	2m	67	GLU
48	2q	68	ARG
50	2s	81	ARG
17	1V	79	VAL
26	14	49	PHE
26	14	53	GLU
33	1b	124	SER
33	1b	126	GLU
35	1d	173	TRP
41	1j	79	ARG
44	1m	67	GLU
48	1q	68	ARG
51	1t	100	ILE
8	2I	40	THR
11	2P	44	GLY
11	2P	45	LEU
17	2V	79	VAL
26	24	45	GLY
33	2b	21	ARG
38	2g	55	GLY
42	2k	49	GLY
51	2t	95	ALA
20	1Y	54	LYS
23	11	3	LYS
36	1e	85	GLY
42	1k	77	MET
51	1t	10	LEU
6	2G	43	LEU
9	2N	2	LYS
11	2P	38	GLN
21	2Z	51	ALA
21	2Z	144	LEU
33	2b	8	LYS
36	2e	37	ARG
43	2l	105	TYR
45	2n	19	ARG
49	2r	36	ASN
4	1E	52	LEU
11	1P	38	GLN
33	1b	231	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	3	ASN
41	1j	77	PRO
51	1t	96	GLY
51	1t	102	GLY
4	2E	52	LEU
26	24	48	ARG
44	2m	106	ASN
48	2q	67	LYS
38	1g	52	GLU
42	1k	105	VAL
5	2F	21	ALA
6	2G	42	GLY
6	2G	51	ARG
7	2H	126	PRO
18	2W	60	ASN
33	2b	20	GLU
10	1O	5	GLN
14	2S	84	GLN
33	2b	9	GLU
36	2e	77	PRO
11	2P	122	PRO
25	23	59	VAL
42	1k	49	GLY
14	2S	109	GLY
26	24	29	PRO
39	2h	73	ASP
51	2t	47	GLY
36	1e	69	VAL
21	2Z	171	ILE
41	2j	37	PRO
33	1b	125	PRO

5.3.2 Protein sidechains [i](#)

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	203 (94%)	12 (6%)	21	33
3	2D	215/218 (99%)	202 (94%)	13 (6%)	19	30
4	1E	164/166 (99%)	157 (96%)	7 (4%)	29	44
4	2E	164/166 (99%)	158 (96%)	6 (4%)	34	50
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	17
5	2F	159/166 (96%)	151 (95%)	8 (5%)	24	38
6	1G	143/156 (92%)	133 (93%)	10 (7%)	15	23
6	2G	143/156 (92%)	127 (89%)	16 (11%)	6	8
7	1H	144/148 (97%)	142 (99%)	2 (1%)	67	81
7	2H	144/148 (97%)	131 (91%)	13 (9%)	9	14
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2	2
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4	6
9	1N	118/119 (99%)	109 (92%)	9 (8%)	13	21
9	2N	118/119 (99%)	109 (92%)	9 (8%)	13	21
10	1O	100/100 (100%)	98 (98%)	2 (2%)	55	73
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	59
11	1P	115/116 (99%)	107 (93%)	8 (7%)	15	23
11	2P	115/116 (99%)	105 (91%)	10 (9%)	10	15
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	44	63
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	44	63
13	1R	101/101 (100%)	96 (95%)	5 (5%)	24	38
13	2R	101/101 (100%)	98 (97%)	3 (3%)	41	59
14	1S	86/88 (98%)	78 (91%)	8 (9%)	9	13
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4	5
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	44
15	2T	113/127 (89%)	109 (96%)	4 (4%)	36	52
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	56
16	2U	93/94 (99%)	88 (95%)	5 (5%)	22	34
17	1V	80/82 (98%)	74 (92%)	6 (8%)	13	21
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21	33
18	2W	90/92 (98%)	84 (93%)	6 (7%)	16	25
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	48
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	48
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	19	30
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8	13
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	14
21	2Z	137/179 (76%)	127 (93%)	10 (7%)	14	21
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	57
23	11	80/83 (96%)	80 (100%)	0	100	100
23	21	80/83 (96%)	75 (94%)	5 (6%)	18	28
24	12	65/67 (97%)	63 (97%)	2 (3%)	40	57
24	22	65/67 (97%)	63 (97%)	2 (3%)	40	57
25	13	51/52 (98%)	45 (88%)	6 (12%)	5	7
25	23	50/52 (96%)	49 (98%)	1 (2%)	55	73
26	14	59/63 (94%)	55 (93%)	4 (7%)	16	24
26	24	53/63 (84%)	46 (87%)	7 (13%)	4	5
27	15	50/52 (96%)	47 (94%)	3 (6%)	19	30
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	47
28	16	51/52 (98%)	47 (92%)	4 (8%)	12	20
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	4
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	11
29	27	41/42 (98%)	38 (93%)	3 (7%)	14	21
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	21
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	13
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	32 (94%)	2 (6%)	19	30
33	1b	192/220 (87%)	175 (91%)	17 (9%)	9	14
33	2b	187/220 (85%)	169 (90%)	18 (10%)	8	12
34	1c	142/188 (76%)	130 (92%)	12 (8%)	10	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	2c	140/188 (74%)	127 (91%)	13 (9%)	9	13
35	1d	169/181 (93%)	155 (92%)	14 (8%)	11	16
35	2d	173/181 (96%)	157 (91%)	16 (9%)	9	13
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6	10
36	2e	114/123 (93%)	101 (89%)	13 (11%)	5	8
37	1f	84/90 (93%)	79 (94%)	5 (6%)	19	30
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	40
38	1g	119/127 (94%)	103 (87%)	16 (13%)	4	5
38	2g	120/127 (94%)	112 (93%)	8 (7%)	16	25
39	1h	114/119 (96%)	109 (96%)	5 (4%)	28	43
39	2h	114/119 (96%)	109 (96%)	5 (4%)	28	43
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	8
40	2i	89/99 (90%)	74 (83%)	15 (17%)	2	2
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6	10
41	2j	69/92 (75%)	60 (87%)	9 (13%)	4	5
42	1k	82/99 (83%)	75 (92%)	7 (8%)	10	15
42	2k	83/99 (84%)	78 (94%)	5 (6%)	19	30
43	1l	96/108 (89%)	91 (95%)	5 (5%)	23	36
43	2l	96/108 (89%)	92 (96%)	4 (4%)	30	45
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	9
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	7
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	17
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	6
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	64
46	2o	78/80 (98%)	73 (94%)	5 (6%)	17	27
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7	10
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	10
48	1q	94/97 (97%)	91 (97%)	3 (3%)	39	56
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	21
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	53
49	2r	59/77 (77%)	56 (95%)	3 (5%)	24	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	1s	69/80 (86%)	65 (94%)	4 (6%)	20	31
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	14
51	1t	70/82 (85%)	65 (93%)	5 (7%)	14	22
51	2t	70/82 (85%)	65 (93%)	5 (7%)	14	22
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	33
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	8
All	All	9303/10064 (92%)	8644 (93%)	659 (7%)	14	22

All (659) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	12	SER
3	1D	37	LEU
3	1D	99	ASP
3	1D	106	ILE
3	1D	173	VAL
3	1D	200	ASP
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	273	ARG
3	1D	275	LYS
4	1E	12	THR
4	1E	47	VAL
4	1E	49	LEU
4	1E	73	GLU
4	1E	113	PHE
4	1E	116	VAL
4	1E	184	VAL
5	1F	12	LEU
5	1F	24	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	106	ARG
5	1F	112	MET
5	1F	140	LEU
5	1F	144	LYS
5	1F	158	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	162	LEU
5	1F	168	ARG
5	1F	192	LEU
6	1G	3	LEU
6	1G	5	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	126	ASP
6	1G	133	LEU
6	1G	139	LEU
6	1G	148	MET
6	1G	149	VAL
7	1H	84	SER
7	1H	119	GLU
8	1I	2	LYS
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	40	THR
8	1I	41	GLU
8	1I	47	LEU
8	1I	50	ARG
8	1I	76	THR
8	1I	77	LEU
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	105	HIS
8	1I	108	THR
8	1I	109	ILE
8	1I	123	LEU
8	1I	129	THR
9	1N	2	LYS
9	1N	5	VAL
9	1N	12	ARG
9	1N	28	THR
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	67	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	1N	96	GLU
10	1O	28	SER
10	1O	106	LEU
11	1P	7	ARG
11	1P	45	LEU
11	1P	76	LYS
11	1P	90	ARG
11	1P	95	VAL
11	1P	98	GLU
11	1P	147	LEU
11	1P	149	GLU
12	1Q	8	LYS
12	1Q	75	THR
12	1Q	109	VAL
13	1R	6	SER
13	1R	15	SER
13	1R	36	THR
13	1R	67	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	25	ARG
14	1S	53	SER
14	1S	68	GLN
14	1S	69	VAL
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	36	GLU
15	1T	49	VAL
15	1T	96	ARG
15	1T	128	GLU
16	1U	74	LEU
16	1U	95	LEU
16	1U	117	GLN
17	1V	10	LYS
17	1V	28	GLU
17	1V	46	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	85	LYS
18	1W	11	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	1W	17	VAL
18	1W	19	LEU
18	1W	60	ASN
18	1W	63	ASP
19	1X	72	LYS
19	1X	88	LYS
19	1X	92	LEU
20	1Y	1	MET
20	1Y	64	GLU
20	1Y	67	LEU
20	1Y	72	VAL
20	1Y	99	CYS
21	1Z	49	ARG
21	1Z	53	ILE
21	1Z	61	LEU
21	1Z	77	ASP
21	1Z	87	ASP
21	1Z	122	ARG
21	1Z	129	SER
21	1Z	138	GLU
21	1Z	149	SER
21	1Z	154	ASP
21	1Z	170	THR
21	1Z	171	ILE
24	12	19	VAL
24	12	65	ASN
25	13	23	LEU
25	13	34	GLU
25	13	35	ARG
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	49	PHE
26	14	53	GLU
26	14	63	TYR
26	14	67	TYR
27	15	6	VAL
27	15	40	LYS
27	15	55	ARG
28	16	4	GLU
28	16	5	VAL
28	16	19	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	16	48	VAL
29	17	24	THR
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	29	LYS
30	18	31	HIS
30	18	34	TRP
33	1b	8	LYS
33	1b	12	GLU
33	1b	16	HIS
33	1b	21	ARG
33	1b	23	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	54	THR
33	1b	67	THR
33	1b	80	ILE
33	1b	97	TRP
33	1b	130	ARG
33	1b	133	LYS
33	1b	150	SER
33	1b	160	ASP
33	1b	200	ILE
33	1b	208	ILE
34	1c	3	ASN
34	1c	15	THR
34	1c	17	ASP
34	1c	20	SER
34	1c	58	GLU
34	1c	66	VAL
34	1c	70	VAL
34	1c	77	ILE
34	1c	178	LEU
34	1c	179	ARG
34	1c	195	VAL
34	1c	207	VAL
35	1d	10	ARG
35	1d	59	ARG
35	1d	61	LYS
35	1d	70	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	119	GLN
35	1d	135	LEU
35	1d	140	VAL
35	1d	141	ARG
35	1d	158	ILE
35	1d	177	ASP
35	1d	178	VAL
35	1d	179	GLU
35	1d	181	MET
35	1d	194	LEU
36	1e	10	MET
36	1e	16	THR
36	1e	20	GLN
36	1e	24	ARG
36	1e	31	LEU
36	1e	41	VAL
36	1e	45	PHE
36	1e	56	GLN
36	1e	63	ARG
36	1e	67	VAL
36	1e	91	LEU
36	1e	131	ILE
37	1f	55	ASP
37	1f	57	GLN
37	1f	70	ASP
37	1f	78	GLU
37	1f	98	LEU
38	1g	12	LEU
38	1g	16	LEU
38	1g	22	LEU
38	1g	24	THR
38	1g	32	ARG
38	1g	50	ILE
38	1g	61	VAL
38	1g	76	ARG
38	1g	85	TYR
38	1g	94	ARG
38	1g	98	SER
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	114	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	1g	115	ARG
39	1h	19	VAL
39	1h	25	ASP
39	1h	52	ASP
39	1h	54	ASP
39	1h	133	LEU
40	1i	17	VAL
40	1i	23	ASN
40	1i	47	LEU
40	1i	53	VAL
40	1i	54	ASP
40	1i	83	ARG
40	1i	96	LEU
40	1i	103	THR
40	1i	105	ASP
40	1i	128	ARG
41	1j	8	LEU
41	1j	38	ILE
41	1j	46	ARG
41	1j	81	THR
41	1j	92	THR
41	1j	98	ILE
41	1j	100	THR
42	1k	14	VAL
42	1k	33	THR
42	1k	48	ILE
42	1k	84	VAL
42	1k	87	THR
42	1k	109	VAL
42	1k	114	VAL
43	1l	18	VAL
43	1l	22	SER
43	1l	33	ARG
43	1l	83	VAL
43	1l	116	SER
44	1m	4	ILE
44	1m	14	ARG
44	1m	15	VAL
44	1m	43	THR
44	1m	49	THR
44	1m	70	LEU
44	1m	98	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	1m	106	ASN
44	1m	109	THR
44	1m	122	LYS
45	1n	3	ARG
45	1n	13	THR
45	1n	18	VAL
45	1n	33	VAL
46	1o	39	LEU
46	1o	76	GLU
47	1p	20	VAL
47	1p	27	LYS
47	1p	43	LYS
47	1p	45	THR
47	1p	53	VAL
47	1p	67	THR
47	1p	76	GLN
48	1q	11	VAL
48	1q	52	LYS
48	1q	89	LEU
49	1r	36	ASN
49	1r	42	ARG
50	1s	12	ASP
50	1s	28	LYS
50	1s	35	SER
50	1s	37	ARG
51	1t	10	LEU
51	1t	13	LEU
51	1t	24	LEU
51	1t	53	LEU
51	1t	100	ILE
52	1u	15	ARG
3	2D	3	VAL
3	2D	14	ARG
3	2D	38	LYS
3	2D	88	ARG
3	2D	142	VAL
3	2D	173	VAL
3	2D	200	ASP
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2D	259	THR
3	2D	275	LYS
4	2E	7	VAL
4	2E	38	THR
4	2E	73	GLU
4	2E	90	THR
4	2E	116	VAL
4	2E	119	ARG
5	2F	33	LEU
5	2F	53	THR
5	2F	60	SER
5	2F	70	THR
5	2F	158	THR
5	2F	160	ASN
5	2F	192	LEU
5	2F	200	GLU
6	2G	21	ARG
6	2G	28	VAL
6	2G	31	VAL
6	2G	45	GLU
6	2G	49	ASP
6	2G	51	ARG
6	2G	53	LEU
6	2G	58	GLN
6	2G	79	ASN
6	2G	91	ARG
6	2G	123	ASN
6	2G	126	ASP
6	2G	140	ILE
6	2G	145	THR
6	2G	165	THR
6	2G	170	ARG
7	2H	3	ARG
7	2H	6	ARG
7	2H	15	VAL
7	2H	16	SER
7	2H	44	VAL
7	2H	51	ARG
7	2H	70	THR
7	2H	71	LEU
7	2H	88	LEU
7	2H	103	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	2H	122	THR
7	2H	129	THR
7	2H	141	VAL
8	2I	14	ASP
8	2I	15	VAL
8	2I	19	VAL
8	2I	38	LEU
8	2I	58	LEU
8	2I	61	ARG
8	2I	68	LEU
8	2I	82	ARG
8	2I	102	SER
8	2I	117	GLU
8	2I	121	LYS
8	2I	122	GLU
8	2I	127	VAL
9	2N	5	VAL
9	2N	15	LEU
9	2N	22	THR
9	2N	28	THR
9	2N	38	HIS
9	2N	48	MET
9	2N	61	ARG
9	2N	73	THR
9	2N	121	LYS
10	2O	19	ILE
10	2O	98	VAL
10	2O	113	LYS
11	2P	7	ARG
11	2P	45	LEU
11	2P	77	ARG
11	2P	95	VAL
11	2P	98	GLU
11	2P	121	LYS
11	2P	135	LEU
11	2P	147	LEU
11	2P	148	LEU
11	2P	149	GLU
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	133	ARG
13	2R	6	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	2R	15	SER
13	2R	114	VAL
14	2S	15	ARG
14	2S	21	THR
14	2S	23	ARG
14	2S	27	SER
14	2S	35	ILE
14	2S	36	TYR
14	2S	43	GLU
14	2S	58	LEU
14	2S	80	LEU
14	2S	83	LYS
14	2S	110	LEU
15	2T	72	VAL
15	2T	74	ARG
15	2T	96	ARG
15	2T	115	ARG
16	2U	5	LYS
16	2U	27	LEU
16	2U	74	LEU
16	2U	78	THR
16	2U	95	LEU
17	2V	7	THR
17	2V	28	GLU
17	2V	53	GLU
17	2V	79	VAL
17	2V	98	GLU
18	2W	4	LYS
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	67	ASP
19	2X	60	ARG
19	2X	66	LEU
19	2X	81	VAL
20	2Y	1	MET
20	2Y	6	HIS
20	2Y	9	LYS
20	2Y	11	ASP
20	2Y	14	LEU
20	2Y	47	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	2Y	72	VAL
20	2Y	99	CYS
21	2Z	61	LEU
21	2Z	71	VAL
21	2Z	121	HIS
21	2Z	128	VAL
21	2Z	136	PHE
21	2Z	148	ASP
21	2Z	150	LEU
21	2Z	154	ASP
21	2Z	157	LEU
21	2Z	170	THR
22	20	9	SER
22	20	74	ARG
23	21	21	ARG
23	21	35	THR
23	21	40	ARG
23	21	81	LYS
23	21	92	LYS
24	22	53	LEU
24	22	70	GLN
25	23	56	VAL
26	24	1	MET
26	24	13	ARG
26	24	27	THR
26	24	34	GLU
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR
27	25	6	VAL
27	25	40	LYS
28	26	6	ARG
28	26	9	LEU
28	26	19	ARG
28	26	20	ASN
28	26	23	THR
28	26	29	ASN
28	26	50	ARG
29	27	1	MET
29	27	43	THR
29	27	46	VAL
30	28	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	28	31	HIS
30	28	34	TRP
30	28	37	SER
30	28	46	ARG
31	29	6	SER
31	29	7	VAL
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	10	LEU
33	2b	16	HIS
33	2b	23	ARG
33	2b	76	GLN
33	2b	94	ASN
33	2b	109	SER
33	2b	117	GLU
33	2b	127	ILE
33	2b	153	ARG
33	2b	185	ILE
33	2b	189	ASP
33	2b	223	ILE
33	2b	224	GLN
33	2b	229	VAL
33	2b	236	TYR
34	2c	16	ARG
34	2c	44	GLU
34	2c	46	GLU
34	2c	57	ILE
34	2c	69	HIS
34	2c	72	LYS
34	2c	91	LEU
34	2c	105	GLU
34	2c	112	SER
34	2c	119	ARG
34	2c	132	ARG
34	2c	190	ARG
34	2c	191	THR
35	2d	28	SER
35	2d	31	CYS
35	2d	34	GLU
35	2d	47	ARG
35	2d	52	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	53	ASP
35	2d	58	LEU
35	2d	59	ARG
35	2d	76	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	155	LEU
35	2d	162	LEU
35	2d	188	LEU
35	2d	190	ASP
35	2d	193	ASP
36	2e	6	PHE
36	2e	12	LEU
36	2e	13	ILE
36	2e	18	ARG
36	2e	45	PHE
36	2e	51	VAL
36	2e	55	VAL
36	2e	72	GLN
36	2e	75	THR
36	2e	78	HIS
36	2e	115	VAL
36	2e	119	LEU
36	2e	149	GLU
37	2f	21	LEU
37	2f	69	GLU
37	2f	92	LYS
37	2f	93	SER
38	2g	9	VAL
38	2g	15	ASP
38	2g	51	GLN
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	110	GLN
38	2g	135	VAL
39	2h	23	SER
39	2h	39	LEU
39	2h	52	ASP
39	2h	56	LYS
39	2h	133	LEU
40	2i	7	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	2i	32	ASP
40	2i	38	GLN
40	2i	40	LEU
40	2i	50	LEU
40	2i	54	ASP
40	2i	65	VAL
40	2i	89	ASN
40	2i	99	LEU
40	2i	102	LEU
40	2i	103	THR
40	2i	104	ARG
40	2i	108	VAL
40	2i	113	LYS
40	2i	128	ARG
41	2j	8	LEU
41	2j	13	HIS
41	2j	38	ILE
41	2j	49	VAL
41	2j	65	LEU
41	2j	72	VAL
41	2j	73	ASP
41	2j	89	ASP
41	2j	100	THR
42	2k	14	VAL
42	2k	79	SER
42	2k	105	VAL
42	2k	109	VAL
42	2k	126	ARG
43	2l	18	VAL
43	2l	83	VAL
43	2l	104	VAL
43	2l	118	SER
44	2m	4	ILE
44	2m	19	LEU
44	2m	27	LYS
44	2m	47	ASP
44	2m	50	GLU
44	2m	81	LEU
44	2m	93	ARG
44	2m	106	ASN
44	2m	108	ARG
44	2m	114	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	2m	122	LYS
45	2n	3	ARG
45	2n	18	VAL
45	2n	22	THR
45	2n	33	VAL
45	2n	56	VAL
45	2n	60	SER
46	2o	3	ILE
46	2o	26	GLU
46	2o	39	LEU
46	2o	47	LYS
46	2o	76	GLU
47	2p	20	VAL
47	2p	21	VAL
47	2p	45	THR
47	2p	60	LEU
47	2p	67	THR
47	2p	73	LEU
47	2p	74	LEU
48	2q	5	VAL
48	2q	7	THR
48	2q	9	VAL
48	2q	19	VAL
48	2q	52	LYS
48	2q	83	ASP
48	2q	85	VAL
49	2r	31	LEU
49	2r	37	VAL
49	2r	82	THR
50	2s	37	ARG
50	2s	43	GLU
50	2s	56	GLN
50	2s	58	VAL
50	2s	79	THR
50	2s	81	ARG
51	2t	15	ARG
51	2t	45	GLN
51	2t	50	GLU
51	2t	51	GLU
51	2t	93	GLU
52	2u	6	ARG
52	2u	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
4	1E	48	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
8	1I	105	HIS
9	1N	8	GLN
9	1N	131	GLN
12	1Q	89	ASN
14	1S	68	GLN
16	1U	81	HIS
19	1X	31	HIS
19	1X	82	GLN
21	1Z	55	HIS
21	1Z	73	GLN
21	1Z	151	HIS
24	12	46	GLN
25	13	32	GLN
33	1b	40	HIS
33	1b	78	GLN
33	1b	95	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	118	GLN
34	1c	162	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
36	1e	20	GLN
36	1e	65	ASN
36	1e	78	HIS
37	1f	57	GLN
37	1f	100	ASN
38	1g	28	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	1m	92	HIS
47	1p	13	HIS
47	1p	76	GLN
49	1r	63	GLN
50	1s	47	HIS
50	1s	83	HIS
51	1t	42	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	160	ASN
6	2G	58	GLN
6	2G	108	ASN
6	2G	121	ASN
7	2H	74	ASN
8	2I	139	GLN
9	2N	8	GLN
9	2N	56	ASN
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	13	GLN
12	2Q	89	ASN
12	2Q	123	HIS
13	2R	61	HIS
14	2S	38	GLN
14	2S	84	GLN
15	2T	43	GLN
15	2T	58	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	34	ASN
21	2Z	73	GLN
21	2Z	121	HIS
24	22	70	GLN
26	24	46	GLN
30	28	35	GLN
33	2b	40	HIS
33	2b	76	GLN
33	2b	94	ASN
33	2b	135	GLN
33	2b	140	HIS
34	2c	98	ASN
34	2c	162	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
36	2e	72	GLN
36	2e	73	ASN
37	2f	100	ASN
38	2g	28	ASN
40	2i	3	GLN
40	2i	38	GLN
40	2i	58	HIS
41	2j	62	HIS
41	2j	69	ASN
42	2k	117	ASN
43	2l	78	GLN
43	2l	99	HIS
44	2m	62	ASN
44	2m	77	ASN
45	2n	49	HIS
46	2o	62	GLN
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	430 (15%)	30 (1%)
1	2A	2789/2915 (95%)	462 (16%)	26 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	31 (26%)	0
32	1a	1494/1521 (98%)	241 (16%)	0
32	2a	1498/1521 (98%)	272 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	70/76 (92%)	23 (32%)	0
54	2w	67/76 (88%)	20 (29%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	8 (10%)	0
56	1y	71/76 (93%)	34 (47%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
56	2y	69/76 (90%)	24 (34%)	0
All	All	9331/9620 (96%)	1560 (16%)	56 (0%)

All (1560) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	58	G
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	181	A
1	1A	188	G
1	1A	196	A
1	1A	197	A
1	1A	200	U
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(A)	A
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(B)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	357	A
1	1A	363	G
1	1A	363(B)	G
1	1A	370	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	455	C
1	1A	467	G
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	568	U
1	1A	573	G
1	1A	575	A
1	1A	593	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	615	G
1	1A	627	A
1	1A	634	C
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	654	A
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	762	U
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	881	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	890	A
1	1A	892	G
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	899	A
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	990	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1041	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1064	C
1	1A	1067	A
1	1A	1068	G
1	1A	1069	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1083	U
1	1A	1085	A
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1099	G
1	1A	1101	U
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1132	A
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1220	A
1	1A	1236	G
1	1A	1244	G
1	1A	1248	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1384	A
1	1A	1385	G
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1539	G
1	1A	1540	U
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1648	C
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1745	C
1	1A	1756	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A
1	1A	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2098	U
1	1A	2102	U
1	1A	2108	C
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2117	A
1	1A	2119	A
1	1A	2120	G
1	1A	2121	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2138	C
1	1A	2142	C
1	1A	2144	U
1	1A	2146	C
1	1A	2148	G
1	1A	2150	U
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2189	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2358	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2449	U
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2582	G
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2727	G
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A
1	1A	2825	C
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	13	A
2	1B	50	G
2	1B	56	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	6	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	145	G
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(D)	C
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	220	G
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	330	C
32	1a	332	G
32	1a	342	C
32	1a	344	A
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	483	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	536	C
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	630	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	666	G
32	1a	672	U
32	1a	687	A
32	1a	688	G
32	1a	693	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	695	A
32	1a	722	A
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	749	C
32	1a	753	A
32	1a	755	G
32	1a	759	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	870	U
32	1a	873	A
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1037	C
32	1a	1039	C
32	1a	1044	A
32	1a	1053	G
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1133	G
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1158	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1159	U
32	1a	1165	C
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1222	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1446	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	6	G
54	1w	8	4SU
54	1w	11	C
54	1w	12	U
54	1w	15	G
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	27	G
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	66	U
54	1w	67	C
54	1w	70	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	19	G
55	1x	20	U
55	1x	47	U
55	1x	61	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	1y	2	C
56	1y	5	G
56	1y	6	G
56	1y	7	A
56	1y	8	4SU
56	1y	11	C
56	1y	13	C
56	1y	14	A
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	28	G
56	1y	34	G
56	1y	35	A
56	1y	40	C
56	1y	44	G
56	1y	45	U
56	1y	46	G7M
56	1y	47	U
56	1y	48	C
56	1y	49	C
56	1y	51	U
56	1y	57	G
56	1y	58	A
56	1y	59	U
56	1y	60	U
56	1y	61	C
56	1y	65	G
56	1y	66	U
56	1y	67	C
56	1y	69	G
56	1y	70	G
56	1y	72	C
56	1y	76	A
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	55	G
1	2A	61	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	141	A
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	271(I)	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	311	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	354	G
1	2A	363	G
1	2A	363(B)	G
1	2A	380	U
1	2A	386	G
1	2A	411	G
1	2A	421	U
1	2A	422	A
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	606	U
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	645	C
1	2A	648	G
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(D)	C
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	936	C
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1116	C
1	2A	1126	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1142	U
1	2A	1148	A
1	2A	1170	G
1	2A	1171	G
1	2A	1195	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1244	G
1	2A	1252	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1435	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1543	C
1	2A	1547	C
1	2A	1554	A
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1717	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2080	G
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2141	G
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2165	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2171	A
1	2A	2172	U
1	2A	2178	C
1	2A	2181	G
1	2A	2182	G
1	2A	2185	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2267	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2282	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2372	G
1	2A	2376	A
1	2A	2379	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2383	G
1	2A	2385	C
1	2A	2400	G
1	2A	2402	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2480	C
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2530	A
1	2A	2534	A
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2630	G
1	2A	2634	G
1	2A	2646	C
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	5	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	23	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	25	A
2	2B	30	C
2	2B	33	G
2	2B	34	U
2	2B	40	U
2	2B	41	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	84	C
2	2B	85	G
2	2B	89	G
2	2B	105	A
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	119	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	31	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	89	C
32	2a	96	U
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	129(A)	G
32	2a	131	C
32	2a	144	G
32	2a	163	C
32	2a	182	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	231	G
32	2a	245	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	414	A
32	2a	421	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	475	G
32	2a	476	G
32	2a	477	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	601	C
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	702	A
32	2a	703	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	777	A
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	873	A
32	2a	887	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	963	G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	984	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1042	G
32	2a	1050	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1091	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1126	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1172	C
32	2a	1181	G
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1260	C
32	2a	1264	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1320	C
32	2a	1323	G
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1380	U
32	2a	1382	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1457	G
32	2a	1492	A
32	2a	1497	G
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1532	U
53	2v	24	A
54	2w	4	C
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	45	U
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	62	C
54	2w	64	A
54	2w	65	G
54	2w	66	U
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	72	C
54	2w	73	A
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	20	U
55	2x	47	U
55	2x	48	C
55	2x	61	C
56	2y	2	C
56	2y	15	G
56	2y	19	G
56	2y	23	A
56	2y	27	G
56	2y	40	C
56	2y	41	C
56	2y	43	C
56	2y	45	U
56	2y	46	G7M
56	2y	47	U
56	2y	48	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	2y	49	C
56	2y	52	G
56	2y	53	G
56	2y	54	5MU
56	2y	55	PSU
56	2y	56	C
56	2y	58	A
56	2y	59	U
56	2y	63	G
56	2y	65	G
56	2y	69	G
56	2y	70	G

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2430	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	195	A
1	2A	196	A
1	2A	228	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	746	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2156	G
1	2A	2439	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.12	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	28,32,35	2.18	7 (25%)
32	PSU	1a	516	32	18,21,22	1.34	2 (11%)	22,30,33	1.82	5 (22%)
55	5MU	1x	54	55,57	19,22,23	1.40	5 (26%)	28,32,35	1.99	6 (21%)
54	MIA	2w	37	54	20,27,32	1.83	3 (15%)	22,39,47	1.85	7 (31%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	4 (18%)
32	UR3	1a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.50	2 (7%)
32	UR3	2a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.45	1 (3%)
55	31H	2x	76	55,57	28,34,35	1.05	3 (10%)	23,47,50	1.58	4 (17%)
54	4SU	2w	8	54	18,21,22	1.63	3 (16%)	26,30,33	2.72	5 (19%)
56	PSU	1y	32	56	18,21,22	1.32	2 (11%)	22,30,33	1.81	3 (13%)
56	4SU	2y	8	56	18,21,22	1.63	4 (22%)	26,30,33	2.33	6 (23%)
54	PSU	2w	55	54	18,21,22	1.34	2 (11%)	22,30,33	1.83	3 (13%)
32	4OC	1a	1402	32	20,23,24	0.73	0	26,32,35	0.95	1 (3%)
56	PSU	1y	39	56	18,21,22	1.41	2 (11%)	22,30,33	1.68	3 (13%)
54	PSU	2w	32	54	18,21,22	1.35	2 (11%)	22,30,33	1.81	3 (13%)
56	4SU	1y	8	56	18,21,22	1.68	4 (22%)	26,30,33	2.04	5 (19%)
32	MA6	2a	1519	32	19,26,27	0.84	0	18,38,41	1.63	2 (11%)
1	8AH	1A	2503	1,57	20,26,27	0.82	1 (5%)	23,39,42	2.14	4 (17%)
55	4SU	1x	8	55	18,21,22	2.21	5 (27%)	26,30,33	1.72	6 (23%)
56	PSU	2y	39	56	18,21,22	1.38	2 (11%)	22,30,33	1.64	3 (13%)
1	OMG	2A	2251	1,55	18,26,27	0.93	1 (5%)	19,38,41	1.14	3 (15%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.09	2 (12%)
1	PSU	1A	1917	1	18,21,22	1.32	2 (11%)	22,30,33	1.89	3 (13%)
32	4OC	2a	1402	32	20,23,24	0.78	0	26,32,35	1.06	2 (7%)
1	5MU	1A	1939	1,57	19,22,23	1.35	5 (26%)	28,32,35	2.17	6 (21%)
1	PSU	1A	1911	1	18,21,22	1.41	2 (11%)	22,30,33	1.90	3 (13%)
56	MIA	1y	37	56	18,24,32	1.19	2 (11%)	18,35,47	1.21	2 (11%)
1	OMC	1A	1920	1	19,22,23	0.84	0	26,31,34	0.84	0
56	5MU	2y	54	56	19,22,23	1.48	4 (21%)	28,32,35	1.98	6 (21%)
1	OMC	2A	1920	1	19,22,23	0.82	0	26,31,34	0.91	1 (3%)
55	31H	1x	76	55,57	28,34,35	1.07	3 (10%)	23,47,50	1.64	4 (17%)
54	MIA	1w	37	54	24,31,32	2.23	3 (12%)	26,44,47	2.33	9 (34%)
32	PSU	2a	516	32	18,21,22	1.31	2 (11%)	22,30,33	1.83	3 (13%)
32	MA6	2a	1518	32	19,26,27	0.82	0	18,38,41	1.45	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	1w	32	54,57	18,21,22	1.28	2 (11%)	22,30,33	1.81	3 (13%)
32	5MC	1a	1407	32	18,22,23	0.91	2 (11%)	26,32,35	1.07	3 (11%)
1	PSU	2A	2605	1	18,21,22	1.40	3 (16%)	22,30,33	1.92	4 (18%)
1	5MC	1A	1962	1	18,22,23	0.97	2 (11%)	26,32,35	1.19	2 (7%)
1	2MU	2A	2552	1	19,22,24	1.29	3 (15%)	26,31,36	1.77	6 (23%)
32	M2G	2a	966	32	20,27,28	1.35	3 (15%)	22,40,43	1.05	2 (9%)
54	G7M	2w	46	54	20,26,27	1.25	1 (5%)	17,39,42	0.63	0
54	PSU	2w	39	54	18,21,22	1.37	2 (11%)	22,30,33	1.58	3 (13%)
1	OMG	1A	2251	1,57,55	18,26,27	0.98	1 (5%)	19,38,41	1.08	3 (15%)
32	5MC	1a	967	32	18,22,23	0.97	2 (11%)	26,32,35	1.14	2 (7%)
32	5MC	1a	1404	32	18,22,23	1.05	2 (11%)	26,32,35	1.17	4 (15%)
55	4SU	2x	8	55	18,21,22	2.05	6 (33%)	26,30,33	1.42	5 (19%)
55	PSU	1x	55	55	18,21,22	1.32	2 (11%)	22,30,33	1.88	4 (18%)
32	MA6	1a	1518	32	19,26,27	0.83	0	18,38,41	1.48	2 (11%)
55	5MC	1x	32	55	18,22,23	0.98	2 (11%)	26,32,35	1.25	3 (11%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	22,30,33	1.82	3 (13%)
54	PSU	1w	55	54	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
32	5MC	2a	1404	32	18,22,23	0.99	2 (11%)	26,32,35	1.16	3 (11%)
56	PSU	2y	55	56	18,21,22	1.30	3 (16%)	22,30,33	1.85	4 (18%)
1	2MU	1A	2552	1,57	19,22,24	1.17	2 (10%)	26,31,36	1.88	6 (23%)
1	5MC	1A	1942	1	18,22,23	0.93	2 (11%)	26,32,35	1.19	4 (15%)
54	5MU	1w	54	54	19,22,23	1.37	4 (21%)	28,32,35	1.92	6 (21%)
55	5MC	2x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.24	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	6 (31%)	28,32,35	2.16	6 (21%)
43	0TD	1l	92	43	7,9,10	4.79	2 (28%)	6,11,13	7.46	2 (33%)
54	F3N	2w	76	1,54	30,36,37	1.45	5 (16%)	29,51,54	1.22	1 (3%)
32	5MC	2a	967	32	18,22,23	0.93	2 (11%)	26,32,35	1.19	3 (11%)
1	5MU	2A	1939	1,57	19,22,23	1.40	4 (21%)	28,32,35	2.28	6 (21%)
55	5MU	2x	54	55	19,22,23	1.41	6 (31%)	28,32,35	2.12	6 (21%)
56	G7M	2y	46	56	20,26,27	1.43	3 (15%)	17,39,42	0.83	1 (5%)
32	M2G	1a	966	32	20,27,28	1.38	3 (15%)	22,40,43	1.03	2 (9%)
32	5MC	1a	1400	32	18,22,23	0.94	2 (11%)	26,32,35	1.14	3 (11%)
32	G7M	1a	527	32,57	20,26,27	1.20	2 (10%)	17,39,42	0.68	0
32	5MC	2a	1400	32	18,22,23	0.97	2 (11%)	26,32,35	1.24	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	2A	1962	1,57	18,22,23	0.96	2 (11%)	26,32,35	1.18	2 (7%)
54	4SU	1w	8	54	18,21,22	1.67	4 (22%)	26,30,33	1.84	4 (15%)
32	MA6	1a	1519	32	19,26,27	0.84	0	18,38,41	1.61	2 (11%)
56	PSU	1y	55	56	18,21,22	1.38	2 (11%)	22,30,33	1.92	4 (18%)
56	G7M	1y	46	56	20,26,27	1.43	2 (10%)	17,39,42	0.67	0
54	5MU	2w	54	54	19,22,23	1.36	4 (21%)	28,32,35	1.90	6 (21%)
32	2MG	2a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	0.99	2 (12%)
54	G7M	1w	46	54	20,26,27	1.23	2 (10%)	17,39,42	0.70	0
32	5MC	2a	1407	32	18,22,23	0.97	2 (11%)	26,32,35	1.11	2 (7%)
1	8AH	2A	2503	1,57	20,26,27	0.85	1 (5%)	23,39,42	1.89	4 (17%)
43	0TD	2l	92	43	7,9,10	4.76	1 (14%)	6,11,13	1.91	2 (33%)
56	MIA	2y	37	56	18,24,32	1.16	2 (11%)	18,35,47	1.30	2 (11%)
54	PSU	1w	39	54	18,21,22	1.38	2 (11%)	22,30,33	1.69	3 (13%)
56	PSU	2y	32	56	18,21,22	1.30	2 (11%)	22,30,33	1.80	3 (13%)
56	5MU	1y	54	56	19,22,23	1.39	5 (26%)	28,32,35	2.14	7 (25%)
54	F3N	1w	76	1,54	30,36,37	1.57	6 (20%)	29,51,54	1.31	2 (6%)
32	G7M	2a	527	32,57	20,26,27	1.29	2 (10%)	17,39,42	0.47	0
1	PSU	1A	2605	1,57	18,21,22	1.32	2 (11%)	22,30,33	1.88	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,57	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,57	-	3/18/40/41	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	1/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	2/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	8AH	1A	2503	1,57	-	2/3/25/26	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	2/3/25/34	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
55	31H	1x	76	55,57	-	3/18/40/41	0/3/3/3
54	MIA	1w	37	54	-	3/11/33/34	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
54	PSU	1w	32	54,57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1	-	0/9/27/28	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,57,55	-	0/5/27/28	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	2y	55	56	-	6/7/25/26	0/2/2/2
1	2MU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
54	F3N	2w	76	1,54	-	1/15/37/38	0/4/4/4
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	2/3/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,57	-	3/3/25/26	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	2/3/25/26	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/5/27/28	0/3/3/3
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	8AH	2A	2503	1,57	-	1/3/25/26	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
56	MIA	2y	37	56	-	3/3/25/34	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	1,54	-	2/15/37/38	0/4/4/4
32	G7M	2a	527	32,57	-	3/3/25/26	0/3/3/3
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.28	1.69	1.82
43	1l	92	0TD	CB-SB	-12.15	1.69	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.34	1.53	1.32
54	2w	37	MIA	C2-S10	-6.77	1.70	1.75
54	1w	37	MIA	C2-S10	-6.57	1.70	1.75
55	1x	8	4SU	C4-N3	-5.41	1.31	1.37
54	1w	76	F3N	CB-CG	-5.07	1.39	1.51
55	2x	8	4SU	C4-N3	-5.05	1.32	1.37
54	2w	76	F3N	CB-CG	-4.77	1.39	1.51
54	2w	8	4SU	C4-S4	-4.58	1.59	1.68
55	1x	8	4SU	C4-S4	-4.34	1.60	1.68
32	2a	966	M2G	C2-N3	4.33	1.36	1.30
56	2y	46	G7M	C5-C4	4.27	1.47	1.39
56	2y	8	4SU	C4-S4	-4.24	1.60	1.68
56	1y	46	G7M	C5-C4	4.21	1.47	1.39
56	1y	8	4SU	C4-S4	-4.19	1.60	1.68
54	1w	8	4SU	C4-S4	-4.10	1.60	1.68
32	1a	966	M2G	C2-N3	4.10	1.35	1.30
56	1y	39	PSU	C6-C5	4.06	1.40	1.35
55	2x	8	4SU	C4-S4	-4.03	1.60	1.68
54	2w	46	G7M	C5-C4	3.96	1.47	1.39
55	1x	8	4SU	C2-N3	-3.87	1.31	1.38
56	2y	39	PSU	C6-C5	3.81	1.39	1.35
56	1y	55	PSU	C6-C5	3.80	1.39	1.35
32	2a	527	G7M	C5-C4	3.79	1.46	1.39
54	1w	46	G7M	C5-C4	3.77	1.46	1.39
32	1a	527	G7M	C5-C4	3.75	1.46	1.39
54	2w	55	PSU	C6-C5	3.73	1.39	1.35
54	2w	39	PSU	C6-C5	3.70	1.39	1.35
1	1A	1911	PSU	C6-C5	3.67	1.39	1.35
54	1w	55	PSU	C6-C5	3.65	1.39	1.35
56	1y	32	PSU	C6-C5	3.57	1.39	1.35
54	1w	76	F3N	O4'-C1'	3.47	1.45	1.41
54	2w	32	PSU	C6-C5	3.45	1.39	1.35
1	2A	2605	PSU	C6-C5	3.44	1.39	1.35
55	1x	8	4SU	C5-C4	-3.44	1.38	1.42
56	2y	32	PSU	C6-C5	3.43	1.39	1.35
1	2A	1911	PSU	C6-C5	3.41	1.39	1.35
32	2a	516	PSU	C6-C5	3.38	1.39	1.35
55	2x	55	PSU	C6-C5	3.37	1.39	1.35
32	1a	516	PSU	C6-C5	3.35	1.39	1.35
54	1w	32	PSU	C6-C5	3.31	1.39	1.35
1	2A	1917	PSU	C6-C5	3.28	1.39	1.35
55	2x	8	4SU	C2-N3	-3.28	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1917	PSU	C6-C5	3.23	1.39	1.35
54	1w	8	4SU	C4-N3	-3.22	1.34	1.37
54	1w	39	PSU	C6-C5	3.19	1.39	1.35
56	2y	54	5MU	C6-C5	3.15	1.39	1.34
54	2w	76	F3N	O4'-C1'	3.00	1.45	1.41
1	2A	1915	5MU	C6-C5	2.98	1.39	1.34
55	1x	55	PSU	C6-C5	2.96	1.38	1.35
32	2a	1404	5MC	C6-C5	2.95	1.39	1.34
55	2x	8	4SU	C5-C4	-2.95	1.38	1.42
1	2A	1939	5MU	C6-C5	2.94	1.39	1.34
54	1w	76	F3N	C5-C4	-2.93	1.33	1.40
56	1y	37	MIA	C5-C4	2.92	1.48	1.40
1	1A	1939	5MU	C6-C5	2.91	1.39	1.34
56	1y	8	4SU	C4-N3	-2.87	1.34	1.37
54	2w	37	MIA	C5-C4	2.86	1.48	1.40
1	2A	1939	5MU	C4-N3	-2.86	1.33	1.38
56	2y	37	MIA	C5-C4	2.85	1.48	1.40
55	1x	54	5MU	C4-N3	-2.85	1.33	1.38
56	2y	8	4SU	C4-N3	-2.82	1.34	1.37
54	2w	76	F3N	C5-C4	-2.82	1.33	1.40
54	2w	8	4SU	C4-N3	-2.82	1.34	1.37
32	1a	967	5MC	C6-C5	2.81	1.39	1.34
55	1x	32	5MC	C6-C5	2.80	1.39	1.34
32	1a	966	M2G	C2-N2	2.79	1.40	1.35
54	1w	54	5MU	C6-C5	2.79	1.39	1.34
54	1w	39	PSU	C4-N3	-2.77	1.33	1.38
55	2x	76	31H	C5-C4	-2.77	1.33	1.40
55	2x	32	5MC	C6-C5	2.77	1.39	1.34
55	1x	54	5MU	C6-C5	2.77	1.39	1.34
56	1y	37	MIA	C2-N3	2.77	1.36	1.32
1	1A	2605	PSU	C4-N3	-2.77	1.33	1.38
55	2x	54	5MU	C6-C5	2.75	1.39	1.34
54	2w	39	PSU	C4-N3	-2.75	1.33	1.38
1	1A	1915	5MU	C2-N1	2.75	1.42	1.38
32	1a	1400	5MC	C6-C5	2.74	1.39	1.34
56	1y	54	5MU	C6-C5	2.72	1.39	1.34
55	2x	55	PSU	C4-N3	-2.71	1.33	1.38
1	2A	1942	5MC	C6-C5	2.70	1.39	1.34
1	1A	1962	5MC	C6-C5	2.69	1.39	1.34
32	1a	1404	5MC	C6-C5	2.68	1.39	1.34
55	1x	76	31H	C5-C4	-2.67	1.33	1.40
56	1y	46	G7M	C6-N1	-2.67	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	46	G7M	C6-N1	-2.67	1.33	1.37
54	2w	54	5MU	C6-C5	2.67	1.39	1.34
1	2A	2552	2MU	C4-N3	-2.66	1.33	1.38
32	2a	1407	5MC	C6-C5	2.66	1.39	1.34
1	1A	2552	2MU	C4-N3	-2.66	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.65	1.33	1.38
56	1y	54	5MU	C4-C5	2.64	1.49	1.44
54	1w	37	MIA	C5-C4	2.64	1.47	1.40
55	2x	54	5MU	C4-N3	-2.63	1.34	1.38
1	2A	1962	5MC	C6-C5	2.63	1.38	1.34
56	2y	37	MIA	C2-N3	2.63	1.36	1.32
56	2y	54	5MU	C2-N1	2.62	1.42	1.38
54	2w	54	5MU	C4-N3	-2.62	1.34	1.38
56	2y	55	PSU	C4-N3	-2.62	1.34	1.38
32	1a	516	PSU	C4-N3	-2.61	1.34	1.38
54	1w	76	F3N	C6-C5	-2.61	1.33	1.43
1	1A	1939	5MU	C4-N3	-2.61	1.34	1.38
32	2a	527	G7M	C6-N1	-2.60	1.34	1.37
56	2y	54	5MU	C4-C5	2.59	1.49	1.44
55	2x	76	31H	C6-C5	-2.58	1.33	1.43
1	2A	1915	5MU	C4-N3	-2.58	1.34	1.38
32	2a	966	M2G	C2-N2	2.58	1.40	1.35
1	1A	1911	PSU	C4-N3	-2.58	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.57	1.34	1.38
32	2a	1400	5MC	C6-C5	2.57	1.38	1.34
56	1y	8	4SU	C5-C4	-2.57	1.39	1.42
32	1a	1207	2MG	C6-N1	-2.57	1.34	1.37
32	2a	1207	2MG	C6-N1	-2.57	1.34	1.37
55	1x	55	PSU	C4-N3	-2.56	1.34	1.38
56	1y	39	PSU	C4-N3	-2.55	1.34	1.38
54	1w	55	PSU	C4-N3	-2.51	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.50	1.34	1.37
1	2A	2251	OMG	C6-N1	-2.50	1.34	1.37
56	2y	39	PSU	C4-N3	-2.49	1.34	1.38
1	1A	1942	5MC	C6-C5	2.49	1.38	1.34
32	1a	1404	5MC	C6-N1	-2.49	1.33	1.38
1	2A	1915	5MU	C4-C5	2.47	1.48	1.44
1	2A	1911	PSU	C4-N3	-2.47	1.34	1.38
32	1a	1407	5MC	C6-C5	2.47	1.38	1.34
56	2y	54	5MU	C4-N3	-2.47	1.34	1.38
32	2a	967	5MC	C6-C5	2.45	1.38	1.34
1	2A	1915	5MU	C2-N1	2.44	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	32	5MC	C6-N1	-2.44	1.33	1.38
1	1A	1915	5MU	C6-C5	2.44	1.38	1.34
56	2y	8	4SU	C2-N1	2.43	1.42	1.38
54	2w	55	PSU	C4-N3	-2.43	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.42	1.33	1.38
54	2w	76	F3N	C6-C5	-2.42	1.34	1.43
55	2x	54	5MU	C4-C5	2.41	1.48	1.44
1	2A	2503	8AH	C5-C4	2.41	1.47	1.40
54	1w	46	G7M	C6-N1	-2.41	1.34	1.37
1	1A	1915	5MU	C4-N3	-2.40	1.34	1.38
56	1y	32	PSU	C4-N3	-2.40	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.40	1.34	1.38
56	1y	55	PSU	C4-N3	-2.39	1.34	1.38
32	1a	1498	UR3	C2-N1	2.39	1.42	1.38
1	1A	1942	5MC	C6-N1	-2.39	1.34	1.38
56	1y	54	5MU	C2-N1	2.38	1.42	1.38
1	1A	1917	PSU	C4-N3	-2.38	1.34	1.38
32	1a	966	M2G	C6-N1	-2.38	1.34	1.37
55	1x	76	31H	C6-C5	-2.37	1.34	1.43
54	1w	54	5MU	C4-N3	-2.37	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.35	1.34	1.38
54	2w	32	PSU	C4-N3	-2.35	1.34	1.38
56	2y	55	PSU	C6-C5	2.34	1.38	1.35
1	2A	1939	5MU	C6-N1	-2.32	1.34	1.38
54	1w	32	PSU	C4-N3	-2.31	1.34	1.38
54	1w	8	4SU	C5-C4	-2.31	1.39	1.42
32	2a	1400	5MC	C6-N1	-2.30	1.34	1.38
32	2a	1498	UR3	C2-N1	2.30	1.41	1.38
54	1w	8	4SU	C2-N3	-2.30	1.33	1.38
54	1w	54	5MU	C4-C5	2.30	1.48	1.44
56	1y	8	4SU	C2-N1	2.30	1.42	1.38
56	1y	54	5MU	C4-N3	-2.30	1.34	1.38
32	2a	516	PSU	C4-N3	-2.29	1.34	1.38
54	2w	37	MIA	C2-N3	2.29	1.37	1.34
1	2A	1942	5MC	C6-N1	-2.29	1.34	1.38
32	2a	967	5MC	C6-N1	-2.28	1.34	1.38
56	2y	8	4SU	C5-C4	-2.26	1.39	1.42
1	2A	1939	5MU	C4-C5	2.25	1.48	1.44
55	1x	76	31H	C5-N7	-2.25	1.31	1.39
55	2x	32	5MC	C6-N1	-2.24	1.34	1.38
55	1x	54	5MU	C4-C5	2.24	1.48	1.44
1	2A	2552	2MU	C5-C4	2.23	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C4-C5	2.23	1.48	1.44
54	1w	76	F3N	C2'-C3'	-2.22	1.49	1.53
54	2w	54	5MU	C4-C5	2.22	1.48	1.44
56	2y	32	PSU	C4-N3	-2.22	1.34	1.38
55	1x	8	4SU	O2-C2	2.21	1.27	1.23
32	1a	1407	5MC	C6-N1	-2.19	1.34	1.38
32	1a	967	5MC	C6-N1	-2.19	1.34	1.38
43	1l	92	0TD	CB-CG	2.18	1.55	1.52
1	2A	1915	5MU	C6-N1	-2.18	1.34	1.38
54	2w	76	F3N	C5-N7	-2.18	1.31	1.39
32	1a	1400	5MC	C6-N1	-2.17	1.34	1.38
55	2x	54	5MU	C2-N1	2.17	1.41	1.38
56	2y	55	PSU	C2-N1	-2.17	1.33	1.36
1	1A	2552	2MU	C2-N3	-2.17	1.34	1.38
54	1w	54	5MU	C2-N1	2.16	1.41	1.38
1	2A	2605	PSU	C2-N3	-2.15	1.33	1.37
32	2a	1404	5MC	C6-N1	-2.15	1.34	1.38
1	2A	2552	2MU	C2-N3	-2.15	1.34	1.38
32	1a	1498	UR3	C6-C5	2.15	1.40	1.35
1	1A	1915	5MU	C6-N1	-2.15	1.34	1.38
1	1A	1915	5MU	C4-C5	2.14	1.48	1.44
55	2x	54	5MU	C6-N1	-2.14	1.34	1.38
56	1y	54	5MU	C6-N1	-2.12	1.34	1.38
32	2a	966	M2G	C6-N1	-2.12	1.34	1.37
55	2x	76	31H	C5-N7	-2.12	1.32	1.39
55	2x	8	4SU	O2-C2	2.11	1.26	1.23
56	2y	46	G7M	C2-N3	2.11	1.38	1.33
55	1x	54	5MU	C2-N3	-2.11	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.10	1.34	1.38
1	1A	2503	8AH	C5-C4	2.09	1.46	1.40
32	1a	527	G7M	C6-N1	-2.08	1.34	1.37
1	1A	2605	PSU	C2-N1	-2.07	1.33	1.36
54	1w	76	F3N	C5-N7	-2.07	1.32	1.39
1	1A	1939	5MU	C6-N1	-2.06	1.34	1.38
55	2x	54	5MU	C2-N3	-2.05	1.34	1.38
54	2w	8	4SU	C5-C4	-2.04	1.39	1.42
1	2A	1915	5MU	C2-N3	-2.04	1.34	1.38
55	1x	54	5MU	C6-N1	-2.03	1.34	1.38
55	2x	8	4SU	C6-C5	2.02	1.39	1.35
54	2w	54	5MU	C2-N3	-2.01	1.34	1.38

