



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:18 PM GMT

PDB ID : 4Y4P
Title : Crystal structure of the Thermus thermophilus 70S ribosome with rRNA modifications and bound to mRNA and A-, P- and E-site tRNAs at 2.5Å resolution
Authors : Polikanov, Y.S.; Melnikov, S.V.; Soll, D.; Steitz, T.A.
Deposited on : 2015-02-10
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

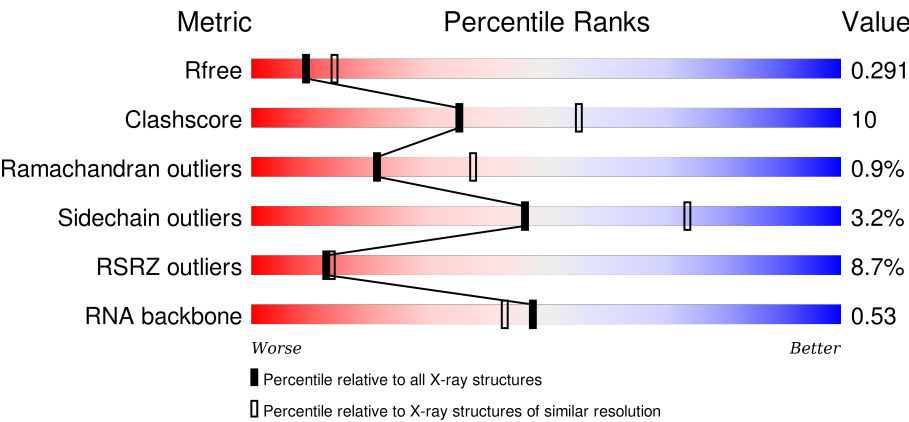
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div><div>3%</div><div>63%28%7%..</div></div>
1	2A	2915	<div><div>3%</div><div>52%34%9%..</div></div>
2	1B	121	<div><div></div><div>72%23%..</div></div>
2	2B	121	<div><div>2%</div><div>36%45%18%..</div></div>

Continued on next page...

Continued from previous page...

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



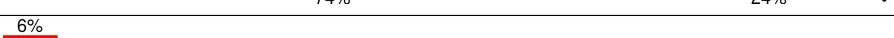
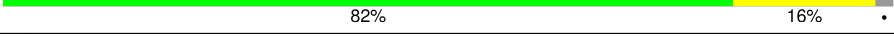

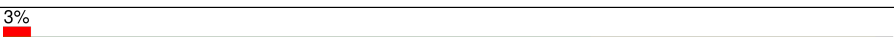
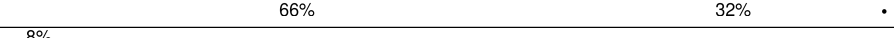


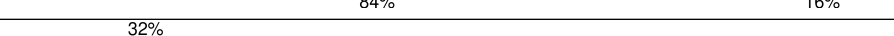


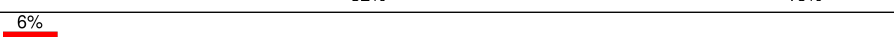



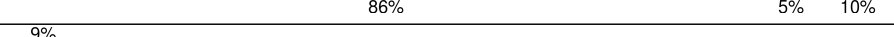


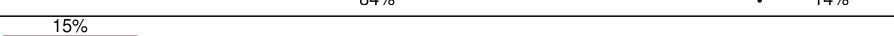
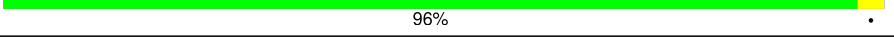
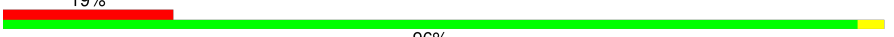
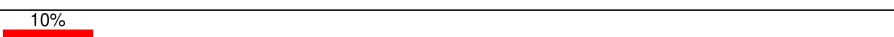
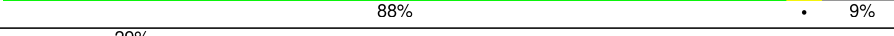

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	16	101	-	-	-	X
56	MG	1A	3013	-	-	-	X
56	MG	1A	3016	-	-	-	X
56	MG	1A	3055	-	-	-	X
56	MG	1A	3056	-	-	-	X
56	MG	1A	3063	-	-	-	X
56	MG	1A	3068	-	-	-	X
56	MG	1A	3095	-	-	-	X
56	MG	1A	3104	-	-	-	X
56	MG	1A	3125	-	-	-	X
56	MG	1A	3151	-	-	-	X
56	MG	1A	3162	-	-	-	X
56	MG	1A	3165	-	-	-	X
56	MG	1A	3171	-	-	-	X
56	MG	1A	3177	-	-	-	X
56	MG	1A	3185	-	-	-	X
56	MG	1A	3189	-	-	-	X
56	MG	1A	3194	-	-	-	X
56	MG	1A	3200	-	-	-	X
56	MG	1A	3248	-	-	-	X
56	MG	1A	3252	-	-	-	X
56	MG	1A	3280	-	-	-	X
56	MG	1A	3306	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	3307	-	-	-	X
56	MG	1A	3309	-	-	-	X
56	MG	1A	3311	-	-	-	X
56	MG	1A	3313	-	-	-	X
56	MG	1A	3338	-	-	-	X
56	MG	1A	3347	-	-	-	X
56	MG	1A	3351	-	-	-	X
56	MG	1A	3354	-	-	-	X
56	MG	1A	