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-17.74	70.35	102.44
54	2w	8	4SU	C4-N3-C2	-8.89	118.71	127.34
1	1A	2503	8AH	C2-N3-C4	7.29	121.44	115.52
56	2y	8	4SU	C4-N3-C2	-7.28	120.27	127.34
54	1w	37	MIA	C12-C13-C14	-6.97	113.57	127.14
54	2w	8	4SU	C5-C4-N3	6.83	121.02	114.69
1	2A	2503	8AH	C2-N3-C4	6.19	120.55	115.52
56	1y	55	PSU	N1-C2-N3	6.14	122.09	115.13
1	1A	1911	PSU	N1-C2-N3	6.07	122.01	115.13
1	2A	1911	PSU	N1-C2-N3	6.00	121.93	115.13
55	2x	55	PSU	N1-C2-N3	5.99	121.91	115.13
32	2a	1498	UR3	C4-N3-C2	-5.94	118.97	124.56
55	1x	55	PSU	N1-C2-N3	5.94	121.86	115.13
1	2A	2605	PSU	N1-C2-N3	5.90	121.81	115.13
32	1a	1498	UR3	C4-N3-C2	-5.88	119.02	124.56
54	1w	55	PSU	N1-C2-N3	5.87	121.78	115.13
55	1x	76	31H	N3-C2-N1	-5.82	119.58	128.68
56	1y	8	4SU	C4-N3-C2	-5.79	121.71	127.34
1	2A	1917	PSU	N1-C2-N3	5.78	121.68	115.13
32	1a	516	PSU	N1-C2-N3	5.75	121.64	115.13
1	2A	1939	5MU	C4-N3-C2	-5.75	119.91	127.35
54	2w	32	PSU	N1-C2-N3	5.74	121.64	115.13
54	2w	76	F3N	N3-C2-N1	-5.74	119.71	128.68
54	2w	55	PSU	N1-C2-N3	5.72	121.61	115.13
1	1A	1917	PSU	N1-C2-N3	5.70	121.59	115.13
56	2y	8	4SU	C5-C4-N3	5.67	119.95	114.69
55	2x	76	31H	N3-C2-N1	-5.63	119.89	128.68
32	2a	516	PSU	N1-C2-N3	5.62	121.50	115.13
56	1y	32	PSU	N1-C2-N3	5.62	121.50	115.13
1	1A	2605	PSU	N1-C2-N3	5.61	121.48	115.13
54	1w	32	PSU	N1-C2-N3	5.57	121.44	115.13
56	2y	32	PSU	N1-C2-N3	5.56	121.43	115.13
1	1A	1939	5MU	C5-C4-N3	5.52	120.02	115.31
54	1w	8	4SU	C4-N3-C2	-5.50	122.00	127.34
1	1A	1915	5MU	C4-N3-C2	-5.48	120.26	127.35
1	2A	1915	5MU	C4-N3-C2	-5.48	120.26	127.35
1	1A	2552	2MU	N3-C2-N1	5.47	122.14	114.89
54	1w	76	F3N	N3-C2-N1	-5.46	120.14	128.68
56	1y	39	PSU	N1-C2-N3	5.44	121.29	115.13
54	1w	39	PSU	N1-C2-N3	5.42	121.27	115.13
56	1y	8	4SU	C5-C4-N3	5.41	119.71	114.69
55	2x	54	5MU	C4-N3-C2	-5.34	120.44	127.35
56	1y	54	5MU	C4-N3-C2	-5.33	120.45	127.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	55	PSU	N1-C2-N3	5.32	121.16	115.13
1	1A	1939	5MU	C4-N3-C2	-5.31	120.47	127.35
1	2A	1915	5MU	N3-C2-N1	5.23	121.84	114.89
56	2y	39	PSU	N1-C2-N3	5.20	121.02	115.13
1	2A	1939	5MU	N3-C2-N1	5.17	121.75	114.89
55	2x	54	5MU	N3-C2-N1	5.14	121.71	114.89
1	2A	1939	5MU	C5-C4-N3	5.12	119.68	115.31
32	2a	1519	MA6	N3-C2-N1	-5.07	120.76	128.68
1	1A	1915	5MU	N3-C2-N1	5.02	121.56	114.89
54	2w	8	4SU	N3-C2-N1	4.99	121.52	114.89
1	2A	2552	2MU	N3-C2-N1	4.99	121.51	114.89
32	2a	1518	MA6	N3-C2-N1	-4.98	120.89	128.68
56	2y	54	5MU	N3-C2-N1	4.97	121.49	114.89
55	1x	54	5MU	N3-C2-N1	4.93	121.43	114.89
32	1a	1519	MA6	N3-C2-N1	-4.92	120.99	128.68
56	2y	54	5MU	C4-N3-C2	-4.91	121.00	127.35
54	1w	8	4SU	C5-C4-N3	4.91	119.24	114.69
55	1x	54	5MU	C4-N3-C2	-4.90	121.01	127.35
1	1A	1915	5MU	C5-C4-N3	4.83	119.43	115.31
56	1y	54	5MU	N3-C2-N1	4.80	121.26	114.89
32	1a	1518	MA6	N3-C2-N1	-4.78	121.21	128.68
1	2A	1915	5MU	C5-C4-N3	4.78	119.39	115.31
56	1y	54	5MU	C5-C4-N3	4.77	119.38	115.31
1	1A	2503	8AH	C5-C6-N1	-4.76	117.88	121.01
54	2w	39	PSU	N1-C2-N3	4.75	120.51	115.13
1	1A	2552	2MU	C4-N3-C2	-4.74	120.33	126.58
56	2y	8	4SU	N3-C2-N1	4.64	121.05	114.89
54	1w	54	5MU	C4-N3-C2	-4.60	121.40	127.35
54	1w	54	5MU	N3-C2-N1	4.55	120.93	114.89
1	2A	1939	5MU	C5-C6-N1	-4.53	118.67	123.34
1	1A	1915	5MU	O4-C4-C5	-4.49	119.69	124.90
54	2w	54	5MU	C4-N3-C2	-4.49	121.54	127.35
55	2x	54	5MU	C5-C4-N3	4.48	119.14	115.31
1	2A	1939	5MU	O4-C4-C5	-4.43	119.76	124.90
1	2A	2552	2MU	C4-N3-C2	-4.43	120.74	126.58
1	1A	1939	5MU	N3-C2-N1	4.43	120.77	114.89
54	2w	54	5MU	C5-C4-N3	4.33	119.00	115.31
1	1A	1939	5MU	O4-C4-C5	-4.28	119.94	124.90
55	1x	54	5MU	C5-C4-N3	4.22	118.91	115.31
54	1w	54	5MU	O4-C4-C5	-4.21	120.02	124.90
56	2y	54	5MU	C5-C4-N3	4.19	118.89	115.31
55	1x	8	4SU	C6-C5-C4	-4.19	116.32	119.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2605	PSU	C4-N3-C2	-4.19	120.30	126.34
55	2x	55	PSU	C4-N3-C2	-4.19	120.31	126.34
54	2w	54	5MU	N3-C2-N1	4.19	120.45	114.89
1	1A	1939	5MU	C5-C6-N1	-4.18	119.04	123.34
1	2A	2503	8AH	C5-C6-N1	-4.14	118.29	121.01
1	2A	1915	5MU	O4-C4-C5	-4.14	120.11	124.90
54	1w	54	5MU	C5-C4-N3	4.13	118.84	115.31
55	1x	32	5MC	C5-C6-N1	-4.11	119.11	123.34
54	2w	8	4SU	C5-C4-S4	-4.09	119.19	124.47
1	1A	2605	PSU	C4-N3-C2	-4.07	120.48	126.34
56	1y	54	5MU	O4-C4-C5	-4.04	120.22	124.90
55	2x	32	5MC	C5-C6-N1	-4.04	119.18	123.34
54	1w	37	MIA	C5-C6-N1	-4.03	117.46	120.81
55	2x	54	5MU	O4-C4-C5	-4.02	120.24	124.90
54	2w	54	5MU	O4-C4-C5	-4.00	120.27	124.90
54	1w	37	MIA	C15-C14-C13	-3.98	111.13	122.65
55	1x	55	PSU	C4-N3-C2	-3.95	120.64	126.34
1	2A	1911	PSU	C4-N3-C2	-3.93	120.67	126.34
55	2x	54	5MU	C5-C6-N1	-3.93	119.30	123.34
54	1w	37	MIA	C2-N3-C4	3.92	120.72	115.32
1	1A	1962	5MC	C5-C6-N1	-3.90	119.33	123.34
1	1A	1911	PSU	C4-N3-C2	-3.90	120.73	126.34
54	2w	8	4SU	O2-C2-N1	-3.88	117.62	122.79
55	1x	8	4SU	O2-C2-N1	3.87	127.93	122.79
32	1a	516	PSU	C4-N3-C2	-3.87	120.77	126.34
1	1A	1917	PSU	C4-N3-C2	-3.86	120.78	126.34
56	1y	55	PSU	O2-C2-N1	-3.86	118.54	122.79
54	2w	37	MIA	C2-N3-C4	3.85	120.64	115.32
32	2a	516	PSU	C4-N3-C2	-3.85	120.79	126.34
1	2A	1915	5MU	C5-C6-N1	-3.82	119.41	123.34
54	2w	37	MIA	C5-C6-N1	-3.81	117.65	120.81
56	1y	8	4SU	C5-C4-S4	-3.79	119.58	124.47
55	1x	54	5MU	C5-C6-N1	-3.79	119.44	123.34
54	2w	32	PSU	C4-N3-C2	-3.76	120.91	126.34
56	2y	54	5MU	O4-C4-C5	-3.76	120.54	124.90
1	1A	1917	PSU	O2-C2-N1	-3.75	118.67	122.79
54	1w	32	PSU	C4-N3-C2	-3.72	120.97	126.34
1	2A	1962	5MC	C5-C6-N1	-3.71	119.52	123.34
54	1w	55	PSU	C4-N3-C2	-3.71	120.99	126.34
54	2w	55	PSU	C4-N3-C2	-3.71	121.00	126.34
56	1y	32	PSU	C4-N3-C2	-3.70	121.01	126.34
56	2y	32	PSU	O2-C2-N1	-3.67	118.75	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	967	5MC	C5-C6-N1	-3.67	119.56	123.34
54	1w	8	4SU	N3-C2-N1	3.67	119.76	114.89
1	1A	2552	2MU	O2-C2-N1	-3.66	117.92	122.79
55	1x	54	5MU	O4-C4-C5	-3.65	120.67	124.90
32	2a	1404	5MC	C5-C6-N1	-3.65	119.58	123.34
56	2y	54	5MU	C5-C6-N1	-3.64	119.60	123.34
1	2A	1917	PSU	C4-N3-C2	-3.64	121.10	126.34
56	2y	55	PSU	C4-N3-C2	-3.62	121.13	126.34
56	1y	55	PSU	C4-N3-C2	-3.61	121.14	126.34
56	2y	55	PSU	O2-C2-N1	-3.60	118.83	122.79
56	2y	8	4SU	C5-C4-S4	-3.60	119.83	124.47
32	1a	967	5MC	C5-C6-N1	-3.59	119.64	123.34
32	2a	1400	5MC	C5-C6-N1	-3.52	119.72	123.34
56	1y	8	4SU	N3-C2-N1	3.50	119.54	114.89
54	2w	54	5MU	C5-C6-N1	-3.50	119.74	123.34
56	2y	32	PSU	C4-N3-C2	-3.50	121.30	126.34
56	1y	54	5MU	C5-C6-N1	-3.48	119.76	123.34
54	1w	32	PSU	O2-C2-N1	-3.47	118.97	122.79
32	2a	1407	5MC	C5-C6-N1	-3.44	119.80	123.34
43	1l	92	0TD	OD2-CG-CB	3.43	120.57	113.15
55	1x	8	4SU	C5-C4-N3	3.41	117.85	114.69
1	2A	1917	PSU	O2-C2-N1	-3.39	119.06	122.79
32	1a	1407	5MC	C5-C6-N1	-3.38	119.87	123.34
1	1A	2605	PSU	O2-C2-N1	-3.33	119.12	122.79
43	2l	92	0TD	OD2-CG-CB	3.33	120.35	113.15
56	2y	37	MIA	N3-C2-N1	-3.33	123.47	128.68
54	1w	37	MIA	C16-C14-C13	-3.32	113.04	122.65
32	1a	1519	MA6	C4-C5-N7	-3.32	105.94	109.40
32	1a	1518	MA6	C4-C5-N7	-3.30	105.96	109.40
32	2a	1519	MA6	C4-C5-N7	-3.29	105.97	109.40
54	2w	37	MIA	C12-N6-C6	-3.29	120.04	122.87
56	1y	39	PSU	C4-N3-C2	-3.28	121.62	126.34
54	1w	39	PSU	C4-N3-C2	-3.27	121.63	126.34
55	1x	8	4SU	S4-C4-N3	-3.24	117.02	120.21
32	1a	1400	5MC	C5-C6-N1	-3.22	120.03	123.34
1	2A	1911	PSU	O2-C2-N1	-3.21	119.26	122.79
1	1A	1911	PSU	O2-C2-N1	-3.20	119.27	122.79
56	1y	37	MIA	N3-C2-N1	-3.20	123.68	128.68
32	2a	516	PSU	O2-C2-N1	-3.19	119.28	122.79
1	1A	1915	5MU	C5-C6-N1	-3.18	120.06	123.34
1	1A	1942	5MC	C5-C6-N1	-3.17	120.08	123.34
54	2w	32	PSU	O2-C2-N1	-3.15	119.33	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	39	PSU	C4-N3-C2	-3.14	121.81	126.34
54	1w	55	PSU	O2-C2-N1	-3.14	119.33	122.79
56	1y	32	PSU	O2-C2-N1	-3.14	119.33	122.79
56	2y	55	PSU	C6-C5-C4	-3.13	116.01	118.20
56	2y	39	PSU	C4-N3-C2	-3.12	121.84	126.34
55	2x	8	4SU	C5-C4-N3	3.11	117.57	114.69
1	1A	2503	8AH	C4-C5-N7	-3.09	106.34	109.47
1	2A	1942	5MC	C5-C6-N1	-3.09	120.16	123.34
55	1x	55	PSU	O2-C2-N1	-3.06	119.42	122.79
54	1w	54	5MU	C5-C6-N1	-3.05	120.20	123.34
1	2A	1939	5MU	O2-C2-N1	-3.04	118.75	122.79
55	2x	8	4SU	C1'-N1-C2	3.01	123.03	117.57
55	2x	8	4SU	C6-C5-C4	-3.00	117.35	119.95
54	2w	55	PSU	O2-C2-N1	-2.96	119.53	122.79
32	1a	1404	5MC	C5-C6-N1	-2.93	120.33	123.34
55	2x	55	PSU	O2-C2-N1	-2.93	119.57	122.79
55	1x	54	5MU	O2-C2-N1	-2.92	118.90	122.79
1	1A	1942	5MC	C5-C4-N3	-2.90	118.54	121.67
1	2A	2552	2MU	O2-C2-N1	-2.89	118.94	122.79
32	2a	1407	5MC	C5-C4-N3	-2.89	118.56	121.67
54	1w	8	4SU	C5-C4-S4	-2.88	120.75	124.47
1	1A	2552	2MU	C5-C4-N3	2.87	119.13	114.84
55	1x	32	5MC	C5-C4-N3	-2.86	118.58	121.67
54	1w	37	MIA	C2-N1-C6	2.86	122.30	117.19
55	1x	76	31H	O4'-C1'-C2'	-2.85	102.75	106.93
56	1y	8	4SU	C1'-N1-C2	2.84	122.72	117.57
55	2x	54	5MU	O2-C2-N1	-2.79	119.08	122.79
54	2w	37	MIA	C11-S10-C2	-2.79	100.19	102.27
1	1A	1939	5MU	O2-C2-N1	-2.76	119.12	122.79
32	2a	1518	MA6	C4-C5-N7	-2.75	106.53	109.40
1	1A	2552	2MU	O4-C4-C5	-2.75	120.32	125.16
1	2A	2552	2MU	C5-C4-N3	2.75	118.96	114.84
32	1a	1404	5MC	C5-C4-N3	-2.75	118.71	121.67
55	2x	76	31H	O4'-C1'-C2'	-2.74	102.92	106.93
1	2A	2503	8AH	C2-N1-C6	2.72	122.33	118.08
56	2y	37	MIA	C4-C5-N7	-2.70	106.58	109.40
32	1a	1400	5MC	C5-C4-N3	-2.70	118.77	121.67
55	1x	8	4SU	C1'-N1-C2	2.69	122.45	117.57
1	2A	1942	5MC	C5-C4-N3	-2.68	118.78	121.67
1	2A	2605	PSU	O2-C2-N1	-2.68	119.84	122.79
54	1w	39	PSU	O2-C2-N1	-2.65	119.88	122.79
55	2x	8	4SU	O2-C2-N1	2.63	126.28	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	8AH	C2-N1-C6	2.62	122.17	118.08
54	1w	37	MIA	C11-S10-C2	-2.62	100.31	102.27
1	2A	1962	5MC	C5-C4-N3	-2.61	118.85	121.67
55	2x	32	5MC	C5-C4-N3	-2.58	118.89	121.67
56	2y	8	4SU	C1'-N1-C2	2.58	122.24	117.57
32	1a	1207	2MG	C8-N7-C5	2.56	107.87	102.99
43	2l	92	0TD	OD1-CG-CB	-2.54	117.13	122.44
54	2w	37	MIA	C2-N1-C6	2.53	121.72	117.19
32	1a	1404	5MC	CM5-C5-C6	-2.52	119.48	122.85
32	1a	1402	4OC	C6-C5-C4	2.50	120.02	116.96
54	1w	37	MIA	C4-C5-N7	-2.50	106.79	109.40
32	2a	1404	5MC	C5-C4-N3	-2.48	118.99	121.67
55	2x	8	4SU	S4-C4-N3	-2.48	117.77	120.21
32	1a	516	PSU	O2-C2-N1	-2.47	120.07	122.79
1	1A	1962	5MC	C5-C4-N3	-2.43	119.05	121.67
1	2A	2552	2MU	O4-C4-C5	-2.43	120.89	125.16
1	1A	2605	PSU	C5-C6-N1	-2.40	118.50	122.11
56	1y	54	5MU	O2-C2-N1	-2.40	119.59	122.79
32	2a	966	M2G	C8-N7-C5	2.40	107.55	102.99
56	2y	8	4SU	O2-C2-N1	-2.39	119.61	122.79
56	1y	54	5MU	C5M-C5-C4	2.39	121.40	118.77
1	2A	2251	OMG	C5-C6-N1	2.38	118.16	113.95
32	1a	967	5MC	C5-C4-N3	-2.38	119.11	121.67
1	2A	1915	5MU	O2-C2-N1	-2.37	119.64	122.79
1	1A	1915	5MU	O2-C2-N1	-2.37	119.64	122.79
1	2A	2552	2MU	C2'-C1'-N1	-2.35	109.66	114.22
32	1a	1407	5MC	C5-C4-N3	-2.35	119.14	121.67
1	1A	1942	5MC	CM5-C5-C6	-2.33	119.74	122.85
32	2a	1402	4OC	C6-C5-C4	2.33	119.81	116.96
32	2a	967	5MC	C5-C4-N3	-2.32	119.17	121.67
54	2w	39	PSU	C6-C5-C4	-2.31	116.58	118.20
54	2w	37	MIA	C1'-N9-C4	2.31	130.69	126.64
54	1w	54	5MU	O2-C2-N1	-2.31	119.72	122.79
55	1x	76	31H	O2'-C2'-C3'	2.29	116.78	111.16
32	2a	1207	2MG	C8-N7-C5	2.28	107.33	102.99
32	2a	1404	5MC	O2-C2-N3	-2.28	118.63	122.33
54	2w	54	5MU	O2-C2-N1	-2.27	119.78	122.79
1	2A	2605	PSU	C5-C6-N1	-2.26	118.72	122.11
1	2A	2251	OMG	C8-N7-C5	2.26	107.29	102.99
32	1a	966	M2G	C5-C6-N1	2.26	117.94	113.95
32	2a	1402	4OC	CM4-N4-C4	-2.26	118.04	122.45
32	2a	1400	5MC	O2-C2-N3	-2.25	118.67	122.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1920	OMC	O2-C2-N3	-2.24	118.68	122.33
54	1w	76	F3N	O2'-C2'-C3'	-2.24	105.67	111.16
32	2a	1400	5MC	C5-C4-N3	-2.23	119.27	121.67
32	1a	1498	UR3	C1'-N1-C2	2.22	120.74	116.99
55	2x	55	PSU	C5-C6-N1	-2.20	118.80	122.11
55	1x	8	4SU	O2-C2-N3	-2.19	117.42	121.50
32	2a	1400	5MC	C1'-N1-C6	-2.19	117.48	121.12
1	2A	2251	OMG	O6-C6-C5	-2.19	120.10	124.37
1	1A	2251	OMG	C8-N7-C5	2.18	107.15	102.99
32	1a	1400	5MC	O2-C2-N3	-2.17	118.80	122.33
55	2x	76	31H	CA-N-CN	-2.17	119.49	122.82
32	2a	967	5MC	CM5-C5-C6	-2.17	119.95	122.85
55	2x	32	5MC	O2-C2-N3	-2.16	118.83	122.33
32	1a	1207	2MG	C5-C6-N1	2.16	117.76	113.95
1	1A	2251	OMG	C5-C6-N1	2.16	117.76	113.95
54	1w	37	MIA	N3-C2-N1	-2.15	123.03	126.98
1	2A	2503	8AH	C4-C5-N7	-2.15	107.29	109.47
32	1a	1404	5MC	O2-C2-N3	-2.15	118.84	122.33
55	2x	76	31H	OCN-CN-N	-2.13	119.65	125.27
56	1y	55	PSU	O4'-C1'-C2'	2.13	108.15	105.14
32	1a	966	M2G	C8-N7-C5	2.12	107.03	102.99
54	2w	37	MIA	C4-C5-N7	-2.12	107.19	109.40
32	1a	516	PSU	O4'-C1'-C2'	2.10	108.11	105.14
56	2y	54	5MU	O2-C2-N1	-2.09	120.00	122.79
56	2y	39	PSU	O2-C2-N1	-2.07	120.51	122.79
32	1a	1407	5MC	CM5-C5-C6	-2.07	120.08	122.85
55	1x	32	5MC	O2-C2-N3	-2.07	118.97	122.33
1	1A	1942	5MC	O2-C2-N3	-2.06	118.98	122.33
32	2a	966	M2G	C5-C6-N1	2.06	117.59	113.95
55	1x	55	PSU	C5-C6-N1	-2.06	119.02	122.11
55	1x	76	31H	CA-N-CN	-2.05	119.68	122.82
32	1a	516	PSU	C5-C6-N1	-2.04	119.05	122.11
1	1A	2552	2MU	C2'-C1'-N1	-2.04	110.26	114.22
1	1A	2251	OMG	O6-C6-C5	-2.03	120.41	124.37
1	1A	1915	5MU	C5M-C5-C4	2.03	121.00	118.77
56	1y	39	PSU	O2-C2-N1	-2.02	120.56	122.79
56	2y	46	G7M	C3'-C2'-C1'	2.02	104.02	100.98
1	2A	1911	PSU	O4'-C1'-C2'	2.02	107.99	105.14
32	2a	1207	2MG	C5-C6-N1	2.01	117.51	113.95
56	1y	37	MIA	C4-C5-N7	-2.00	107.31	109.40

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	527	G7M	C3'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C15
54	1w	76	F3N	C3'-C4'-C5'-O5'
55	1x	76	31H	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'
56	1y	37	MIA	C3'-C4'-C5'-O5'
56	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1207	2MG	N3-C2-N2-CM2
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB
54	2w	37	MIA	N1-C6-N6-C12
55	2x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
56	2y	37	MIA	C3'-C4'-C5'-O5'
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
56	2y	55	PSU	C2'-C1'-C5-C4
56	2y	55	PSU	C2'-C1'-C5-C6
56	2y	55	PSU	O4'-C1'-C5-C6
56	2y	55	PSU	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	1w	76	F3N	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
56	1y	8	4SU	C3'-C4'-C5'-O5'
56	1y	37	MIA	O4'-C4'-C5'-O5'
56	2y	37	MIA	O4'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
56	2y	46	G7M	O4'-C4'-C5'-O5'
56	2y	46	G7M	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
54	2w	76	F3N	N-CA-CB-CG
54	1w	46	G7M	C4'-C5'-O5'-P
55	2x	76	31H	C4'-C5'-O5'-P
55	1x	76	31H	C4'-C5'-O5'-P
54	2w	46	G7M	C4'-C5'-O5'-P
56	2y	37	MIA	C4'-C5'-O5'-P
1	1A	1915	5MU	O4'-C4'-C5'-O5'
32	2a	527	G7M	C4'-C5'-O5'-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1A	2503	8AH	C4'-C5'-O5'-P
32	2a	1519	MA6	C3'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
54	1w	37	MIA	N1-C2-S10-C11
54	1w	37	MIA	N3-C2-S10-C11
56	1y	55	PSU	O4'-C1'-C5-C4
56	2y	55	PSU	O4'-C1'-C5-C4
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	527	G7M	C4'-C5'-O5'-P
56	1y	46	G7M	C3'-C4'-C5'-O5'
54	2w	37	MIA	C5-C6-N6-C12
56	2y	8	4SU	C2'-C1'-N1-C2
32	2a	1402	4OC	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	2503	8AH	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	8AH	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
32	2a	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2685 ligands modelled in this entry, 2681 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	TYK	2A	3798	1	67,67,67	1.81	8 (11%)	83,97,97	1.49	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	TYK	1A	4101	1	67,67,67	1.74	6 (8%)	83,97,97	1.31	14 (16%)
61	SF4	2d	303	35	0,12,12	-	-	-	-	-
61	SF4	1d	501	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	TYK	2A	3798	1	-	4/67/126/126	1/3/4/4
59	TYK	1A	4101	1	-	2/67/126/126	1/3/4/4
61	SF4	2d	303	35	-	-	0/6/5/5
61	SF4	1d	501	35	-	-	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	2A	3798	TYK	C14-C13	-8.12	1.37	1.50
59	1A	4101	TYK	C8-C9	-7.66	1.38	1.51
59	2A	3798	TYK	C8-C9	-7.64	1.38	1.51
59	1A	4101	TYK	C14-C13	-7.46	1.39	1.50
59	2A	3798	TYK	C2-C1	-4.72	1.41	1.50
59	1A	4101	TYK	C2-C1	-4.32	1.42	1.50
59	2A	3798	TYK	C11-C12	-3.22	1.39	1.45
59	1A	4101	TYK	C11-C12	-2.87	1.39	1.45
59	2A	3798	TYK	O5B-C1B	2.45	1.48	1.42
59	2A	3798	TYK	C2A-C3A	-2.25	1.49	1.53
59	2A	3798	TYK	O1C-C1C	2.23	1.44	1.40
59	1A	4101	TYK	C3B-C4B	2.11	1.57	1.53
59	1A	4101	TYK	C11-C10	2.02	1.39	1.33
59	2A	3798	TYK	C2B-C1B	2.00	1.56	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	2A	3798	TYK	C10-C11-C12	-4.31	119.72	126.23
59	1A	4101	TYK	C3B-C2B-C1B	-4.24	106.69	114.82
59	2A	3798	TYK	C1B-O4A-C4A	3.81	122.36	114.66
59	2A	3798	TYK	C3B-C2B-C1B	-3.63	107.85	114.82
59	2A	3798	TYK	O4B-C4B-C5B	-3.62	103.04	109.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	2A	3798	TYK	O5B-C5B-C6B	3.06	113.31	106.70
59	1A	4101	TYK	O5B-C5B-C6B	2.87	112.91	106.70
59	1A	4101	TYK	C23-O1C-C1C	-2.78	108.31	113.74
59	2A	3798	TYK	O15-C15-C16	-2.78	102.48	106.92
59	2A	3798	TYK	C18-C4-C3	-2.72	106.91	111.17
59	1A	4101	TYK	O20-C20-C19	-2.69	117.58	125.43
59	1A	4101	TYK	O4B-C4B-C5B	-2.66	104.73	109.39
59	2A	3798	TYK	C1A-O1A-C5	-2.63	111.45	117.96
59	2A	3798	TYK	C1A-O5A-C5A	-2.62	109.16	113.67
59	1A	4101	TYK	C7C-O2C-C2C	-2.61	107.67	114.52
59	2A	3798	TYK	C7C-O2C-C2C	-2.54	107.87	114.52
59	2A	3798	TYK	O20-C20-C19	-2.44	118.32	125.43
59	1A	4101	TYK	C18-C4-C3	-2.40	107.41	111.17
59	1A	4101	TYK	C10-C11-C12	-2.39	122.62	126.23
59	1A	4101	TYK	C1A-O5A-C5A	-2.32	109.69	113.67
59	2A	3798	TYK	C6C-C5C-C4C	-2.28	108.85	113.07
59	1A	4101	TYK	C22-C12-C11	2.25	121.62	118.08
59	2A	3798	TYK	O15-C15-C14	2.17	112.19	107.42
59	1A	4101	TYK	O3B-C3B-C4B	2.15	111.47	107.48
59	1A	4101	TYK	C1B-O4A-C4A	2.10	118.91	114.66
59	1A	4101	TYK	C17-C16-C15	-2.09	107.51	113.27
59	2A	3798	TYK	C17-C16-C15	-2.05	107.61	113.27
59	1A	4101	TYK	O4A-C4A-C3A	-2.01	103.94	109.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

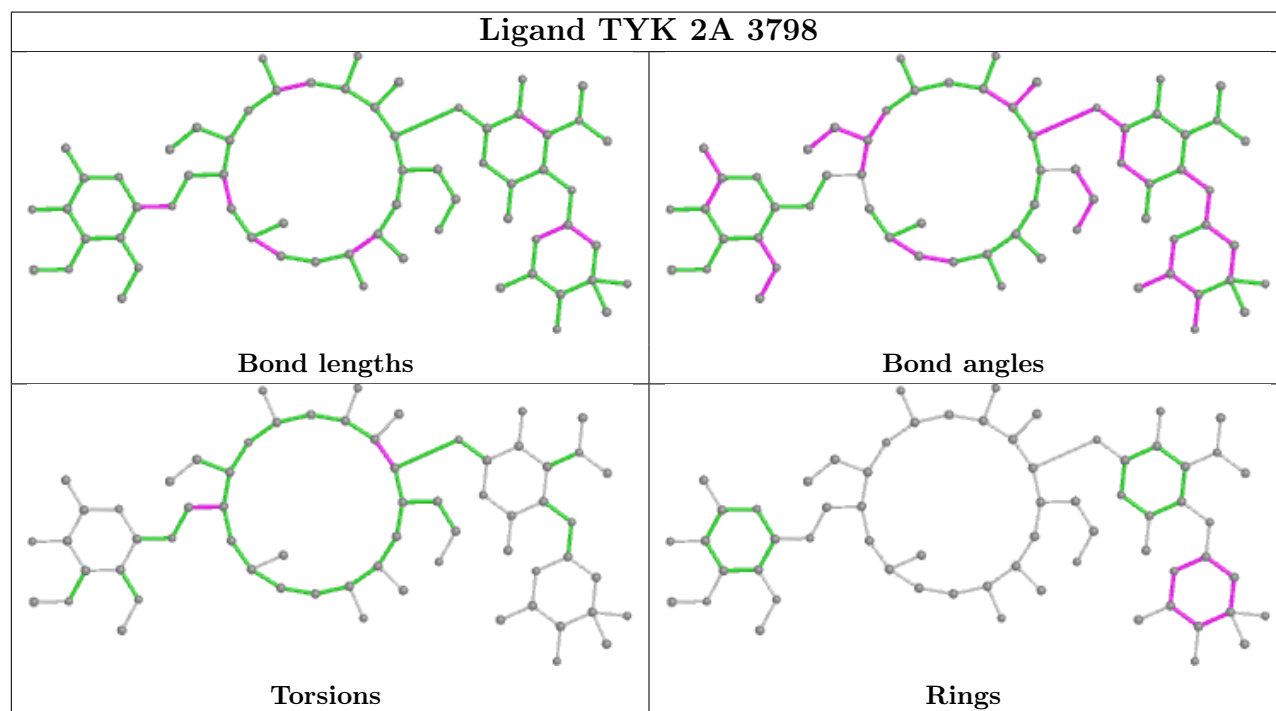
Mol	Chain	Res	Type	Atoms
59	1A	4101	TYK	C15-C14-C23-O1C
59	2A	3798	TYK	C15-C14-C23-O1C
59	1A	4101	TYK	C18-C4-C5-C6
59	2A	3798	TYK	C18-C4-C5-C6
59	2A	3798	TYK	C3-C4-C5-O1A
59	2A	3798	TYK	C3-C4-C5-C6

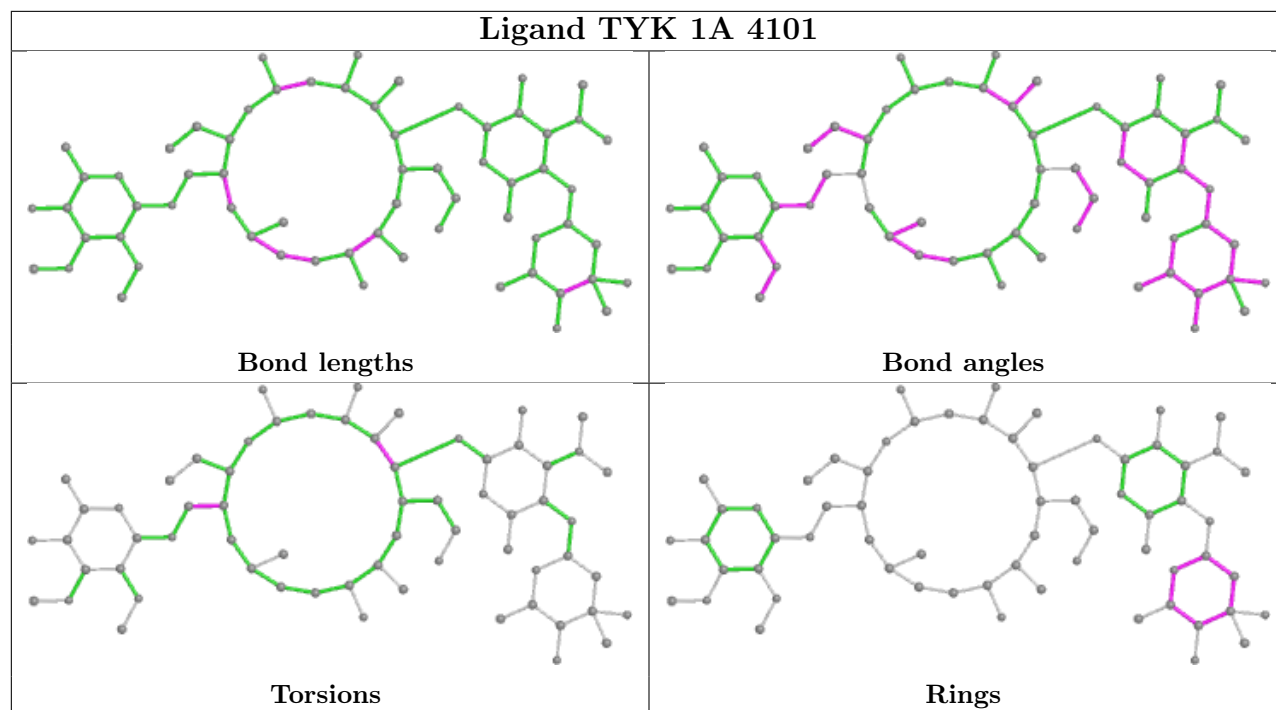
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	2A	3798	TYK	C1B-C2B-C3B-C4B-C5B-O5B
59	1A	4101	TYK	C1B-C2B-C3B-C4B-C5B-O5B

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.11	136 (4%) 30 27	20, 36, 98, 108	0
1	2A	2789/2915 (95%)	0.03	94 (3%) 45 41	33, 57, 95, 107	0
2	1B	120/121 (99%)	-0.45	0 100 100	29, 48, 63, 89	0
2	2B	120/121 (99%)	-0.69	0 100 100	61, 75, 84, 91	0
3	1D	275/276 (99%)	0.39	6 (2%) 62 57	21, 37, 52, 77	0
3	2D	275/276 (99%)	0.49	3 (1%) 80 79	33, 50, 62, 82	0
4	1E	204/206 (99%)	0.11	1 (0%) 91 91	20, 39, 59, 76	0
4	2E	204/206 (99%)	0.13	0 100 100	38, 59, 72, 81	0
5	1F	202/210 (96%)	0.24	1 (0%) 91 91	19, 41, 66, 84	0
5	2F	202/210 (96%)	0.43	4 (1%) 65 60	37, 66, 79, 87	0
6	1G	181/182 (99%)	-0.16	0 100 100	39, 56, 71, 81	0
6	2G	181/182 (99%)	0.74	28 (15%) 2 1	67, 77, 85, 94	0
7	1H	174/180 (96%)	-0.10	1 (0%) 89 89	36, 53, 67, 73	0
7	2H	174/180 (96%)	1.85	74 (42%) 0 0	69, 83, 90, 95	0
8	1I	146/148 (98%)	-0.06	0 100 100	46, 72, 80, 83	0
8	2I	146/148 (98%)	0.44	8 (5%) 25 21	53, 73, 80, 85	0
9	1N	140/140 (100%)	0.14	0 100 100	25, 38, 61, 67	0
9	2N	140/140 (100%)	0.48	4 (2%) 51 48	48, 66, 79, 85	0
10	1O	122/122 (100%)	0.12	0 100 100	28, 39, 57, 61	0
10	2O	122/122 (100%)	0.51	3 (2%) 57 53	47, 58, 70, 76	0
11	1P	149/150 (99%)	0.27	2 (1%) 77 75	23, 45, 68, 73	0
11	2P	149/150 (99%)	1.14	32 (21%) 0 0	40, 65, 80, 89	0
12	1Q	141/141 (100%)	0.03	0 100 100	25, 39, 55, 72	0
12	2Q	141/141 (100%)	0.24	1 (0%) 87 87	48, 66, 77, 81	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%)	0.19	0 100 100	25, 34, 46, 56	0
13	2R	118/118 (100%)	0.35	3 (2%) 57 53	44, 53, 63, 70	0
14	1S	110/112 (98%)	-0.12	0 100 100	38, 49, 60, 66	0
14	2S	110/112 (98%)	0.06	2 (1%) 68 65	61, 70, 78, 84	0
15	1T	131/146 (89%)	0.26	1 (0%) 86 85	33, 44, 68, 78	0
15	2T	131/146 (89%)	0.70	9 (6%) 16 13	52, 62, 75, 82	0
16	1U	116/118 (98%)	0.17	0 100 100	22, 30, 44, 64	0
16	2U	116/118 (98%)	0.33	1 (0%) 84 83	44, 62, 72, 77	0
17	1V	101/101 (100%)	0.19	0 100 100	23, 38, 55, 65	0
17	2V	101/101 (100%)	0.36	4 (3%) 38 34	43, 71, 77, 83	0
18	1W	112/113 (99%)	0.03	1 (0%) 84 83	25, 32, 49, 85	0
18	2W	112/113 (99%)	0.14	0 100 100	40, 51, 69, 86	0
19	1X	95/96 (98%)	-0.02	1 (1%) 80 79	26, 38, 62, 77	0
19	2X	95/96 (98%)	0.31	3 (3%) 47 44	45, 58, 75, 82	0
20	1Y	107/110 (97%)	-0.09	0 100 100	36, 50, 67, 80	0
20	2Y	107/110 (97%)	0.34	5 (4%) 31 28	58, 71, 80, 86	0
21	1Z	154/206 (74%)	0.06	4 (2%) 56 52	38, 64, 83, 91	0
21	2Z	160/206 (77%)	0.66	19 (11%) 4 3	64, 81, 88, 92	0
22	10	83/85 (97%)	0.04	0 100 100	29, 37, 50, 67	0
22	20	83/85 (97%)	0.13	0 100 100	47, 61, 73, 78	0
23	11	97/98 (98%)	0.37	2 (2%) 63 59	29, 47, 71, 75	0
23	21	97/98 (98%)	0.57	6 (6%) 20 17	39, 55, 75, 84	0
24	12	70/72 (97%)	0.03	0 100 100	35, 48, 59, 76	0
24	22	70/72 (97%)	-0.06	0 100 100	58, 69, 76, 80	0
25	13	59/60 (98%)	0.24	1 (1%) 70 67	26, 36, 62, 79	0
25	23	59/60 (98%)	0.83	5 (8%) 10 8	57, 66, 79, 87	0
26	14	69/71 (97%)	0.27	6 (8%) 10 8	52, 73, 88, 89	0
26	24	69/71 (97%)	1.27	16 (23%) 0 0	75, 84, 92, 94	0
27	15	59/60 (98%)	0.10	1 (1%) 70 67	20, 32, 51, 54	0
27	25	59/60 (98%)	0.18	3 (5%) 28 25	39, 54, 66, 78	0
28	16	53/54 (98%)	0.11	0 100 100	33, 43, 57, 60	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%)	0.51	3 (5%) 23 20	51, 60, 68, 72	0
29	17	48/49 (97%)	0.26	1 (2%) 63 59	24, 29, 54, 63	0
29	27	48/49 (97%)	0.54	4 (8%) 11 9	35, 42, 64, 74	0
30	18	64/65 (98%)	0.16	0 100 100	29, 34, 42, 56	0
30	28	64/65 (98%)	0.75	3 (4%) 31 28	44, 55, 62, 65	0
31	19	37/37 (100%)	-0.04	0 100 100	30, 38, 54, 61	0
31	29	37/37 (100%)	0.54	4 (10%) 5 4	60, 68, 77, 83	0
32	1a	1488/1521 (97%)	-0.22	27 (1%) 68 65	34, 64, 92, 105	0
32	2a	1491/1521 (98%)	0.02	66 (4%) 34 31	49, 75, 95, 106	0
33	1b	231/256 (90%)	0.73	28 (12%) 4 3	62, 77, 87, 92	0
33	2b	231/256 (90%)	1.77	82 (35%) 0 0	73, 83, 89, 92	0
34	1c	206/239 (86%)	-0.00	1 (0%) 91 91	56, 68, 79, 86	0
34	2c	206/239 (86%)	1.69	78 (37%) 0 0	73, 82, 88, 91	0
35	1d	208/209 (99%)	0.51	11 (5%) 26 23	52, 67, 76, 82	0
35	2d	208/209 (99%)	0.64	12 (5%) 23 19	59, 71, 79, 82	0
36	1e	148/162 (91%)	0.14	0 100 100	48, 62, 72, 80	0
36	2e	148/162 (91%)	0.88	22 (14%) 2 1	65, 75, 81, 86	0
37	1f	100/101 (99%)	0.46	5 (5%) 28 25	52, 65, 72, 77	0
37	2f	100/101 (99%)	0.26	1 (1%) 82 81	49, 67, 75, 82	0
38	1g	155/156 (99%)	0.36	10 (6%) 18 16	59, 70, 84, 88	0
38	2g	155/156 (99%)	1.23	34 (21%) 0 0	68, 78, 87, 92	0
39	1h	137/138 (99%)	0.74	14 (10%) 6 4	52, 65, 72, 76	0
39	2h	137/138 (99%)	0.54	13 (9%) 8 6	65, 74, 80, 83	0
40	1i	127/128 (99%)	0.42	8 (6%) 20 17	50, 74, 83, 87	0
40	2i	127/128 (99%)	2.24	71 (55%) 0 0	71, 83, 88, 92	0
41	1j	97/105 (92%)	0.77	14 (14%) 2 1	53, 76, 84, 91	0
41	2j	96/105 (91%)	2.16	46 (47%) 0 0	74, 84, 90, 92	0
42	1k	114/129 (88%)	0.67	8 (7%) 16 13	41, 66, 76, 80	0
42	2k	114/129 (88%)	0.14	1 (0%) 84 83	52, 72, 79, 82	0
43	1l	121/132 (91%)	0.15	0 100 100	41, 50, 63, 71	0
43	2l	121/132 (91%)	0.30	3 (2%) 57 53	50, 66, 75, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	-0.15	3 (2%) 59 54	53, 67, 76, 88	0
44	2m	122/126 (96%)	1.34	28 (22%) 0 0	67, 80, 85, 88	0
45	1n	60/61 (98%)	0.18	0 100 100	54, 64, 71, 76	0
45	2n	60/61 (98%)	3.66	43 (71%) 0 0	73, 82, 87, 90	0
46	1o	88/89 (98%)	0.70	5 (5%) 23 20	47, 63, 72, 79	0
46	2o	88/89 (98%)	0.23	0 100 100	59, 70, 80, 85	0
47	1p	82/88 (93%)	0.11	0 100 100	58, 69, 77, 86	0
47	2p	82/88 (93%)	0.37	3 (3%) 41 38	59, 69, 77, 81	0
48	1q	99/105 (94%)	1.11	15 (15%) 2 1	48, 66, 75, 76	0
48	2q	99/105 (94%)	0.58	6 (6%) 21 18	62, 72, 80, 81	0
49	1r	68/88 (77%)	1.31	17 (25%) 0 0	53, 64, 76, 77	0
49	2r	68/88 (77%)	0.23	1 (1%) 73 71	59, 69, 78, 83	0
50	1s	83/93 (89%)	0.33	3 (3%) 42 39	59, 69, 79, 84	0
50	2s	83/93 (89%)	2.06	37 (44%) 0 0	78, 83, 89, 95	0
51	1t	96/106 (90%)	1.10	15 (15%) 2 1	61, 68, 78, 82	0
51	2t	96/106 (90%)	1.43	27 (28%) 0 0	60, 70, 81, 87	0
52	1u	23/27 (85%)	0.42	0 100 100	59, 64, 70, 74	0
52	2u	23/27 (85%)	2.83	18 (78%) 0 0	74, 78, 83, 89	0
53	1v	13/24 (54%)	0.62	2 (15%) 2 1	47, 51, 92, 98	0
53	2v	13/24 (54%)	0.44	2 (15%) 2 1	63, 73, 96, 102	0
54	1w	66/76 (86%)	0.22	6 (9%) 9 7	29, 86, 98, 103	0
54	2w	64/76 (84%)	0.12	7 (10%) 5 4	48, 91, 100, 102	0
55	1x	72/77 (93%)	-0.20	1 (1%) 75 73	25, 58, 78, 91	0
55	2x	72/77 (93%)	-0.29	0 100 100	42, 73, 87, 97	0
56	1y	67/76 (88%)	3.40	58 (86%) 0 0	58, 99, 103, 105	0
56	2y	66/76 (86%)	4.24	64 (96%) 0 0	69, 101, 103, 105	0
All	All	20871/21748 (95%)	0.31	1422 (6%) 17 14	19, 63, 89, 108	0

All (1422) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	653	A	16.8
1	2A	652(U)	G	14.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	652(V)	C	14.5
1	2A	652(V)	C	14.2
1	2A	652(C)	G	13.9
1	1A	652(C)	G	13.0
1	1A	653	A	12.8
1	2A	652(T)	C	12.6
1	1A	652(S)	C	12.5
45	2n	38	GLY	11.8
1	1A	652(U)	G	11.2
44	2m	123	ALA	11.0
1	2A	654	A	10.8
44	2m	124	PRO	10.7
45	2n	39	LEU	9.8
45	2n	25	VAL	9.6
1	1A	654	A	9.6
1	1A	652(E)	G	9.3
1	1A	652(T)	C	9.2
45	2n	34	TYR	9.1
1	2A	652(D)	C	9.0
54	2w	71	G	9.0
45	2n	10	ALA	8.4
1	1A	652(F)	G	8.3
32	2a	1030(B)	C	7.9
1	2A	652(E)	G	7.7
45	2n	2	ALA	7.6
1	1A	1509	C	7.6
44	1m	124	PRO	7.5
32	1a	1030(A)	G	7.5
1	1A	2159	G	7.4
38	1g	80	VAL	7.4
32	1a	1030(B)	C	7.4
38	2g	154	TYR	7.3
52	2u	16	GLY	7.2
1	2A	884	C	7.1
1	2A	2802	G	7.1
56	2y	36	A	7.1
41	2j	47	PHE	7.1
32	2a	1257	U	7.0
1	1A	2130	U	6.9
41	2j	65	LEU	6.9
1	1A	2174	C	6.8
56	1y	47	U	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	652(D)	C	6.7
32	2a	1030(A)	G	6.6
56	2y	52	G	6.6
32	2a	1030(C)	G	6.6
56	2y	29	G	6.5
56	2y	44	G	6.5
45	2n	11	LYS	6.4
38	2g	40	ALA	6.4
1	2A	883	G	6.4
33	2b	121	LEU	6.4
33	2b	122	PHE	6.4
56	2y	1	G	6.4
40	2i	90	PRO	6.4
33	2b	165	VAL	6.4
1	1A	2129	C	6.3
1	2A	885	C	6.3
44	2m	122	LYS	6.3
56	1y	35	A	6.3
33	2b	70	PHE	6.3
1	2A	2146	C	6.2
32	1a	1030(C)	G	6.2
54	1w	70	G	6.2
3	1D	276	LYS	6.2
38	2g	42	ILE	6.1
56	1y	20	U	6.1
33	2b	69	LEU	6.1
1	2A	1509	C	6.1
56	1y	24	G	6.1
40	2i	19	LEU	6.1
56	2y	34	G	6.1
56	2y	47	U	6.1
50	2s	80	TYR	6.1
26	24	50	VAL	6.0
45	2n	35	ARG	6.0
26	24	63	TYR	6.0
56	1y	36	A	6.0
33	2b	187	LEU	5.9
1	1A	2181	G	5.9
1	1A	2160	G	5.8
56	2y	21	A	5.8
56	1y	56	C	5.8
32	2a	1030(D)	A	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
56	2y	64	A	5.8
41	2j	66	ARG	5.8
7	2H	47	GLU	5.7
56	2y	53	G	5.7
50	2s	12	ASP	5.7
56	2y	73	A	5.7
50	2s	71	LEU	5.7
56	1y	1	G	5.7
45	2n	37	PHE	5.7
48	1q	98	LEU	5.7
56	2y	65	G	5.6
45	2n	6	LEU	5.6
7	2H	48	GLY	5.6
40	2i	14	VAL	5.6
32	2a	1001(A)	G	5.6
56	1y	63	G	5.6
56	2y	35	A	5.5
51	1t	55	ILE	5.5
1	2A	229	A	5.5
56	2y	28	G	5.5
1	1A	2145	C	5.5
56	2y	63	G	5.5
23	11	2	SER	5.5
32	2a	1021	G	5.5
56	1y	53	G	5.5
1	1A	2128	C	5.5
44	2m	42	ALA	5.4
33	2b	92	TYR	5.4
26	24	51	ASP	5.4
34	2c	198	VAL	5.4
1	1A	2131	G	5.4
40	2i	36	TYR	5.4
45	2n	53	LEU	5.3
1	1A	884	C	5.3
1	1A	2115	G	5.3
1	1A	2143	C	5.3
1	1A	2173	A	5.3
1	2A	2133	G	5.3
32	2a	1031	G	5.3
56	2y	15	G	5.3
44	2m	102	ARG	5.2
34	2c	32	LEU	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
56	1y	12	U	5.2
33	2b	227	GLY	5.2
34	2c	87	LEU	5.2
33	2b	214	ILE	5.2
34	2c	101	LEU	5.2
45	2n	29	ARG	5.2
56	2y	57	G	5.2
1	1A	1094	U	5.2
56	1y	51	U	5.2
1	1A	1096	A	5.2
20	2Y	1	MET	5.1
41	2j	63	PHE	5.1
3	1D	2	ALA	5.1
56	2y	13	C	5.1
32	2a	1036	G	5.1
45	2n	30	ALA	5.1
1	1A	2132	U	5.1
1	1A	2146	C	5.1
33	1b	188	ALA	5.0
32	2a	1033	G	5.0
7	2H	45	VAL	5.0
32	2a	1030	C	5.0
1	1A	2109	U	5.0
33	2b	211	ILE	5.0
34	2c	8	ILE	5.0
41	2j	72	VAL	5.0
56	2y	6	G	5.0
56	1y	21	A	5.0
26	24	49	PHE	5.0
26	24	32	TYR	5.0
1	1A	2166	G	5.0
32	2a	1032	G	5.0
1	1A	2170	A	5.0
32	1a	1030	C	5.0
56	1y	23	A	5.0
56	2y	24	G	5.0
1	1A	2108	C	4.9
56	1y	75	C	4.9
41	2j	44	VAL	4.9
1	1A	2141	G	4.9
33	2b	71	VAL	4.9
1	2A	2128	C	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	156	TRP	4.9
54	2w	72	C	4.9
1	1A	2169	A	4.9
34	2c	53	ALA	4.9
56	2y	74	C	4.9
1	2A	2147	G	4.9
54	1w	71	G	4.9
32	2a	1005	A	4.8
33	2b	185	ILE	4.8
1	1A	2140	C	4.8
1	1A	2162	G	4.8
56	1y	5	G	4.8
56	2y	22	G	4.8
45	2n	50	LYS	4.8
1	2A	2167	U	4.8
45	2n	23	ARG	4.8
1	1A	2158	A	4.8
23	2l	28	GLY	4.7
32	2a	1034	G	4.7
50	2s	48	THR	4.7
45	2n	36	PHE	4.7
45	2n	42	ILE	4.7
56	2y	23	A	4.7
1	2A	2154	G	4.7
56	1y	22	G	4.7
1	1A	2175	C	4.7
1	2A	2145	C	4.7
41	2j	11	PHE	4.7
45	2n	12	ARG	4.7
56	1y	19	G	4.7
7	2H	35	VAL	4.7
56	2y	25	C	4.7
1	2A	2160	G	4.6
7	2H	24	VAL	4.6
7	2H	52	VAL	4.6
32	1a	1257	U	4.6
34	2c	23	TYR	4.6
1	1A	2125	G	4.6
56	2y	71	G	4.6
41	2j	68	HIS	4.6
1	2A	2801(A)	A	4.6
1	2A	888	C	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	201	TYR	4.6
19	2X	92	LEU	4.6
3	2D	38	LYS	4.6
1	1A	1176	G	4.5
1	2A	2127	G	4.5
54	2w	70	G	4.5
11	2P	15	ARG	4.5
33	2b	66	GLY	4.5
56	2y	43	C	4.5
21	2Z	153	SER	4.5
1	1A	2107	C	4.5
1	2A	2793	G	4.5
38	2g	82	GLY	4.5
1	1A	885	C	4.5
34	2c	60	ALA	4.5
49	1r	42	ARG	4.5
54	1w	20	U	4.5
1	1A	2114	A	4.5
38	1g	81	GLY	4.5
38	1g	85	TYR	4.5
1	1A	1057	A	4.5
11	2P	91	PHE	4.5
56	1y	71	G	4.5
1	1A	2112	G	4.4
1	1A	2133	G	4.4
1	1A	2161	C	4.4
32	1a	1031	G	4.4
56	2y	72	C	4.4
1	1A	2151	G	4.4
1	2A	2123	G	4.4
7	2H	6	ARG	4.4
56	2y	45	U	4.4
11	2P	123	LEU	4.4
50	2s	13	ASP	4.4
21	2Z	139	VAL	4.4
1	1A	2110	G	4.4
3	1D	275	LYS	4.4
41	2j	40	LEU	4.3
45	2n	51	GLY	4.3
40	2i	109	VAL	4.3
56	1y	52	G	4.3
40	2i	40	LEU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
56	1y	57	G	4.3
26	24	55	ARG	4.3
33	2b	152	PHE	4.3
45	2n	22	THR	4.3
7	2H	72	ILE	4.3
56	1y	64	A	4.3
1	1A	2111	C	4.3
56	1y	62	C	4.3
21	2Z	144	LEU	4.3
50	2s	67	VAL	4.3
51	2t	25	ARG	4.3
32	2a	1026	G	4.3
21	1Z	1	MET	4.3
7	2H	7	LEU	4.2
56	2y	26	A	4.2
56	2y	27	G	4.2
1	2A	2111	C	4.2
56	1y	50	U	4.2
1	2A	2174	C	4.2
56	2y	51	U	4.2
1	1A	2105	C	4.2
44	2m	66	LEU	4.2
56	2y	70	G	4.2
40	2i	33	PHE	4.2
33	2b	201	ILE	4.2
38	1g	79	ARG	4.2
56	2y	62	C	4.2
1	1A	2127	G	4.2
32	2a	1024	G	4.2
33	2b	118	LEU	4.2
33	2b	81	VAL	4.2
1	1A	2134	A	4.2
32	2a	1035	A	4.2
37	1f	46	ARG	4.1
41	2j	62	HIS	4.1
44	2m	4	ILE	4.1
1	1A	2113	U	4.1
56	2y	48	C	4.1
56	2y	5	G	4.1
7	2H	115	VAL	4.1
56	2y	66	U	4.1
38	2g	79	ARG	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	49	VAL	4.1
1	2A	2112	G	4.1
41	2j	71	LEU	4.1
43	2l	64	TYR	4.1
23	2l	2	SER	4.1
56	2y	12	U	4.1
1	2A	2125	G	4.1
33	2b	51	LEU	4.1
33	2b	232	PRO	4.1
38	2g	81	GLY	4.1
44	2m	78	ILE	4.1
32	1a	1036	G	4.1
1	2A	2803	C	4.1
50	2s	31	ILE	4.1
1	2A	2166	G	4.1
40	2i	10	ARG	4.0
34	2c	39	ILE	4.0
33	2b	67	THR	4.0
56	2y	2	C	4.0
40	2i	63	ILE	4.0
1	1A	1066	U	4.0
1	2A	2804	C	4.0
45	2n	55	GLY	4.0
52	2u	15	ARG	4.0
1	1A	2104	G	4.0
32	2a	1023	G	4.0
44	2m	7	VAL	4.0
1	1A	1064	C	4.0
39	1h	112	LEU	4.0
41	2j	6	ILE	4.0
45	2n	7	ILE	4.0
34	2c	71	ALA	4.0
1	1A	2165	G	4.0
32	1a	1029	C	4.0
34	2c	33	LEU	4.0
32	1a	1030(D)	A	4.0
26	24	54	GLY	4.0
56	1y	3	C	3.9
7	2H	102	ALA	3.9
6	2G	142	PRO	3.9
1	1A	2180	U	3.9
45	2n	31	ARG	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	2u	6	ARG	3.9
52	2u	22	ARG	3.9
40	2i	59	PHE	3.9
38	2g	80	VAL	3.9
41	2j	88	LEU	3.9
52	2u	17	THR	3.9
51	2t	63	ILE	3.9
1	1A	2897	U	3.9
49	1r	39	VAL	3.9
50	2s	70	LYS	3.9
40	2i	27	THR	3.9
1	2A	2175	C	3.9
40	2i	9	ARG	3.9
40	2i	62	TYR	3.9
6	2G	49	ASP	3.9
11	2P	125	VAL	3.9
40	2i	102	LEU	3.9
26	24	68	ARG	3.9
53	1v	12	A	3.9
38	1g	156	TRP	3.9
1	2A	2896	C	3.9
56	1y	2	C	3.9
1	2A	2165	G	3.9
21	2Z	155	LEU	3.9
41	2j	48	THR	3.9
34	2c	206	GLU	3.9
1	2A	2164	C	3.9
7	2H	44	VAL	3.8
36	2e	6	PHE	3.8
33	2b	215	LEU	3.8
26	24	57	GLU	3.8
32	1a	204	U	3.8
6	2G	39	ILE	3.8
38	1g	153	HIS	3.8
1	1A	2138	C	3.8
1	1A	2803	C	3.8
44	2m	41	PRO	3.8
1	2A	2168	G	3.8
33	2b	164	VAL	3.8
3	2D	276	LYS	3.8
33	1b	133	LYS	3.8
41	2j	10	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	84	ASN	3.8
6	2G	146	TYR	3.8
1	2A	2897	U	3.8
7	2H	51	ARG	3.8
1	2A	882	G	3.8
8	2I	75	LEU	3.8
35	1d	180	GLY	3.8
40	2i	106	ALA	3.8
41	2j	13	HIS	3.8
49	1r	78	LEU	3.8
1	1A	1095	A	3.8
1	2A	2126	A	3.8
45	2n	46	GLU	3.8
1	1A	2147	G	3.7
1	1A	2177	C	3.7
1	1A	1098	A	3.7
41	2j	85	LEU	3.7
50	2s	50	ALA	3.7
56	1y	15	G	3.7
56	1y	34	G	3.7
56	1y	13	C	3.7
50	2s	36	ARG	3.7
56	2y	31	A	3.7
1	1A	2123	G	3.7
56	1y	6	G	3.7
50	2s	14	HIS	3.7
45	2n	56	VAL	3.7
44	2m	121	LYS	3.7
34	2c	145	GLY	3.7
50	2s	30	LEU	3.7
1	1A	2106	G	3.7
56	2y	69	G	3.7
56	2y	58	A	3.7
56	2y	61	C	3.7
40	2i	7	THR	3.7
7	2H	133	VAL	3.7
31	29	17	ILE	3.7
52	2u	2	GLY	3.7
1	1A	1059	G	3.7
1	1A	2135	A	3.6
56	2y	9	A	3.6
45	2n	16	PHE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1447	A	3.6
38	2g	43	PHE	3.6
34	2c	170	GLN	3.6
52	2u	14	TRP	3.6
42	1k	25	TYR	3.6
51	1t	47	GLY	3.6
38	2g	32	ARG	3.6
33	2b	115	LEU	3.6
53	1v	13	A	3.6
34	2c	96	GLY	3.6
40	2i	43	ALA	3.6
25	23	30	ARG	3.6
1	1A	2185	C	3.6
44	2m	90	LEU	3.6
34	2c	51	GLY	3.6
1	1A	1068	G	3.6
56	2y	18	G	3.6
34	2c	182	ILE	3.6
1	1A	1082	U	3.6
1	2A	2113	U	3.6
56	2y	50	U	3.6
41	2j	38	ILE	3.6
38	1g	154	TYR	3.6
6	2G	139	LEU	3.6
33	2b	226	ARG	3.5
38	2g	16	LEU	3.6
1	2A	2144	U	3.5
34	2c	105	GLU	3.5
35	1d	179	GLU	3.5
50	2s	62	ILE	3.5
8	2I	12	LEU	3.5
26	24	67	TYR	3.5
45	2n	26	ARG	3.5
7	2H	32	GLU	3.5
32	1a	1027	C	3.5
32	2a	1007	C	3.5
32	2a	1027	C	3.5
56	1y	49	C	3.5
56	1y	74	C	3.5
51	1t	45	GLN	3.5
50	2s	63	THR	3.5
34	2c	204	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	1r	85	LEU	3.5
32	2a	1003	G	3.5
56	2y	68	C	3.5
29	27	47	ARG	3.5
34	2c	14	ILE	3.5
42	1k	14	VAL	3.5
50	2s	15	LEU	3.5
1	1A	2154	G	3.5
1	2A	2159	G	3.5
1	1A	2178	C	3.5
35	1d	167	GLY	3.5
33	1b	211	ILE	3.5
1	1A	2167	U	3.5
7	2H	105	LEU	3.5
33	2b	68	ILE	3.5
56	1y	27	G	3.5
56	2y	30	G	3.5
32	2a	91	C	3.5
34	2c	115	LEU	3.5
35	1d	110	PHE	3.5
33	2b	114	ARG	3.5
7	2H	34	GLU	3.5
35	1d	158	ILE	3.5
6	2G	3	LEU	3.5
51	2t	13	LEU	3.5
1	1A	897	C	3.5
1	1A	2117	A	3.5
1	1A	2801(A)	A	3.5
35	2d	168	ARG	3.5
56	1y	44	G	3.5
34	2c	48	TYR	3.5
23	11	98	LEU	3.5
26	14	68	ARG	3.5
32	1a	1035	A	3.4
32	2a	1006	C	3.4
44	2m	87	TYR	3.4
45	2n	21	TYR	3.4
32	1a	1003	G	3.4
45	2n	54	PRO	3.4
34	2c	186	PHE	3.4
1	2A	272(A)	U	3.4
1	2A	2794	C	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	140	ASP	3.4
36	2e	63	ARG	3.4
41	2j	46	ARG	3.4
11	2P	78	PRO	3.4
56	2y	33	U	3.4
1	2A	2179	C	3.4
33	2b	112	VAL	3.4
52	2u	10	ARG	3.4
32	1a	1025	U	3.4
38	2g	120	ILE	3.4
45	2n	13	THR	3.4
32	2a	1002	G	3.4
1	1A	1060	U	3.4
56	1y	45	U	3.4
1	1A	2142	C	3.4
40	2i	61	ALA	3.4
1	1A	896	A	3.4
1	1A	2121	G	3.4
7	2H	31	GLY	3.4
1	2A	2131	G	3.3
1	2A	2155	G	3.3
36	2e	8	GLU	3.3
41	2j	9	ARG	3.3
11	2P	124	LYS	3.3
32	2a	1357	A	3.3
38	2g	59	LEU	3.3
1	1A	888	C	3.3
48	1q	90	ILE	3.3
11	2P	79	ARG	3.3
1	2A	2792	G	3.3
15	2T	48	ILE	3.3
33	2b	139	LYS	3.3
33	2b	90	MET	3.3
7	2H	98	LEU	3.3
53	2v	12	A	3.3
32	1a	1024	G	3.3
50	1s	71	LEU	3.3
1	1A	1065	U	3.3
33	2b	8	LYS	3.3
40	2i	66	ARG	3.3
48	1q	36	ILE	3.3
1	1A	2124	G	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	48	MET	3.3
33	2b	131	PRO	3.3
56	1y	61	C	3.3
45	2n	57	ARG	3.3
50	2s	38	SER	3.3
40	2i	5	TYR	3.3
34	2c	57	ILE	3.3
51	1t	38	LYS	3.3
1	1A	2168	G	3.3
34	2c	154	SER	3.2
26	14	59	PHE	3.2
52	2u	21	TYR	3.2
11	2P	94	GLU	3.2
52	2u	12	LYS	3.2
56	2y	76	A	3.2
48	1q	97	SER	3.2
51	2t	9	ASN	3.2
7	2H	37	VAL	3.2
32	1a	1032	G	3.2
32	2a	80	G	3.2
41	2j	92	THR	3.2
54	2w	4	C	3.2
56	2y	75	C	3.2
7	2H	121	ILE	3.2
33	2b	127	ILE	3.2
40	2i	15	ALA	3.2
40	2i	115	GLY	3.2
50	2s	68	GLY	3.2
36	2e	109	ILE	3.2
56	2y	4	C	3.2
34	2c	50	ALA	3.2
7	2H	103	LEU	3.2
7	2H	128	PRO	3.2
51	2t	24	LEU	3.2
40	2i	26	VAL	3.2
1	1A	1081	U	3.2
1	1A	2189	U	3.2
1	2A	2132	U	3.2
32	2a	1149	C	3.2
56	2y	59	U	3.2
33	1b	19	HIS	3.2
7	2H	43	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	136	VAL	3.2
1	2A	887	A	3.2
45	2n	24	CYS	3.2
56	2y	14	A	3.2
29	27	48	LYS	3.2
56	2y	10	G	3.2
33	1b	214	ILE	3.2
45	2n	61	TRP	3.2
1	1A	2116	G	3.2
35	2d	164	ALA	3.2
38	2g	46	ALA	3.2
11	2P	109	GLY	3.2
34	2c	21	ARG	3.2
35	2d	160	GLN	3.2
32	1a	841	U	3.1
11	2P	101	VAL	3.1
32	2a	470	C	3.1
32	2a	1039	C	3.1
56	2y	19	G	3.1
7	2H	123	PHE	3.1
1	1A	1175	U	3.1
1	1A	2188	C	3.1
6	2G	140	ILE	3.1
15	2T	111	ARG	3.1
33	2b	89	GLY	3.1
33	2b	94	ASN	3.1
49	1r	24	ALA	3.1
40	2i	49	PRO	3.1
51	2t	98	PRO	3.1
52	2u	13	ILE	3.1
7	2H	55	PRO	3.1
20	2Y	55	TYR	3.1
45	2n	17	LYS	3.1
7	2H	124	GLU	3.1
26	24	59	PHE	3.1
1	2A	2130	U	3.1
15	2T	125	ARG	3.1
34	2c	59	ARG	3.1
1	2A	2143	C	3.1
33	2b	75	LYS	3.1
7	2H	141	VAL	3.1
40	2i	65	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
51	1t	83	ARG	3.1
1	2A	2115	G	3.1
41	2j	67	THR	3.1
7	2H	125	VAL	3.1
40	2i	17	VAL	3.1
1	2A	2170	A	3.1
33	1b	187	LEU	3.1
56	1y	67	C	3.1
6	2G	144	ILE	3.1
7	2H	148	ILE	3.1
15	2T	22	PHE	3.0
40	2i	53	VAL	3.0
1	1A	2896	C	3.0
33	1b	78	GLN	3.0
54	2w	73	A	3.0
33	1b	227	GLY	3.0
35	2d	23	GLY	3.0
40	2i	57	GLY	3.0
34	2c	63	ASN	3.0
50	2s	35	SER	3.0
34	2c	100	ALA	3.0
1	2A	2138	C	3.0
56	2y	42	C	3.0
42	2k	25	TYR	3.0
56	1y	14	A	3.0
32	2a	1025	U	3.0
20	2Y	90	LEU	3.0
38	2g	58	PRO	3.0
40	2i	30	GLY	3.0
7	2H	13	LYS	3.0
1	1A	2137	C	3.0
1	2A	2129	C	3.0
1	2A	2177	C	3.0
40	2i	42	ARG	3.0
1	1A	2122	U	3.0
39	2h	133	LEU	3.0
51	1t	43	LEU	3.0
33	2b	223	ILE	3.0
41	2j	74	ILE	3.0
47	2p	19	ILE	3.0
51	1t	41	ILE	3.0
40	2i	93	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	1r	29	PHE	3.0
1	2A	2110	G	3.0
40	2i	105	ASP	3.0
54	2w	44	G	3.0
33	2b	161	ALA	3.0
41	1j	18	ALA	3.0
5	1F	17	ARG	3.0
41	2j	45	ARG	3.0
35	1d	138	TYR	3.0
33	2b	221	LEU	3.0
44	1m	2	ALA	3.0
1	1A	1058	G	3.0
7	2H	29	PRO	3.0
1	1A	1508	A	3.0
50	2s	52	TYR	3.0
36	2e	90	VAL	3.0
33	2b	120	ALA	3.0
38	2g	14	PRO	3.0
1	1A	2120	G	2.9
1	1A	2182	G	2.9
32	2a	1001	A	2.9
39	1h	58	TYR	2.9
40	2i	69	GLY	2.9
51	2t	83	ARG	2.9
52	2u	23	PRO	2.9
32	1a	1023	G	2.9
34	2c	184	TYR	2.9
40	2i	20	ARG	2.9
41	2j	15	THR	2.9
48	1q	7	THR	2.9
33	2b	101	MET	2.9
41	2j	96	ILE	2.9
26	24	66	SER	2.9
33	2b	17	PHE	2.9
9	2N	61	ARG	2.9
44	2m	65	LYS	2.9
44	2m	120	LYS	2.9
7	2H	94	TYR	2.9
7	2H	50	VAL	2.9
36	2e	10	MET	2.9
42	1k	82	VAL	2.9
1	2A	2116	G	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2124	G	2.9
34	2c	22	TRP	2.9
34	2c	6	HIS	2.9
34	2c	124	ILE	2.9
34	2c	134	ILE	2.9
44	2m	119	GLY	2.9
6	2G	149	VAL	2.9
40	2i	114	TYR	2.9
41	2j	34	VAL	2.9
33	2b	111	ARG	2.9
51	2t	17	ARG	2.9
1	2A	2114	A	2.9
40	2i	37	PHE	2.9
26	24	52	THR	2.9
26	24	30	GLU	2.9
40	2i	78	LYS	2.9
38	2g	115	ARG	2.9
49	1r	75	ILE	2.9
21	2Z	170	THR	2.9
39	2h	17	THR	2.9
6	2G	92	VAL	2.9
7	2H	17	VAL	2.9
17	2V	72	VAL	2.9
38	2g	13	GLN	2.9
33	2b	65	GLY	2.9
40	2i	6	GLY	2.9
50	2s	69	HIS	2.9
33	2b	58	ILE	2.9
51	2t	29	LYS	2.9
1	1A	2157	G	2.9
40	2i	28	VAL	2.9
44	1m	123	ALA	2.9
11	2P	93	GLY	2.8
34	2c	155	GLY	2.8
34	2c	185	GLY	2.8
33	2b	233	SER	2.8
51	1t	63	ILE	2.8
1	2A	886	C	2.8
6	2G	62	LEU	2.8
33	2b	218	ALA	2.8
40	2i	82	ALA	2.8
1	1A	2119	A	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	149	LEU	2.8
52	2u	24	ARG	2.8
40	2i	75	ASP	2.8
7	2H	41	MET	2.8
25	23	29	ARG	2.8
1	1A	229	A	2.8
1	1A	883	G	2.8
1	1A	2144	U	2.8
1	1A	2172	U	2.8
49	1r	51	LEU	2.8
50	2s	22	LEU	2.8
41	2j	7	LYS	2.8
1	1A	2163	C	2.8
32	2a	1223	C	2.8
32	2a	1452	C	2.8
41	2j	43	ARG	2.8
33	2b	55	PHE	2.8
33	2b	98	LEU	2.8
40	1i	19	LEU	2.8
38	2g	24	THR	2.8
41	2j	87	THR	2.8
34	2c	13	GLY	2.8
41	2j	26	ALA	2.8
34	2c	126	ARG	2.8
40	2i	88	TYR	2.8
6	2G	102	PHE	2.8
11	2P	106	LEU	2.8
52	2u	11	GLY	2.8
11	2P	103	ALA	2.8
40	2i	86	VAL	2.8
40	2i	108	VAL	2.8
51	2t	59	ALA	2.8
1	2A	652(B)	A	2.8
33	1b	61	LEU	2.8
6	2G	37	VAL	2.8
56	2y	60	U	2.8
33	2b	63	MET	2.8
34	2c	28	GLN	2.8
39	1h	6	ILE	2.8
39	2h	83	ILE	2.8
41	1j	8	LEU	2.8
1	2A	894	C	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	88	ARG	2.8
7	2H	145	ALA	2.7
50	2s	27	GLU	2.7
50	2s	47	HIS	2.7
44	2m	23	TYR	2.7
33	2b	97	TRP	2.7
44	2m	13	LYS	2.7
6	2G	157	ILE	2.7
7	2H	101	ARG	2.7
56	2y	3	C	2.7
41	2j	27	ALA	2.7
11	2P	102	ARG	2.7
33	1b	11	LEU	2.7
50	2s	84	GLY	2.7
7	2H	10	PRO	2.7
27	15	60	VAL	2.7
42	1k	80	VAL	2.7
29	27	1	MET	2.7
41	2j	12	ASP	2.7
44	2m	92	HIS	2.7
54	1w	72	C	2.7
11	2P	130	PHE	2.7
33	1b	215	LEU	2.7
38	2g	36	LYS	2.7
40	2i	64	THR	2.7
40	2i	21	PRO	2.7
9	2N	140	VAL	2.7
46	1o	88	ARG	2.7
1	1A	2164	C	2.7
1	1A	2179	C	2.7
56	2y	38	A	2.7
33	2b	145	LEU	2.7
34	2c	102	ASN	2.7
1	2A	271(K)	U	2.7
56	1y	18	G	2.7
50	2s	49	ILE	2.7
52	2u	8	THR	2.7
33	2b	88	ALA	2.7
33	2b	216	SER	2.7
40	2i	72	GLY	2.7
29	17	48	LYS	2.7
34	2c	91	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	47	LEU	2.7
41	1j	71	LEU	2.7
56	1y	11	C	2.7
32	2a	204	U	2.7
40	2i	55	ALA	2.7
33	2b	72	GLY	2.7
33	2b	228	GLY	2.7
36	2e	9	LYS	2.7
40	1i	59	PHE	2.7
50	1s	15	LEU	2.7
1	1A	887	A	2.7
1	2A	896	A	2.7
1	2A	2134	A	2.7
9	2N	9	VAL	2.7
32	1a	1001(A)	G	2.7
34	2c	207	VAL	2.7
36	2e	60	TYR	2.7
37	2f	59	TYR	2.7
42	1k	92	GLU	2.7
6	2G	136	ARG	2.7
33	1b	43	ASP	2.7
33	2b	222	ILE	2.7
41	1j	38	ILE	2.7
7	2H	56	SER	2.7
45	2n	4	LYS	2.7
15	2T	131	ALA	2.6
32	1a	1532	U	2.6
32	2a	1020	U	2.6
35	2d	167	GLY	2.6
51	2t	101	GLY	2.6
7	2H	19	VAL	2.6
50	2s	45	VAL	2.6
1	1A	2171	A	2.6
1	2A	2117	A	2.6
1	2A	892	G	2.6
32	1a	1026	G	2.6
32	2a	79	G	2.6
7	2H	84	SER	2.6
33	1b	33	TYR	2.6
33	1b	79	ASP	2.6
34	2c	65	ALA	2.6
45	2n	14	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1446	U	2.6
33	1b	165	VAL	2.6
34	2c	66	VAL	2.6
35	2d	105	VAL	2.6
56	1y	59	U	2.6
56	2y	41	C	2.6
33	2b	133	LYS	2.6
39	1h	119	LEU	2.6
40	2i	79	LEU	2.6
41	1j	85	LEU	2.6
51	2t	20	LEU	2.6
32	2a	1248	A	2.6
48	1q	38	ARG	2.6
33	2b	135	GLN	2.6
40	1i	8	GLY	2.6
40	2i	24	GLY	2.6
40	2i	23	ASN	2.6
40	2i	41	VAL	2.6
56	2y	49	C	2.6
32	2a	1287	A	2.6
56	1y	58	A	2.6
40	2i	127	LYS	2.6
39	2h	93	VAL	2.6
32	2a	202	U	2.6
41	2j	93	GLY	2.6
38	2g	27	ILE	2.6
41	2j	98	ILE	2.6
7	2H	164	TYR	2.6
40	2i	92	TYR	2.6
44	2m	60	VAL	2.6
23	2l	98	LEU	2.6
51	2t	99	LEU	2.6
33	2b	163	PHE	2.6
51	2t	21	LYS	2.6
25	13	60	GLU	2.6
28	26	54	ILE	2.6
34	1c	100	ALA	2.6
41	2j	18	ALA	2.6
39	2h	129	VAL	2.6
1	1A	1070	A	2.6
38	2g	63	LYS	2.6
45	2n	40	CYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	19	GLU	2.6
32	2a	1022	G	2.6
50	2s	40	ILE	2.6
3	1D	5	LYS	2.6
34	2c	72	LYS	2.6
7	2H	113	VAL	2.6
21	2Z	96	VAL	2.6
21	2Z	145	GLU	2.6
33	1b	213	LEU	2.6
39	1h	133	LEU	2.6
41	2j	64	GLU	2.6
1	2A	2169	A	2.6
32	2a	1250	A	2.6
27	25	29	THR	2.5
33	1b	132	LYS	2.5
41	2j	75	ILE	2.5
56	1y	33	U	2.5
1	1A	2152	G	2.5
1	1A	2186	G	2.5
48	1q	45	HIS	2.5
7	2H	46	GLU	2.5
5	2F	37	VAL	2.5
33	1b	93	VAL	2.5
35	1d	104	VAL	2.5
38	2g	4	ARG	2.5
41	2j	29	ARG	2.5
50	2s	37	ARG	2.5
51	2t	22	ARG	2.5
6	2G	41	GLN	2.5
1	2A	2158	A	2.5
8	2I	4	ILE	2.5
11	1P	149	GLU	2.5
11	2P	140	ALA	2.5
34	2c	200	ALA	2.5
26	14	54	GLY	2.5
34	2c	64	VAL	2.5
40	2i	8	GLY	2.5
32	2a	1220	G	2.5
52	2u	9	ARG	2.5
37	1f	60	PHE	2.5
7	2H	162	ILE	2.5
33	1b	77	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
51	2t	28	ALA	2.5
1	2A	2109	U	2.5
21	2Z	156	LYS	2.5
33	2b	157	ARG	2.5
47	2p	74	LEU	2.5
34	2c	20	SER	2.5
1	2A	1533	G	2.5
32	1a	1034	G	2.5
54	1w	44	G	2.5
33	2b	7	VAL	2.5
35	1d	157	LEU	2.5
38	2g	22	LEU	2.5
56	1y	60	U	2.5
15	1T	108	ARG	2.5
36	2e	120	THR	2.5
32	1a	1028	C	2.5
51	2t	41	ILE	2.5
6	2G	152	LEU	2.5
26	14	57	GLU	2.5
41	2j	94	VAL	2.5
43	2l	39	VAL	2.5
33	2b	105	PHE	2.5
56	1y	66	U	2.5
43	2l	28	LYS	2.5
7	2H	8	PRO	2.5
15	2T	126	ALA	2.5
49	1r	25	THR	2.5
4	1E	195	LEU	2.5
1	1A	2136	C	2.5
1	1A	2139	C	2.5
32	2a	1249	C	2.5
34	2c	55	VAL	2.5
36	2e	115	VAL	2.5
1	2A	2162	G	2.5
32	2a	1131	G	2.5
56	1y	65	G	2.5
40	2i	83	ARG	2.5
51	1t	75	ASN	2.5
51	2t	57	ARG	2.5
11	2P	149	GLU	2.5
48	1q	28	PRO	2.5
1	2A	2135	A	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	2h	112	LEU	2.5
56	2y	7	A	2.5
7	2H	25	LYS	2.5
34	2c	49	SER	2.5
38	2g	26	PHE	2.5
6	2G	181	ARG	2.5
49	1r	54	ARG	2.5
50	2s	66	MET	2.5
1	1A	2187	G	2.5
32	2a	1150	U	2.4
40	2i	70	LYS	2.4
40	2i	81	ILE	2.4
49	1r	31	LEU	2.4
51	1t	72	LEU	2.4
1	2A	2176	A	2.4
27	25	60	VAL	2.4
28	26	5	VAL	2.4
50	2s	41	VAL	2.4
28	26	28	ARG	2.4
51	2t	23	ARG	2.4
34	2c	142	MET	2.4
32	2a	1028	C	2.4
56	1y	48	C	2.4
40	1i	49	PRO	2.4
1	1A	271(K)	U	2.4
1	2A	2805	G	2.4
33	2b	188	ALA	2.4
34	2c	92	ALA	2.4
50	2s	39	THR	2.4
41	1j	34	VAL	2.4
48	2q	75	ARG	2.4
40	2i	35	GLU	2.4
21	2Z	68	PRO	2.4
51	2t	16	HIS	2.4
30	28	41	ILE	2.4
44	2m	71	ARG	2.4
11	2P	126	VAL	2.4
32	2a	1224	G	2.4
44	2m	98	VAL	2.4
40	2i	125	TYR	2.4
7	2H	33	LEU	2.4
32	2a	1038	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	28	LYS	2.4
33	2b	219	VAL	2.4
37	1f	57	GLN	2.4
56	1y	29	G	2.4
46	1o	57	LEU	2.4
19	2X	8	ILE	2.4
40	2i	77	ILE	2.4
1	1A	1097	U	2.4
1	1A	2118	U	2.4
40	1i	14	VAL	2.4
7	2H	23	ARG	2.4
11	2P	110	TYR	2.4
1	1A	2156	G	2.4
33	2b	207	ALA	2.4
7	1H	2	SER	2.4
39	1h	100	ILE	2.4
10	2O	99	PHE	2.4
48	2q	9	VAL	2.4
1	1A	1067	A	2.4
35	2d	68	TYR	2.4
49	1r	34	TYR	2.4
50	2s	42	PRO	2.4
7	2H	96	ALA	2.4
34	2c	196	LEU	2.4
40	2i	85	LEU	2.4
34	2c	205	GLY	2.4
13	2R	66	VAL	2.4
25	23	6	VAL	2.4
35	1d	122	ARG	2.4
36	2e	105	VAL	2.4
1	1A	886	C	2.3
32	1a	1447	A	2.3
32	2a	1116	C	2.3
41	2j	91	PRO	2.3
46	1o	56	LEU	2.3
34	2c	80	GLY	2.3
11	2P	144	GLU	2.3
35	2d	179	GLU	2.3
41	1j	9	ARG	2.3
45	2n	8	GLU	2.3
31	29	16	VAL	2.3
34	2c	75	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1356	G	2.3
33	1b	31	TYR	2.3
39	1h	57	PRO	2.3
48	2q	95	TYR	2.3
6	2G	133	LEU	2.3
34	2c	62	ASP	2.3
32	2a	1037	C	2.3
33	2b	210	SER	2.3
40	1i	50	LEU	2.3
31	29	19	ARG	2.3
33	1b	200	ILE	2.3
33	2b	146	GLN	2.3
36	2e	56	GLN	2.3
7	2H	30	LYS	2.3
1	2A	1170	G	2.3
51	1t	84	LEU	2.3
54	1w	69	G	2.3
32	2a	1532	U	2.3
33	1b	21	ARG	2.3
34	2c	189	ALA	2.3
41	1j	20	ALA	2.3
33	2b	162	ILE	2.3
12	2Q	104	PHE	2.3
36	2e	84	PHE	2.3
38	2g	51	GLN	2.3
11	1P	15	ARG	2.3
33	2b	183	PRO	2.3
34	2c	42	LEU	2.3
38	2g	41	ARG	2.3
34	2c	61	ALA	2.3
32	2a	90	U	2.3
11	2P	108	LYS	2.3
30	28	29	LYS	2.3
33	2b	74	LYS	2.3
33	1b	17	PHE	2.3
56	1y	7	A	2.3
40	2i	16	ARG	2.3
11	2P	97	PRO	2.3
41	1j	68	HIS	2.3
11	2P	120	ALA	2.3
36	2e	133	TYR	2.3
38	2g	7	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	2h	65	TYR	2.3
51	1t	59	ALA	2.3
1	1A	1078	U	2.3
7	2H	89	ILE	2.3
30	28	16	ILE	2.3
39	2h	134	ILE	2.3
10	2O	10	VAL	2.3
49	1r	38	GLU	2.3
1	1A	2101	G	2.3
1	2A	614(B)	G	2.3
32	2a	999	C	2.3
44	2m	64	TRP	2.3
33	1b	232	PRO	2.3
51	2t	68	LYS	2.3
11	2P	6	LEU	2.3
13	2R	70	LEU	2.3
14	2S	58	LEU	2.3
48	2q	22	LEU	2.3
7	2H	122	THR	2.3
7	2H	165	ALA	2.3
35	2d	20	TYR	2.3
50	2s	56	GLN	2.3
3	1D	176	ARG	2.3
7	2H	76	VAL	2.3
7	2H	99	VAL	2.3
23	2l	30	VAL	2.3
45	2n	18	VAL	2.3
48	1q	77	VAL	2.3
44	2m	24	GLY	2.3
16	2U	2	PRO	2.3
41	2j	37	PRO	2.3
50	2s	76	PRO	2.3
51	2t	26	ASN	2.3
56	1y	28	G	2.3
41	2j	32	ALA	2.3
40	2i	4	TYR	2.3
6	2G	51	ARG	2.3
49	1r	43	PHE	2.3
51	1t	89	ARG	2.3
21	2Z	141	VAL	2.3
33	2b	184	VAL	2.3
34	2c	56	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	32	VAL	2.3
36	2e	148	VAL	2.3
48	2q	23	VAL	2.3
21	2Z	24	LEU	2.2
39	1h	2	LEU	2.2
44	2m	12	ASN	2.2
1	1A	1080	C	2.2
1	2A	2104	G	2.2
7	2H	54	ARG	2.2
56	1y	25	C	2.2
56	1y	30	G	2.2
33	2b	205	ASP	2.2
36	2e	76	ILE	2.2
38	2g	62	PHE	2.2
7	2H	14	GLY	2.2
56	1y	76	A	2.2
6	2G	138	GLN	2.2
7	2H	21	PRO	2.2
7	2H	36	PRO	2.2
7	2H	65	HIS	2.2
32	2a	1358	U	2.2
37	1f	98	LEU	2.2
7	2H	97	ARG	2.2
20	2Y	50	ARG	2.2
44	2m	103	THR	2.2
41	2j	89	ASP	2.2
7	2H	4	ILE	2.2
8	2I	13	GLY	2.2
18	1W	112	GLY	2.2
21	2Z	57	ILE	2.2
32	2a	1296	C	2.2
38	1g	42	ILE	2.2
56	1y	4	C	2.2
56	2y	56	C	2.2
50	2s	9	VAL	2.2
33	2b	124	SER	2.2
32	2a	1256	A	2.2
34	2c	52	LEU	2.2
38	2g	10	ARG	2.2
38	2g	119	ARG	2.2
51	2t	12	ALA	2.2
21	2Z	148	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	1j	89	ASP	2.2
7	2H	159	GLU	2.2
15	2T	63	VAL	2.2
29	27	46	VAL	2.2
56	2y	67	C	2.2
1	1A	2802	G	2.2
39	1h	101	PRO	2.2
48	1q	53	LEU	2.2
32	2a	1004	A	2.2
40	2i	38	GLN	2.2
48	1q	14	LYS	2.2
34	2c	138	VAL	2.2
45	2n	33	VAL	2.2
48	2q	85	VAL	2.2
7	2H	42	ARG	2.2
8	2I	68	LEU	2.2
17	2V	71	LEU	2.2
1	1A	2794	C	2.2
21	2Z	62	PRO	2.2
39	1h	39	LEU	2.2
38	2g	117	ALA	2.2
1	1A	2155	G	2.2
23	2I	81	LYS	2.2
41	2j	17	ASP	2.2
48	1q	16	GLN	2.2
52	2u	5	ASP	2.2
32	1a	1002	G	2.2
1	1A	1054	A	2.2
1	2A	2173	A	2.2
56	1y	38	A	2.2
7	2H	26	VAL	2.2
17	2V	5	VAL	2.2
21	1Z	133	ILE	2.2
21	2Z	126	VAL	2.2
38	2g	50	ILE	2.2
50	1s	40	ILE	2.2
11	2P	122	PRO	2.2
33	2b	113	HIS	2.2
39	1h	127	LEU	2.2
41	1j	10	GLY	2.2
1	2A	881	G	2.2
7	2H	107	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	2Y	45	VAL	2.2
1	1A	655	A	2.2
6	2G	43	LEU	2.2
36	2e	12	LEU	2.2
36	2e	142	LEU	2.2
5	2F	21	ALA	2.2
19	1X	94	GLY	2.2
34	2c	159	GLY	2.2
40	1i	76	ALA	2.2
40	2i	122	ALA	2.2
10	2O	14	THR	2.2
19	2X	68	ARG	2.2
1	2A	2895	U	2.1
21	1Z	149	SER	2.1
35	1d	198	VAL	2.1
39	2h	95	VAL	2.1
6	2G	34	LEU	2.1
56	1y	31	A	2.1
6	2G	29	TRP	2.1
8	2I	3	VAL	2.1
11	2P	83	VAL	2.1
26	24	56	VAL	2.1
52	2u	18	TYR	2.1
51	2t	84	LEU	2.1
7	2H	100	GLY	2.1
9	2N	57	ALA	2.1
33	2b	77	ALA	2.1
42	1k	64	ALA	2.1
1	1A	1093	G	2.1
1	2A	2121	G	2.1
33	1b	129	GLU	2.1
47	2p	80	PHE	2.1
45	2n	32	SER	2.1
51	2t	45	GLN	2.1
15	2T	52	ILE	2.1
33	1b	222	ILE	2.1
6	2G	150	ASP	2.1
17	2V	101	GLY	2.1
34	2c	38	ARG	2.1
42	1k	91	ARG	2.1
56	1y	72	C	2.1
40	2i	13	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	18	TRP	2.1
41	1j	21	GLN	2.1
1	1A	1063	G	2.1
32	1a	1033	G	2.1
32	2a	1202	G	2.1
50	2s	4	SER	2.1
7	2H	157	TYR	2.1
35	2d	180	GLY	2.1
36	2e	34	VAL	2.1
45	2n	58	LYS	2.1
32	2a	92	C	2.1
34	2c	143	GLU	2.1
8	2I	1	MET	2.1
11	2P	111	ARG	2.1
34	2c	83	ARG	2.1
5	2F	181	LEU	2.1
11	2P	95	VAL	2.1
39	2h	79	VAL	2.1
51	1t	53	LEU	2.1
1	2A	2141	G	2.1
7	2H	18	GLU	2.1
32	2a	977	A	2.1
56	1y	70	G	2.1
1	1A	2103	C	2.1
13	2R	68	ARG	2.1
26	14	55	ARG	2.1
34	2c	190	ARG	2.1
46	1o	68	ARG	2.1
48	1q	27	PHE	2.1
7	2H	161	GLY	2.1
39	2h	66	GLY	2.1
6	2G	48	GLU	2.1
6	2G	28	VAL	2.1
41	1j	90	LEU	2.1
39	1h	35	ILE	2.1
1	1A	2126	A	2.1
1	2A	2171	A	2.1
32	1a	1531	A	2.1
32	2a	998	G	2.1
40	1i	106	ALA	2.1
40	2i	52	ALA	2.1
3	1D	200	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	2F	202	PHE	2.1
33	1b	126	GLU	2.1
33	2b	79	ASP	2.1
6	2G	160	VAL	2.1
33	2b	155	LEU	2.1
39	1h	61	VAL	2.1
41	1j	98	ILE	2.1
31	29	15	LYS	2.1
33	2b	29	ALA	2.1
36	2e	138	ALA	2.1
51	2t	77	ALA	2.1
15	2T	115	ARG	2.1
38	2g	78	ARG	2.1
11	2P	92	GLU	2.1
35	2d	156	GLU	2.1
1	1A	882	G	2.0
1	2A	614(A)	U	2.0
34	2c	78	GLY	2.1
56	1y	73	A	2.1
14	2S	32	LEU	2.0
7	2H	144	VAL	2.0
26	14	50	VAL	2.0
48	1q	95	TYR	2.0
35	1d	163	GLU	2.0
42	1k	117	ASN	2.0
23	21	22	GLY	2.0
35	2d	90	GLY	2.0
48	1q	52	LYS	2.0
27	25	58	LEU	2.0
32	2a	1219	U	2.0
39	2h	2	LEU	2.0
49	2r	66	LEU	2.0
55	1x	47	U	2.0
1	2A	2181	G	2.0
32	2a	1442	G	2.0
34	2c	79	ARG	2.0
11	2P	12	ALA	2.0
34	2c	180	ALA	2.0
26	24	69	LYS	2.0
33	2b	60	ASP	2.0
34	2c	197	GLY	2.0
36	2e	99	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	1r	68	LYS	2.0
33	1b	48	MET	2.0
8	2I	38	LEU	2.0
11	2P	45	LEU	2.0
34	2c	47	LEU	2.0
45	2n	44	LEU	2.0
49	1r	40	LEU	2.0
51	1t	91	LEU	2.0
1	2A	1026	U	2.0
21	1Z	165	VAL	2.0
34	2c	58	GLU	2.0
38	1g	78	ARG	2.0
39	1h	122	ARG	2.0
39	2h	61	VAL	2.0
40	2i	44	VAL	2.0
41	2j	39	PRO	2.0
44	2m	17	VAL	2.0
54	2w	45	U	2.0
46	1o	69	TYR	2.0
53	2v	13	A	2.0
1	1A	1076	C	2.0
1	2A	274	G	2.0
1	2A	2188	C	2.0
3	2D	153	ALA	2.0
21	2Z	152	ALA	2.0
37	1f	99	ALA	2.0
40	2i	87	GLN	2.0
11	2P	105	LEU	2.0
25	23	23	LEU	2.0
49	1r	79	LEU	2.0
21	2Z	100	VAL	2.0
21	2Z	167	PRO	2.0
25	23	16	PRO	2.0
51	2t	14	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	4SU	2y	8	20/21	0.61	0.30	95,104,112,126	0
56	PSU	1y	55	20/21	0.66	0.49	96,101,106,114	0
56	5MU	1y	54	21/22	0.73	0.50	89,99,104,118	0
56	G7M	2y	46	24/25	0.74	0.41	86,99,105,120	0
56	MIA	2y	37	22/30	0.77	0.41	83,97,109,123	0
56	PSU	2y	55	20/21	0.77	0.33	89,97,106,108	0
56	PSU	2y	32	20/21	0.78	0.42	86,98,107,115	0
54	G7M	2w	46	24/25	0.78	0.18	84,94,109,123	0
56	PSU	1y	39	20/21	0.79	0.30	83,94,107,109	0
56	5MU	2y	54	21/22	0.79	0.44	91,96,106,126	0
56	G7M	1y	46	24/25	0.79	0.36	91,99,104,117	0
56	PSU	2y	39	20/21	0.81	0.35	90,95,104,111	0
54	G7M	1w	46	24/25	0.81	0.15	78,88,100,121	0
56	PSU	1y	32	20/21	0.82	0.36	88,96,106,112	0
54	4SU	2w	8	20/21	0.85	0.14	90,94,105,108	0
54	PSU	2w	55	20/21	0.87	0.12	77,83,94,96	0
56	4SU	1y	8	20/21	0.87	0.25	93,97,105,116	0
54	4SU	1w	8	20/21	0.87	0.16	71,85,92,94	0
56	MIA	1y	37	22/30	0.87	0.24	86,93,100,113	0
32	2MG	2a	1207	24/25	0.90	0.16	76,83,86,90	0
55	4SU	2x	8	20/21	0.91	0.17	64,75,83,83	0
54	MIA	2w	37	25/30	0.91	0.18	68,76,85,103	0
55	PSU	2x	55	20/21	0.92	0.14	69,75,84,86	0
54	PSU	2w	32	20/21	0.92	0.17	76,84,91,92	0
32	G7M	2a	527	24/25	0.93	0.18	61,67,71,76	0
32	5MC	2a	967	21/22	0.93	0.14	62,66,76,82	0
54	5MU	2w	54	21/22	0.93	0.13	74,80,84,89	0
54	PSU	1w	55	20/21	0.93	0.14	61,73,81,81	0
43	0TD	1l	92	10/11	0.93	0.15	41,49,50,61	0
55	5MU	2x	54	21/22	0.93	0.16	72,79,84,96	0
32	PSU	2a	516	20/21	0.93	0.16	61,71,78,79	0
54	PSU	1w	32	20/21	0.94	0.13	60,65,74,77	0
54	PSU	2w	39	20/21	0.94	0.19	62,78,85,85	0
54	MIA	1w	37	29/30	0.94	0.22	43,53,70,87	0
55	PSU	1x	55	20/21	0.94	0.15	49,56,67,70	0
32	M2G	2a	966	25/26	0.94	0.18	55,65,76,81	0
55	5MC	2x	32	21/22	0.95	0.18	63,69,78,80	0
55	4SU	1x	8	20/21	0.95	0.19	52,60,67,77	0
32	5MC	2a	1400	21/22	0.95	0.19	63,71,76,80	0
32	4OC	2a	1402	22/23	0.95	0.17	55,60,66,71	0
43	0TD	2l	92	10/11	0.95	0.17	61,65,67,78	0
1	5MU	1A	1915	21/22	0.95	0.21	42,51,55,55	0
1	5MU	2A	1915	21/22	0.95	0.18	57,64,73,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	M2G	1a	966	25/26	0.96	0.15	46,50,57,61	0
32	5MC	2a	1407	21/22	0.96	0.19	50,57,61,65	0
32	MA6	2a	1518	24/25	0.96	0.19	49,60,69,69	0
32	MA6	2a	1519	24/25	0.96	0.18	55,61,67,71	0
55	31H	2x	76	32/33	0.96	0.22	36,46,54,63	0
1	PSU	2A	1911	20/21	0.96	0.18	52,62,67,71	0
55	31H	1x	76	32/33	0.96	0.20	22,26,37,41	10
54	5MU	1w	54	21/22	0.96	0.16	46,62,67,69	0
1	PSU	2A	1917	20/21	0.96	0.18	54,61,69,72	0
1	5MC	2A	1962	21/22	0.96	0.22	39,51,58,67	0
32	5MC	1a	1400	21/22	0.97	0.17	39,47,49,50	0
32	5MC	1a	1404	21/22	0.97	0.18	33,39,42,45	0
32	G7M	1a	527	24/25	0.97	0.15	36,42,50,50	0
32	PSU	1a	516	20/21	0.97	0.16	51,55,58,59	0
32	5MC	2a	1404	21/22	0.97	0.16	53,57,62,66	0
55	5MC	1x	32	21/22	0.97	0.17	51,53,59,70	0
54	F3N	2w	76	33/34	0.97	0.23	38,43,48,51	0
1	PSU	1A	1911	20/21	0.97	0.20	42,46,49,50	0
32	UR3	2a	1498	21/22	0.97	0.21	52,58,61,65	0
55	5MU	1x	54	21/22	0.97	0.15	55,61,65,70	0
32	5MC	1a	967	21/22	0.97	0.14	45,51,59,61	0
1	PSU	1A	1917	20/21	0.97	0.17	39,45,50,52	0
32	2MG	1a	1207	24/25	0.97	0.14	61,67,71,71	0
1	OMC	2A	1920	21/22	0.97	0.18	53,61,63,65	0
1	5MC	2A	1942	21/22	0.97	0.20	43,53,57,62	0
54	PSU	1w	39	20/21	0.97	0.16	53,61,67,76	0
1	2MU	2A	2552	21/23	0.97	0.19	35,41,45,55	0
1	PSU	2A	2605	20/21	0.97	0.19	30,38,42,44	0
32	4OC	1a	1402	22/23	0.98	0.17	38,45,48,49	0
1	OMC	1A	1920	21/22	0.98	0.20	35,43,45,52	0
32	5MC	1a	1407	21/22	0.98	0.18	30,39,42,43	0
1	5MU	1A	1939	21/22	0.98	0.19	21,28,30,32	0
1	5MU	2A	1939	21/22	0.98	0.20	32,38,42,45	0
1	5MC	1A	1942	21/22	0.98	0.21	34,39,43,51	0
32	UR3	1a	1498	21/22	0.98	0.17	36,41,45,46	0
1	5MC	1A	1962	21/22	0.98	0.20	24,32,37,42	0
54	F3N	1w	76	33/34	0.98	0.22	22,25,30,32	0
1	OMG	2A	2251	24/25	0.98	0.20	35,43,45,51	0
1	8AH	2A	2503	24/25	0.98	0.22	32,38,44,45	0
1	2MU	1A	2552	21/23	0.98	0.21	23,27,34,36	0
32	MA6	1a	1518	24/25	0.98	0.21	31,39,45,46	0
1	PSU	1A	2605	20/21	0.98	0.20	23,26,31,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MA6	1a	1519	24/25	0.98	0.20	35,42,45,47	0
1	8AH	1A	2503	24/25	0.99	0.19	15,21,26,27	0
1	OMG	1A	2251	24/25	0.99	0.18	22,25,28,30	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3735	1/1	0.34	0.10	79,79,79,79	0
57	MG	1a	1792	1/1	0.44	0.21	74,74,74,74	0
57	MG	2A	3516	1/1	0.45	0.20	40,40,40,40	0
57	MG	2a	1808	1/1	0.45	0.11	91,91,91,91	0
57	MG	1a	1796	1/1	0.46	0.27	67,67,67,67	0
57	MG	2A	3271	1/1	0.47	0.26	73,73,73,73	0
57	MG	1A	3395	1/1	0.47	0.28	69,69,69,69	0
57	MG	1a	1704	1/1	0.48	0.38	72,72,72,72	0
57	MG	1A	3979	1/1	0.49	0.16	70,70,70,70	0
57	MG	2A	3216	1/1	0.49	0.25	73,73,73,73	0
57	MG	2A	3001	1/1	0.50	0.33	59,59,59,59	0
57	MG	1a	1673	1/1	0.51	0.20	77,77,77,77	0
57	MG	2A	3077	1/1	0.53	0.49	60,60,60,60	0
57	MG	2v	102	1/1	0.53	0.41	80,80,80,80	0
57	MG	1O	201	1/1	0.55	0.33	72,72,72,72	0
57	MG	2A	3143	1/1	0.55	0.26	72,72,72,72	0
57	MG	1A	4076	1/1	0.56	0.16	70,70,70,70	0
57	MG	2A	3282	1/1	0.56	0.16	76,76,76,76	0
57	MG	1A	3375	1/1	0.56	0.21	74,74,74,74	0
57	MG	2A	3547	1/1	0.58	0.30	72,72,72,72	0
57	MG	1A	3970	1/1	0.58	0.26	47,47,47,47	0
57	MG	2a	1650	1/1	0.58	0.16	66,66,66,66	0
57	MG	2A	3159	1/1	0.58	0.17	82,82,82,82	0
57	MG	1A	3491	1/1	0.58	0.35	64,64,64,64	0
57	MG	2a	1628	1/1	0.59	0.17	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3235	1/1	0.60	0.32	68,68,68,68	0
57	MG	2a	1696	1/1	0.60	0.19	74,74,74,74	0
57	MG	2y	102	1/1	0.60	0.23	75,75,75,75	0
57	MG	1A	3431	1/1	0.61	0.18	66,66,66,66	0
57	MG	2A	3058	1/1	0.62	0.23	68,68,68,68	0
57	MG	1A	4042	1/1	0.62	0.17	70,70,70,70	0
57	MG	2a	1642	1/1	0.62	0.33	73,73,73,73	0
57	MG	2A	3711	1/1	0.62	0.23	47,47,47,47	0
57	MG	2A	3482	1/1	0.63	0.14	69,69,69,69	0
57	MG	1A	3732	1/1	0.64	0.25	70,70,70,70	0
57	MG	2a	1781	1/1	0.64	0.15	81,81,81,81	0
57	MG	1A	3373	1/1	0.64	0.27	69,69,69,69	0
57	MG	1x	108	1/1	0.64	0.27	67,67,67,67	0
57	MG	1a	1778	1/1	0.64	0.17	78,78,78,78	0
57	MG	1A	4029	1/1	0.65	0.27	27,27,27,27	0
57	MG	1A	3766	1/1	0.65	0.30	51,51,51,51	0
57	MG	2a	1768	1/1	0.65	0.17	69,69,69,69	0
57	MG	1A	3670	1/1	0.65	0.28	62,62,62,62	0
57	MG	2A	3065	1/1	0.65	0.25	64,64,64,64	0
57	MG	1A	3747	1/1	0.65	0.17	82,82,82,82	0
57	MG	1V	205	1/1	0.65	0.39	63,63,63,63	0
57	MG	2A	3019	1/1	0.66	0.12	79,79,79,79	0
57	MG	2A	3690	1/1	0.66	0.15	58,58,58,58	0
57	MG	2A	3347	1/1	0.66	0.19	70,70,70,70	0
57	MG	1A	3794	1/1	0.66	0.18	59,59,59,59	0
57	MG	2B	202	1/1	0.66	0.35	70,70,70,70	0
57	MG	2T	201	1/1	0.66	0.34	70,70,70,70	0
57	MG	2q	202	1/1	0.66	0.09	82,82,82,82	0
57	MG	2a	1619	1/1	0.66	0.26	71,71,71,71	0
57	MG	1A	3930	1/1	0.66	0.08	62,62,62,62	0
57	MG	2A	3775	1/1	0.67	0.36	73,73,73,73	0
57	MG	1A	3432	1/1	0.67	0.16	64,64,64,64	0
57	MG	2A	3573	1/1	0.67	0.28	68,68,68,68	0
57	MG	2A	3359	1/1	0.67	0.76	73,73,73,73	0
57	MG	1A	3888	1/1	0.67	0.08	70,70,70,70	0
57	MG	1A	3641	1/1	0.67	0.14	43,43,43,43	0
57	MG	2A	3762	1/1	0.67	0.23	53,53,53,53	0
57	MG	2A	3176	1/1	0.68	0.33	63,63,63,63	0
57	MG	2V	202	1/1	0.68	0.27	67,67,67,67	0
57	MG	2W	201	1/1	0.68	0.14	67,67,67,67	0
57	MG	1A	4078	1/1	0.68	0.28	62,62,62,62	0
57	MG	2A	3231	1/1	0.68	0.15	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3804	1/1	0.68	0.24	69,69,69,69	0
57	MG	2A	3639	1/1	0.68	0.19	72,72,72,72	0
57	MG	1x	111	1/1	0.68	0.31	70,70,70,70	0
57	MG	2A	3119	1/1	0.68	0.15	69,69,69,69	0
57	MG	2A	3298	1/1	0.68	0.14	76,76,76,76	0
57	MG	1A	3235	1/1	0.68	0.21	71,71,71,71	0
57	MG	1a	1604	1/1	0.68	0.12	58,58,58,58	0
57	MG	2A	3415	1/1	0.68	0.20	71,71,71,71	0
57	MG	2B	204	1/1	0.68	0.11	75,75,75,75	0
57	MG	2A	3156	1/1	0.69	0.19	76,76,76,76	0
57	MG	1A	3876	1/1	0.69	0.14	61,61,61,61	0
57	MG	1a	1647	1/1	0.69	0.21	67,67,67,67	0
57	MG	2A	3606	1/1	0.69	0.14	66,66,66,66	0
57	MG	2A	3181	1/1	0.69	0.26	65,65,65,65	0
57	MG	2A	3675	1/1	0.69	0.40	69,69,69,69	0
57	MG	1U	210	1/1	0.69	0.43	55,55,55,55	0
57	MG	1A	3990	1/1	0.69	0.10	54,54,54,54	0
57	MG	2A	3155	1/1	0.69	0.33	67,67,67,67	0
57	MG	1a	1694	1/1	0.70	0.20	63,63,63,63	0
57	MG	2A	3173	1/1	0.70	0.29	70,70,70,70	0
57	MG	2A	3382	1/1	0.70	0.32	72,72,72,72	0
57	MG	2a	1710	1/1	0.70	0.15	79,79,79,79	0
57	MG	2a	1716	1/1	0.70	0.21	63,63,63,63	0
57	MG	2A	3400	1/1	0.70	0.23	73,73,73,73	0
57	MG	1A	3477	1/1	0.70	0.16	74,74,74,74	0
57	MG	2A	3450	1/1	0.70	0.22	49,49,49,49	0
57	MG	2A	3703	1/1	0.70	0.12	63,63,63,63	0
57	MG	1A	3793	1/1	0.70	0.17	57,57,57,57	0
57	MG	1A	4095	1/1	0.70	0.16	47,47,47,47	0
57	MG	2A	3260	1/1	0.71	0.18	67,67,67,67	0
57	MG	1a	1615	1/1	0.71	0.14	56,56,56,56	0
57	MG	1A	3428	1/1	0.71	0.18	57,57,57,57	0
57	MG	1a	1666	1/1	0.71	0.21	72,72,72,72	0
57	MG	2A	3043	1/1	0.71	0.32	70,70,70,70	0
57	MG	2A	3784	1/1	0.71	0.21	70,70,70,70	0
57	MG	2A	3584	1/1	0.71	0.17	69,69,69,69	0
57	MG	1A	3898	1/1	0.71	0.16	35,35,35,35	0
57	MG	2B	214	1/1	0.71	0.24	66,66,66,66	0
57	MG	2P	202	1/1	0.71	0.31	66,66,66,66	0
57	MG	1A	3885	1/1	0.71	0.14	43,43,43,43	0
57	MG	2A	3236	1/1	0.71	0.27	63,63,63,63	0
57	MG	2A	3257	1/1	0.71	0.24	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3308	1/1	0.72	0.13	50,50,50,50	0
57	MG	2a	1633	1/1	0.72	0.13	73,73,73,73	0
57	MG	1A	3561	1/1	0.72	0.22	39,39,39,39	0
57	MG	2A	3548	1/1	0.72	0.47	65,65,65,65	0
57	MG	2A	3100	1/1	0.72	0.14	70,70,70,70	0
57	MG	1A	4023	1/1	0.72	0.20	50,50,50,50	0
57	MG	1A	3796	1/1	0.72	0.18	49,49,49,49	0
57	MG	2A	3614	1/1	0.72	0.22	63,63,63,63	0
57	MG	1A	3620	1/1	0.72	0.13	65,65,65,65	0
57	MG	14	101	1/1	0.72	0.13	80,80,80,80	0
57	MG	1a	1755	1/1	0.72	0.13	64,64,64,64	0
57	MG	1A	3427	1/1	0.72	0.52	55,55,55,55	0
57	MG	2A	3509	1/1	0.72	0.13	68,68,68,68	0
57	MG	2A	3086	1/1	0.73	0.26	44,44,44,44	0
57	MG	2A	3395	1/1	0.73	0.48	58,58,58,58	0
57	MG	2A	3580	1/1	0.73	0.21	55,55,55,55	0
57	MG	2A	3399	1/1	0.73	0.20	83,83,83,83	0
57	MG	1A	3795	1/1	0.73	0.28	60,60,60,60	0
57	MG	1A	3909	1/1	0.73	0.50	85,85,85,85	0
57	MG	1A	3126	1/1	0.73	0.30	48,48,48,48	0
57	MG	10	109	1/1	0.73	0.22	69,69,69,69	0
57	MG	2a	1779	1/1	0.73	0.16	71,71,71,71	0
57	MG	1A	3158	1/1	0.73	0.18	62,62,62,62	0
57	MG	1F	315	1/1	0.73	0.49	58,58,58,58	0
57	MG	2A	3360	1/1	0.73	0.26	67,67,67,67	0
57	MG	2a	1604	1/1	0.73	0.10	73,73,73,73	0
57	MG	2A	3717	1/1	0.73	0.12	64,64,64,64	0
57	MG	1A	3371	1/1	0.74	0.19	54,54,54,54	0
57	MG	2A	3091	1/1	0.74	0.22	70,70,70,70	0
57	MG	1A	3806	1/1	0.74	0.17	58,58,58,58	0
57	MG	1A	3829	1/1	0.74	0.10	37,37,37,37	0
57	MG	1A	3258	1/1	0.74	0.21	55,55,55,55	0
57	MG	1a	1802	1/1	0.74	0.12	84,84,84,84	0
57	MG	1A	3445	1/1	0.74	0.15	58,58,58,58	0
57	MG	1A	3476	1/1	0.74	0.21	49,49,49,49	0
57	MG	1A	3139	1/1	0.74	0.22	47,47,47,47	0
57	MG	2a	1745	1/1	0.74	0.09	75,75,75,75	0
57	MG	2B	208	1/1	0.74	0.19	56,56,56,56	0
57	MG	1A	3904	1/1	0.74	0.08	74,74,74,74	0
57	MG	1A	3689	1/1	0.74	0.12	56,56,56,56	0
57	MG	1B	227	1/1	0.74	0.15	81,81,81,81	0
57	MG	2T	202	1/1	0.74	0.17	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
57	MG	1E	307	1/1	0.74	0.13	67,67,67,67	0
57	MG	1A	3724	1/1	0.74	0.19	45,45,45,45	0
60	ZN	24	501	1/1	0.74	0.10	126,126,126,126	0
57	MG	2A	3035	1/1	0.75	0.24	69,69,69,69	0
57	MG	1A	3327	1/1	0.75	0.49	59,59,59,59	0
57	MG	2a	1691	1/1	0.75	0.29	76,76,76,76	0
57	MG	2A	3247	1/1	0.75	0.25	65,65,65,65	0
57	MG	2A	3248	1/1	0.75	0.25	57,57,57,57	0
57	MG	1a	1654	1/1	0.75	0.10	61,61,61,61	0
57	MG	1B	214	1/1	0.75	0.15	59,59,59,59	0
57	MG	1A	3297	1/1	0.75	0.24	58,58,58,58	0
57	MG	1A	3583	1/1	0.75	0.17	58,58,58,58	0
57	MG	1A	3309	1/1	0.75	0.13	58,58,58,58	0
57	MG	2a	1795	1/1	0.75	0.48	72,72,72,72	0
57	MG	2a	1798	1/1	0.75	0.35	73,73,73,73	0
57	MG	2A	3343	1/1	0.75	0.15	64,64,64,64	0
57	MG	2a	1812	1/1	0.75	0.12	65,65,65,65	0
57	MG	2A	3203	1/1	0.75	0.42	54,54,54,54	0
57	MG	1A	4011	1/1	0.75	0.15	51,51,51,51	0
57	MG	2x	105	1/1	0.75	0.21	65,65,65,65	0
57	MG	1a	1777	1/1	0.75	0.09	85,85,85,85	0
57	MG	2a	1637	1/1	0.75	0.14	64,64,64,64	0
57	MG	1b	301	1/1	0.76	0.09	68,68,68,68	0
57	MG	1A	3454	1/1	0.76	0.23	36,36,36,36	0
57	MG	1D	311	1/1	0.76	0.25	55,55,55,55	0
57	MG	2a	1674	1/1	0.76	0.26	59,59,59,59	0
57	MG	2A	3151	1/1	0.76	0.27	45,45,45,45	0
57	MG	1a	1747	1/1	0.76	0.15	59,59,59,59	0
57	MG	1A	3467	1/1	0.76	0.49	60,60,60,60	0
57	MG	2A	3518	1/1	0.76	0.15	51,51,51,51	0
57	MG	2a	1722	1/1	0.76	0.08	62,62,62,62	0
57	MG	1a	1764	1/1	0.76	0.18	48,48,48,48	0
57	MG	1A	3374	1/1	0.76	0.34	61,61,61,61	0
57	MG	1A	3277	1/1	0.76	0.15	64,64,64,64	0
57	MG	2A	3177	1/1	0.76	0.75	80,80,80,80	0
57	MG	2A	3344	1/1	0.76	0.20	63,63,63,63	0
57	MG	1T	201	1/1	0.76	0.21	65,65,65,65	0
57	MG	2A	3193	1/1	0.76	0.18	55,55,55,55	0
57	MG	1B	213	1/1	0.76	0.23	73,73,73,73	0
57	MG	2A	3645	1/1	0.76	0.30	48,48,48,48	0
57	MG	2a	1610	1/1	0.76	0.36	78,78,78,78	0
57	MG	2A	3215	1/1	0.76	0.25	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3388	1/1	0.76	0.44	70,70,70,70	0
57	MG	1a	1809	1/1	0.76	0.17	69,69,69,69	0
57	MG	2A	3167	1/1	0.77	0.27	57,57,57,57	0
57	MG	1A	3621	1/1	0.77	0.16	38,38,38,38	0
57	MG	1A	3694	1/1	0.77	0.14	57,57,57,57	0
57	MG	2A	3783	1/1	0.77	0.30	75,75,75,75	0
57	MG	2A	3562	1/1	0.77	0.16	68,68,68,68	0
57	MG	1A	3607	1/1	0.77	0.16	68,68,68,68	0
57	MG	2A	3576	1/1	0.77	0.28	42,42,42,42	0
57	MG	2A	3251	1/1	0.77	0.25	62,62,62,62	0
57	MG	1a	1662	1/1	0.77	0.27	71,71,71,71	0
57	MG	2D	303	1/1	0.77	0.27	61,61,61,61	0
57	MG	2D	306	1/1	0.77	0.77	54,54,54,54	0
57	MG	2A	3047	1/1	0.77	0.27	69,69,69,69	0
57	MG	1A	4049	1/1	0.77	0.18	44,44,44,44	0
57	MG	2A	3636	1/1	0.77	0.24	67,67,67,67	0
57	MG	2A	3412	1/1	0.77	0.14	57,57,57,57	0
57	MG	1a	1667	1/1	0.77	0.14	50,50,50,50	0
57	MG	20	102	1/1	0.77	0.28	73,73,73,73	0
57	MG	2a	1819	1/1	0.77	0.09	69,69,69,69	0
57	MG	2A	3290	1/1	0.77	0.16	64,64,64,64	0
57	MG	2A	3074	1/1	0.77	0.17	63,63,63,63	0
57	MG	2A	3483	1/1	0.77	0.16	84,84,84,84	0
57	MG	2A	3299	1/1	0.77	0.21	75,75,75,75	0
57	MG	1A	3378	1/1	0.77	0.30	62,62,62,62	0
57	MG	1T	202	1/1	0.78	0.31	54,54,54,54	0
57	MG	2A	3346	1/1	0.78	0.36	68,68,68,68	0
57	MG	2A	3092	1/1	0.78	0.29	65,65,65,65	0
57	MG	2a	1652	1/1	0.78	0.10	73,73,73,73	0
57	MG	2A	3792	1/1	0.78	0.06	77,77,77,77	0
57	MG	2A	3793	1/1	0.78	0.07	64,64,64,64	0
57	MG	1A	3256	1/1	0.78	0.14	56,56,56,56	0
57	MG	2a	1707	1/1	0.78	0.10	76,76,76,76	0
57	MG	1A	3988	1/1	0.78	0.17	51,51,51,51	0
57	MG	1A	4045	1/1	0.78	0.10	44,44,44,44	0
57	MG	2A	3238	1/1	0.78	0.29	60,60,60,60	0
57	MG	2a	1726	1/1	0.78	0.13	66,66,66,66	0
57	MG	1A	3333	1/1	0.78	0.16	60,60,60,60	0
57	MG	18	107	1/1	0.78	0.43	70,70,70,70	0
57	MG	1A	4066	1/1	0.78	0.14	52,52,52,52	0
57	MG	1A	3677	1/1	0.78	0.18	42,42,42,42	0
57	MG	2A	3662	1/1	0.78	0.42	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
57	MG	1a	1768	1/1	0.78	0.15	53,53,53,53	0
57	MG	2A	3686	1/1	0.78	0.08	55,55,55,55	0
57	MG	1a	1772	1/1	0.78	0.09	77,77,77,77	0
57	MG	1I	201	1/1	0.78	0.14	65,65,65,65	0
57	MG	2f	202	1/1	0.78	0.23	76,76,76,76	0
57	MG	1A	3025	1/1	0.78	0.18	55,55,55,55	0
57	MG	1a	1779	1/1	0.78	0.09	75,75,75,75	0
57	MG	2a	1620	1/1	0.78	0.22	76,76,76,76	0
57	MG	1A	4028	1/1	0.78	0.13	62,62,62,62	0
57	MG	1a	1663	1/1	0.78	0.20	68,68,68,68	0
57	MG	1a	1743	1/1	0.79	0.08	81,81,81,81	0
57	MG	1A	4075	1/1	0.79	0.15	62,62,62,62	0
57	MG	2a	1632	1/1	0.79	0.37	74,74,74,74	0
57	MG	1A	3276	1/1	0.79	0.22	45,45,45,45	0
57	MG	1A	3975	1/1	0.79	0.20	61,61,61,61	0
57	MG	2a	1638	1/1	0.79	0.14	82,82,82,82	0
57	MG	2A	3078	1/1	0.79	0.14	58,58,58,58	0
57	MG	2A	3430	1/1	0.79	0.13	39,39,39,39	0
57	MG	2A	3754	1/1	0.79	0.17	77,77,77,77	0
57	MG	1A	3840	1/1	0.79	0.20	48,48,48,48	0
57	MG	2a	1686	1/1	0.79	0.19	72,72,72,72	0
57	MG	2A	3478	1/1	0.79	0.25	50,50,50,50	0
57	MG	1A	3849	1/1	0.79	0.12	35,35,35,35	0
57	MG	1a	1612	1/1	0.79	0.10	66,66,66,66	0
57	MG	1A	3643	1/1	0.79	0.23	72,72,72,72	0
57	MG	2A	3253	1/1	0.79	0.25	72,72,72,72	0
57	MG	1a	1639	1/1	0.79	0.31	67,67,67,67	0
57	MG	2A	3132	1/1	0.79	0.17	64,64,64,64	0
57	MG	2A	3262	1/1	0.79	0.15	71,71,71,71	0
57	MG	2a	1749	1/1	0.79	0.06	78,78,78,78	0
57	MG	2a	1767	1/1	0.79	0.36	69,69,69,69	0
57	MG	2B	209	1/1	0.79	0.19	69,69,69,69	0
57	MG	2a	1777	1/1	0.79	0.12	75,75,75,75	0
57	MG	1A	3526	1/1	0.79	0.31	56,56,56,56	0
57	MG	1A	3243	1/1	0.79	0.36	41,41,41,41	0
57	MG	1A	3246	1/1	0.79	0.29	28,28,28,28	0
57	MG	1A	3305	1/1	0.79	0.18	63,63,63,63	0
57	MG	1A	3908	1/1	0.79	0.08	53,53,53,53	0
57	MG	1A	3222	1/1	0.79	0.25	63,63,63,63	0
57	MG	1A	3239	1/1	0.79	0.20	64,64,64,64	0
57	MG	1A	4063	1/1	0.79	0.19	71,71,71,71	0
57	MG	1a	1697	1/1	0.79	0.15	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
57	MG	1A	3943	1/1	0.79	0.23	33,33,33,33	0
57	MG	2w	106	1/1	0.79	0.15	75,75,75,75	0
57	MG	2a	1606	1/1	0.79	0.11	74,74,74,74	0
57	MG	1a	1711	1/1	0.79	0.21	55,55,55,55	0
57	MG	1a	1727	1/1	0.79	0.14	64,64,64,64	0
57	MG	1Y	201	1/1	0.80	0.16	69,69,69,69	0
57	MG	1A	3204	1/1	0.80	0.14	53,53,53,53	0
57	MG	2A	3264	1/1	0.80	0.31	69,69,69,69	0
57	MG	1A	3933	1/1	0.80	0.12	66,66,66,66	0
57	MG	2A	3057	1/1	0.80	0.14	65,65,65,65	0
57	MG	2a	1693	1/1	0.80	0.24	65,65,65,65	0
57	MG	1A	3821	1/1	0.80	0.17	56,56,56,56	0
57	MG	1A	3962	1/1	0.80	0.22	58,58,58,58	0
57	MG	1a	1681	1/1	0.80	0.20	57,57,57,57	0
57	MG	2A	3185	1/1	0.80	0.18	63,63,63,63	0
57	MG	1a	1688	1/1	0.80	0.23	51,51,51,51	0
57	MG	2A	3199	1/1	0.80	0.41	55,55,55,55	0
57	MG	2A	3590	1/1	0.80	0.23	50,50,50,50	0
57	MG	1a	1785	1/1	0.80	0.21	59,59,59,59	0
57	MG	1A	3485	1/1	0.80	0.17	65,65,65,65	0
57	MG	1A	3434	1/1	0.80	0.40	60,60,60,60	0
57	MG	2A	3369	1/1	0.80	0.20	70,70,70,70	0
57	MG	1a	1622	1/1	0.80	0.19	65,65,65,65	0
57	MG	1a	1626	1/1	0.80	0.23	59,59,59,59	0
57	MG	2a	1784	1/1	0.80	0.15	65,65,65,65	0
57	MG	2A	3671	1/1	0.80	0.16	73,73,73,73	0
57	MG	2A	3105	1/1	0.80	0.35	55,55,55,55	0
57	MG	2A	3106	1/1	0.80	0.26	59,59,59,59	0
57	MG	2a	1611	1/1	0.80	0.13	75,75,75,75	0
57	MG	2a	1816	1/1	0.80	0.14	81,81,81,81	0
57	MG	2A	3244	1/1	0.80	0.23	63,63,63,63	0
57	MG	1a	1720	1/1	0.80	0.23	44,44,44,44	0
57	MG	1A	4044	1/1	0.80	0.21	59,59,59,59	0
57	MG	1A	3514	1/1	0.80	0.45	48,48,48,48	0
57	MG	2A	3731	1/1	0.80	0.11	59,59,59,59	0
57	MG	2x	102	1/1	0.80	0.34	82,82,82,82	0
57	MG	2A	3470	1/1	0.80	0.15	39,39,39,39	0
57	MG	2x	107	1/1	0.80	0.17	64,64,64,64	0
57	MG	1A	3016	1/1	0.80	0.53	66,66,66,66	0
57	MG	1a	1752	1/1	0.80	0.11	63,63,63,63	0
57	MG	2A	3753	1/1	0.81	0.16	66,66,66,66	0
57	MG	1A	3739	1/1	0.81	0.15	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3627	1/1	0.81	0.11	43,43,43,43	0
57	MG	2A	3774	1/1	0.81	0.40	68,68,68,68	0
57	MG	1A	3866	1/1	0.81	0.18	44,44,44,44	0
57	MG	1A	3413	1/1	0.81	0.38	67,67,67,67	0
57	MG	2A	3498	1/1	0.81	0.11	79,79,79,79	0
57	MG	2A	3785	1/1	0.81	0.19	57,57,57,57	0
57	MG	1A	3536	1/1	0.81	0.20	63,63,63,63	0
57	MG	1A	3314	1/1	0.81	0.28	54,54,54,54	0
57	MG	1A	3337	1/1	0.81	0.41	36,36,36,36	0
57	MG	2A	3071	1/1	0.81	0.28	60,60,60,60	0
57	MG	1A	3680	1/1	0.81	0.22	56,56,56,56	0
57	MG	2A	3183	1/1	0.81	0.21	56,56,56,56	0
57	MG	2a	1761	1/1	0.81	0.12	73,73,73,73	0
57	MG	1B	208	1/1	0.81	0.11	65,65,65,65	0
57	MG	2A	3309	1/1	0.81	0.16	66,66,66,66	0
57	MG	2A	3339	1/1	0.81	0.26	58,58,58,58	0
57	MG	2A	3186	1/1	0.81	0.21	57,57,57,57	0
57	MG	2A	3190	1/1	0.81	0.37	60,60,60,60	0
57	MG	1l	103	1/1	0.81	0.11	42,42,42,42	0
57	MG	1B	210	1/1	0.81	0.25	51,51,51,51	0
57	MG	2A	3354	1/1	0.81	0.33	65,65,65,65	0
57	MG	1A	3600	1/1	0.81	0.10	66,66,66,66	0
57	MG	2a	1811	1/1	0.81	0.08	70,70,70,70	0
57	MG	1A	3282	1/1	0.81	0.15	46,46,46,46	0
57	MG	1A	3915	1/1	0.81	0.23	62,62,62,62	0
57	MG	1B	229	1/1	0.81	0.11	75,75,75,75	0
57	MG	2A	3392	1/1	0.81	0.09	47,47,47,47	0
57	MG	2A	3232	1/1	0.81	0.22	66,66,66,66	0
57	MG	1x	106	1/1	0.81	0.23	61,61,61,61	0
57	MG	2A	3699	1/1	0.81	0.16	59,59,59,59	0
57	MG	1A	3456	1/1	0.81	0.14	58,58,58,58	0
57	MG	2A	3121	1/1	0.81	0.39	42,42,42,42	0
57	MG	1A	3459	1/1	0.81	0.15	52,52,52,52	0
57	MG	2A	3137	1/1	0.81	0.15	58,58,58,58	0
57	MG	1a	1745	1/1	0.81	0.17	74,74,74,74	0
57	MG	1A	4064	1/1	0.82	0.19	64,64,64,64	0
57	MG	1A	3446	1/1	0.82	0.19	65,65,65,65	0
57	MG	1A	3414	1/1	0.82	0.14	51,51,51,51	0
57	MG	2A	3039	1/1	0.82	0.13	56,56,56,56	0
57	MG	2a	1643	1/1	0.82	0.18	73,73,73,73	0
57	MG	1A	3704	1/1	0.82	0.17	61,61,61,61	0
57	MG	1a	1762	1/1	0.82	0.12	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3903	1/1	0.82	0.14	61,61,61,61	0
57	MG	1A	3287	1/1	0.82	0.19	30,30,30,30	0
57	MG	1B	206	1/1	0.82	0.14	47,47,47,47	0
57	MG	2A	3472	1/1	0.82	0.21	47,47,47,47	0
57	MG	2a	1695	1/1	0.82	0.26	67,67,67,67	0
57	MG	2A	3769	1/1	0.82	0.09	71,71,71,71	0
57	MG	2a	1700	1/1	0.82	0.12	82,82,82,82	0
57	MG	1A	4012	1/1	0.82	0.14	67,67,67,67	0
57	MG	2a	1708	1/1	0.82	0.15	62,62,62,62	0
57	MG	1A	3808	1/1	0.82	0.20	22,22,22,22	0
57	MG	2A	3266	1/1	0.82	0.18	69,69,69,69	0
57	MG	2a	1717	1/1	0.82	0.12	75,75,75,75	0
57	MG	2a	1720	1/1	0.82	0.17	68,68,68,68	0
57	MG	2A	3487	1/1	0.82	0.21	63,63,63,63	0
57	MG	1a	1682	1/1	0.82	0.35	62,62,62,62	0
57	MG	2A	3788	1/1	0.82	0.23	64,64,64,64	0
57	MG	2a	1748	1/1	0.82	0.17	78,78,78,78	0
57	MG	1a	1687	1/1	0.82	0.29	55,55,55,55	0
57	MG	2A	3283	1/1	0.82	0.15	83,83,83,83	0
57	MG	2A	3797	1/1	0.82	0.15	69,69,69,69	0
57	MG	2A	3517	1/1	0.82	0.20	51,51,51,51	0
57	MG	2a	1773	1/1	0.82	0.09	68,68,68,68	0
57	MG	2A	3289	1/1	0.82	0.18	62,62,62,62	0
57	MG	1A	3381	1/1	0.82	0.17	57,57,57,57	0
57	MG	2A	3294	1/1	0.82	0.23	69,69,69,69	0
57	MG	1A	3196	1/1	0.82	0.18	53,53,53,53	0
57	MG	2a	1793	1/1	0.82	0.27	64,64,64,64	0
57	MG	1A	3663	1/1	0.82	0.18	28,28,28,28	0
57	MG	2A	3196	1/1	0.82	0.24	74,74,74,74	0
57	MG	2A	3330	1/1	0.82	0.27	56,56,56,56	0
57	MG	1a	1806	1/1	0.82	0.12	60,60,60,60	0
57	MG	1A	3841	1/1	0.82	0.24	24,24,24,24	0
57	MG	2A	3605	1/1	0.82	0.27	67,67,67,67	0
57	MG	2A	3211	1/1	0.82	0.25	49,49,49,49	0
57	MG	2A	3214	1/1	0.82	0.09	77,77,77,77	0
57	MG	2A	3634	1/1	0.82	0.12	45,45,45,45	0
57	MG	1A	3394	1/1	0.82	0.18	69,69,69,69	0
57	MG	2A	3353	1/1	0.82	0.36	81,81,81,81	0
57	MG	1A	3335	1/1	0.82	0.23	56,56,56,56	0
57	MG	2x	104	1/1	0.82	0.60	72,72,72,72	0
57	MG	2A	3223	1/1	0.82	0.27	63,63,63,63	0
57	MG	1a	1623	1/1	0.82	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
57	MG	1A	3315	1/1	0.82	0.18	61,61,61,61	0
57	MG	2A	3134	1/1	0.82	0.27	63,63,63,63	0
57	MG	2A	3055	1/1	0.83	0.23	57,57,57,57	0
57	MG	1A	3924	1/1	0.83	0.58	55,55,55,55	0
57	MG	1F	311	1/1	0.83	0.23	46,46,46,46	0
57	MG	1A	3827	1/1	0.83	0.17	37,37,37,37	0
57	MG	1G	203	1/1	0.83	0.11	68,68,68,68	0
57	MG	1A	3271	1/1	0.83	0.65	40,40,40,40	0
57	MG	1A	3648	1/1	0.83	0.17	20,20,20,20	0
57	MG	2A	3195	1/1	0.83	0.21	56,56,56,56	0
57	MG	1A	3205	1/1	0.83	0.11	48,48,48,48	0
57	MG	1a	1672	1/1	0.83	0.20	70,70,70,70	0
57	MG	1A	3783	1/1	0.83	0.14	49,49,49,49	0
57	MG	2A	3321	1/1	0.83	0.16	64,64,64,64	0
57	MG	2A	3568	1/1	0.83	0.28	60,60,60,60	0
57	MG	1A	3859	1/1	0.83	0.22	50,50,50,50	0
57	MG	2A	3574	1/1	0.83	0.26	71,71,71,71	0
57	MG	2A	3095	1/1	0.83	0.22	75,75,75,75	0
57	MG	1A	3785	1/1	0.83	0.20	55,55,55,55	0
57	MG	2B	213	1/1	0.83	0.17	65,65,65,65	0
57	MG	1A	3786	1/1	0.83	0.23	47,47,47,47	0
57	MG	2A	3217	1/1	0.83	0.14	70,70,70,70	0
57	MG	2a	1766	1/1	0.83	0.22	61,61,61,61	0
57	MG	2A	3593	1/1	0.83	0.35	63,63,63,63	0
57	MG	2F	308	1/1	0.83	0.29	69,69,69,69	0
57	MG	2a	1770	1/1	0.83	0.28	70,70,70,70	0
57	MG	1Z	301	1/1	0.83	0.14	67,67,67,67	0
57	MG	2A	3224	1/1	0.83	0.17	65,65,65,65	0
57	MG	2A	3610	1/1	0.83	0.15	39,39,39,39	0
57	MG	2A	3225	1/1	0.83	0.21	75,75,75,75	0
57	MG	2A	3230	1/1	0.83	0.15	81,81,81,81	0
57	MG	2a	1788	1/1	0.83	0.16	83,83,83,83	0
57	MG	1B	203	1/1	0.83	0.36	66,66,66,66	0
57	MG	2I	101	1/1	0.83	0.16	54,54,54,54	0
57	MG	1A	3185	1/1	0.83	0.14	57,57,57,57	0
57	MG	1w	104	1/1	0.83	0.37	81,81,81,81	0
57	MG	1A	3247	1/1	0.83	0.26	42,42,42,42	0
57	MG	1A	3096	1/1	0.83	0.12	65,65,65,65	0
57	MG	2A	3673	1/1	0.83	0.11	49,49,49,49	0
57	MG	1a	1717	1/1	0.83	0.14	67,67,67,67	0
57	MG	1B	211	1/1	0.83	0.27	64,64,64,64	0
57	MG	2I	201	1/1	0.83	0.20	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3061	1/1	0.83	0.19	59,59,59,59	0
57	MG	2A	3025	1/1	0.83	0.14	63,63,63,63	0
57	MG	2a	1636	1/1	0.83	0.17	69,69,69,69	0
57	MG	1A	3259	1/1	0.83	0.16	40,40,40,40	0
57	MG	1A	3306	1/1	0.83	0.22	58,58,58,58	0
57	MG	2A	3461	1/1	0.83	0.13	57,57,57,57	0
57	MG	1A	3507	1/1	0.83	0.86	53,53,53,53	0
57	MG	2a	1646	1/1	0.83	0.48	61,61,61,61	0
57	MG	1A	3367	1/1	0.83	0.13	47,47,47,47	0
57	MG	2A	3102	1/1	0.84	0.09	66,66,66,66	0
57	MG	1A	4054	1/1	0.84	0.22	64,64,64,64	0
57	MG	1a	1800	1/1	0.84	0.13	76,76,76,76	0
57	MG	1O	204	1/1	0.84	0.20	71,71,71,71	0
57	MG	1Q	204	1/1	0.84	0.15	54,54,54,54	0
57	MG	2a	1626	1/1	0.84	0.27	77,77,77,77	0
57	MG	1A	3823	1/1	0.84	0.19	29,29,29,29	0
57	MG	1a	1812	1/1	0.84	0.18	67,67,67,67	0
57	MG	2A	3582	1/1	0.84	0.13	70,70,70,70	0
57	MG	1a	1813	1/1	0.84	0.10	47,47,47,47	0
57	MG	1A	3481	1/1	0.84	0.33	56,56,56,56	0
57	MG	2A	3144	1/1	0.84	0.53	44,44,44,44	0
57	MG	1A	3401	1/1	0.84	0.30	56,56,56,56	0
57	MG	1x	101	1/1	0.84	0.20	60,60,60,60	0
57	MG	1A	3406	1/1	0.84	0.33	41,41,41,41	0
57	MG	1A	3953	1/1	0.84	0.22	60,60,60,60	0
57	MG	2A	3160	1/1	0.84	0.28	63,63,63,63	0
57	MG	2A	3161	1/1	0.84	0.16	57,57,57,57	0
57	MG	2A	3313	1/1	0.84	0.27	63,63,63,63	0
57	MG	2A	3314	1/1	0.84	0.26	74,74,74,74	0
57	MG	1A	3632	1/1	0.84	0.17	29,29,29,29	0
57	MG	2A	3664	1/1	0.84	0.28	71,71,71,71	0
57	MG	10	102	1/1	0.84	0.14	66,66,66,66	0
57	MG	2A	3335	1/1	0.84	0.36	62,62,62,62	0
57	MG	2A	3011	1/1	0.84	0.16	46,46,46,46	0
57	MG	1a	1710	1/1	0.84	0.09	57,57,57,57	0
57	MG	2A	3023	1/1	0.84	0.29	71,71,71,71	0
57	MG	2a	1714	1/1	0.84	0.13	74,74,74,74	0
57	MG	2A	3695	1/1	0.84	0.13	70,70,70,70	0
57	MG	1A	3844	1/1	0.84	0.20	30,30,30,30	0
57	MG	2A	3026	1/1	0.84	0.22	43,43,43,43	0
57	MG	2A	3348	1/1	0.84	0.33	58,58,58,58	0
57	MG	2A	3350	1/1	0.84	0.34	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2A	3029	1/1	0.84	0.28	48,48,48,48	0
57	MG	2A	3187	1/1	0.84	0.14	63,63,63,63	0
57	MG	1A	3637	1/1	0.84	0.07	45,45,45,45	0
57	MG	1A	3039	1/1	0.84	0.25	63,63,63,63	0
57	MG	2A	3367	1/1	0.84	0.20	74,74,74,74	0
57	MG	1A	3513	1/1	0.84	0.28	50,50,50,50	0
57	MG	1A	3452	1/1	0.84	0.24	65,65,65,65	0
57	MG	2A	3050	1/1	0.84	0.17	65,65,65,65	0
57	MG	1A	3993	1/1	0.84	0.21	50,50,50,50	0
57	MG	1A	3340	1/1	0.84	0.24	49,49,49,49	0
57	MG	1A	3423	1/1	0.84	0.28	65,65,65,65	0
57	MG	2A	3410	1/1	0.84	0.15	76,76,76,76	0
57	MG	1A	4020	1/1	0.84	0.17	47,47,47,47	0
57	MG	2A	3069	1/1	0.84	0.23	52,52,52,52	0
57	MG	1A	3892	1/1	0.84	0.13	62,62,62,62	0
57	MG	2A	3072	1/1	0.84	0.12	57,57,57,57	0
57	MG	1a	1627	1/1	0.84	0.09	63,63,63,63	0
57	MG	2A	3466	1/1	0.84	0.23	40,40,40,40	0
57	MG	1A	3558	1/1	0.84	0.16	55,55,55,55	0
57	MG	1A	3320	1/1	0.84	0.33	56,56,56,56	0
57	MG	2A	3080	1/1	0.84	0.34	66,66,66,66	0
57	MG	2A	3085	1/1	0.84	0.25	47,47,47,47	0
57	MG	2A	3233	1/1	0.84	0.12	69,69,69,69	0
57	MG	2F	302	1/1	0.84	0.21	74,74,74,74	0
57	MG	1a	1648	1/1	0.84	0.26	66,66,66,66	0
57	MG	1A	3201	1/1	0.84	0.24	49,49,49,49	0
57	MG	2A	3501	1/1	0.84	0.26	63,63,63,63	0
57	MG	1A	3060	1/1	0.84	0.20	39,39,39,39	0
57	MG	2A	3514	1/1	0.84	0.09	65,65,65,65	0
57	MG	2A	3241	1/1	0.84	0.26	63,63,63,63	0
57	MG	1A	3193	1/1	0.84	0.21	47,47,47,47	0
57	MG	2x	108	1/1	0.84	0.19	56,56,56,56	0
57	MG	2A	3099	1/1	0.84	0.19	77,77,77,77	0
60	ZN	14	102	1/1	0.84	0.05	100,100,100,100	0
57	MG	1A	3709	1/1	0.84	0.16	44,44,44,44	0
57	MG	28	102	1/1	0.85	0.18	69,69,69,69	0
57	MG	1A	3138	1/1	0.85	0.14	57,57,57,57	0
57	MG	2A	3296	1/1	0.85	0.20	75,75,75,75	0
57	MG	2A	3579	1/1	0.85	0.15	58,58,58,58	0
57	MG	1A	3716	1/1	0.85	0.15	44,44,44,44	0
57	MG	1A	4060	1/1	0.85	0.17	53,53,53,53	0
57	MG	1A	3936	1/1	0.85	0.13	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3589	1/1	0.85	0.15	54,54,54,54	0
57	MG	1A	3940	1/1	0.85	0.14	51,51,51,51	0
57	MG	1A	3349	1/1	0.85	0.18	40,40,40,40	0
57	MG	1A	4067	1/1	0.85	0.20	59,59,59,59	0
57	MG	1A	3944	1/1	0.85	0.18	27,27,27,27	0
57	MG	2A	3609	1/1	0.85	0.28	40,40,40,40	0
57	MG	1A	3946	1/1	0.85	0.17	28,28,28,28	0
57	MG	2A	3198	1/1	0.85	0.26	69,69,69,69	0
57	MG	2A	3619	1/1	0.85	0.18	40,40,40,40	0
57	MG	2A	3341	1/1	0.85	0.47	71,71,71,71	0
57	MG	1A	3952	1/1	0.85	0.12	48,48,48,48	0
57	MG	2A	3202	1/1	0.85	0.28	50,50,50,50	0
57	MG	2a	1661	1/1	0.85	0.33	59,59,59,59	0
57	MG	1A	3626	1/1	0.85	0.13	32,32,32,32	0
57	MG	2A	3648	1/1	0.85	0.17	46,46,46,46	0
57	MG	2A	3205	1/1	0.85	0.62	47,47,47,47	0
57	MG	2A	3206	1/1	0.85	0.30	45,45,45,45	0
57	MG	1A	3960	1/1	0.85	0.10	65,65,65,65	0
57	MG	1A	3262	1/1	0.85	0.15	51,51,51,51	0
57	MG	1A	3226	1/1	0.85	0.33	31,31,31,31	0
57	MG	2a	1704	1/1	0.85	0.18	69,69,69,69	0
57	MG	1A	3528	1/1	0.85	0.17	57,57,57,57	0
57	MG	1A	3034	1/1	0.85	0.14	46,46,46,46	0
57	MG	2A	3362	1/1	0.85	0.21	50,50,50,50	0
57	MG	2a	1712	1/1	0.85	0.23	51,51,51,51	0
57	MG	2A	3366	1/1	0.85	0.30	46,46,46,46	0
57	MG	1A	3981	1/1	0.85	0.11	69,69,69,69	0
57	MG	1A	3546	1/1	0.85	0.18	44,44,44,44	0
57	MG	1A	3647	1/1	0.85	0.23	24,24,24,24	0
57	MG	2A	3227	1/1	0.85	0.23	71,71,71,71	0
57	MG	2A	3229	1/1	0.85	0.22	72,72,72,72	0
57	MG	2a	1728	1/1	0.85	0.17	64,64,64,64	0
57	MG	2A	3749	1/1	0.85	0.09	58,58,58,58	0
57	MG	1A	3992	1/1	0.85	0.15	53,53,53,53	0
57	MG	1A	3556	1/1	0.85	0.24	72,72,72,72	0
57	MG	2a	1754	1/1	0.85	0.25	49,49,49,49	0
57	MG	2A	3402	1/1	0.85	0.12	71,71,71,71	0
57	MG	1A	4006	1/1	0.85	0.11	59,59,59,59	0
57	MG	1A	4007	1/1	0.85	0.26	77,77,77,77	0
57	MG	1t	201	1/1	0.85	0.10	57,57,57,57	0
57	MG	2A	3778	1/1	0.85	0.10	60,60,60,60	0
57	MG	1w	103	1/1	0.85	0.30	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
57	MG	2A	3436	1/1	0.85	0.22	66,66,66,66	0
57	MG	1A	3653	1/1	0.85	0.10	37,37,37,37	0
57	MG	1A	3402	1/1	0.85	0.22	61,61,61,61	0
57	MG	2a	1783	1/1	0.85	0.17	66,66,66,66	0
57	MG	1x	103	1/1	0.85	0.27	55,55,55,55	0
57	MG	2A	3245	1/1	0.85	0.60	73,73,73,73	0
57	MG	1A	4018	1/1	0.85	0.21	72,72,72,72	0
57	MG	2B	201	1/1	0.85	0.14	69,69,69,69	0
57	MG	1A	3307	1/1	0.85	0.14	60,60,60,60	0
57	MG	1A	3238	1/1	0.85	0.39	41,41,41,41	0
57	MG	1a	1690	1/1	0.85	0.25	69,69,69,69	0
57	MG	1A	3584	1/1	0.85	0.25	30,30,30,30	0
57	MG	2B	212	1/1	0.85	0.24	65,65,65,65	0
57	MG	2A	3258	1/1	0.85	0.24	51,51,51,51	0
57	MG	2A	3013	1/1	0.85	0.16	78,78,78,78	0
57	MG	2f	203	1/1	0.85	0.13	75,75,75,75	0
57	MG	2k	201	1/1	0.85	0.31	66,66,66,66	0
57	MG	2D	302	1/1	0.85	0.33	66,66,66,66	0
57	MG	2A	3261	1/1	0.85	0.19	56,56,56,56	0
57	MG	1R	205	1/1	0.85	0.28	36,36,36,36	0
57	MG	1A	3089	1/1	0.85	0.10	76,76,76,76	0
57	MG	1A	3494	1/1	0.85	0.35	69,69,69,69	0
57	MG	2A	3267	1/1	0.85	0.22	64,64,64,64	0
57	MG	2A	3165	1/1	0.85	0.17	67,67,67,67	0
57	MG	1U	209	1/1	0.85	0.70	37,37,37,37	0
57	MG	1A	3916	1/1	0.85	0.08	23,23,23,23	0
57	MG	2A	3567	1/1	0.85	0.12	59,59,59,59	0
57	MG	1A	3617	1/1	0.85	0.17	25,25,25,25	0
57	MG	1a	1721	1/1	0.85	0.15	39,39,39,39	0
57	MG	2A	3515	1/1	0.86	0.16	34,34,34,34	0
57	MG	1a	1814	1/1	0.86	0.18	65,65,65,65	0
57	MG	1A	3867	1/1	0.86	0.19	33,33,33,33	0
57	MG	1A	3379	1/1	0.86	0.51	47,47,47,47	0
57	MG	1a	1651	1/1	0.86	0.11	54,54,54,54	0
57	MG	1A	3495	1/1	0.86	0.29	59,59,59,59	0
57	MG	2A	3557	1/1	0.86	0.16	83,83,83,83	0
57	MG	2A	3560	1/1	0.86	0.07	74,74,74,74	0
57	MG	2A	3278	1/1	0.86	0.23	59,59,59,59	0
57	MG	25	103	1/1	0.86	0.23	63,63,63,63	0
57	MG	2A	3566	1/1	0.86	0.12	33,33,33,33	0
57	MG	1a	1659	1/1	0.86	0.70	61,61,61,61	0
57	MG	1A	3500	1/1	0.86	0.19	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
57	MG	1A	3111	1/1	0.86	0.33	39,39,39,39	0
57	MG	2A	3171	1/1	0.86	0.39	70,70,70,70	0
57	MG	1B	219	1/1	0.86	0.20	34,34,34,34	0
57	MG	1A	3001	1/1	0.86	0.09	43,43,43,43	0
57	MG	2A	3297	1/1	0.86	0.33	69,69,69,69	0
57	MG	1A	3996	1/1	0.86	0.11	53,53,53,53	0
57	MG	2a	1630	1/1	0.86	0.17	68,68,68,68	0
57	MG	2A	3180	1/1	0.86	0.11	60,60,60,60	0
57	MG	2A	3307	1/1	0.86	0.42	71,71,71,71	0
57	MG	2A	3003	1/1	0.86	0.51	57,57,57,57	0
57	MG	2A	3182	1/1	0.86	0.12	64,64,64,64	0
57	MG	1B	232	1/1	0.86	0.16	68,68,68,68	0
57	MG	2A	3315	1/1	0.86	0.14	65,65,65,65	0
57	MG	2A	3317	1/1	0.86	0.22	58,58,58,58	0
57	MG	1B	233	1/1	0.86	0.10	61,61,61,61	0
57	MG	2A	3611	1/1	0.86	0.16	55,55,55,55	0
57	MG	2A	3326	1/1	0.86	0.22	63,63,63,63	0
57	MG	2A	3618	1/1	0.86	0.18	47,47,47,47	0
57	MG	2a	1664	1/1	0.86	0.07	64,64,64,64	0
57	MG	2a	1666	1/1	0.86	0.33	68,68,68,68	0
57	MG	1A	3997	1/1	0.86	0.15	53,53,53,53	0
57	MG	2A	3626	1/1	0.86	0.12	62,62,62,62	0
57	MG	2A	3630	1/1	0.86	0.21	65,65,65,65	0
57	MG	1A	4000	1/1	0.86	0.17	33,33,33,33	0
57	MG	1F	308	1/1	0.86	0.11	50,50,50,50	0
57	MG	1A	3902	1/1	0.86	0.13	47,47,47,47	0
57	MG	1A	3441	1/1	0.86	0.15	64,64,64,64	0
57	MG	1A	3163	1/1	0.86	0.25	59,59,59,59	0
57	MG	2A	3656	1/1	0.86	0.16	56,56,56,56	0
57	MG	2A	3036	1/1	0.86	0.14	66,66,66,66	0
57	MG	1A	3359	1/1	0.86	0.38	36,36,36,36	0
57	MG	1A	4013	1/1	0.86	0.32	41,41,41,41	0
57	MG	1A	3203	1/1	0.86	0.09	40,40,40,40	0
57	MG	1A	3911	1/1	0.86	0.08	43,43,43,43	0
57	MG	1A	3912	1/1	0.86	0.15	64,64,64,64	0
57	MG	2A	3056	1/1	0.86	0.13	73,73,73,73	0
57	MG	2a	1721	1/1	0.86	0.14	76,76,76,76	0
57	MG	2A	3692	1/1	0.86	0.15	71,71,71,71	0
57	MG	2a	1723	1/1	0.86	0.22	80,80,80,80	0
57	MG	2A	3213	1/1	0.86	0.30	72,72,72,72	0
57	MG	1A	3541	1/1	0.86	0.22	65,65,65,65	0
57	MG	1a	1725	1/1	0.86	0.15	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
57	MG	1A	3178	1/1	0.86	0.08	74,74,74,74	0
57	MG	1A	3372	1/1	0.86	0.74	53,53,53,53	0
57	MG	2A	3381	1/1	0.86	0.30	50,50,50,50	0
57	MG	2a	1760	1/1	0.86	0.22	54,54,54,54	0
57	MG	2A	3733	1/1	0.86	0.21	68,68,68,68	0
57	MG	2A	3219	1/1	0.86	0.22	49,49,49,49	0
57	MG	2A	3385	1/1	0.86	0.21	73,73,73,73	0
57	MG	1A	3927	1/1	0.86	0.14	65,65,65,65	0
57	MG	1A	3929	1/1	0.86	0.18	65,65,65,65	0
57	MG	1A	3080	1/1	0.86	0.21	34,34,34,34	0
57	MG	2A	3765	1/1	0.86	0.06	63,63,63,63	0
57	MG	1A	3244	1/1	0.86	0.14	59,59,59,59	0
57	MG	1A	3573	1/1	0.86	0.18	35,35,35,35	0
57	MG	10	105	1/1	0.86	0.56	43,43,43,43	0
57	MG	2A	3776	1/1	0.86	0.16	67,67,67,67	0
57	MG	1a	1767	1/1	0.86	0.07	59,59,59,59	0
57	MG	2a	1790	1/1	0.86	0.25	75,75,75,75	0
57	MG	2A	3413	1/1	0.86	0.21	38,38,38,38	0
57	MG	1A	3419	1/1	0.86	0.17	66,66,66,66	0
57	MG	1A	3701	1/1	0.86	0.15	19,19,19,19	0
57	MG	1A	3334	1/1	0.86	0.14	53,53,53,53	0
57	MG	1A	3376	1/1	0.86	0.16	42,42,42,42	0
57	MG	1A	3275	1/1	0.86	0.16	53,53,53,53	0
57	MG	1A	3723	1/1	0.86	0.21	26,26,26,26	0
57	MG	1A	3488	1/1	0.86	0.27	60,60,60,60	0
57	MG	1a	1795	1/1	0.86	0.10	68,68,68,68	0
57	MG	2A	3477	1/1	0.86	0.28	50,50,50,50	0
57	MG	1A	3861	1/1	0.86	0.23	37,37,37,37	0
57	MG	1a	1799	1/1	0.86	0.13	73,73,73,73	0
57	MG	2B	211	1/1	0.86	0.26	76,76,76,76	0
57	MG	1A	4098	1/1	0.86	0.14	51,51,51,51	0
57	MG	2w	103	1/1	0.86	0.25	70,70,70,70	0
57	MG	1B	201	1/1	0.86	0.11	51,51,51,51	0
57	MG	1A	3863	1/1	0.86	0.17	44,44,44,44	0
57	MG	1a	1629	1/1	0.86	0.30	69,69,69,69	0
57	MG	1a	1636	1/1	0.86	0.12	57,57,57,57	0
57	MG	1A	3429	1/1	0.86	0.17	50,50,50,50	0
57	MG	2D	307	1/1	0.86	0.16	68,68,68,68	0
57	MG	2D	308	1/1	0.86	0.18	59,59,59,59	0
57	MG	2E	301	1/1	0.86	0.21	68,68,68,68	0
57	MG	2E	305	1/1	0.86	0.15	63,63,63,63	0
57	MG	1A	3399	1/1	0.87	0.34	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
57	MG	2A	3293	1/1	0.87	0.24	67,67,67,67	0
57	MG	2A	3094	1/1	0.87	0.13	67,67,67,67	0
57	MG	1A	3763	1/1	0.87	0.14	32,32,32,32	0
57	MG	2A	3096	1/1	0.87	0.09	62,62,62,62	0
57	MG	1x	107	1/1	0.87	0.26	72,72,72,72	0
57	MG	1A	3051	1/1	0.87	0.15	54,54,54,54	0
57	MG	2A	3301	1/1	0.87	0.19	67,67,67,67	0
57	MG	2A	3304	1/1	0.87	0.12	62,62,62,62	0
57	MG	1A	4039	1/1	0.87	0.13	48,48,48,48	0
57	MG	2A	3103	1/1	0.87	0.23	68,68,68,68	0
57	MG	2A	3507	1/1	0.87	0.08	61,61,61,61	0
57	MG	1a	1624	1/1	0.87	0.12	46,46,46,46	0
57	MG	1A	3223	1/1	0.87	0.25	57,57,57,57	0
57	MG	1A	3529	1/1	0.87	0.12	56,56,56,56	0
57	MG	1E	310	1/1	0.87	0.09	39,39,39,39	0
57	MG	1A	3405	1/1	0.87	0.30	62,62,62,62	0
57	MG	2A	3322	1/1	0.87	0.22	57,57,57,57	0
57	MG	2A	3542	1/1	0.87	0.23	72,72,72,72	0
57	MG	2A	3325	1/1	0.87	0.14	67,67,67,67	0
57	MG	2A	3020	1/1	0.87	0.25	49,49,49,49	0
57	MG	2A	3549	1/1	0.87	0.12	53,53,53,53	0
57	MG	1A	3540	1/1	0.87	0.31	59,59,59,59	0
57	MG	2a	1719	1/1	0.87	0.11	69,69,69,69	0
57	MG	1A	3026	1/1	0.87	0.23	65,65,65,65	0
57	MG	1A	3046	1/1	0.87	0.12	35,35,35,35	0
57	MG	2A	3150	1/1	0.87	0.14	63,63,63,63	0
57	MG	1A	3468	1/1	0.87	0.20	54,54,54,54	0
57	MG	2a	1725	1/1	0.87	0.07	84,84,84,84	0
57	MG	2A	3030	1/1	0.87	0.28	63,63,63,63	0
57	MG	2a	1727	1/1	0.87	0.14	71,71,71,71	0
57	MG	1A	3146	1/1	0.87	0.40	34,34,34,34	0
57	MG	1O	203	1/1	0.87	0.25	55,55,55,55	0
57	MG	2A	3575	1/1	0.87	0.24	60,60,60,60	0
57	MG	1A	3984	1/1	0.87	0.09	43,43,43,43	0
57	MG	2a	1751	1/1	0.87	0.21	60,60,60,60	0
57	MG	1A	3199	1/1	0.87	0.13	71,71,71,71	0
57	MG	2A	3351	1/1	0.87	0.30	57,57,57,57	0
57	MG	2A	3239	1/1	0.87	0.22	55,55,55,55	0
57	MG	1A	3326	1/1	0.87	0.39	62,62,62,62	0
57	MG	2A	3357	1/1	0.87	0.35	58,58,58,58	0
57	MG	2A	3166	1/1	0.87	0.17	65,65,65,65	0
57	MG	1A	3148	1/1	0.87	0.12	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3053	1/1	0.87	0.15	58,58,58,58	0
57	MG	2A	3364	1/1	0.87	0.35	54,54,54,54	0
57	MG	1A	3068	1/1	0.87	0.18	58,58,58,58	0
57	MG	1A	3159	1/1	0.87	0.15	40,40,40,40	0
57	MG	1A	3124	1/1	0.87	0.23	37,37,37,37	0
57	MG	2G	201	1/1	0.87	0.07	77,77,77,77	0
57	MG	2a	1786	1/1	0.87	0.24	68,68,68,68	0
57	MG	2N	201	1/1	0.87	0.32	85,85,85,85	0
57	MG	1A	3384	1/1	0.87	0.17	51,51,51,51	0
57	MG	1A	3299	1/1	0.87	0.45	37,37,37,37	0
57	MG	2A	3259	1/1	0.87	0.20	65,65,65,65	0
57	MG	2A	3391	1/1	0.87	0.13	61,61,61,61	0
57	MG	2a	1804	1/1	0.87	0.26	65,65,65,65	0
57	MG	1B	204	1/1	0.87	0.21	44,44,44,44	0
57	MG	2A	3631	1/1	0.87	0.24	86,86,86,86	0
57	MG	1A	3843	1/1	0.87	0.19	31,31,31,31	0
57	MG	2a	1815	1/1	0.87	0.08	67,67,67,67	0
57	MG	1A	4008	1/1	0.87	0.13	18,18,18,18	0
57	MG	2A	3637	1/1	0.87	0.13	54,54,54,54	0
57	MG	2a	1602	1/1	0.87	0.10	81,81,81,81	0
57	MG	10	106	1/1	0.87	0.28	64,64,64,64	0
57	MG	2A	3643	1/1	0.87	0.12	71,71,71,71	0
57	MG	1A	3251	1/1	0.87	0.22	64,64,64,64	0
57	MG	1A	3511	1/1	0.87	0.29	58,58,58,58	0
57	MG	2a	1616	1/1	0.87	0.14	79,79,79,79	0
57	MG	1v	101	1/1	0.87	0.28	82,82,82,82	0
57	MG	2A	3194	1/1	0.87	0.16	59,59,59,59	0
57	MG	1A	3854	1/1	0.87	0.15	58,58,58,58	0
57	MG	1A	3858	1/1	0.87	0.10	56,56,56,56	0
57	MG	2A	3288	1/1	0.87	0.11	57,57,57,57	0
57	MG	2A	3441	1/1	0.87	0.30	59,59,59,59	0
57	MG	2A	3678	1/1	0.87	0.16	68,68,68,68	0
57	MG	2y	101	1/1	0.87	0.14	81,81,81,81	0
57	MG	1A	3216	1/1	0.87	0.15	53,53,53,53	0
57	MG	2A	3688	1/1	0.87	0.15	50,50,50,50	0
57	MG	2A	3451	1/1	0.87	0.15	42,42,42,42	0
57	MG	1a	1741	1/1	0.88	0.17	58,58,58,58	0
57	MG	2A	3494	1/1	0.88	0.22	76,76,76,76	0
57	MG	1A	4040	1/1	0.88	0.12	67,67,67,67	0
57	MG	2A	3249	1/1	0.88	0.18	55,55,55,55	0
57	MG	2A	3087	1/1	0.88	0.28	69,69,69,69	0
57	MG	2A	3088	1/1	0.88	0.12	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2F	303	1/1	0.88	0.35	54,54,54,54	0
57	MG	1U	205	1/1	0.88	0.35	36,36,36,36	0
57	MG	1A	3449	1/1	0.88	0.43	48,48,48,48	0
57	MG	1A	3272	1/1	0.88	0.37	46,46,46,46	0
57	MG	1A	3918	1/1	0.88	0.11	65,65,65,65	0
57	MG	1A	3101	1/1	0.88	0.15	31,31,31,31	0
57	MG	1A	4051	1/1	0.88	0.25	57,57,57,57	0
57	MG	2A	3543	1/1	0.88	0.23	35,35,35,35	0
57	MG	1A	3416	1/1	0.88	0.16	67,67,67,67	0
57	MG	2A	3101	1/1	0.88	0.09	50,50,50,50	0
57	MG	10	103	1/1	0.88	0.36	52,52,52,52	0
57	MG	25	101	1/1	0.88	0.30	67,67,67,67	0
57	MG	2A	3552	1/1	0.88	0.22	39,39,39,39	0
57	MG	1A	3088	1/1	0.88	0.26	53,53,53,53	0
57	MG	28	104	1/1	0.88	0.25	58,58,58,58	0
57	MG	1a	1773	1/1	0.88	0.08	63,63,63,63	0
57	MG	2A	3279	1/1	0.88	0.50	60,60,60,60	0
57	MG	2A	3564	1/1	0.88	0.21	75,75,75,75	0
57	MG	2A	3280	1/1	0.88	0.21	47,47,47,47	0
57	MG	1A	3208	1/1	0.88	0.20	50,50,50,50	0
57	MG	2a	1614	1/1	0.88	0.11	63,63,63,63	0
57	MG	2A	3112	1/1	0.88	0.12	75,75,75,75	0
57	MG	1A	3533	1/1	0.88	0.20	38,38,38,38	0
57	MG	11	102	1/1	0.88	0.29	60,60,60,60	0
57	MG	2A	3126	1/1	0.88	0.09	61,61,61,61	0
57	MG	2A	3291	1/1	0.88	0.17	67,67,67,67	0
57	MG	1A	3424	1/1	0.88	0.23	60,60,60,60	0
57	MG	1a	1791	1/1	0.88	0.13	69,69,69,69	0
57	MG	11	105	1/1	0.88	0.18	53,53,53,53	0
57	MG	12	102	1/1	0.88	0.14	50,50,50,50	0
57	MG	12	103	1/1	0.88	0.20	43,43,43,43	0
57	MG	2A	3146	1/1	0.88	0.17	66,66,66,66	0
57	MG	2a	1639	1/1	0.88	0.19	71,71,71,71	0
57	MG	2A	3147	1/1	0.88	0.16	56,56,56,56	0
57	MG	2A	3303	1/1	0.88	0.15	72,72,72,72	0
57	MG	1A	3538	1/1	0.88	0.14	68,68,68,68	0
57	MG	15	101	1/1	0.88	0.23	39,39,39,39	0
57	MG	16	101	1/1	0.88	0.41	52,52,52,52	0
57	MG	18	104	1/1	0.88	0.37	41,41,41,41	0
57	MG	1A	4074	1/1	0.88	0.18	62,62,62,62	0
57	MG	1A	3209	1/1	0.88	0.40	44,44,44,44	0
57	MG	1A	3654	1/1	0.88	0.15	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1684	1/1	0.88	0.17	67,67,67,67	0
57	MG	1A	3313	1/1	0.88	0.18	53,53,53,53	0
57	MG	1A	4086	1/1	0.88	0.10	40,40,40,40	0
57	MG	2A	3324	1/1	0.88	0.63	55,55,55,55	0
57	MG	1A	3949	1/1	0.88	0.13	57,57,57,57	0
57	MG	1A	4097	1/1	0.88	0.10	46,46,46,46	0
57	MG	1A	3479	1/1	0.88	0.14	67,67,67,67	0
57	MG	2a	1701	1/1	0.88	0.23	51,51,51,51	0
57	MG	2A	3334	1/1	0.88	0.42	54,54,54,54	0
57	MG	1A	3555	1/1	0.88	0.30	54,54,54,54	0
57	MG	1A	3260	1/1	0.88	0.52	47,47,47,47	0
57	MG	1x	102	1/1	0.88	0.21	70,70,70,70	0
57	MG	2A	3652	1/1	0.88	0.08	54,54,54,54	0
57	MG	1A	3557	1/1	0.88	0.45	66,66,66,66	0
57	MG	2A	3658	1/1	0.88	0.17	67,67,67,67	0
57	MG	1A	3294	1/1	0.88	0.20	63,63,63,63	0
57	MG	1a	1640	1/1	0.88	0.22	61,61,61,61	0
57	MG	1A	3855	1/1	0.88	0.28	34,34,34,34	0
57	MG	1A	3234	1/1	0.88	0.34	52,52,52,52	0
57	MG	1y	101	1/1	0.88	0.32	55,55,55,55	0
57	MG	2A	3677	1/1	0.88	0.15	60,60,60,60	0
57	MG	1A	3563	1/1	0.88	0.21	25,25,25,25	0
57	MG	1A	3565	1/1	0.88	0.13	23,23,23,23	0
57	MG	2A	3687	1/1	0.88	0.31	70,70,70,70	0
57	MG	1A	3567	1/1	0.88	0.13	30,30,30,30	0
57	MG	2a	1738	1/1	0.88	0.09	75,75,75,75	0
57	MG	2a	1739	1/1	0.88	0.14	69,69,69,69	0
57	MG	2a	1744	1/1	0.88	0.15	64,64,64,64	0
57	MG	2A	3689	1/1	0.88	0.22	54,54,54,54	0
57	MG	1A	3720	1/1	0.88	0.16	29,29,29,29	0
57	MG	2A	3358	1/1	0.88	0.35	52,52,52,52	0
57	MG	2A	3694	1/1	0.88	0.15	64,64,64,64	0
57	MG	1A	3722	1/1	0.88	0.20	30,30,30,30	0
57	MG	2A	3197	1/1	0.88	0.40	58,58,58,58	0
57	MG	1a	1665	1/1	0.88	0.11	65,65,65,65	0
57	MG	2A	3707	1/1	0.88	0.17	51,51,51,51	0
57	MG	1A	3871	1/1	0.88	0.20	24,24,24,24	0
57	MG	1A	3994	1/1	0.88	0.13	29,29,29,29	0
57	MG	2A	3730	1/1	0.88	0.08	63,63,63,63	0
57	MG	1A	3873	1/1	0.88	0.26	42,42,42,42	0
57	MG	2A	3027	1/1	0.88	0.16	45,45,45,45	0
57	MG	1A	3571	1/1	0.88	0.12	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
57	MG	2A	3745	1/1	0.88	0.15	57,57,57,57	0
57	MG	1a	1679	1/1	0.88	0.38	47,47,47,47	0
57	MG	1A	3298	1/1	0.88	0.31	39,39,39,39	0
57	MG	1A	3439	1/1	0.88	0.38	46,46,46,46	0
57	MG	2A	3757	1/1	0.88	0.09	64,64,64,64	0
57	MG	1a	1684	1/1	0.88	0.06	68,68,68,68	0
57	MG	1a	1686	1/1	0.88	0.19	62,62,62,62	0
57	MG	2A	3768	1/1	0.88	0.12	72,72,72,72	0
57	MG	2A	3046	1/1	0.88	0.18	70,70,70,70	0
57	MG	1F	305	1/1	0.88	0.59	60,60,60,60	0
57	MG	2a	1805	1/1	0.88	0.26	58,58,58,58	0
57	MG	2A	3221	1/1	0.88	0.23	65,65,65,65	0
57	MG	2a	1810	1/1	0.88	0.20	77,77,77,77	0
57	MG	2A	3403	1/1	0.88	0.45	56,56,56,56	0
57	MG	1A	3210	1/1	0.88	0.20	49,49,49,49	0
57	MG	2A	3782	1/1	0.88	0.11	54,54,54,54	0
57	MG	2A	3051	1/1	0.88	0.29	56,56,56,56	0
57	MG	2a	1818	1/1	0.88	0.08	72,72,72,72	0
57	MG	1A	3586	1/1	0.88	0.08	33,33,33,33	0
57	MG	1a	1692	1/1	0.88	0.09	69,69,69,69	0
57	MG	1A	3900	1/1	0.88	0.23	65,65,65,65	0
57	MG	1A	3587	1/1	0.88	0.07	41,41,41,41	0
57	MG	2A	3439	1/1	0.88	0.14	68,68,68,68	0
57	MG	2A	3794	1/1	0.88	0.14	47,47,47,47	0
57	MG	1A	3498	1/1	0.88	0.15	63,63,63,63	0
57	MG	2A	3448	1/1	0.88	0.22	47,47,47,47	0
57	MG	1A	3776	1/1	0.88	0.12	46,46,46,46	0
57	MG	1A	3905	1/1	0.88	0.08	62,62,62,62	0
57	MG	2x	103	1/1	0.88	0.23	65,65,65,65	0
57	MG	1A	3328	1/1	0.88	0.17	57,57,57,57	0
57	MG	1A	3332	1/1	0.88	0.24	66,66,66,66	0
57	MG	1A	3509	1/1	0.88	0.24	35,35,35,35	0
57	MG	1R	206	1/1	0.88	0.12	71,71,71,71	0
57	MG	1A	3792	1/1	0.88	0.12	28,28,28,28	0
57	MG	1a	1733	1/1	0.88	0.17	71,71,71,71	0
57	MG	2A	3081	1/1	0.88	0.21	52,52,52,52	0
57	MG	2A	3246	1/1	0.88	0.13	68,68,68,68	0
57	MG	1H	201	1/1	0.89	0.21	48,48,48,48	0
57	MG	2P	201	1/1	0.89	0.29	63,63,63,63	0
57	MG	2A	3168	1/1	0.89	0.23	49,49,49,49	0
57	MG	2Q	201	1/1	0.89	0.07	65,65,65,65	0
57	MG	2R	202	1/1	0.89	0.16	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
57	MG	2A	3005	1/1	0.89	0.33	56,56,56,56	0
57	MG	1A	3330	1/1	0.89	0.48	39,39,39,39	0
57	MG	2A	3565	1/1	0.89	0.13	66,66,66,66	0
57	MG	1A	3910	1/1	0.89	0.16	67,67,67,67	0
57	MG	1A	3212	1/1	0.89	0.21	45,45,45,45	0
57	MG	2A	3305	1/1	0.89	0.15	58,58,58,58	0
57	MG	2A	3570	1/1	0.89	0.12	73,73,73,73	0
57	MG	1A	4032	1/1	0.89	0.20	40,40,40,40	0
57	MG	1A	4033	1/1	0.89	0.21	60,60,60,60	0
57	MG	2A	3312	1/1	0.89	0.25	69,69,69,69	0
57	MG	1A	3301	1/1	0.89	0.27	39,39,39,39	0
57	MG	2A	3578	1/1	0.89	0.16	69,69,69,69	0
57	MG	1A	3807	1/1	0.89	0.19	43,43,43,43	0
57	MG	2A	3184	1/1	0.89	0.22	66,66,66,66	0
57	MG	1A	3668	1/1	0.89	0.19	61,61,61,61	0
57	MG	2A	3583	1/1	0.89	0.16	43,43,43,43	0
57	MG	2A	3319	1/1	0.89	0.13	73,73,73,73	0
57	MG	2a	1617	1/1	0.89	0.24	57,57,57,57	0
57	MG	2a	1618	1/1	0.89	0.15	71,71,71,71	0
57	MG	2A	3320	1/1	0.89	0.26	69,69,69,69	0
57	MG	1A	3810	1/1	0.89	0.14	69,69,69,69	0
57	MG	2a	1623	1/1	0.89	0.29	63,63,63,63	0
57	MG	1a	1698	1/1	0.89	0.21	63,63,63,63	0
57	MG	2A	3596	1/1	0.89	0.21	56,56,56,56	0
57	MG	1A	3815	1/1	0.89	0.10	57,57,57,57	0
57	MG	2A	3192	1/1	0.89	0.34	45,45,45,45	0
57	MG	1A	3490	1/1	0.89	0.21	49,49,49,49	0
57	MG	1A	3024	1/1	0.89	0.29	35,35,35,35	0
57	MG	1a	1712	1/1	0.89	0.16	31,31,31,31	0
57	MG	1A	3157	1/1	0.89	0.12	52,52,52,52	0
57	MG	1W	202	1/1	0.89	0.13	57,57,57,57	0
57	MG	1A	3681	1/1	0.89	0.17	62,62,62,62	0
57	MG	1a	1723	1/1	0.89	0.17	58,58,58,58	0
57	MG	2a	1644	1/1	0.89	0.10	83,83,83,83	0
57	MG	1A	3934	1/1	0.89	0.09	61,61,61,61	0
57	MG	1a	1726	1/1	0.89	0.12	52,52,52,52	0
57	MG	1A	3438	1/1	0.89	0.19	45,45,45,45	0
57	MG	2a	1654	1/1	0.89	0.13	64,64,64,64	0
57	MG	1a	1728	1/1	0.89	0.29	67,67,67,67	0
57	MG	1A	3497	1/1	0.89	0.16	47,47,47,47	0
57	MG	2a	1665	1/1	0.89	0.37	64,64,64,64	0
57	MG	2A	3063	1/1	0.89	0.17	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
57	MG	1A	3697	1/1	0.89	0.07	53,53,53,53	0
57	MG	1A	3191	1/1	0.89	0.12	40,40,40,40	0
57	MG	1A	3440	1/1	0.89	0.23	46,46,46,46	0
57	MG	2a	1689	1/1	0.89	0.33	67,67,67,67	0
57	MG	1A	3015	1/1	0.89	0.26	37,37,37,37	0
57	MG	1A	3443	1/1	0.89	0.24	43,43,43,43	0
57	MG	2A	3075	1/1	0.89	0.21	57,57,57,57	0
57	MG	1A	3444	1/1	0.89	0.15	57,57,57,57	0
57	MG	2A	3363	1/1	0.89	0.34	65,65,65,65	0
57	MG	2A	3666	1/1	0.89	0.08	72,72,72,72	0
57	MG	1A	4087	1/1	0.89	0.16	51,51,51,51	0
57	MG	1A	4091	1/1	0.89	0.27	40,40,40,40	0
57	MG	1A	3342	1/1	0.89	0.46	60,60,60,60	0
57	MG	1A	3601	1/1	0.89	0.11	70,70,70,70	0
57	MG	2A	3376	1/1	0.89	0.44	62,62,62,62	0
57	MG	2a	1713	1/1	0.89	0.13	68,68,68,68	0
57	MG	1A	3233	1/1	0.89	0.19	47,47,47,47	0
57	MG	1A	3865	1/1	0.89	0.14	47,47,47,47	0
57	MG	1a	1775	1/1	0.89	0.06	62,62,62,62	0
57	MG	2A	3386	1/1	0.89	0.15	56,56,56,56	0
57	MG	1A	3613	1/1	0.89	0.13	43,43,43,43	0
57	MG	1a	1603	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	3615	1/1	0.89	0.14	36,36,36,36	0
57	MG	2A	3397	1/1	0.89	0.33	62,62,62,62	0
57	MG	1a	1610	1/1	0.89	0.17	65,65,65,65	0
57	MG	1A	3516	1/1	0.89	0.21	33,33,33,33	0
57	MG	2A	3240	1/1	0.89	0.16	63,63,63,63	0
57	MG	2A	3098	1/1	0.89	0.18	49,49,49,49	0
57	MG	2a	1737	1/1	0.89	0.13	52,52,52,52	0
57	MG	2A	3713	1/1	0.89	0.20	50,50,50,50	0
57	MG	2A	3714	1/1	0.89	0.12	52,52,52,52	0
57	MG	2A	3407	1/1	0.89	0.16	66,66,66,66	0
57	MG	2A	3242	1/1	0.89	0.10	66,66,66,66	0
57	MG	1A	3312	1/1	0.89	0.22	49,49,49,49	0
57	MG	1A	3252	1/1	0.89	0.15	46,46,46,46	0
57	MG	1A	3880	1/1	0.89	0.19	51,51,51,51	0
57	MG	2A	3416	1/1	0.89	0.21	35,35,35,35	0
57	MG	2A	3425	1/1	0.89	0.09	73,73,73,73	0
57	MG	1A	3882	1/1	0.89	0.14	43,43,43,43	0
57	MG	1A	3768	1/1	0.89	0.14	45,45,45,45	0
57	MG	1B	217	1/1	0.89	0.08	52,52,52,52	0
57	MG	1A	3409	1/1	0.89	0.46	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
57	MG	2A	3447	1/1	0.89	0.23	41,41,41,41	0
57	MG	2A	3252	1/1	0.89	0.40	62,62,62,62	0
57	MG	2A	3108	1/1	0.89	0.19	40,40,40,40	0
57	MG	1a	1633	1/1	0.89	0.18	58,58,58,58	0
57	MG	1a	1811	1/1	0.89	0.35	61,61,61,61	0
57	MG	2A	3463	1/1	0.89	0.32	53,53,53,53	0
57	MG	2A	3777	1/1	0.89	0.12	70,70,70,70	0
57	MG	1B	222	1/1	0.89	0.20	56,56,56,56	0
57	MG	2A	3124	1/1	0.89	0.35	46,46,46,46	0
57	MG	1A	3283	1/1	0.89	0.38	50,50,50,50	0
57	MG	1A	3144	1/1	0.89	0.34	32,32,32,32	0
57	MG	1A	4005	1/1	0.89	0.21	26,26,26,26	0
57	MG	2A	3481	1/1	0.89	0.14	52,52,52,52	0
57	MG	2A	3791	1/1	0.89	0.07	71,71,71,71	0
57	MG	2A	3265	1/1	0.89	0.18	60,60,60,60	0
57	MG	1A	3293	1/1	0.89	0.10	57,57,57,57	0
57	MG	2A	3138	1/1	0.89	0.23	45,45,45,45	0
57	MG	1A	3789	1/1	0.89	0.27	60,60,60,60	0
57	MG	2A	3274	1/1	0.89	0.51	74,74,74,74	0
57	MG	2A	3275	1/1	0.89	0.25	78,78,78,78	0
57	MG	1E	302	1/1	0.89	0.26	36,36,36,36	0
57	MG	2a	1817	1/1	0.89	0.14	54,54,54,54	0
57	MG	1a	1657	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3510	1/1	0.89	0.14	51,51,51,51	0
57	MG	1E	305	1/1	0.89	0.19	28,28,28,28	0
57	MG	1A	3321	1/1	0.89	0.27	41,41,41,41	0
57	MG	1A	3197	1/1	0.89	0.18	39,39,39,39	0
57	MG	2A	3286	1/1	0.89	0.21	61,61,61,61	0
57	MG	2B	215	1/1	0.89	0.16	66,66,66,66	0
57	MG	2v	101	1/1	0.89	0.19	78,78,78,78	0
57	MG	1A	3237	1/1	0.89	0.09	56,56,56,56	0
57	MG	2A	3526	1/1	0.89	0.16	65,65,65,65	0
57	MG	2A	3529	1/1	0.89	0.08	62,62,62,62	0
57	MG	2A	3534	1/1	0.89	0.26	63,63,63,63	0
57	MG	1F	307	1/1	0.89	0.16	38,38,38,38	0
57	MG	1A	3906	1/1	0.89	0.17	48,48,48,48	0
57	MG	2A	3544	1/1	0.89	0.20	50,50,50,50	0
57	MG	1x	109	1/1	0.89	0.33	71,71,71,71	0
57	MG	1A	4014	1/1	0.89	0.22	29,29,29,29	0
57	MG	2F	304	1/1	0.89	0.17	49,49,49,49	0
57	MG	2F	305	1/1	0.89	0.11	63,63,63,63	0
57	MG	1A	3907	1/1	0.89	0.09	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	ZN	2Y	202	1/1	0.89	0.12	105,105,105,105	0
57	MG	1A	3133	1/1	0.89	0.18	48,48,48,48	0
57	MG	2A	3561	1/1	0.90	0.27	67,67,67,67	0
57	MG	1A	4055	1/1	0.90	0.13	58,58,58,58	0
57	MG	1A	3598	1/1	0.90	0.14	19,19,19,19	0
57	MG	1A	4062	1/1	0.90	0.11	48,48,48,48	0
57	MG	1A	3346	1/1	0.90	0.30	38,38,38,38	0
57	MG	1A	3099	1/1	0.90	0.36	54,54,54,54	0
57	MG	1A	3422	1/1	0.90	0.24	48,48,48,48	0
57	MG	20	101	1/1	0.90	0.11	63,63,63,63	0
57	MG	2A	3158	1/1	0.90	0.27	70,70,70,70	0
57	MG	17	104	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	3019	1/1	0.90	0.20	48,48,48,48	0
57	MG	1A	3493	1/1	0.90	0.34	49,49,49,49	0
57	MG	1A	3922	1/1	0.90	0.17	49,49,49,49	0
57	MG	1A	3006	1/1	0.90	0.19	55,55,55,55	0
57	MG	1A	4077	1/1	0.90	0.06	61,61,61,61	0
57	MG	1A	3925	1/1	0.90	0.13	56,56,56,56	0
57	MG	2a	1605	1/1	0.90	0.23	69,69,69,69	0
57	MG	1A	3618	1/1	0.90	0.18	21,21,21,21	0
57	MG	1a	1620	1/1	0.90	0.14	50,50,50,50	0
57	MG	2A	3175	1/1	0.90	0.52	65,65,65,65	0
57	MG	2a	1612	1/1	0.90	0.09	60,60,60,60	0
57	MG	2A	3586	1/1	0.90	0.07	67,67,67,67	0
57	MG	2a	1615	1/1	0.90	0.44	62,62,62,62	0
57	MG	1A	3114	1/1	0.90	0.23	43,43,43,43	0
57	MG	1A	3175	1/1	0.90	0.14	38,38,38,38	0
57	MG	1A	4093	1/1	0.90	0.31	49,49,49,49	0
57	MG	1A	4094	1/1	0.90	0.34	42,42,42,42	0
57	MG	1A	3224	1/1	0.90	0.52	50,50,50,50	0
57	MG	1A	3430	1/1	0.90	0.33	69,69,69,69	0
57	MG	1a	1630	1/1	0.90	0.25	71,71,71,71	0
57	MG	1A	3935	1/1	0.90	0.12	39,39,39,39	0
57	MG	1A	3074	1/1	0.90	0.25	42,42,42,42	0
57	MG	2a	1631	1/1	0.90	0.25	66,66,66,66	0
57	MG	2A	3613	1/1	0.90	0.47	56,56,56,56	0
57	MG	1A	3052	1/1	0.90	0.23	51,51,51,51	0
57	MG	1A	3817	1/1	0.90	0.10	61,61,61,61	0
57	MG	2A	3191	1/1	0.90	0.19	56,56,56,56	0
57	MG	1A	3127	1/1	0.90	0.43	41,41,41,41	0
57	MG	1A	3822	1/1	0.90	0.21	61,61,61,61	0
57	MG	1A	3947	1/1	0.90	0.20	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
57	MG	2A	3017	1/1	0.90	0.31	61,61,61,61	0
57	MG	1A	3083	1/1	0.90	0.20	39,39,39,39	0
57	MG	1B	212	1/1	0.90	0.21	60,60,60,60	0
57	MG	2A	3638	1/1	0.90	0.07	68,68,68,68	0
57	MG	1A	3646	1/1	0.90	0.22	34,34,34,34	0
57	MG	1A	3134	1/1	0.90	0.26	41,41,41,41	0
57	MG	1A	3830	1/1	0.90	0.44	45,45,45,45	0
57	MG	1A	3085	1/1	0.90	0.17	54,54,54,54	0
57	MG	1A	3086	1/1	0.90	0.17	59,59,59,59	0
57	MG	1B	224	1/1	0.90	0.24	57,57,57,57	0
57	MG	1A	3291	1/1	0.90	0.22	61,61,61,61	0
57	MG	2a	1682	1/1	0.90	0.43	60,60,60,60	0
57	MG	1A	3389	1/1	0.90	0.33	38,38,38,38	0
57	MG	1a	1676	1/1	0.90	0.19	73,73,73,73	0
57	MG	2A	3379	1/1	0.90	0.32	58,58,58,58	0
57	MG	1a	1677	1/1	0.90	0.30	41,41,41,41	0
57	MG	1A	3665	1/1	0.90	0.18	43,43,43,43	0
57	MG	1A	3390	1/1	0.90	0.27	37,37,37,37	0
57	MG	1A	3985	1/1	0.90	0.13	57,57,57,57	0
57	MG	1A	3143	1/1	0.90	0.49	39,39,39,39	0
57	MG	2A	3680	1/1	0.90	0.16	63,63,63,63	0
57	MG	1A	3537	1/1	0.90	0.34	45,45,45,45	0
57	MG	1A	3447	1/1	0.90	0.22	50,50,50,50	0
57	MG	1A	3056	1/1	0.90	0.20	37,37,37,37	0
57	MG	1A	3451	1/1	0.90	0.69	46,46,46,46	0
57	MG	1A	3545	1/1	0.90	0.45	61,61,61,61	0
57	MG	1A	3396	1/1	0.90	0.14	53,53,53,53	0
57	MG	2A	3064	1/1	0.90	0.19	49,49,49,49	0
57	MG	2a	1715	1/1	0.90	0.53	60,60,60,60	0
57	MG	1A	3058	1/1	0.90	0.28	54,54,54,54	0
57	MG	1F	312	1/1	0.90	0.11	54,54,54,54	0
57	MG	1F	313	1/1	0.90	0.19	32,32,32,32	0
57	MG	2A	3704	1/1	0.90	0.05	72,72,72,72	0
57	MG	1a	1705	1/1	0.90	0.13	55,55,55,55	0
57	MG	2A	3073	1/1	0.90	0.25	49,49,49,49	0
57	MG	1A	3042	1/1	0.90	0.34	35,35,35,35	0
57	MG	1A	3249	1/1	0.90	0.19	40,40,40,40	0
57	MG	2A	3076	1/1	0.90	0.20	52,52,52,52	0
57	MG	2A	3432	1/1	0.90	0.14	30,30,30,30	0
57	MG	2A	3433	1/1	0.90	0.14	45,45,45,45	0
57	MG	2a	1732	1/1	0.90	0.16	83,83,83,83	0
57	MG	1A	3461	1/1	0.90	0.13	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
57	MG	2A	3734	1/1	0.90	0.22	24,24,24,24	0
57	MG	2A	3243	1/1	0.90	0.11	77,77,77,77	0
57	MG	2A	3742	1/1	0.90	0.20	48,48,48,48	0
57	MG	1A	3877	1/1	0.90	0.18	33,33,33,33	0
57	MG	1N	201	1/1	0.90	0.48	45,45,45,45	0
57	MG	1A	3878	1/1	0.90	0.10	48,48,48,48	0
57	MG	1A	3463	1/1	0.90	0.16	55,55,55,55	0
57	MG	2A	3755	1/1	0.90	0.21	62,62,62,62	0
57	MG	1A	3881	1/1	0.90	0.18	26,26,26,26	0
57	MG	2A	3758	1/1	0.90	0.19	50,50,50,50	0
57	MG	1O	205	1/1	0.90	0.14	48,48,48,48	0
57	MG	1P	203	1/1	0.90	0.48	32,32,32,32	0
57	MG	1A	3339	1/1	0.90	0.48	48,48,48,48	0
57	MG	1A	3150	1/1	0.90	0.25	48,48,48,48	0
57	MG	1a	1737	1/1	0.90	0.15	56,56,56,56	0
57	MG	1A	3471	1/1	0.90	0.60	40,40,40,40	0
57	MG	1S	203	1/1	0.90	0.22	67,67,67,67	0
57	MG	1A	3891	1/1	0.90	0.13	33,33,33,33	0
57	MG	1A	4026	1/1	0.90	0.24	46,46,46,46	0
57	MG	1A	3726	1/1	0.90	0.15	31,31,31,31	0
57	MG	2a	1785	1/1	0.90	0.25	66,66,66,66	0
57	MG	2A	3484	1/1	0.90	0.25	32,32,32,32	0
57	MG	2A	3485	1/1	0.90	0.14	67,67,67,67	0
57	MG	1U	207	1/1	0.90	0.47	38,38,38,38	0
57	MG	2a	1791	1/1	0.90	0.15	79,79,79,79	0
57	MG	2A	3489	1/1	0.90	0.27	60,60,60,60	0
57	MG	1A	3895	1/1	0.90	0.09	53,53,53,53	0
57	MG	2a	1797	1/1	0.90	0.18	54,54,54,54	0
57	MG	1A	3568	1/1	0.90	0.14	50,50,50,50	0
57	MG	2a	1799	1/1	0.90	0.22	60,60,60,60	0
57	MG	1A	3738	1/1	0.90	0.14	48,48,48,48	0
57	MG	1A	4034	1/1	0.90	0.22	48,48,48,48	0
57	MG	2A	3795	1/1	0.90	0.15	71,71,71,71	0
57	MG	1a	1770	1/1	0.90	0.18	53,53,53,53	0
57	MG	1A	4035	1/1	0.90	0.33	58,58,58,58	0
57	MG	2A	3512	1/1	0.90	0.13	53,53,53,53	0
57	MG	2A	3276	1/1	0.90	0.17	52,52,52,52	0
57	MG	2A	3115	1/1	0.90	0.16	61,61,61,61	0
57	MG	1A	3474	1/1	0.90	0.15	54,54,54,54	0
57	MG	2A	3120	1/1	0.90	0.10	53,53,53,53	0
57	MG	1A	3475	1/1	0.90	0.23	60,60,60,60	0
57	MG	2a	1820	1/1	0.90	0.10	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3519	1/1	0.90	0.34	50,50,50,50	0
57	MG	2A	3523	1/1	0.90	0.13	59,59,59,59	0
57	MG	1A	3152	1/1	0.90	0.19	42,42,42,42	0
57	MG	2A	3125	1/1	0.90	0.26	44,44,44,44	0
57	MG	1A	3411	1/1	0.90	0.14	58,58,58,58	0
57	MG	2A	3536	1/1	0.90	0.29	46,46,46,46	0
57	MG	2A	3538	1/1	0.90	0.13	41,41,41,41	0
57	MG	2A	3539	1/1	0.90	0.24	47,47,47,47	0
57	MG	2A	3541	1/1	0.90	0.38	63,63,63,63	0
57	MG	2E	302	1/1	0.90	0.11	55,55,55,55	0
57	MG	2A	3131	1/1	0.90	0.35	53,53,53,53	0
57	MG	2E	306	1/1	0.90	0.19	54,54,54,54	0
57	MG	1A	3343	1/1	0.90	0.18	45,45,45,45	0
57	MG	10	107	1/1	0.90	0.17	54,54,54,54	0
57	MG	2A	3292	1/1	0.90	0.21	58,58,58,58	0
57	MG	1a	1786	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3773	1/1	0.90	0.07	58,58,58,58	0
57	MG	2A	3140	1/1	0.90	0.06	73,73,73,73	0
57	MG	1A	3344	1/1	0.90	0.44	45,45,45,45	0
57	MG	1A	3596	1/1	0.90	0.18	35,35,35,35	0
57	MG	1a	1708	1/1	0.91	0.15	60,60,60,60	0
57	MG	2F	301	1/1	0.91	0.18	47,47,47,47	0
57	MG	1A	3552	1/1	0.91	0.34	42,42,42,42	0
57	MG	2A	3079	1/1	0.91	0.23	58,58,58,58	0
57	MG	1A	3696	1/1	0.91	0.18	66,66,66,66	0
57	MG	2A	3525	1/1	0.91	0.20	35,35,35,35	0
57	MG	2F	307	1/1	0.91	0.52	51,51,51,51	0
57	MG	1A	3554	1/1	0.91	0.11	63,63,63,63	0
57	MG	1a	1716	1/1	0.91	0.08	69,69,69,69	0
57	MG	1A	3137	1/1	0.91	0.17	51,51,51,51	0
57	MG	1A	3874	1/1	0.91	0.18	52,52,52,52	0
57	MG	1A	3227	1/1	0.91	0.19	29,29,29,29	0
57	MG	2A	3089	1/1	0.91	0.17	46,46,46,46	0
57	MG	2A	3090	1/1	0.91	0.14	51,51,51,51	0
57	MG	1R	203	1/1	0.91	0.64	38,38,38,38	0
57	MG	2A	3277	1/1	0.91	0.29	72,72,72,72	0
57	MG	1A	3002	1/1	0.91	0.19	60,60,60,60	0
57	MG	2A	3093	1/1	0.91	0.14	28,28,28,28	0
57	MG	1A	3711	1/1	0.91	0.18	27,27,27,27	0
57	MG	1S	202	1/1	0.91	0.13	54,54,54,54	0
57	MG	1A	3712	1/1	0.91	0.23	61,61,61,61	0
57	MG	1A	3267	1/1	0.91	0.26	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
57	MG	1A	3348	1/1	0.91	0.17	61,61,61,61	0
57	MG	27	102	1/1	0.91	0.20	57,57,57,57	0
57	MG	28	101	1/1	0.91	0.32	70,70,70,70	0
57	MG	1a	1738	1/1	0.91	0.23	76,76,76,76	0
57	MG	1a	1739	1/1	0.91	0.14	67,67,67,67	0
57	MG	1a	1740	1/1	0.91	0.21	43,43,43,43	0
57	MG	1A	4030	1/1	0.91	0.18	43,43,43,43	0
57	MG	1A	3202	1/1	0.91	0.27	36,36,36,36	0
57	MG	1A	3352	1/1	0.91	0.13	47,47,47,47	0
57	MG	1A	3119	1/1	0.91	0.37	32,32,32,32	0
57	MG	1A	3420	1/1	0.91	0.23	43,43,43,43	0
57	MG	1A	3731	1/1	0.91	0.07	40,40,40,40	0
57	MG	1a	1761	1/1	0.91	0.24	58,58,58,58	0
57	MG	2A	3300	1/1	0.91	0.18	64,64,64,64	0
57	MG	1X	102	1/1	0.91	0.29	37,37,37,37	0
57	MG	2A	3302	1/1	0.91	0.78	57,57,57,57	0
57	MG	1A	3897	1/1	0.91	0.17	18,18,18,18	0
57	MG	1A	3361	1/1	0.91	0.27	33,33,33,33	0
57	MG	1A	3483	1/1	0.91	0.29	35,35,35,35	0
57	MG	1A	3484	1/1	0.91	0.38	44,44,44,44	0
57	MG	1A	3740	1/1	0.91	0.07	71,71,71,71	0
57	MG	2a	1627	1/1	0.91	0.28	45,45,45,45	0
57	MG	1A	3742	1/1	0.91	0.08	35,35,35,35	0
57	MG	2A	3588	1/1	0.91	0.13	60,60,60,60	0
57	MG	2A	3133	1/1	0.91	0.12	60,60,60,60	0
57	MG	1A	3744	1/1	0.91	0.10	42,42,42,42	0
57	MG	10	108	1/1	0.91	0.41	70,70,70,70	0
57	MG	1A	3745	1/1	0.91	0.08	39,39,39,39	0
57	MG	2A	3600	1/1	0.91	0.20	58,58,58,58	0
57	MG	2A	3318	1/1	0.91	0.14	61,61,61,61	0
57	MG	1A	3363	1/1	0.91	0.48	41,41,41,41	0
57	MG	1A	3755	1/1	0.91	0.15	42,42,42,42	0
57	MG	1A	3757	1/1	0.91	0.07	61,61,61,61	0
57	MG	1a	1787	1/1	0.91	0.11	52,52,52,52	0
57	MG	2a	1645	1/1	0.91	0.33	70,70,70,70	0
57	MG	12	101	1/1	0.91	0.15	38,38,38,38	0
57	MG	2a	1647	1/1	0.91	0.26	78,78,78,78	0
57	MG	2A	3148	1/1	0.91	0.35	46,46,46,46	0
57	MG	2A	3615	1/1	0.91	0.31	68,68,68,68	0
57	MG	1A	3366	1/1	0.91	0.11	44,44,44,44	0
57	MG	2a	1658	1/1	0.91	0.27	57,57,57,57	0
57	MG	2A	3327	1/1	0.91	0.22	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2A	3622	1/1	0.91	0.26	48,48,48,48	0
57	MG	2A	3625	1/1	0.91	0.20	50,50,50,50	0
57	MG	1a	1793	1/1	0.91	0.15	65,65,65,65	0
57	MG	2A	3153	1/1	0.91	0.18	48,48,48,48	0
57	MG	2a	1680	1/1	0.91	0.12	66,66,66,66	0
57	MG	1A	3425	1/1	0.91	0.26	37,37,37,37	0
57	MG	2a	1683	1/1	0.91	0.09	75,75,75,75	0
57	MG	2A	3633	1/1	0.91	0.11	64,64,64,64	0
57	MG	13	103	1/1	0.91	0.12	59,59,59,59	0
57	MG	13	104	1/1	0.91	0.18	55,55,55,55	0
57	MG	1A	3097	1/1	0.91	0.13	37,37,37,37	0
57	MG	1a	1801	1/1	0.91	0.21	56,56,56,56	0
57	MG	2a	1694	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	3492	1/1	0.91	0.20	24,24,24,24	0
57	MG	2A	3640	1/1	0.91	0.07	68,68,68,68	0
57	MG	2a	1699	1/1	0.91	0.28	57,57,57,57	0
57	MG	15	104	1/1	0.91	0.40	40,40,40,40	0
57	MG	1A	3775	1/1	0.91	0.12	45,45,45,45	0
57	MG	1a	1810	1/1	0.91	0.10	56,56,56,56	0
57	MG	1A	3368	1/1	0.91	0.14	43,43,43,43	0
57	MG	1A	3166	1/1	0.91	0.42	60,60,60,60	0
57	MG	1A	3923	1/1	0.91	0.28	50,50,50,50	0
57	MG	2a	1711	1/1	0.91	0.09	83,83,83,83	0
57	MG	2A	3174	1/1	0.91	0.35	60,60,60,60	0
57	MG	1A	4082	1/1	0.91	0.38	33,33,33,33	0
57	MG	1A	3603	1/1	0.91	0.17	32,32,32,32	0
57	MG	1A	3125	1/1	0.91	0.09	64,64,64,64	0
57	MG	1A	3612	1/1	0.91	0.16	46,46,46,46	0
57	MG	1A	3928	1/1	0.91	0.10	59,59,59,59	0
57	MG	1A	3496	1/1	0.91	0.33	54,54,54,54	0
57	MG	2A	3365	1/1	0.91	0.26	69,69,69,69	0
57	MG	1A	3318	1/1	0.91	0.39	54,54,54,54	0
57	MG	1A	3280	1/1	0.91	0.17	39,39,39,39	0
57	MG	2A	3368	1/1	0.91	0.62	57,57,57,57	0
57	MG	1A	3240	1/1	0.91	0.18	48,48,48,48	0
57	MG	1x	104	1/1	0.91	0.13	66,66,66,66	0
57	MG	1A	4100	1/1	0.91	0.28	53,53,53,53	0
57	MG	1A	3501	1/1	0.91	0.35	32,32,32,32	0
57	MG	2a	1729	1/1	0.91	0.17	74,74,74,74	0
57	MG	1A	3798	1/1	0.91	0.23	51,51,51,51	0
57	MG	2a	1733	1/1	0.91	0.15	72,72,72,72	0
57	MG	1A	3803	1/1	0.91	0.12	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
57	MG	1A	3435	1/1	0.91	0.15	56,56,56,56	0
57	MG	2A	3390	1/1	0.91	0.15	64,64,64,64	0
57	MG	2a	1740	1/1	0.91	0.12	56,56,56,56	0
57	MG	1A	3076	1/1	0.91	0.39	42,42,42,42	0
57	MG	1a	1638	1/1	0.91	0.08	60,60,60,60	0
57	MG	2A	3002	1/1	0.91	0.40	49,49,49,49	0
57	MG	1A	3510	1/1	0.91	0.23	54,54,54,54	0
57	MG	1A	3179	1/1	0.91	0.20	38,38,38,38	0
57	MG	2A	3007	1/1	0.91	0.11	59,59,59,59	0
57	MG	2a	1755	1/1	0.91	0.21	46,46,46,46	0
57	MG	1a	1645	1/1	0.91	0.17	54,54,54,54	0
57	MG	1A	3147	1/1	0.91	0.43	38,38,38,38	0
57	MG	2a	1765	1/1	0.91	0.12	67,67,67,67	0
57	MG	2A	3405	1/1	0.91	0.25	61,61,61,61	0
57	MG	1A	3638	1/1	0.91	0.15	31,31,31,31	0
57	MG	1A	3079	1/1	0.91	0.46	33,33,33,33	0
57	MG	2A	3209	1/1	0.91	0.17	47,47,47,47	0
57	MG	2A	3743	1/1	0.91	0.16	70,70,70,70	0
57	MG	2A	3210	1/1	0.91	0.32	63,63,63,63	0
57	MG	1A	3818	1/1	0.91	0.07	41,41,41,41	0
57	MG	2A	3751	1/1	0.91	0.09	65,65,65,65	0
57	MG	2a	1782	1/1	0.91	0.21	70,70,70,70	0
57	MG	1a	1656	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3419	1/1	0.91	0.32	61,61,61,61	0
57	MG	1A	3331	1/1	0.91	0.19	56,56,56,56	0
57	MG	1A	3964	1/1	0.91	0.17	24,24,24,24	0
57	MG	1a	1660	1/1	0.91	0.10	60,60,60,60	0
57	MG	1A	3517	1/1	0.91	0.26	23,23,23,23	0
57	MG	1A	3973	1/1	0.91	0.06	54,54,54,54	0
57	MG	2A	3033	1/1	0.91	0.50	55,55,55,55	0
57	MG	2a	1794	1/1	0.91	0.31	67,67,67,67	0
57	MG	2A	3222	1/1	0.91	0.19	62,62,62,62	0
57	MG	1A	3974	1/1	0.91	0.15	62,62,62,62	0
57	MG	1B	231	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	3218	1/1	0.91	0.41	36,36,36,36	0
57	MG	1A	3219	1/1	0.91	0.52	33,33,33,33	0
57	MG	2A	3452	1/1	0.91	0.14	39,39,39,39	0
57	MG	2a	1806	1/1	0.91	0.20	53,53,53,53	0
57	MG	2A	3460	1/1	0.91	0.26	51,51,51,51	0
57	MG	2A	3044	1/1	0.91	0.23	58,58,58,58	0
57	MG	1A	3103	1/1	0.91	0.49	34,34,34,34	0
57	MG	1A	3983	1/1	0.91	0.16	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	1A	3091	1/1	0.91	0.12	32,32,32,32	0
57	MG	1A	3656	1/1	0.91	0.10	31,31,31,31	0
57	MG	2A	3052	1/1	0.91	0.21	59,59,59,59	0
57	MG	1A	3336	1/1	0.91	0.15	51,51,51,51	0
57	MG	1A	3664	1/1	0.91	0.22	38,38,38,38	0
57	MG	1A	3991	1/1	0.91	0.08	56,56,56,56	0
57	MG	2d	301	1/1	0.91	0.11	69,69,69,69	0
57	MG	1A	3300	1/1	0.91	0.21	56,56,56,56	0
57	MG	1A	3397	1/1	0.91	0.46	42,42,42,42	0
57	MG	2A	3061	1/1	0.91	0.20	37,37,37,37	0
57	MG	1A	3153	1/1	0.91	0.21	32,32,32,32	0
57	MG	1A	3673	1/1	0.91	0.08	37,37,37,37	0
57	MG	1a	1691	1/1	0.91	0.18	56,56,56,56	0
57	MG	2A	3497	1/1	0.91	0.10	40,40,40,40	0
57	MG	2A	3066	1/1	0.91	0.14	68,68,68,68	0
57	MG	2A	3067	1/1	0.91	0.27	51,51,51,51	0
57	MG	2A	3502	1/1	0.91	0.12	67,67,67,67	0
57	MG	2A	3503	1/1	0.91	0.15	40,40,40,40	0
57	MG	2D	301	1/1	0.91	0.17	42,42,42,42	0
57	MG	1A	3400	1/1	0.91	0.19	46,46,46,46	0
57	MG	2A	3508	1/1	0.91	0.13	76,76,76,76	0
57	MG	1A	3304	1/1	0.91	0.27	45,45,45,45	0
57	MG	1a	1696	1/1	0.91	0.23	57,57,57,57	0
57	MG	1G	205	1/1	0.91	0.17	49,49,49,49	0
57	MG	1A	3341	1/1	0.91	0.23	35,35,35,35	0
57	MG	1A	3547	1/1	0.91	0.14	42,42,42,42	0
57	MG	1A	3690	1/1	0.91	0.17	62,62,62,62	0
57	MG	1A	3480	1/1	0.92	0.12	52,52,52,52	0
57	MG	1A	3171	1/1	0.92	0.19	34,34,34,34	0
57	MG	1a	1763	1/1	0.92	0.20	64,64,64,64	0
57	MG	1A	3839	1/1	0.92	0.14	30,30,30,30	0
57	MG	1A	3614	1/1	0.92	0.22	50,50,50,50	0
57	MG	1A	3715	1/1	0.92	0.17	20,20,20,20	0
57	MG	1A	3365	1/1	0.92	0.19	42,42,42,42	0
57	MG	1a	1771	1/1	0.92	0.13	45,45,45,45	0
57	MG	1A	3718	1/1	0.92	0.19	20,20,20,20	0
57	MG	1A	3957	1/1	0.92	0.12	26,26,26,26	0
57	MG	2A	3545	1/1	0.92	0.14	50,50,50,50	0
57	MG	2A	3295	1/1	0.92	0.09	70,70,70,70	0
57	MG	2A	3116	1/1	0.92	0.24	65,65,65,65	0
57	MG	15	106	1/1	0.92	0.09	61,61,61,61	0
57	MG	1A	3719	1/1	0.92	0.16	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3554	1/1	0.92	0.33	63,63,63,63	0
57	MG	1A	4099	1/1	0.92	0.34	53,53,53,53	0
57	MG	2A	3559	1/1	0.92	0.12	67,67,67,67	0
57	MG	2A	3122	1/1	0.92	0.18	44,44,44,44	0
57	MG	1A	3084	1/1	0.92	0.54	45,45,45,45	0
57	MG	1a	1780	1/1	0.92	0.19	64,64,64,64	0
57	MG	1a	1782	1/1	0.92	0.14	54,54,54,54	0
57	MG	1a	1784	1/1	0.92	0.11	46,46,46,46	0
57	MG	1A	3721	1/1	0.92	0.15	42,42,42,42	0
57	MG	1a	1602	1/1	0.92	0.11	71,71,71,71	0
57	MG	2A	3308	1/1	0.92	0.17	70,70,70,70	0
57	MG	1A	3968	1/1	0.92	0.10	37,37,37,37	0
57	MG	1A	3230	1/1	0.92	0.40	28,28,28,28	0
57	MG	1a	1605	1/1	0.92	0.09	62,62,62,62	0
57	MG	1A	3198	1/1	0.92	0.14	59,59,59,59	0
57	MG	2a	1608	1/1	0.92	0.14	67,67,67,67	0
57	MG	1A	3542	1/1	0.92	0.26	37,37,37,37	0
57	MG	2A	3316	1/1	0.92	0.12	75,75,75,75	0
57	MG	1A	3623	1/1	0.92	0.26	30,30,30,30	0
57	MG	2a	1613	1/1	0.92	0.16	53,53,53,53	0
57	MG	1a	1797	1/1	0.92	0.09	66,66,66,66	0
57	MG	1A	3727	1/1	0.92	0.15	26,26,26,26	0
57	MG	1a	1621	1/1	0.92	0.09	43,43,43,43	0
57	MG	1A	3370	1/1	0.92	0.18	52,52,52,52	0
57	MG	1A	3255	1/1	0.92	0.32	46,46,46,46	0
57	MG	1a	1803	1/1	0.92	0.10	50,50,50,50	0
57	MG	1A	3736	1/1	0.92	0.15	33,33,33,33	0
57	MG	2a	1622	1/1	0.92	0.19	59,59,59,59	0
57	MG	1a	1808	1/1	0.92	0.14	67,67,67,67	0
57	MG	2a	1624	1/1	0.92	0.36	64,64,64,64	0
57	MG	2A	3591	1/1	0.92	0.06	66,66,66,66	0
57	MG	2A	3157	1/1	0.92	0.17	76,76,76,76	0
57	MG	1A	3737	1/1	0.92	0.13	50,50,50,50	0
57	MG	1A	3631	1/1	0.92	0.17	17,17,17,17	0
57	MG	2A	3602	1/1	0.92	0.15	31,31,31,31	0
57	MG	2A	3603	1/1	0.92	0.15	76,76,76,76	0
57	MG	1B	221	1/1	0.92	0.30	56,56,56,56	0
57	MG	2a	1634	1/1	0.92	0.27	62,62,62,62	0
57	MG	1A	3285	1/1	0.92	0.36	52,52,52,52	0
57	MG	2A	3340	1/1	0.92	0.37	56,56,56,56	0
57	MG	2A	3164	1/1	0.92	0.20	66,66,66,66	0
57	MG	1a	1631	1/1	0.92	0.28	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
57	MG	1A	3636	1/1	0.92	0.20	56,56,56,56	0
57	MG	1a	1634	1/1	0.92	0.15	74,74,74,74	0
57	MG	1r	101	1/1	0.92	0.18	69,69,69,69	0
57	MG	2A	3617	1/1	0.92	0.23	58,58,58,58	0
57	MG	2A	3169	1/1	0.92	0.18	40,40,40,40	0
57	MG	1B	225	1/1	0.92	0.17	37,37,37,37	0
57	MG	1a	1637	1/1	0.92	0.23	57,57,57,57	0
57	MG	1w	101	1/1	0.92	0.21	43,43,43,43	0
57	MG	2a	1653	1/1	0.92	0.17	47,47,47,47	0
57	MG	1A	3549	1/1	0.92	0.24	59,59,59,59	0
57	MG	2a	1655	1/1	0.92	0.14	68,68,68,68	0
57	MG	2A	3628	1/1	0.92	0.19	76,76,76,76	0
57	MG	2a	1659	1/1	0.92	0.09	64,64,64,64	0
57	MG	2a	1660	1/1	0.92	0.29	42,42,42,42	0
57	MG	2A	3629	1/1	0.92	0.23	61,61,61,61	0
57	MG	2A	3356	1/1	0.92	0.40	53,53,53,53	0
57	MG	1A	3018	1/1	0.92	0.21	50,50,50,50	0
57	MG	1w	105	1/1	0.92	0.08	68,68,68,68	0
57	MG	1A	3288	1/1	0.92	0.24	42,42,42,42	0
57	MG	1a	1641	1/1	0.92	0.08	61,61,61,61	0
57	MG	2A	3361	1/1	0.92	0.22	54,54,54,54	0
57	MG	1a	1642	1/1	0.92	0.21	64,64,64,64	0
57	MG	1A	3415	1/1	0.92	0.57	55,55,55,55	0
57	MG	1A	3645	1/1	0.92	0.17	29,29,29,29	0
57	MG	2a	1688	1/1	0.92	0.10	71,71,71,71	0
57	MG	1D	309	1/1	0.92	0.30	52,52,52,52	0
57	MG	1a	1650	1/1	0.92	0.10	44,44,44,44	0
57	MG	1A	3887	1/1	0.92	0.07	39,39,39,39	0
57	MG	2A	3189	1/1	0.92	0.16	64,64,64,64	0
57	MG	1a	1652	1/1	0.92	0.15	45,45,45,45	0
57	MG	2A	3657	1/1	0.92	0.17	49,49,49,49	0
57	MG	2a	1697	1/1	0.92	0.11	81,81,81,81	0
57	MG	2a	1698	1/1	0.92	0.08	74,74,74,74	0
57	MG	2A	3374	1/1	0.92	0.16	40,40,40,40	0
57	MG	2A	3659	1/1	0.92	0.10	69,69,69,69	0
57	MG	2A	3660	1/1	0.92	0.18	42,42,42,42	0
57	MG	1x	112	1/1	0.92	0.11	72,72,72,72	0
57	MG	2A	3378	1/1	0.92	0.15	59,59,59,59	0
57	MG	1A	4001	1/1	0.92	0.17	29,29,29,29	0
57	MG	2A	3668	1/1	0.92	0.10	56,56,56,56	0
57	MG	2A	3669	1/1	0.92	0.06	73,73,73,73	0
57	MG	1A	4003	1/1	0.92	0.17	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
57	MG	1A	3214	1/1	0.92	0.20	49,49,49,49	0
57	MG	2A	3383	1/1	0.92	0.23	42,42,42,42	0
57	MG	1A	3417	1/1	0.92	0.28	45,45,45,45	0
57	MG	1A	3453	1/1	0.92	0.43	48,48,48,48	0
57	MG	2A	3388	1/1	0.92	0.18	66,66,66,66	0
57	MG	1A	3292	1/1	0.92	0.32	47,47,47,47	0
57	MG	1A	4009	1/1	0.92	0.27	56,56,56,56	0
57	MG	1a	1664	1/1	0.92	0.20	64,64,64,64	0
57	MG	2A	3014	1/1	0.92	0.24	50,50,50,50	0
57	MG	2A	3015	1/1	0.92	0.20	58,58,58,58	0
57	MG	1A	4010	1/1	0.92	0.11	58,58,58,58	0
57	MG	1A	3896	1/1	0.92	0.11	36,36,36,36	0
57	MG	1A	3772	1/1	0.92	0.12	30,30,30,30	0
57	MG	1A	3316	1/1	0.92	0.11	55,55,55,55	0
57	MG	2A	3404	1/1	0.92	0.11	63,63,63,63	0
57	MG	2a	1730	1/1	0.92	0.12	87,87,87,87	0
57	MG	1A	3503	1/1	0.92	0.19	44,44,44,44	0
57	MG	2A	3706	1/1	0.92	0.14	39,39,39,39	0
57	MG	1a	1674	1/1	0.92	0.18	67,67,67,67	0
57	MG	2A	3409	1/1	0.92	0.17	54,54,54,54	0
57	MG	1A	4016	1/1	0.92	0.10	25,25,25,25	0
57	MG	1A	3661	1/1	0.92	0.16	46,46,46,46	0
57	MG	2a	1741	1/1	0.92	0.10	77,77,77,77	0
57	MG	1A	3782	1/1	0.92	0.11	34,34,34,34	0
57	MG	2A	3719	1/1	0.92	0.12	56,56,56,56	0
57	MG	2A	3720	1/1	0.92	0.15	58,58,58,58	0
57	MG	1A	3215	1/1	0.92	0.17	48,48,48,48	0
57	MG	2A	3218	1/1	0.92	0.14	58,58,58,58	0
57	MG	2a	1753	1/1	0.92	0.33	52,52,52,52	0
57	MG	1A	3319	1/1	0.92	0.10	67,67,67,67	0
57	MG	1A	3032	1/1	0.92	0.43	27,27,27,27	0
57	MG	2a	1759	1/1	0.92	0.12	81,81,81,81	0
57	MG	2A	3427	1/1	0.92	0.28	74,74,74,74	0
57	MG	2A	3736	1/1	0.92	0.09	56,56,56,56	0
57	MG	2A	3739	1/1	0.92	0.17	52,52,52,52	0
57	MG	2A	3740	1/1	0.92	0.17	62,62,62,62	0
57	MG	1A	3667	1/1	0.92	0.11	57,57,57,57	0
57	MG	1A	3107	1/1	0.92	0.16	33,33,33,33	0
57	MG	1A	3669	1/1	0.92	0.07	61,61,61,61	0
57	MG	2A	3746	1/1	0.92	0.11	55,55,55,55	0
57	MG	2a	1776	1/1	0.92	0.32	75,75,75,75	0
57	MG	1a	1689	1/1	0.92	0.22	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
57	MG	1P	205	1/1	0.92	0.38	41,41,41,41	0
57	MG	2A	3752	1/1	0.92	0.07	71,71,71,71	0
57	MG	1A	3576	1/1	0.92	0.14	41,41,41,41	0
57	MG	1A	3187	1/1	0.92	0.55	37,37,37,37	0
57	MG	1A	3674	1/1	0.92	0.19	58,58,58,58	0
57	MG	2A	3449	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	4037	1/1	0.92	0.14	58,58,58,58	0
57	MG	2A	3760	1/1	0.92	0.23	73,73,73,73	0
57	MG	2A	3761	1/1	0.92	0.09	57,57,57,57	0
57	MG	1A	3675	1/1	0.92	0.27	49,49,49,49	0
57	MG	1A	3801	1/1	0.92	0.07	53,53,53,53	0
57	MG	2A	3459	1/1	0.92	0.26	38,38,38,38	0
57	MG	1a	1699	1/1	0.92	0.23	51,51,51,51	0
57	MG	1A	3110	1/1	0.92	0.24	35,35,35,35	0
57	MG	1A	3354	1/1	0.92	0.35	43,43,43,43	0
57	MG	1U	203	1/1	0.92	0.59	53,53,53,53	0
57	MG	1A	3022	1/1	0.92	0.12	17,17,17,17	0
57	MG	1A	3521	1/1	0.92	0.26	40,40,40,40	0
57	MG	2A	3476	1/1	0.92	0.14	71,71,71,71	0
57	MG	1A	3360	1/1	0.92	0.16	57,57,57,57	0
57	MG	1A	3207	1/1	0.92	0.17	36,36,36,36	0
57	MG	1V	204	1/1	0.92	0.14	49,49,49,49	0
57	MG	2A	3787	1/1	0.92	0.08	58,58,58,58	0
57	MG	1A	3398	1/1	0.92	0.25	45,45,45,45	0
57	MG	1W	201	1/1	0.92	0.34	49,49,49,49	0
57	MG	1A	3531	1/1	0.92	0.27	42,42,42,42	0
57	MG	1a	1724	1/1	0.92	0.19	59,59,59,59	0
57	MG	1W	204	1/1	0.92	0.17	38,38,38,38	0
57	MG	1A	3698	1/1	0.92	0.22	25,25,25,25	0
57	MG	2a	1821	1/1	0.92	0.05	66,66,66,66	0
57	MG	2A	3493	1/1	0.92	0.06	64,64,64,64	0
57	MG	2f	201	1/1	0.92	0.24	49,49,49,49	0
57	MG	1X	106	1/1	0.92	0.13	34,34,34,34	0
57	MG	1A	3820	1/1	0.92	0.21	56,56,56,56	0
57	MG	1a	1730	1/1	0.92	0.12	54,54,54,54	0
57	MG	1A	3605	1/1	0.92	0.11	27,27,27,27	0
57	MG	1a	1734	1/1	0.92	0.08	76,76,76,76	0
57	MG	2t	201	1/1	0.92	0.07	58,58,58,58	0
57	MG	2A	3082	1/1	0.92	0.07	78,78,78,78	0
57	MG	2A	3505	1/1	0.92	0.18	59,59,59,59	0
57	MG	1a	1736	1/1	0.92	0.19	54,54,54,54	0
57	MG	2w	105	1/1	0.92	0.39	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
57	MG	1A	3702	1/1	0.92	0.19	67,67,67,67	0
57	MG	1A	3532	1/1	0.92	0.44	46,46,46,46	0
57	MG	1A	4071	1/1	0.92	0.09	59,59,59,59	0
57	MG	1A	4073	1/1	0.92	0.13	66,66,66,66	0
57	MG	1A	3938	1/1	0.92	0.09	66,66,66,66	0
57	MG	1A	3939	1/1	0.92	0.15	65,65,65,65	0
57	MG	1a	1744	1/1	0.92	0.16	43,43,43,43	0
57	MG	1A	3706	1/1	0.92	0.16	40,40,40,40	0
57	MG	1A	3941	1/1	0.92	0.24	18,18,18,18	0
57	MG	1A	3942	1/1	0.92	0.16	31,31,31,31	0
57	MG	1a	1754	1/1	0.92	0.09	64,64,64,64	0
57	MG	1A	4079	1/1	0.92	0.21	48,48,48,48	0
57	MG	1A	3356	1/1	0.93	0.28	34,34,34,34	0
57	MG	1A	3845	1/1	0.93	0.13	29,29,29,29	0
57	MG	2A	3604	1/1	0.93	0.26	76,76,76,76	0
57	MG	1a	1713	1/1	0.93	0.22	37,37,37,37	0
57	MG	2A	3040	1/1	0.93	0.09	60,60,60,60	0
57	MG	2A	3201	1/1	0.93	0.11	59,59,59,59	0
57	MG	2a	1607	1/1	0.93	0.29	69,69,69,69	0
57	MG	1A	3639	1/1	0.93	0.19	61,61,61,61	0
57	MG	10	104	1/1	0.93	0.27	44,44,44,44	0
57	MG	1a	1718	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3375	1/1	0.93	0.14	69,69,69,69	0
57	MG	1A	3852	1/1	0.93	0.16	23,23,23,23	0
57	MG	2A	3208	1/1	0.93	0.14	54,54,54,54	0
57	MG	2A	3048	1/1	0.93	0.11	48,48,48,48	0
57	MG	2A	3049	1/1	0.93	0.08	67,67,67,67	0
57	MG	2A	3620	1/1	0.93	0.24	71,71,71,71	0
57	MG	1A	3082	1/1	0.93	0.07	52,52,52,52	0
57	MG	1A	3948	1/1	0.93	0.22	40,40,40,40	0
57	MG	1A	3183	1/1	0.93	0.43	45,45,45,45	0
57	MG	1A	3856	1/1	0.93	0.19	49,49,49,49	0
57	MG	1A	4083	1/1	0.93	0.33	31,31,31,31	0
57	MG	1A	3011	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3066	1/1	0.93	0.31	31,31,31,31	0
57	MG	1A	3958	1/1	0.93	0.07	37,37,37,37	0
57	MG	2A	3394	1/1	0.93	0.24	57,57,57,57	0
57	MG	2A	3635	1/1	0.93	0.07	68,68,68,68	0
57	MG	1a	1732	1/1	0.93	0.12	53,53,53,53	0
57	MG	2A	3062	1/1	0.93	0.22	55,55,55,55	0
57	MG	1A	3364	1/1	0.93	0.28	34,34,34,34	0
57	MG	1A	3017	1/1	0.93	0.24	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1635	1/1	0.93	0.09	69,69,69,69	0
57	MG	1a	1735	1/1	0.93	0.20	58,58,58,58	0
57	MG	2A	3226	1/1	0.93	0.20	59,59,59,59	0
57	MG	1A	3963	1/1	0.93	0.13	34,34,34,34	0
57	MG	2A	3228	1/1	0.93	0.14	54,54,54,54	0
57	MG	2a	1640	1/1	0.93	0.12	67,67,67,67	0
57	MG	2a	1641	1/1	0.93	0.07	67,67,67,67	0
57	MG	1A	4096	1/1	0.93	0.14	50,50,50,50	0
57	MG	2A	3654	1/1	0.93	0.22	58,58,58,58	0
57	MG	1A	3071	1/1	0.93	0.42	47,47,47,47	0
57	MG	1A	3562	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3969	1/1	0.93	0.12	37,37,37,37	0
57	MG	15	105	1/1	0.93	0.18	43,43,43,43	0
57	MG	2a	1648	1/1	0.93	0.08	66,66,66,66	0
57	MG	1a	1742	1/1	0.93	0.11	65,65,65,65	0
57	MG	2A	3661	1/1	0.93	0.18	41,41,41,41	0
57	MG	1A	3407	1/1	0.93	0.31	43,43,43,43	0
57	MG	2A	3663	1/1	0.93	0.10	66,66,66,66	0
57	MG	2A	3418	1/1	0.93	0.22	28,28,28,28	0
57	MG	2a	1656	1/1	0.93	0.26	63,63,63,63	0
57	MG	2A	3665	1/1	0.93	0.06	70,70,70,70	0
57	MG	1A	3749	1/1	0.93	0.20	47,47,47,47	0
57	MG	2A	3423	1/1	0.93	0.14	64,64,64,64	0
57	MG	1A	3658	1/1	0.93	0.24	31,31,31,31	0
57	MG	2a	1662	1/1	0.93	0.07	51,51,51,51	0
57	MG	17	105	1/1	0.93	0.16	50,50,50,50	0
57	MG	18	101	1/1	0.93	0.52	53,53,53,53	0
57	MG	18	102	1/1	0.93	0.19	39,39,39,39	0
57	MG	2a	1668	1/1	0.93	0.09	58,58,58,58	0
57	MG	2a	1670	1/1	0.93	0.08	74,74,74,74	0
57	MG	1A	3263	1/1	0.93	0.40	39,39,39,39	0
57	MG	18	106	1/1	0.93	0.23	53,53,53,53	0
57	MG	2A	3438	1/1	0.93	0.19	69,69,69,69	0
57	MG	2A	3682	1/1	0.93	0.11	67,67,67,67	0
57	MG	1A	3978	1/1	0.93	0.07	66,66,66,66	0
57	MG	1a	1601	1/1	0.93	0.29	55,55,55,55	0
57	MG	1A	3875	1/1	0.93	0.08	31,31,31,31	0
57	MG	1A	3762	1/1	0.93	0.08	37,37,37,37	0
57	MG	1A	3264	1/1	0.93	0.25	49,49,49,49	0
57	MG	1A	3450	1/1	0.93	0.21	43,43,43,43	0
57	MG	1A	3194	1/1	0.93	0.14	22,22,22,22	0
57	MG	1A	3986	1/1	0.93	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
57	MG	2A	3697	1/1	0.93	0.06	72,72,72,72	0
57	MG	2A	3457	1/1	0.93	0.11	71,71,71,71	0
57	MG	2A	3458	1/1	0.93	0.16	46,46,46,46	0
57	MG	2A	3254	1/1	0.93	0.14	67,67,67,67	0
57	MG	1A	3769	1/1	0.93	0.08	57,57,57,57	0
57	MG	1A	3989	1/1	0.93	0.18	58,58,58,58	0
57	MG	1B	220	1/1	0.93	0.21	57,57,57,57	0
57	MG	2A	3465	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3770	1/1	0.93	0.18	68,68,68,68	0
57	MG	1A	3883	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3471	1/1	0.93	0.12	45,45,45,45	0
57	MG	1A	3302	1/1	0.93	0.16	54,54,54,54	0
57	MG	2A	3724	1/1	0.93	0.17	56,56,56,56	0
57	MG	2A	3726	1/1	0.93	0.10	61,61,61,61	0
57	MG	2A	3473	1/1	0.93	0.28	54,54,54,54	0
57	MG	2A	3475	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3053	1/1	0.93	0.14	33,33,33,33	0
57	MG	1A	3579	1/1	0.93	0.10	34,34,34,34	0
57	MG	1A	3890	1/1	0.93	0.13	31,31,31,31	0
57	MG	2A	3479	1/1	0.93	0.13	39,39,39,39	0
57	MG	1A	3508	1/1	0.93	0.25	36,36,36,36	0
57	MG	2A	3268	1/1	0.93	0.16	44,44,44,44	0
57	MG	1A	3781	1/1	0.93	0.14	31,31,31,31	0
57	MG	1A	3893	1/1	0.93	0.15	43,43,43,43	0
57	MG	1A	3020	1/1	0.93	0.21	26,26,26,26	0
57	MG	2A	3109	1/1	0.93	0.31	45,45,45,45	0
57	MG	1A	3455	1/1	0.93	0.24	28,28,28,28	0
57	MG	2A	3113	1/1	0.93	0.17	52,52,52,52	0
57	MG	1A	3784	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3273	1/1	0.93	0.29	51,51,51,51	0
57	MG	2a	1734	1/1	0.93	0.43	70,70,70,70	0
57	MG	2a	1735	1/1	0.93	0.15	52,52,52,52	0
57	MG	2a	1736	1/1	0.93	0.19	56,56,56,56	0
57	MG	2A	3117	1/1	0.93	0.11	54,54,54,54	0
57	MG	1A	3899	1/1	0.93	0.22	66,66,66,66	0
57	MG	1E	308	1/1	0.93	0.27	40,40,40,40	0
57	MG	1A	3589	1/1	0.93	0.20	32,32,32,32	0
57	MG	1A	3901	1/1	0.93	0.07	53,53,53,53	0
57	MG	2A	3123	1/1	0.93	0.16	57,57,57,57	0
57	MG	1a	1644	1/1	0.93	0.07	49,49,49,49	0
57	MG	1A	3679	1/1	0.93	0.14	66,66,66,66	0
57	MG	1a	1804	1/1	0.93	0.20	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3511	1/1	0.93	0.23	41,41,41,41	0
57	MG	1a	1646	1/1	0.93	0.09	54,54,54,54	0
57	MG	2A	3513	1/1	0.93	0.11	76,76,76,76	0
57	MG	1A	3791	1/1	0.93	0.24	40,40,40,40	0
57	MG	2a	1756	1/1	0.93	0.28	59,59,59,59	0
57	MG	1A	3590	1/1	0.93	0.18	24,24,24,24	0
57	MG	1A	3457	1/1	0.93	0.16	39,39,39,39	0
57	MG	1A	3683	1/1	0.93	0.08	62,62,62,62	0
57	MG	1A	3418	1/1	0.93	0.34	54,54,54,54	0
57	MG	2A	3139	1/1	0.93	0.16	61,61,61,61	0
57	MG	2A	3520	1/1	0.93	0.22	41,41,41,41	0
57	MG	2A	3521	1/1	0.93	0.17	45,45,45,45	0
57	MG	2a	1769	1/1	0.93	0.09	64,64,64,64	0
57	MG	1G	202	1/1	0.93	0.24	67,67,67,67	0
57	MG	2a	1772	1/1	0.93	0.17	62,62,62,62	0
57	MG	1A	3241	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3242	1/1	0.93	0.66	57,57,57,57	0
57	MG	2A	3527	1/1	0.93	0.25	59,59,59,59	0
57	MG	1a	1658	1/1	0.93	0.20	65,65,65,65	0
57	MG	2A	3530	1/1	0.93	0.30	39,39,39,39	0
57	MG	1A	4024	1/1	0.93	0.14	22,22,22,22	0
57	MG	1A	3465	1/1	0.93	0.16	52,52,52,52	0
57	MG	1A	3522	1/1	0.93	0.61	38,38,38,38	0
57	MG	1A	3466	1/1	0.93	0.37	56,56,56,56	0
57	MG	2B	206	1/1	0.93	0.21	73,73,73,73	0
57	MG	1A	3914	1/1	0.93	0.14	32,32,32,32	0
57	MG	2A	3154	1/1	0.93	0.10	60,60,60,60	0
57	MG	1A	3608	1/1	0.93	0.14	44,44,44,44	0
57	MG	1A	3611	1/1	0.93	0.18	42,42,42,42	0
57	MG	1P	201	1/1	0.93	0.54	32,32,32,32	0
57	MG	1a	1668	1/1	0.93	0.23	56,56,56,56	0
57	MG	1a	1670	1/1	0.93	0.16	75,75,75,75	0
57	MG	1x	105	1/1	0.93	0.20	63,63,63,63	0
57	MG	1A	3161	1/1	0.93	0.14	38,38,38,38	0
57	MG	2A	3553	1/1	0.93	0.15	61,61,61,61	0
57	MG	2D	304	1/1	0.93	0.19	27,27,27,27	0
57	MG	1A	3920	1/1	0.93	0.26	52,52,52,52	0
57	MG	1Q	202	1/1	0.93	0.17	35,35,35,35	0
57	MG	1A	4036	1/1	0.93	0.14	50,50,50,50	0
57	MG	1A	3921	1/1	0.93	0.12	27,27,27,27	0
57	MG	1A	3311	1/1	0.93	0.09	54,54,54,54	0
57	MG	2a	1813	1/1	0.93	0.22	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2E	304	1/1	0.93	0.22	34,34,34,34	0
57	MG	1A	3278	1/1	0.93	0.26	53,53,53,53	0
57	MG	1A	3472	1/1	0.93	0.37	35,35,35,35	0
57	MG	2E	307	1/1	0.93	0.20	45,45,45,45	0
57	MG	2E	309	1/1	0.93	0.11	67,67,67,67	0
57	MG	1A	3115	1/1	0.93	0.24	38,38,38,38	0
57	MG	1A	3534	1/1	0.93	0.15	40,40,40,40	0
57	MG	1A	3387	1/1	0.93	0.25	51,51,51,51	0
57	MG	1A	4050	1/1	0.93	0.11	61,61,61,61	0
57	MG	1A	3220	1/1	0.93	0.19	51,51,51,51	0
57	MG	2F	306	1/1	0.93	0.41	48,48,48,48	0
57	MG	2A	3012	1/1	0.93	0.21	48,48,48,48	0
57	MG	1A	3078	1/1	0.93	0.22	34,34,34,34	0
57	MG	2q	201	1/1	0.93	0.08	77,77,77,77	0
57	MG	1A	3478	1/1	0.93	0.08	74,74,74,74	0
57	MG	1A	4056	1/1	0.93	0.08	50,50,50,50	0
57	MG	1A	3828	1/1	0.93	0.42	38,38,38,38	0
57	MG	2A	3349	1/1	0.93	0.39	54,54,54,54	0
57	MG	2v	104	1/1	0.93	0.31	62,62,62,62	0
57	MG	1A	3145	1/1	0.93	0.57	39,39,39,39	0
57	MG	1A	3629	1/1	0.93	0.14	21,21,21,21	0
57	MG	1A	3351	1/1	0.93	0.57	47,47,47,47	0
57	MG	2w	107	1/1	0.93	0.17	70,70,70,70	0
57	MG	2x	101	1/1	0.93	0.27	68,68,68,68	0
57	MG	2A	3188	1/1	0.93	0.30	51,51,51,51	0
57	MG	2A	3355	1/1	0.93	0.20	42,42,42,42	0
57	MG	1A	3047	1/1	0.93	0.30	34,34,34,34	0
57	MG	1a	1702	1/1	0.93	0.23	38,38,38,38	0
57	MG	2x	106	1/1	0.93	0.09	67,67,67,67	0
57	MG	1A	3433	1/1	0.93	0.21	47,47,47,47	0
57	MG	1A	3048	1/1	0.93	0.16	27,27,27,27	0
57	MG	1A	4072	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3595	1/1	0.93	0.32	56,56,56,56	0
58	K	1A	3512	1/1	0.93	0.12	54,54,54,54	0
59	TYK	2A	3798	64/64	0.93	0.26	32,46,61,66	0
57	MG	25	104	1/1	0.93	0.16	57,57,57,57	0
57	MG	1Y	202	1/1	0.93	0.54	46,46,46,46	0
57	MG	2A	3034	1/1	0.93	0.25	60,60,60,60	0
60	ZN	29	102	1/1	0.93	0.09	78,78,78,78	0
57	MG	1S	201	1/1	0.94	0.35	44,44,44,44	0
57	MG	28	103	1/1	0.94	0.36	57,57,57,57	0
57	MG	1A	4046	1/1	0.94	0.16	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
57	MG	28	105	1/1	0.94	0.12	63,63,63,63	0
57	MG	29	101	1/1	0.94	0.30	69,69,69,69	0
57	MG	2a	1601	1/1	0.94	0.22	81,81,81,81	0
57	MG	1A	3059	1/1	0.94	0.25	44,44,44,44	0
57	MG	2a	1603	1/1	0.94	0.12	58,58,58,58	0
57	MG	1a	1683	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	3606	1/1	0.94	0.10	31,31,31,31	0
57	MG	2A	3607	1/1	0.94	0.14	50,50,50,50	0
57	MG	1A	3250	1/1	0.94	0.13	51,51,51,51	0
57	MG	2A	3372	1/1	0.94	0.12	59,59,59,59	0
57	MG	2a	1609	1/1	0.94	0.06	71,71,71,71	0
57	MG	1U	202	1/1	0.94	0.29	36,36,36,36	0
57	MG	1A	4052	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	4053	1/1	0.94	0.17	24,24,24,24	0
57	MG	1U	206	1/1	0.94	0.22	33,33,33,33	0
57	MG	1A	3825	1/1	0.94	0.13	38,38,38,38	0
57	MG	2A	3380	1/1	0.94	0.23	58,58,58,58	0
57	MG	1A	3195	1/1	0.94	0.15	34,34,34,34	0
57	MG	2A	3028	1/1	0.94	0.29	50,50,50,50	0
57	MG	1A	3098	1/1	0.94	0.27	35,35,35,35	0
57	MG	2A	3384	1/1	0.94	0.15	63,63,63,63	0
57	MG	2A	3200	1/1	0.94	0.34	60,60,60,60	0
57	MG	2a	1621	1/1	0.94	0.20	61,61,61,61	0
57	MG	1A	3253	1/1	0.94	0.15	60,60,60,60	0
57	MG	1A	3518	1/1	0.94	0.40	54,54,54,54	0
57	MG	1A	3834	1/1	0.94	0.26	49,49,49,49	0
57	MG	1A	3013	1/1	0.94	0.24	29,29,29,29	0
57	MG	1A	3347	1/1	0.94	0.21	47,47,47,47	0
57	MG	2A	3393	1/1	0.94	0.22	43,43,43,43	0
57	MG	2A	3038	1/1	0.94	0.10	70,70,70,70	0
57	MG	1W	205	1/1	0.94	0.09	35,35,35,35	0
57	MG	1W	206	1/1	0.94	0.17	28,28,28,28	0
57	MG	1a	1706	1/1	0.94	0.25	63,63,63,63	0
57	MG	1A	3004	1/1	0.94	0.12	25,25,25,25	0
57	MG	1X	104	1/1	0.94	0.21	40,40,40,40	0
57	MG	1A	3842	1/1	0.94	0.14	23,23,23,23	0
57	MG	1A	3257	1/1	0.94	0.34	58,58,58,58	0
57	MG	1A	3458	1/1	0.94	0.19	55,55,55,55	0
57	MG	2A	3650	1/1	0.94	0.37	47,47,47,47	0
57	MG	1A	3530	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3408	1/1	0.94	0.10	65,65,65,65	0
57	MG	2A	3655	1/1	0.94	0.12	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3847	1/1	0.94	0.14	42,42,42,42	0
57	MG	1A	3950	1/1	0.94	0.08	58,58,58,58	0
57	MG	1a	1719	1/1	0.94	0.06	82,82,82,82	0
57	MG	1A	3951	1/1	0.94	0.22	52,52,52,52	0
57	MG	1A	3033	1/1	0.94	0.71	39,39,39,39	0
57	MG	1A	3460	1/1	0.94	0.09	51,51,51,51	0
57	MG	2A	3417	1/1	0.94	0.22	63,63,63,63	0
57	MG	1A	4081	1/1	0.94	0.07	57,57,57,57	0
57	MG	2A	3059	1/1	0.94	0.36	55,55,55,55	0
57	MG	1A	3954	1/1	0.94	0.25	31,31,31,31	0
57	MG	1A	3733	1/1	0.94	0.11	36,36,36,36	0
57	MG	2A	3426	1/1	0.94	0.11	44,44,44,44	0
57	MG	2a	1657	1/1	0.94	0.07	62,62,62,62	0
57	MG	11	101	1/1	0.94	1.08	39,39,39,39	0
57	MG	2A	3429	1/1	0.94	0.25	67,67,67,67	0
57	MG	2A	3672	1/1	0.94	0.07	65,65,65,65	0
57	MG	1A	3734	1/1	0.94	0.14	27,27,27,27	0
57	MG	1A	3225	1/1	0.94	0.22	61,61,61,61	0
57	MG	11	104	1/1	0.94	0.14	78,78,78,78	0
57	MG	2A	3434	1/1	0.94	0.20	38,38,38,38	0
57	MG	2A	3679	1/1	0.94	0.10	71,71,71,71	0
57	MG	2A	3234	1/1	0.94	0.28	62,62,62,62	0
57	MG	2a	1669	1/1	0.94	0.24	72,72,72,72	0
57	MG	1A	4089	1/1	0.94	0.30	58,58,58,58	0
57	MG	2a	1673	1/1	0.94	0.12	64,64,64,64	0
57	MG	2A	3683	1/1	0.94	0.13	72,72,72,72	0
57	MG	2a	1679	1/1	0.94	0.27	69,69,69,69	0
57	MG	2A	3684	1/1	0.94	0.17	50,50,50,50	0
57	MG	2A	3068	1/1	0.94	0.34	44,44,44,44	0
57	MG	1A	3961	1/1	0.94	0.19	64,64,64,64	0
57	MG	2A	3442	1/1	0.94	0.18	41,41,41,41	0
57	MG	1A	3106	1/1	0.94	0.35	40,40,40,40	0
57	MG	1A	3050	1/1	0.94	0.11	45,45,45,45	0
57	MG	2A	3691	1/1	0.94	0.10	57,57,57,57	0
57	MG	1A	3410	1/1	0.94	0.17	31,31,31,31	0
57	MG	2A	3693	1/1	0.94	0.17	71,71,71,71	0
57	MG	1A	3966	1/1	0.94	0.20	40,40,40,40	0
57	MG	1A	3228	1/1	0.94	0.17	24,24,24,24	0
57	MG	1A	3539	1/1	0.94	0.18	49,49,49,49	0
57	MG	2A	3453	1/1	0.94	0.16	38,38,38,38	0
57	MG	2A	3702	1/1	0.94	0.15	69,69,69,69	0
57	MG	1A	3229	1/1	0.94	0.17	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
57	MG	1A	3470	1/1	0.94	0.59	35,35,35,35	0
57	MG	1A	3108	1/1	0.94	0.29	37,37,37,37	0
57	MG	2a	1702	1/1	0.94	0.27	64,64,64,64	0
57	MG	1A	3872	1/1	0.94	0.16	41,41,41,41	0
57	MG	17	101	1/1	0.94	0.11	32,32,32,32	0
57	MG	2A	3250	1/1	0.94	0.25	57,57,57,57	0
57	MG	2a	1709	1/1	0.94	0.21	72,72,72,72	0
57	MG	1a	1746	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3083	1/1	0.94	0.12	75,75,75,75	0
57	MG	1A	3231	1/1	0.94	0.58	42,42,42,42	0
57	MG	1B	205	1/1	0.94	0.29	58,58,58,58	0
57	MG	2A	3723	1/1	0.94	0.26	43,43,43,43	0
57	MG	2A	3256	1/1	0.94	0.11	73,73,73,73	0
57	MG	1A	3750	1/1	0.94	0.19	53,53,53,53	0
57	MG	2A	3727	1/1	0.94	0.26	50,50,50,50	0
57	MG	2a	1718	1/1	0.94	0.22	82,82,82,82	0
57	MG	2A	3729	1/1	0.94	0.10	74,74,74,74	0
57	MG	2A	3474	1/1	0.94	0.18	78,78,78,78	0
57	MG	1A	3754	1/1	0.94	0.16	19,19,19,19	0
57	MG	1a	1758	1/1	0.94	0.06	63,63,63,63	0
57	MG	1A	3232	1/1	0.94	0.10	46,46,46,46	0
57	MG	18	105	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3756	1/1	0.94	0.06	39,39,39,39	0
57	MG	1A	3142	1/1	0.94	0.16	32,32,32,32	0
57	MG	1a	1765	1/1	0.94	0.14	57,57,57,57	0
57	MG	1a	1766	1/1	0.94	0.15	64,64,64,64	0
57	MG	19	101	1/1	0.94	0.21	52,52,52,52	0
57	MG	2A	3744	1/1	0.94	0.16	43,43,43,43	0
57	MG	2A	3097	1/1	0.94	0.46	50,50,50,50	0
57	MG	2A	3269	1/1	0.94	0.24	66,66,66,66	0
57	MG	2A	3747	1/1	0.94	0.15	58,58,58,58	0
57	MG	1A	3317	1/1	0.94	0.43	41,41,41,41	0
57	MG	1A	3551	1/1	0.94	0.14	33,33,33,33	0
57	MG	1A	3274	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3495	1/1	0.94	0.17	63,63,63,63	0
57	MG	1A	3007	1/1	0.94	0.17	35,35,35,35	0
57	MG	1A	3369	1/1	0.94	0.12	55,55,55,55	0
57	MG	1a	1606	1/1	0.94	0.26	60,60,60,60	0
57	MG	2A	3104	1/1	0.94	0.23	55,55,55,55	0
57	MG	2a	1747	1/1	0.94	0.12	72,72,72,72	0
57	MG	1a	1609	1/1	0.94	0.36	56,56,56,56	0
57	MG	2A	3504	1/1	0.94	0.24	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3281	1/1	0.94	0.24	67,67,67,67	0
57	MG	2A	3763	1/1	0.94	0.22	60,60,60,60	0
57	MG	1A	3206	1/1	0.94	0.11	39,39,39,39	0
57	MG	1A	3236	1/1	0.94	0.30	36,36,36,36	0
57	MG	1a	1614	1/1	0.94	0.24	56,56,56,56	0
57	MG	2a	1757	1/1	0.94	0.23	69,69,69,69	0
57	MG	2A	3111	1/1	0.94	0.33	57,57,57,57	0
57	MG	1A	3325	1/1	0.94	0.27	39,39,39,39	0
57	MG	1a	1616	1/1	0.94	0.13	61,61,61,61	0
57	MG	1A	3559	1/1	0.94	0.28	44,44,44,44	0
57	MG	1A	3560	1/1	0.94	0.17	21,21,21,21	0
57	MG	1A	3999	1/1	0.94	0.26	34,34,34,34	0
57	MG	1A	3780	1/1	0.94	0.11	37,37,37,37	0
57	MG	1A	3666	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	4002	1/1	0.94	0.11	34,34,34,34	0
57	MG	2a	1771	1/1	0.94	0.19	76,76,76,76	0
57	MG	1A	3087	1/1	0.94	0.20	27,27,27,27	0
57	MG	1A	3113	1/1	0.94	0.18	34,34,34,34	0
57	MG	2A	3789	1/1	0.94	0.31	55,55,55,55	0
57	MG	1A	3281	1/1	0.94	0.13	58,58,58,58	0
57	MG	1a	1798	1/1	0.94	0.15	70,70,70,70	0
57	MG	1E	303	1/1	0.94	0.22	36,36,36,36	0
57	MG	2A	3130	1/1	0.94	0.24	43,43,43,43	0
57	MG	1A	3010	1/1	0.94	0.16	31,31,31,31	0
57	MG	1A	3184	1/1	0.94	0.15	30,30,30,30	0
57	MG	1a	1635	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3533	1/1	0.94	0.12	60,60,60,60	0
57	MG	2a	1787	1/1	0.94	0.20	67,67,67,67	0
57	MG	1A	3787	1/1	0.94	0.28	62,62,62,62	0
57	MG	2a	1789	1/1	0.94	0.20	60,60,60,60	0
57	MG	2A	3135	1/1	0.94	0.34	44,44,44,44	0
57	MG	1A	3788	1/1	0.94	0.20	59,59,59,59	0
57	MG	2a	1792	1/1	0.94	0.15	76,76,76,76	0
57	MG	1F	301	1/1	0.94	0.23	34,34,34,34	0
57	MG	1A	3005	1/1	0.94	0.23	45,45,45,45	0
57	MG	1A	3790	1/1	0.94	0.16	70,70,70,70	0
57	MG	2A	3141	1/1	0.94	0.16	50,50,50,50	0
57	MG	2A	3142	1/1	0.94	0.16	62,62,62,62	0
57	MG	1A	3380	1/1	0.94	0.10	68,68,68,68	0
57	MG	2a	1801	1/1	0.94	0.09	83,83,83,83	0
57	MG	2B	216	1/1	0.94	0.14	68,68,68,68	0
57	MG	2A	3546	1/1	0.94	0.15	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3676	1/1	0.94	0.15	45,45,45,45	0
57	MG	1a	1643	1/1	0.94	0.17	67,67,67,67	0
57	MG	1A	3572	1/1	0.94	0.13	21,21,21,21	0
57	MG	1A	3213	1/1	0.94	0.50	45,45,45,45	0
57	MG	2A	3149	1/1	0.94	0.43	72,72,72,72	0
57	MG	1A	3382	1/1	0.94	0.12	59,59,59,59	0
57	MG	1e	201	1/1	0.94	0.12	72,72,72,72	0
57	MG	1f	201	1/1	0.94	0.16	41,41,41,41	0
57	MG	1m	3001	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3329	1/1	0.94	0.27	43,43,43,43	0
57	MG	1A	4021	1/1	0.94	0.21	19,19,19,19	0
57	MG	1A	3437	1/1	0.94	0.11	45,45,45,45	0
57	MG	2E	308	1/1	0.94	0.08	61,61,61,61	0
57	MG	1A	3383	1/1	0.94	0.22	54,54,54,54	0
57	MG	2A	3336	1/1	0.94	0.28	47,47,47,47	0
57	MG	1A	3044	1/1	0.94	0.16	35,35,35,35	0
57	MG	1A	3913	1/1	0.94	0.06	43,43,43,43	0
57	MG	1A	3499	1/1	0.94	0.07	58,58,58,58	0
57	MG	2A	3572	1/1	0.94	0.10	56,56,56,56	0
57	MG	1N	203	1/1	0.94	0.12	44,44,44,44	0
57	MG	1A	3385	1/1	0.94	0.35	63,63,63,63	0
57	MG	1O	202	1/1	0.94	0.30	50,50,50,50	0
57	MG	1A	3386	1/1	0.94	0.20	48,48,48,48	0
57	MG	1A	3045	1/1	0.94	0.15	39,39,39,39	0
57	MG	1A	3919	1/1	0.94	0.22	51,51,51,51	0
57	MG	2w	101	1/1	0.94	0.38	66,66,66,66	0
57	MG	1O	206	1/1	0.94	0.24	65,65,65,65	0
57	MG	2A	3581	1/1	0.94	0.20	64,64,64,64	0
57	MG	2Q	204	1/1	0.94	0.18	77,77,77,77	0
57	MG	2R	201	1/1	0.94	0.34	50,50,50,50	0
57	MG	1A	3594	1/1	0.94	0.08	58,58,58,58	0
57	MG	1A	3504	1/1	0.94	0.37	37,37,37,37	0
57	MG	1P	204	1/1	0.94	0.72	28,28,28,28	0
57	MG	2A	3585	1/1	0.94	0.28	57,57,57,57	0
57	MG	1A	3811	1/1	0.94	0.07	64,64,64,64	0
57	MG	1A	3245	1/1	0.94	0.14	77,77,77,77	0
57	MG	1A	3816	1/1	0.94	0.65	41,41,41,41	0
57	MG	1R	202	1/1	0.94	0.30	37,37,37,37	0
57	MG	21	102	1/1	0.94	0.14	68,68,68,68	0
57	MG	23	102	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3151	1/1	0.94	0.54	39,39,39,39	0
57	MG	1R	204	1/1	0.94	0.21	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
60	ZN	1Y	203	1/1	0.94	0.12	68,68,68,68	0
57	MG	1A	3217	1/1	0.94	0.12	22,22,22,22	0
57	MG	27	101	1/1	0.94	0.27	59,59,59,59	0
57	MG	1A	3391	1/1	0.94	0.20	36,36,36,36	0
57	MG	2A	3008	1/1	0.94	0.20	49,49,49,49	0
60	ZN	2n	501	1/1	0.94	0.07	86,86,86,86	0
57	MG	2A	3454	1/1	0.95	0.17	35,35,35,35	0
57	MG	2A	3118	1/1	0.95	0.18	49,49,49,49	0
57	MG	1A	4068	1/1	0.95	0.29	36,36,36,36	0
57	MG	2a	1629	1/1	0.95	0.31	73,73,73,73	0
57	MG	2A	3272	1/1	0.95	0.30	52,52,52,52	0
57	MG	2A	3676	1/1	0.95	0.07	61,61,61,61	0
57	MG	1A	4069	1/1	0.95	0.09	63,63,63,63	0
57	MG	1A	4070	1/1	0.95	0.15	45,45,45,45	0
57	MG	2A	3462	1/1	0.95	0.23	31,31,31,31	0
57	MG	1A	3771	1/1	0.95	0.14	73,73,73,73	0
57	MG	2A	3681	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3464	1/1	0.95	0.24	59,59,59,59	0
57	MG	1A	3591	1/1	0.95	0.22	54,54,54,54	0
57	MG	1A	3965	1/1	0.95	0.11	32,32,32,32	0
57	MG	2A	3469	1/1	0.95	0.15	39,39,39,39	0
57	MG	1A	3592	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3593	1/1	0.95	0.09	22,22,22,22	0
57	MG	2A	3128	1/1	0.95	0.25	56,56,56,56	0
57	MG	2A	3129	1/1	0.95	0.29	41,41,41,41	0
57	MG	1A	3473	1/1	0.95	0.60	38,38,38,38	0
57	MG	1e	202	1/1	0.95	0.40	58,58,58,58	0
57	MG	1A	3779	1/1	0.95	0.10	30,30,30,30	0
57	MG	1h	201	1/1	0.95	0.29	66,66,66,66	0
57	MG	1T	203	1/1	0.95	0.20	62,62,62,62	0
57	MG	1A	3972	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3595	1/1	0.95	0.15	36,36,36,36	0
57	MG	1a	1669	1/1	0.95	0.18	64,64,64,64	0
57	MG	1U	204	1/1	0.95	0.18	35,35,35,35	0
57	MG	1A	3248	1/1	0.95	0.19	32,32,32,32	0
57	MG	1A	3064	1/1	0.95	0.37	48,48,48,48	0
57	MG	1A	3976	1/1	0.95	0.12	57,57,57,57	0
57	MG	1a	1675	1/1	0.95	0.28	58,58,58,58	0
57	MG	1A	4084	1/1	0.95	0.22	73,73,73,73	0
57	MG	1A	3172	1/1	0.95	0.12	35,35,35,35	0
57	MG	1V	201	1/1	0.95	0.27	28,28,28,28	0
57	MG	1A	3065	1/1	0.95	0.19	14,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4088	1/1	0.95	0.19	75,75,75,75	0
57	MG	1A	3980	1/1	0.95	0.05	54,54,54,54	0
57	MG	1A	3284	1/1	0.95	0.27	41,41,41,41	0
57	MG	1A	4092	1/1	0.95	0.10	72,72,72,72	0
57	MG	1A	3353	1/1	0.95	0.20	55,55,55,55	0
57	MG	1A	3692	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3310	1/1	0.95	0.17	64,64,64,64	0
57	MG	1A	3392	1/1	0.95	0.24	49,49,49,49	0
57	MG	2A	3732	1/1	0.95	0.11	64,64,64,64	0
57	MG	2a	1681	1/1	0.95	0.33	35,35,35,35	0
57	MG	1A	3393	1/1	0.95	0.38	47,47,47,47	0
57	MG	1A	3436	1/1	0.95	0.18	46,46,46,46	0
57	MG	1A	3609	1/1	0.95	0.22	39,39,39,39	0
57	MG	2a	1685	1/1	0.95	0.17	65,65,65,65	0
57	MG	2A	3004	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3737	1/1	0.95	0.18	48,48,48,48	0
57	MG	2A	3738	1/1	0.95	0.10	58,58,58,58	0
57	MG	2a	1690	1/1	0.95	0.08	66,66,66,66	0
57	MG	1A	3700	1/1	0.95	0.18	24,24,24,24	0
57	MG	2a	1692	1/1	0.95	0.12	73,73,73,73	0
57	MG	2A	3163	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3176	1/1	0.95	0.20	48,48,48,48	0
57	MG	10	101	1/1	0.95	0.30	43,43,43,43	0
57	MG	1A	3043	1/1	0.95	0.22	42,42,42,42	0
57	MG	1A	3081	1/1	0.95	0.27	37,37,37,37	0
57	MG	2A	3323	1/1	0.95	0.07	67,67,67,67	0
57	MG	1A	3544	1/1	0.95	0.25	27,27,27,27	0
57	MG	2A	3748	1/1	0.95	0.20	68,68,68,68	0
57	MG	1a	1703	1/1	0.95	0.26	53,53,53,53	0
57	MG	1A	3995	1/1	0.95	0.14	37,37,37,37	0
57	MG	2A	3172	1/1	0.95	0.13	56,56,56,56	0
57	MG	1A	3797	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3707	1/1	0.95	0.14	67,67,67,67	0
57	MG	2A	3331	1/1	0.95	0.37	48,48,48,48	0
57	MG	2A	3333	1/1	0.95	0.26	61,61,61,61	0
57	MG	1B	209	1/1	0.95	0.25	57,57,57,57	0
57	MG	2A	3759	1/1	0.95	0.18	64,64,64,64	0
57	MG	1A	3489	1/1	0.95	0.27	38,38,38,38	0
57	MG	2A	3024	1/1	0.95	0.12	39,39,39,39	0
57	MG	2A	3338	1/1	0.95	0.18	39,39,39,39	0
57	MG	2A	3179	1/1	0.95	0.68	65,65,65,65	0
57	MG	10	110	1/1	0.95	0.07	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
57	MG	2A	3767	1/1	0.95	0.28	66,66,66,66	0
57	MG	1A	3802	1/1	0.95	0.25	50,50,50,50	0
57	MG	2A	3342	1/1	0.95	0.42	54,54,54,54	0
57	MG	2A	3772	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3289	1/1	0.95	0.47	56,56,56,56	0
57	MG	1A	3290	1/1	0.95	0.15	35,35,35,35	0
57	MG	2a	1724	1/1	0.95	0.12	69,69,69,69	0
57	MG	2A	3345	1/1	0.95	0.17	56,56,56,56	0
57	MG	1A	3713	1/1	0.95	0.17	51,51,51,51	0
57	MG	1A	3548	1/1	0.95	0.16	36,36,36,36	0
57	MG	2A	3779	1/1	0.95	0.20	82,82,82,82	0
57	MG	2A	3031	1/1	0.95	0.12	47,47,47,47	0
57	MG	1A	3323	1/1	0.95	0.18	35,35,35,35	0
57	MG	1A	3622	1/1	0.95	0.11	39,39,39,39	0
57	MG	1A	3182	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3624	1/1	0.95	0.12	29,29,29,29	0
57	MG	1B	223	1/1	0.95	0.11	58,58,58,58	0
57	MG	1A	3129	1/1	0.95	0.16	39,39,39,39	0
57	MG	2A	3790	1/1	0.95	0.17	60,60,60,60	0
57	MG	1A	3132	1/1	0.95	0.12	29,29,29,29	0
57	MG	2A	3041	1/1	0.95	0.08	62,62,62,62	0
57	MG	1A	3917	1/1	0.95	0.22	52,52,52,52	0
57	MG	1B	228	1/1	0.95	0.30	77,77,77,77	0
57	MG	2a	1742	1/1	0.95	0.24	47,47,47,47	0
57	MG	2a	1743	1/1	0.95	0.15	69,69,69,69	0
57	MG	1A	3404	1/1	0.95	0.29	37,37,37,37	0
57	MG	2A	3796	1/1	0.95	0.40	77,77,77,77	0
57	MG	1B	230	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3094	1/1	0.95	0.13	66,66,66,66	0
57	MG	1A	3295	1/1	0.95	0.37	63,63,63,63	0
57	MG	2B	203	1/1	0.95	0.15	73,73,73,73	0
57	MG	2a	1752	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3571	1/1	0.95	0.17	46,46,46,46	0
57	MG	2B	205	1/1	0.95	0.17	57,57,57,57	0
57	MG	1A	3211	1/1	0.95	0.20	45,45,45,45	0
57	MG	1D	301	1/1	0.95	0.27	36,36,36,36	0
57	MG	1A	3408	1/1	0.95	0.55	46,46,46,46	0
57	MG	2A	3204	1/1	0.95	0.40	48,48,48,48	0
57	MG	1A	3038	1/1	0.95	0.39	36,36,36,36	0
57	MG	1D	312	1/1	0.95	0.27	39,39,39,39	0
57	MG	2a	1762	1/1	0.95	0.22	63,63,63,63	0
57	MG	2A	3370	1/1	0.95	0.41	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
57	MG	2A	3207	1/1	0.95	0.30	56,56,56,56	0
57	MG	1E	301	1/1	0.95	0.36	36,36,36,36	0
57	MG	2B	218	1/1	0.95	0.20	78,78,78,78	0
57	MG	1A	3826	1/1	0.95	0.26	41,41,41,41	0
57	MG	1A	3189	1/1	0.95	0.50	38,38,38,38	0
57	MG	1E	304	1/1	0.95	0.22	29,29,29,29	0
57	MG	2A	3212	1/1	0.95	0.20	58,58,58,58	0
57	MG	1A	3640	1/1	0.95	0.20	22,22,22,22	0
57	MG	2A	3587	1/1	0.95	0.14	68,68,68,68	0
57	MG	1A	3735	1/1	0.95	0.20	25,25,25,25	0
57	MG	1A	3190	1/1	0.95	0.17	46,46,46,46	0
57	MG	1A	3412	1/1	0.95	0.21	48,48,48,48	0
57	MG	1a	1748	1/1	0.95	0.14	71,71,71,71	0
57	MG	2A	3592	1/1	0.95	0.28	36,36,36,36	0
57	MG	1a	1749	1/1	0.95	0.06	73,73,73,73	0
57	MG	1a	1750	1/1	0.95	0.07	64,64,64,64	0
57	MG	2A	3387	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3597	1/1	0.95	0.13	74,74,74,74	0
57	MG	2A	3598	1/1	0.95	0.17	61,61,61,61	0
57	MG	2A	3599	1/1	0.95	0.20	67,67,67,67	0
57	MG	1a	1751	1/1	0.95	0.17	64,64,64,64	0
57	MG	2A	3601	1/1	0.95	0.08	68,68,68,68	0
57	MG	1A	3644	1/1	0.95	0.17	26,26,26,26	0
57	MG	1a	1753	1/1	0.95	0.10	66,66,66,66	0
57	MG	1F	302	1/1	0.95	0.22	33,33,33,33	0
57	MG	1F	304	1/1	0.95	0.09	69,69,69,69	0
57	MG	1a	1757	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3021	1/1	0.95	0.26	47,47,47,47	0
57	MG	2A	3396	1/1	0.95	0.42	48,48,48,48	0
57	MG	1a	1613	1/1	0.95	0.06	62,62,62,62	0
57	MG	2a	1802	1/1	0.95	0.38	55,55,55,55	0
57	MG	1A	3073	1/1	0.95	0.17	31,31,31,31	0
57	MG	1A	3303	1/1	0.95	0.19	56,56,56,56	0
57	MG	1F	310	1/1	0.95	0.17	29,29,29,29	0
57	MG	2a	1807	1/1	0.95	0.04	69,69,69,69	0
57	MG	1a	1619	1/1	0.95	0.14	51,51,51,51	0
57	MG	2A	3616	1/1	0.95	0.15	49,49,49,49	0
57	MG	1A	3569	1/1	0.95	0.13	39,39,39,39	0
57	MG	2V	201	1/1	0.95	0.87	51,51,51,51	0
57	MG	1A	3650	1/1	0.95	0.11	61,61,61,61	0
57	MG	1A	3338	1/1	0.95	0.62	48,48,48,48	0
57	MG	2X	101	1/1	0.95	0.20	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
57	MG	1A	3748	1/1	0.95	0.19	51,51,51,51	0
57	MG	1G	201	1/1	0.95	0.17	39,39,39,39	0
57	MG	2A	3624	1/1	0.95	0.13	33,33,33,33	0
57	MG	1A	3377	1/1	0.95	0.17	37,37,37,37	0
57	MG	1A	3040	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3627	1/1	0.95	0.21	61,61,61,61	0
57	MG	1a	1628	1/1	0.95	0.14	43,43,43,43	0
57	MG	2A	3414	1/1	0.95	0.26	62,62,62,62	0
57	MG	1G	204	1/1	0.95	0.13	62,62,62,62	0
57	MG	2j	201	1/1	0.95	0.07	74,74,74,74	0
57	MG	1A	3752	1/1	0.95	0.17	20,20,20,20	0
57	MG	1A	3945	1/1	0.95	0.18	26,26,26,26	0
57	MG	1A	3116	1/1	0.95	0.54	45,45,45,45	0
57	MG	1A	3577	1/1	0.95	0.06	56,56,56,56	0
57	MG	2A	3421	1/1	0.95	0.19	39,39,39,39	0
57	MG	1a	1783	1/1	0.95	0.13	64,64,64,64	0
57	MG	1A	3578	1/1	0.95	0.25	35,35,35,35	0
57	MG	1N	205	1/1	0.95	0.19	44,44,44,44	0
57	MG	1A	3162	1/1	0.95	0.27	42,42,42,42	0
57	MG	1A	3758	1/1	0.95	0.10	49,49,49,49	0
57	MG	1A	3862	1/1	0.95	0.17	47,47,47,47	0
57	MG	2A	3431	1/1	0.95	0.23	53,53,53,53	0
57	MG	1A	3036	1/1	0.95	0.19	28,28,28,28	0
57	MG	1A	3520	1/1	0.95	0.40	40,40,40,40	0
57	MG	2A	3653	1/1	0.95	0.26	64,64,64,64	0
57	MG	1a	1794	1/1	0.95	0.15	57,57,57,57	0
57	MG	1A	4059	1/1	0.95	0.20	61,61,61,61	0
57	MG	1A	3765	1/1	0.95	0.22	54,54,54,54	0
57	MG	1A	3123	1/1	0.95	0.30	52,52,52,52	0
57	MG	1A	3767	1/1	0.95	0.14	38,38,38,38	0
57	MG	1A	3168	1/1	0.95	0.24	37,37,37,37	0
57	MG	2A	3443	1/1	0.95	0.12	44,44,44,44	0
57	MG	2A	3445	1/1	0.95	0.25	36,36,36,36	0
57	MG	1A	3345	1/1	0.95	0.10	43,43,43,43	0
59	TYK	1A	4101	64/64	0.95	0.23	16,30,46,51	0
57	MG	2A	3263	1/1	0.95	0.12	73,73,73,73	0
57	MG	1Q	203	1/1	0.95	0.22	52,52,52,52	0
57	MG	1a	1649	1/1	0.95	0.23	46,46,46,46	0
57	MG	1A	3200	1/1	0.95	0.26	36,36,36,36	0
57	MG	1Q	205	1/1	0.95	0.18	46,46,46,46	0
57	MG	1Q	206	1/1	0.95	0.18	43,43,43,43	0
57	MG	2A	3670	1/1	0.95	0.21	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	1649	1/1	0.96	0.27	67,67,67,67	0
57	MG	1A	3009	1/1	0.96	0.12	22,22,22,22	0
57	MG	2A	3110	1/1	0.96	0.10	76,76,76,76	0
57	MG	1D	310	1/1	0.96	0.27	26,26,26,26	0
57	MG	1A	3426	1/1	0.96	0.12	43,43,43,43	0
57	MG	1l	3200	1/1	0.96	0.12	71,71,71,71	0
57	MG	2A	3550	1/1	0.96	0.12	68,68,68,68	0
57	MG	2A	3551	1/1	0.96	0.22	40,40,40,40	0
57	MG	1A	3104	1/1	0.96	0.50	29,29,29,29	0
57	MG	1A	4041	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3177	1/1	0.96	0.18	54,54,54,54	0
57	MG	1A	3649	1/1	0.96	0.15	28,28,28,28	0
57	MG	2A	3558	1/1	0.96	0.09	46,46,46,46	0
57	MG	1a	1695	1/1	0.96	0.14	43,43,43,43	0
57	MG	2A	3389	1/1	0.96	0.15	54,54,54,54	0
57	MG	1w	102	1/1	0.96	0.16	49,49,49,49	0
57	MG	1A	3008	1/1	0.96	0.15	26,26,26,26	0
57	MG	1A	3652	1/1	0.96	0.14	40,40,40,40	0
57	MG	1E	306	1/1	0.96	0.21	23,23,23,23	0
57	MG	2a	1672	1/1	0.96	0.12	56,56,56,56	0
57	MG	2A	3255	1/1	0.96	0.26	65,65,65,65	0
57	MG	1A	4047	1/1	0.96	0.16	55,55,55,55	0
57	MG	2a	1676	1/1	0.96	0.31	61,61,61,61	0
57	MG	13	105	1/1	0.96	0.17	52,52,52,52	0
57	MG	2A	3756	1/1	0.96	0.28	48,48,48,48	0
57	MG	1A	3955	1/1	0.96	0.16	16,16,16,16	0
57	MG	2A	3398	1/1	0.96	0.37	62,62,62,62	0
57	MG	1E	309	1/1	0.96	0.14	51,51,51,51	0
57	MG	1A	3023	1/1	0.96	0.23	55,55,55,55	0
57	MG	2A	3401	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3725	1/1	0.96	0.16	27,27,27,27	0
57	MG	2a	1687	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	3180	1/1	0.96	0.31	50,50,50,50	0
57	MG	2A	3764	1/1	0.96	0.16	73,73,73,73	0
57	MG	2A	3577	1/1	0.96	0.20	53,53,53,53	0
57	MG	1a	1709	1/1	0.96	0.14	41,41,41,41	0
57	MG	1F	303	1/1	0.96	0.19	31,31,31,31	0
57	MG	2A	3406	1/1	0.96	0.18	65,65,65,65	0
57	MG	2A	3770	1/1	0.96	0.10	58,58,58,58	0
57	MG	2A	3771	1/1	0.96	0.12	61,61,61,61	0
57	MG	1A	3310	1/1	0.96	0.20	51,51,51,51	0
57	MG	2A	3773	1/1	0.96	0.14	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	17	102	1/1	0.96	0.17	33,33,33,33	0
57	MG	1A	3729	1/1	0.96	0.17	18,18,18,18	0
57	MG	1a	1715	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	3730	1/1	0.96	0.14	22,22,22,22	0
57	MG	2A	3270	1/1	0.96	0.10	51,51,51,51	0
57	MG	2a	1703	1/1	0.96	0.27	64,64,64,64	0
57	MG	1A	3884	1/1	0.96	0.08	45,45,45,45	0
57	MG	2a	1705	1/1	0.96	0.24	44,44,44,44	0
57	MG	2A	3780	1/1	0.96	0.18	67,67,67,67	0
57	MG	1A	4057	1/1	0.96	0.13	51,51,51,51	0
57	MG	2A	3273	1/1	0.96	0.15	70,70,70,70	0
57	MG	1A	3597	1/1	0.96	0.28	63,63,63,63	0
57	MG	1A	3800	1/1	0.96	0.13	69,69,69,69	0
57	MG	1A	3967	1/1	0.96	0.15	28,28,28,28	0
57	MG	1F	314	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3181	1/1	0.96	0.43	39,39,39,39	0
57	MG	2A	3424	1/1	0.96	0.10	65,65,65,65	0
57	MG	1A	3063	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3505	1/1	0.96	0.20	33,33,33,33	0
57	MG	1A	3971	1/1	0.96	0.14	38,38,38,38	0
57	MG	2A	3428	1/1	0.96	0.14	45,45,45,45	0
57	MG	2A	3016	1/1	0.96	0.38	39,39,39,39	0
57	MG	1A	3469	1/1	0.96	0.28	29,29,29,29	0
57	MG	2A	3284	1/1	0.96	0.21	66,66,66,66	0
57	MG	1A	3805	1/1	0.96	0.12	51,51,51,51	0
57	MG	2A	3287	1/1	0.96	0.42	58,58,58,58	0
57	MG	1a	1731	1/1	0.96	0.13	57,57,57,57	0
57	MG	2A	3435	1/1	0.96	0.26	69,69,69,69	0
57	MG	1A	3035	1/1	0.96	0.22	29,29,29,29	0
57	MG	1a	1608	1/1	0.96	0.11	52,52,52,52	0
57	MG	1A	3054	1/1	0.96	0.14	28,28,28,28	0
57	MG	2A	3612	1/1	0.96	0.29	68,68,68,68	0
57	MG	2B	210	1/1	0.96	0.06	78,78,78,78	0
57	MG	1A	3112	1/1	0.96	0.32	30,30,30,30	0
57	MG	1N	202	1/1	0.96	0.22	45,45,45,45	0
57	MG	1A	3809	1/1	0.96	0.25	45,45,45,45	0
57	MG	2A	3444	1/1	0.96	0.16	70,70,70,70	0
57	MG	1A	3186	1/1	0.96	0.43	33,33,33,33	0
57	MG	2A	3446	1/1	0.96	0.17	45,45,45,45	0
57	MG	1A	3028	1/1	0.96	0.17	41,41,41,41	0
57	MG	2B	219	1/1	0.96	0.17	62,62,62,62	0
57	MG	1A	3812	1/1	0.96	0.22	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3621	1/1	0.96	0.12	34,34,34,34	0
57	MG	1A	3813	1/1	0.96	0.20	32,32,32,32	0
57	MG	2A	3623	1/1	0.96	0.11	69,69,69,69	0
57	MG	2D	305	1/1	0.96	0.84	52,52,52,52	0
57	MG	1A	3057	1/1	0.96	0.08	63,63,63,63	0
57	MG	1A	3743	1/1	0.96	0.11	38,38,38,38	0
57	MG	1A	3261	1/1	0.96	0.22	33,33,33,33	0
57	MG	2A	3170	1/1	0.96	0.08	62,62,62,62	0
57	MG	1A	3987	1/1	0.96	0.15	21,21,21,21	0
57	MG	2E	303	1/1	0.96	0.13	43,43,43,43	0
57	MG	1P	202	1/1	0.96	0.47	26,26,26,26	0
57	MG	1a	1625	1/1	0.96	0.24	52,52,52,52	0
57	MG	1A	3442	1/1	0.96	0.17	57,57,57,57	0
57	MG	2A	3632	1/1	0.96	0.10	61,61,61,61	0
57	MG	1A	3746	1/1	0.96	0.21	16,16,16,16	0
57	MG	1A	3069	1/1	0.96	0.14	27,27,27,27	0
57	MG	1A	3070	1/1	0.96	0.14	33,33,33,33	0
57	MG	2A	3311	1/1	0.96	0.07	65,65,65,65	0
57	MG	2a	1763	1/1	0.96	0.13	67,67,67,67	0
57	MG	2a	1764	1/1	0.96	0.16	66,66,66,66	0
57	MG	1A	3564	1/1	0.96	0.12	53,53,53,53	0
57	MG	1A	3322	1/1	0.96	0.59	39,39,39,39	0
57	MG	1A	4090	1/1	0.96	0.34	31,31,31,31	0
57	MG	2A	3467	1/1	0.96	0.21	63,63,63,63	0
57	MG	2A	3641	1/1	0.96	0.34	41,41,41,41	0
57	MG	2A	3642	1/1	0.96	0.14	69,69,69,69	0
57	MG	2A	3468	1/1	0.96	0.19	39,39,39,39	0
57	MG	1A	3566	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3646	1/1	0.96	0.12	56,56,56,56	0
57	MG	2a	1774	1/1	0.96	0.30	68,68,68,68	0
57	MG	2A	3647	1/1	0.96	0.19	54,54,54,54	0
57	MG	1a	1756	1/1	0.96	0.11	64,64,64,64	0
57	MG	2a	1778	1/1	0.96	0.23	56,56,56,56	0
57	MG	2A	3649	1/1	0.96	0.13	51,51,51,51	0
57	MG	1R	201	1/1	0.96	0.18	43,43,43,43	0
57	MG	1A	3192	1/1	0.96	0.16	29,29,29,29	0
57	MG	1A	3524	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	3525	1/1	0.96	0.20	39,39,39,39	0
57	MG	2U	201	1/1	0.96	0.42	54,54,54,54	0
57	MG	1A	3691	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	3833	1/1	0.96	0.24	32,32,32,32	0
57	MG	1A	3570	1/1	0.96	0.25	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
57	MG	2A	3060	1/1	0.96	0.19	50,50,50,50	0
57	MG	2Y	201	1/1	0.96	0.17	60,60,60,60	0
57	MG	1A	3760	1/1	0.96	0.16	24,24,24,24	0
57	MG	1A	3296	1/1	0.96	0.17	56,56,56,56	0
57	MG	1A	3695	1/1	0.96	0.12	44,44,44,44	0
57	MG	1A	3266	1/1	0.96	0.18	28,28,28,28	0
57	MG	1A	3628	1/1	0.96	0.15	36,36,36,36	0
57	MG	1A	3165	1/1	0.96	0.49	45,45,45,45	0
57	MG	2A	3486	1/1	0.96	0.20	60,60,60,60	0
57	MG	1A	3699	1/1	0.96	0.13	29,29,29,29	0
57	MG	2a	1800	1/1	0.96	0.12	56,56,56,56	0
57	MG	2A	3667	1/1	0.96	0.14	50,50,50,50	0
57	MG	2A	3488	1/1	0.96	0.21	52,52,52,52	0
57	MG	1a	1774	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3491	1/1	0.96	0.06	73,73,73,73	0
57	MG	1A	3926	1/1	0.96	0.08	61,61,61,61	0
57	MG	1A	3486	1/1	0.96	0.30	43,43,43,43	0
57	MG	1A	3848	1/1	0.96	0.16	22,22,22,22	0
57	MG	1A	3487	1/1	0.96	0.21	41,41,41,41	0
57	MG	1a	1653	1/1	0.96	0.27	50,50,50,50	0
57	MG	2A	3499	1/1	0.96	0.18	54,54,54,54	0
57	MG	1A	3851	1/1	0.96	0.12	24,24,24,24	0
57	MG	1a	1655	1/1	0.96	0.18	51,51,51,51	0
57	MG	1A	3118	1/1	0.96	0.24	52,52,52,52	0
57	MG	1A	3853	1/1	0.96	0.23	77,77,77,77	0
57	MG	1V	202	1/1	0.96	0.38	36,36,36,36	0
57	MG	2A	3506	1/1	0.96	0.21	62,62,62,62	0
57	MG	1A	4019	1/1	0.96	0.12	41,41,41,41	0
57	MG	2A	3685	1/1	0.96	0.12	88,88,88,88	0
57	MG	1a	1789	1/1	0.96	0.28	60,60,60,60	0
57	MG	1a	1790	1/1	0.96	0.05	74,74,74,74	0
57	MG	1A	3049	1/1	0.96	0.31	32,32,32,32	0
57	MG	2A	3084	1/1	0.96	0.35	41,41,41,41	0
57	MG	1a	1661	1/1	0.96	0.07	65,65,65,65	0
57	MG	2A	3352	1/1	0.96	0.26	63,63,63,63	0
57	MG	1B	218	1/1	0.96	0.33	46,46,46,46	0
57	MG	1A	3705	1/1	0.96	0.20	36,36,36,36	0
57	MG	1A	3937	1/1	0.96	0.14	53,53,53,53	0
57	MG	1A	3580	1/1	0.96	0.17	27,27,27,27	0
57	MG	1A	4025	1/1	0.96	0.17	53,53,53,53	0
57	MG	2A	3698	1/1	0.96	0.25	54,54,54,54	0
57	MG	2v	103	1/1	0.96	0.27	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
57	MG	1X	101	1/1	0.96	0.35	40,40,40,40	0
57	MG	2A	3700	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3857	1/1	0.96	0.13	34,34,34,34	0
57	MG	1A	4027	1/1	0.96	0.11	49,49,49,49	0
57	MG	1A	3581	1/1	0.96	0.10	39,39,39,39	0
57	MG	2A	3705	1/1	0.96	0.20	51,51,51,51	0
57	MG	1A	3421	1/1	0.96	0.13	52,52,52,52	0
57	MG	1A	3120	1/1	0.96	0.47	35,35,35,35	0
57	MG	2A	3709	1/1	0.96	0.21	36,36,36,36	0
57	MG	1A	4031	1/1	0.96	0.23	40,40,40,40	0
57	MG	2A	3528	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3642	1/1	0.96	0.18	29,29,29,29	0
57	MG	1A	3102	1/1	0.96	0.29	40,40,40,40	0
57	MG	2A	3718	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3864	1/1	0.96	0.12	38,38,38,38	0
57	MG	1a	1678	1/1	0.96	0.28	54,54,54,54	0
57	MG	1A	3714	1/1	0.96	0.18	51,51,51,51	0
57	MG	1B	234	1/1	0.96	0.11	37,37,37,37	0
57	MG	1A	3174	1/1	0.96	0.19	32,32,32,32	0
57	MG	2A	3540	1/1	0.96	0.10	48,48,48,48	0
57	MG	2A	3728	1/1	0.96	0.22	36,36,36,36	0
57	MG	1D	303	1/1	0.96	0.29	39,39,39,39	0
57	MG	1D	305	1/1	0.96	0.21	41,41,41,41	0
57	MG	2A	3107	1/1	0.96	0.12	70,70,70,70	0
57	MG	1D	307	1/1	0.96	0.39	36,36,36,36	0
57	MG	2A	3045	1/1	0.97	0.13	55,55,55,55	0
57	MG	1A	3932	1/1	0.97	0.12	43,43,43,43	0
57	MG	2A	3178	1/1	0.97	0.15	67,67,67,67	0
57	MG	2a	1675	1/1	0.97	0.32	53,53,53,53	0
57	MG	1A	4017	1/1	0.97	0.08	43,43,43,43	0
57	MG	2a	1677	1/1	0.97	0.21	68,68,68,68	0
57	MG	2a	1678	1/1	0.97	0.24	55,55,55,55	0
57	MG	1U	201	1/1	0.97	0.31	30,30,30,30	0
57	MG	2A	3455	1/1	0.97	0.26	35,35,35,35	0
57	MG	2A	3456	1/1	0.97	0.28	51,51,51,51	0
57	MG	1A	3155	1/1	0.97	0.25	27,27,27,27	0
57	MG	1A	3777	1/1	0.97	0.11	26,26,26,26	0
57	MG	1B	215	1/1	0.97	0.12	55,55,55,55	0
57	MG	2A	3786	1/1	0.97	0.09	64,64,64,64	0
57	MG	1A	3778	1/1	0.97	0.13	28,28,28,28	0
57	MG	1A	3221	1/1	0.97	0.12	42,42,42,42	0
57	MG	1A	3350	1/1	0.97	0.21	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3269	1/1	0.97	0.13	30,30,30,30	0
57	MG	1a	1769	1/1	0.97	0.17	58,58,58,58	0
57	MG	1A	3717	1/1	0.97	0.18	41,41,41,41	0
57	MG	1A	3270	1/1	0.97	0.26	33,33,33,33	0
57	MG	1A	3657	1/1	0.97	0.13	55,55,55,55	0
57	MG	1V	203	1/1	0.97	0.29	27,27,27,27	0
57	MG	1A	3324	1/1	0.97	0.27	30,30,30,30	0
57	MG	1A	3659	1/1	0.97	0.10	23,23,23,23	0
57	MG	1B	226	1/1	0.97	0.11	45,45,45,45	0
57	MG	2A	3328	1/1	0.97	0.20	61,61,61,61	0
57	MG	1A	3660	1/1	0.97	0.14	16,16,16,16	0
57	MG	1A	3156	1/1	0.97	0.62	35,35,35,35	0
57	MG	1A	3448	1/1	0.97	0.22	37,37,37,37	0
57	MG	1A	3014	1/1	0.97	0.17	28,28,28,28	0
57	MG	2B	207	1/1	0.97	0.13	65,65,65,65	0
57	MG	1A	3869	1/1	0.97	0.14	25,25,25,25	0
57	MG	1A	3870	1/1	0.97	0.13	26,26,26,26	0
57	MG	2a	1706	1/1	0.97	0.22	61,61,61,61	0
57	MG	1A	3610	1/1	0.97	0.08	41,41,41,41	0
57	MG	2A	3480	1/1	0.97	0.15	31,31,31,31	0
57	MG	1A	3357	1/1	0.97	0.19	27,27,27,27	0
57	MG	1A	3728	1/1	0.97	0.10	54,54,54,54	0
57	MG	1a	1788	1/1	0.97	0.18	50,50,50,50	0
57	MG	1D	302	1/1	0.97	0.64	40,40,40,40	0
57	MG	1A	3523	1/1	0.97	0.74	42,42,42,42	0
57	MG	1D	304	1/1	0.97	0.21	22,22,22,22	0
57	MG	1A	3029	1/1	0.97	0.38	31,31,31,31	0
57	MG	1a	1671	1/1	0.97	0.28	65,65,65,65	0
57	MG	1D	306	1/1	0.97	0.15	29,29,29,29	0
57	MG	2A	3490	1/1	0.97	0.20	35,35,35,35	0
57	MG	1A	3109	1/1	0.97	0.09	33,33,33,33	0
57	MG	2A	3492	1/1	0.97	0.10	59,59,59,59	0
57	MG	2A	3651	1/1	0.97	0.23	51,51,51,51	0
57	MG	1A	4043	1/1	0.97	0.19	55,55,55,55	0
57	MG	1A	3956	1/1	0.97	0.27	38,38,38,38	0
57	MG	1A	3160	1/1	0.97	0.26	35,35,35,35	0
57	MG	1A	3672	1/1	0.97	0.13	63,63,63,63	0
57	MG	1A	3959	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3799	1/1	0.97	0.13	32,32,32,32	0
57	MG	2A	3500	1/1	0.97	0.20	59,59,59,59	0
57	MG	1a	1680	1/1	0.97	0.29	40,40,40,40	0
57	MG	2A	3220	1/1	0.97	0.11	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	2a	1731	1/1	0.97	0.06	70,70,70,70	0
57	MG	1A	3616	1/1	0.97	0.12	25,25,25,25	0
57	MG	1A	3527	1/1	0.97	0.30	34,34,34,34	0
57	MG	1A	3362	1/1	0.97	0.10	29,29,29,29	0
57	MG	1a	1807	1/1	0.97	0.10	70,70,70,70	0
57	MG	1A	3067	1/1	0.97	0.13	16,16,16,16	0
57	MG	1a	1685	1/1	0.97	0.22	61,61,61,61	0
57	MG	1A	3041	1/1	0.97	0.32	30,30,30,30	0
57	MG	1A	3886	1/1	0.97	0.12	12,12,12,12	0
57	MG	1A	3075	1/1	0.97	0.18	33,33,33,33	0
57	MG	1A	3279	1/1	0.97	0.29	30,30,30,30	0
57	MG	13	102	1/1	0.97	0.39	39,39,39,39	0
57	MG	1A	3164	1/1	0.97	0.22	17,17,17,17	0
57	MG	2O	201	1/1	0.97	0.18	51,51,51,51	0
57	MG	1A	3682	1/1	0.97	0.11	57,57,57,57	0
57	MG	2a	1746	1/1	0.97	0.09	64,64,64,64	0
57	MG	2A	3674	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3188	1/1	0.97	0.41	31,31,31,31	0
57	MG	2Q	202	1/1	0.97	0.34	47,47,47,47	0
57	MG	2Q	203	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3684	1/1	0.97	0.21	50,50,50,50	0
57	MG	2A	3371	1/1	0.97	0.19	24,24,24,24	0
57	MG	1A	3894	1/1	0.97	0.06	54,54,54,54	0
57	MG	2A	3373	1/1	0.97	0.62	42,42,42,42	0
57	MG	2A	3237	1/1	0.97	0.33	53,53,53,53	0
57	MG	2A	3522	1/1	0.97	0.08	69,69,69,69	0
57	MG	2a	1758	1/1	0.97	0.12	67,67,67,67	0
57	MG	1F	306	1/1	0.97	0.46	36,36,36,36	0
57	MG	2A	3524	1/1	0.97	0.23	37,37,37,37	0
57	MG	1l	3201	1/1	0.97	0.21	60,60,60,60	0
57	MG	2W	202	1/1	0.97	0.16	47,47,47,47	0
57	MG	2A	3377	1/1	0.97	0.18	37,37,37,37	0
57	MG	2X	102	1/1	0.97	0.15	48,48,48,48	0
57	MG	1A	4065	1/1	0.97	0.10	51,51,51,51	0
57	MG	1p	101	1/1	0.97	0.06	63,63,63,63	0
57	MG	1A	3685	1/1	0.97	0.17	44,44,44,44	0
57	MG	1a	1700	1/1	0.97	0.21	50,50,50,50	0
57	MG	2A	3531	1/1	0.97	0.07	64,64,64,64	0
57	MG	23	101	1/1	0.97	0.12	58,58,58,58	0
57	MG	2A	3532	1/1	0.97	0.21	38,38,38,38	0
57	MG	1a	1701	1/1	0.97	0.28	38,38,38,38	0
57	MG	25	102	1/1	0.97	0.30	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
57	MG	1F	309	1/1	0.97	0.38	29,29,29,29	0
57	MG	2a	1775	1/1	0.97	0.08	78,78,78,78	0
57	MG	1A	3686	1/1	0.97	0.10	48,48,48,48	0
57	MG	1A	3254	1/1	0.97	0.17	34,34,34,34	0
57	MG	2A	3696	1/1	0.97	0.12	73,73,73,73	0
57	MG	1A	3977	1/1	0.97	0.15	56,56,56,56	0
57	MG	2a	1780	1/1	0.97	0.25	62,62,62,62	0
57	MG	1A	3814	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	3462	1/1	0.97	0.27	39,39,39,39	0
57	MG	1A	3090	1/1	0.97	0.29	37,37,37,37	0
57	MG	18	103	1/1	0.97	0.34	33,33,33,33	0
57	MG	1A	3751	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3982	1/1	0.97	0.16	55,55,55,55	0
57	MG	1A	3630	1/1	0.97	0.20	26,26,26,26	0
57	MG	1A	3819	1/1	0.97	0.13	43,43,43,43	0
57	MG	1A	3753	1/1	0.97	0.16	22,22,22,22	0
57	MG	1A	3464	1/1	0.97	0.19	29,29,29,29	0
57	MG	2A	3710	1/1	0.97	0.16	58,58,58,58	0
57	MG	1x	110	1/1	0.97	0.18	22,22,22,22	0
57	MG	2A	3712	1/1	0.97	0.18	40,40,40,40	0
57	MG	1A	3582	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3031	1/1	0.97	0.23	23,23,23,23	0
57	MG	2a	1796	1/1	0.97	0.21	63,63,63,63	0
57	MG	2A	3716	1/1	0.97	0.19	37,37,37,37	0
57	MG	1x	113	1/1	0.97	0.30	62,62,62,62	0
57	MG	1A	3824	1/1	0.97	0.11	42,42,42,42	0
57	MG	2A	3555	1/1	0.97	0.24	50,50,50,50	0
57	MG	2A	3556	1/1	0.97	0.16	62,62,62,62	0
57	MG	1A	3093	1/1	0.97	0.23	47,47,47,47	0
57	MG	1a	1722	1/1	0.97	0.14	35,35,35,35	0
57	MG	2A	3725	1/1	0.97	0.17	42,42,42,42	0
57	MG	2A	3136	1/1	0.97	0.24	32,32,32,32	0
57	MG	1N	204	1/1	0.97	0.69	44,44,44,44	0
57	MG	1A	3149	1/1	0.97	0.27	37,37,37,37	0
57	MG	2a	1809	1/1	0.97	0.31	78,78,78,78	0
57	MG	1A	4085	1/1	0.97	0.07	62,62,62,62	0
57	MG	1A	3759	1/1	0.97	0.09	55,55,55,55	0
57	MG	1a	1611	1/1	0.97	0.14	29,29,29,29	0
57	MG	2a	1625	1/1	0.97	0.16	86,86,86,86	0
57	MG	1A	3543	1/1	0.97	0.25	55,55,55,55	0
57	MG	1A	3761	1/1	0.97	0.20	20,20,20,20	0
57	MG	1A	3588	1/1	0.97	0.13	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3569	1/1	0.97	0.20	61,61,61,61	0
57	MG	2A	3145	1/1	0.97	0.20	55,55,55,55	0
57	MG	1A	3832	1/1	0.97	0.20	37,37,37,37	0
57	MG	1A	3502	1/1	0.97	0.14	28,28,28,28	0
57	MG	1a	1618	1/1	0.97	0.14	36,36,36,36	0
57	MG	2d	302	1/1	0.97	0.24	56,56,56,56	0
57	MG	1A	3998	1/1	0.97	0.18	34,34,34,34	0
57	MG	2A	3741	1/1	0.97	0.19	48,48,48,48	0
57	MG	2A	3018	1/1	0.97	0.23	33,33,33,33	0
57	MG	2A	3420	1/1	0.97	0.26	48,48,48,48	0
57	MG	1A	3764	1/1	0.97	0.54	30,30,30,30	0
57	MG	2A	3422	1/1	0.97	0.11	59,59,59,59	0
57	MG	2A	3152	1/1	0.97	0.12	58,58,58,58	0
57	MG	1A	3836	1/1	0.97	0.40	40,40,40,40	0
57	MG	2A	3021	1/1	0.97	0.11	44,44,44,44	0
57	MG	2A	3285	1/1	0.97	0.16	58,58,58,58	0
57	MG	2A	3750	1/1	0.97	0.08	59,59,59,59	0
57	MG	1A	3105	1/1	0.97	0.11	40,40,40,40	0
57	MG	1Q	201	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3703	1/1	0.97	0.13	46,46,46,46	0
57	MG	2w	102	1/1	0.97	0.23	84,84,84,84	0
57	MG	1A	3173	1/1	0.97	0.18	20,20,20,20	0
57	MG	2w	104	1/1	0.97	0.13	87,87,87,87	0
57	MG	1A	3117	1/1	0.97	0.45	37,37,37,37	0
57	MG	1A	3506	1/1	0.97	0.47	34,34,34,34	0
57	MG	2a	1651	1/1	0.97	0.15	67,67,67,67	0
57	MG	1A	3135	1/1	0.97	0.18	33,33,33,33	0
57	MG	2A	3162	1/1	0.97	0.22	34,34,34,34	0
57	MG	1Q	207	1/1	0.97	0.20	49,49,49,49	0
57	MG	1A	3708	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3437	1/1	0.97	0.10	33,33,33,33	0
57	MG	2A	3594	1/1	0.97	0.09	65,65,65,65	0
57	MG	2A	3032	1/1	0.97	0.15	25,25,25,25	0
57	MG	1B	202	1/1	0.97	0.20	49,49,49,49	0
57	MG	2x	109	1/1	0.97	0.12	70,70,70,70	0
57	MG	1a	1632	1/1	0.97	0.24	23,23,23,23	0
57	MG	1A	3846	1/1	0.97	0.17	46,46,46,46	0
57	MG	1A	3550	1/1	0.97	0.19	52,52,52,52	0
57	MG	1A	3077	1/1	0.97	0.18	36,36,36,36	0
57	MG	1A	3774	1/1	0.97	0.25	32,32,32,32	0
57	MG	1B	207	1/1	0.97	0.13	42,42,42,42	0
57	MG	2a	1667	1/1	0.97	0.11	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
57	MG	1A	3154	1/1	0.97	0.20	30,30,30,30	0
57	MG	1A	3931	1/1	0.97	0.12	72,72,72,72	0
60	ZN	26	501	1/1	0.97	0.12	61,61,61,61	0
57	MG	1A	4015	1/1	0.97	0.07	37,37,37,37	0
57	MG	2a	1671	1/1	0.97	0.23	65,65,65,65	0
57	MG	2A	3537	1/1	0.98	0.29	52,52,52,52	0
57	MG	1A	3167	1/1	0.98	0.28	45,45,45,45	0
57	MG	1A	3837	1/1	0.98	0.07	63,63,63,63	0
57	MG	2A	3701	1/1	0.98	0.09	46,46,46,46	0
57	MG	1A	3838	1/1	0.98	0.13	36,36,36,36	0
57	MG	1W	203	1/1	0.98	0.26	33,33,33,33	0
57	MG	1A	3141	1/1	0.98	0.23	32,32,32,32	0
57	MG	1A	4022	1/1	0.98	0.16	22,22,22,22	0
57	MG	1a	1607	1/1	0.98	0.28	60,60,60,60	0
57	MG	1a	1729	1/1	0.98	0.28	45,45,45,45	0
57	MG	2A	3708	1/1	0.98	0.26	39,39,39,39	0
57	MG	1A	3535	1/1	0.98	0.45	28,28,28,28	0
57	MG	1A	3169	1/1	0.98	0.36	29,29,29,29	0
57	MG	1A	3678	1/1	0.98	0.20	16,16,16,16	0
57	MG	1X	103	1/1	0.98	0.22	44,44,44,44	0
57	MG	1A	3889	1/1	0.98	0.14	23,23,23,23	0
57	MG	1X	105	1/1	0.98	0.16	51,51,51,51	0
57	MG	2A	3715	1/1	0.98	0.15	38,38,38,38	0
57	MG	1A	3515	1/1	0.98	0.28	31,31,31,31	0
57	MG	1A	3585	1/1	0.98	0.12	56,56,56,56	0
57	MG	1a	1805	1/1	0.98	0.20	53,53,53,53	0
57	MG	1A	4080	1/1	0.98	0.33	43,43,43,43	0
57	MG	1a	1617	1/1	0.98	0.18	45,45,45,45	0
57	MG	2A	3721	1/1	0.98	0.08	64,64,64,64	0
57	MG	2A	3722	1/1	0.98	0.18	61,61,61,61	0
57	MG	1A	3037	1/1	0.98	0.19	32,32,32,32	0
57	MG	1Z	302	1/1	0.98	0.27	47,47,47,47	0
57	MG	1A	3130	1/1	0.98	0.13	42,42,42,42	0
57	MG	2B	217	1/1	0.98	0.25	71,71,71,71	0
57	MG	1A	3329	1/1	0.98	0.13	54,54,54,54	0
57	MG	2a	1803	1/1	0.98	0.13	61,61,61,61	0
57	MG	1A	3519	1/1	0.98	0.22	35,35,35,35	0
57	MG	2A	3332	1/1	0.98	0.30	39,39,39,39	0
57	MG	2A	3563	1/1	0.98	0.07	71,71,71,71	0
57	MG	2A	3644	1/1	0.98	0.21	68,68,68,68	0
57	MG	1A	3131	1/1	0.98	0.18	28,28,28,28	0
57	MG	1A	3850	1/1	0.98	0.18	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3114	1/1	0.98	0.05	62,62,62,62	0
57	MG	2A	3411	1/1	0.98	0.12	52,52,52,52	0
57	MG	2A	3042	1/1	0.98	0.30	36,36,36,36	0
57	MG	1A	3403	1/1	0.98	0.44	42,42,42,42	0
57	MG	2a	1814	1/1	0.98	0.08	60,60,60,60	0
57	MG	1A	3687	1/1	0.98	0.16	21,21,21,21	0
57	MG	1A	3651	1/1	0.98	0.21	28,28,28,28	0
57	MG	1A	4038	1/1	0.98	0.16	62,62,62,62	0
57	MG	1A	3619	1/1	0.98	0.18	19,19,19,19	0
57	MG	1A	3092	1/1	0.98	0.20	24,24,24,24	0
57	MG	1A	3265	1/1	0.98	0.52	40,40,40,40	0
57	MG	1A	3693	1/1	0.98	0.11	52,52,52,52	0
57	MG	1n	101	1/1	0.98	0.14	46,46,46,46	0
57	MG	1A	3655	1/1	0.98	0.16	28,28,28,28	0
57	MG	2e	201	1/1	0.98	0.04	73,73,73,73	0
57	MG	1a	1693	1/1	0.98	0.06	61,61,61,61	0
57	MG	2A	3127	1/1	0.98	0.32	44,44,44,44	0
57	MG	2A	3054	1/1	0.98	0.12	45,45,45,45	0
57	MG	1A	3121	1/1	0.98	0.36	33,33,33,33	0
57	MG	1A	3100	1/1	0.98	0.25	41,41,41,41	0
57	MG	1a	1760	1/1	0.98	0.15	49,49,49,49	0
57	MG	1A	3072	1/1	0.98	0.13	39,39,39,39	0
57	MG	1A	3625	1/1	0.98	0.10	21,21,21,21	0
57	MG	1A	4048	1/1	0.98	0.07	61,61,61,61	0
57	MG	1A	3136	1/1	0.98	0.17	16,16,16,16	0
57	MG	1A	3030	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3662	1/1	0.98	0.16	27,27,27,27	0
57	MG	1A	3741	1/1	0.98	0.24	47,47,47,47	0
57	MG	1A	4004	1/1	0.98	0.10	41,41,41,41	0
57	MG	1A	3868	1/1	0.98	0.46	33,33,33,33	0
57	MG	1A	3599	1/1	0.98	0.11	16,16,16,16	0
57	MG	1A	3575	1/1	0.98	0.15	29,29,29,29	0
57	MG	2A	3440	1/1	0.98	0.26	55,55,55,55	0
57	MG	2a	1750	1/1	0.98	0.24	63,63,63,63	0
57	MG	1a	1707	1/1	0.98	0.17	65,65,65,65	0
57	MG	1A	3055	1/1	0.98	0.28	49,49,49,49	0
57	MG	2a	1663	1/1	0.98	0.12	67,67,67,67	0
57	MG	2A	3766	1/1	0.98	0.07	54,54,54,54	0
57	MG	1A	4058	1/1	0.98	0.09	35,35,35,35	0
57	MG	1A	3602	1/1	0.98	0.19	24,24,24,24	0
57	MG	1a	1776	1/1	0.98	0.10	49,49,49,49	0
57	MG	1A	3062	1/1	0.98	0.19	30,30,30,30	0

Continued on next page...

Continued from previous page...

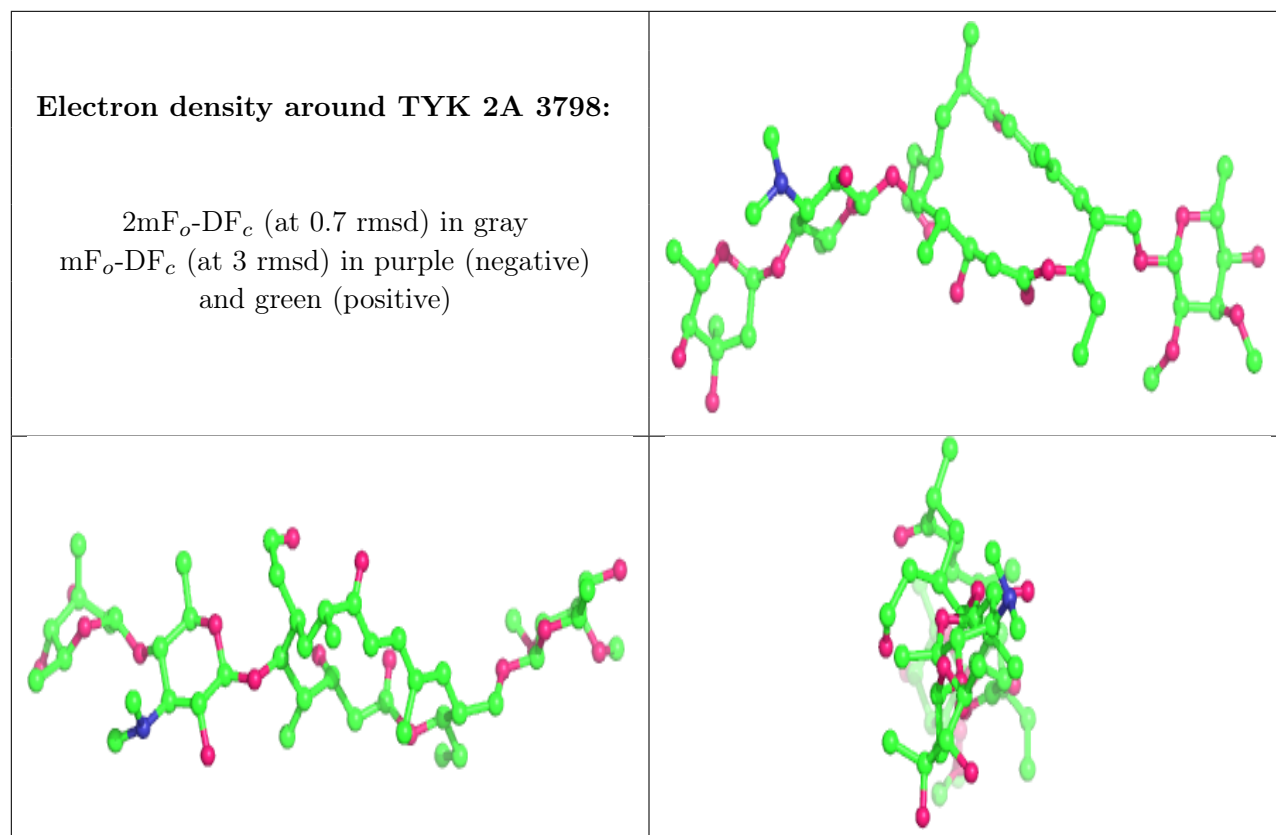
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4061	1/1	0.98	0.16	40,40,40,40	0
57	MG	1A	3634	1/1	0.98	0.16	20,20,20,20	0
57	MG	1a	1714	1/1	0.98	0.16	45,45,45,45	0
57	MG	1a	1781	1/1	0.98	0.13	53,53,53,53	0
57	MG	1U	208	1/1	0.98	0.48	37,37,37,37	0
57	MG	2A	3608	1/1	0.98	0.17	32,32,32,32	0
57	MG	1A	3635	1/1	0.98	0.12	26,26,26,26	0
57	MG	1A	3604	1/1	0.98	0.15	29,29,29,29	0
57	MG	1A	3710	1/1	0.98	0.17	19,19,19,19	0
60	ZN	15	107	1/1	0.98	0.16	43,43,43,43	0
60	ZN	1n	102	1/1	0.98	0.15	57,57,57,57	0
57	MG	2A	3009	1/1	0.98	0.10	40,40,40,40	0
57	MG	1A	3671	1/1	0.98	0.08	21,21,21,21	0
60	ZN	25	105	1/1	0.98	0.19	57,57,57,57	0
57	MG	1A	3358	1/1	0.98	0.07	38,38,38,38	0
57	MG	2A	3535	1/1	0.98	0.17	38,38,38,38	0
57	MG	1A	3140	1/1	0.98	0.22	32,32,32,32	0
57	MG	15	102	1/1	0.99	0.18	36,36,36,36	0
57	MG	15	103	1/1	0.99	0.51	28,28,28,28	0
57	MG	1a	1759	1/1	0.99	0.09	67,67,67,67	0
57	MG	1A	3355	1/1	0.99	0.49	27,27,27,27	0
57	MG	2A	3496	1/1	0.99	0.16	33,33,33,33	0
57	MG	1A	3688	1/1	0.99	0.15	21,21,21,21	0
57	MG	2A	3022	1/1	0.99	0.56	47,47,47,47	0
57	MG	1A	3122	1/1	0.99	0.19	32,32,32,32	0
57	MG	1A	3633	1/1	0.99	0.16	27,27,27,27	0
57	MG	1A	3860	1/1	0.99	0.09	36,36,36,36	0
57	MG	1A	3879	1/1	0.99	0.12	68,68,68,68	0
57	MG	2A	3337	1/1	0.99	0.18	32,32,32,32	0
57	MG	17	103	1/1	0.99	0.14	29,29,29,29	0
57	MG	2A	3306	1/1	0.99	0.14	43,43,43,43	0
57	MG	1A	3268	1/1	0.99	0.24	33,33,33,33	0
57	MG	1A	3170	1/1	0.99	0.19	27,27,27,27	0
57	MG	1A	3286	1/1	0.99	0.19	31,31,31,31	0
57	MG	2A	3781	1/1	0.99	0.15	52,52,52,52	0
57	MG	1A	3128	1/1	0.99	0.17	36,36,36,36	0
57	MG	1A	3003	1/1	0.99	0.13	22,22,22,22	0
57	MG	1A	3831	1/1	0.99	0.20	41,41,41,41	0
57	MG	1A	3482	1/1	0.99	0.37	37,37,37,37	0
57	MG	2A	3006	1/1	0.99	0.17	40,40,40,40	0
57	MG	1A	3574	1/1	0.99	0.20	13,13,13,13	0
57	MG	2A	3037	1/1	0.99	0.15	52,52,52,52	0

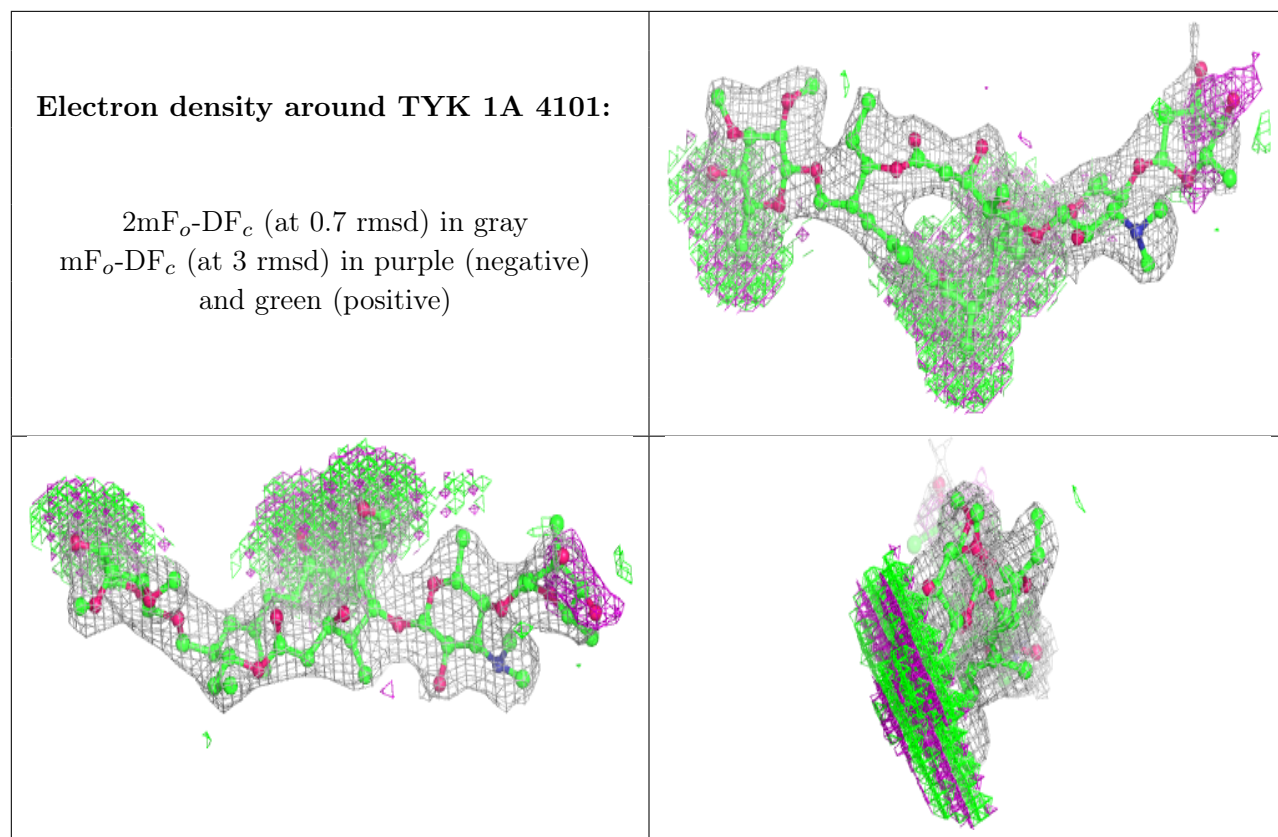
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1B	216	1/1	0.99	0.21	38,38,38,38	0
57	MG	13	101	1/1	0.99	0.15	36,36,36,36	0
57	MG	2A	3070	1/1	0.99	0.20	28,28,28,28	0
60	ZN	19	102	1/1	0.99	0.19	42,42,42,42	0
57	MG	2A	3010	1/1	0.99	0.14	47,47,47,47	0
57	MG	1A	3095	1/1	0.99	0.21	42,42,42,42	0
57	MG	1A	3835	1/1	0.99	0.16	25,25,25,25	0
57	MG	1A	3012	1/1	0.99	0.11	23,23,23,23	0
57	MG	1A	3027	1/1	0.99	0.45	32,32,32,32	0
57	MG	1A	3553	1/1	0.99	0.43	31,31,31,31	0
57	MG	1D	308	1/1	0.99	0.39	47,47,47,47	0
61	SF4	1d	501	8/8	0.99	0.18	56,62,68,68	0
61	SF4	2d	303	8/8	0.99	0.13	67,73,84,84	0
60	ZN	16	102	1/1	1.00	0.16	44,44,44,44	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.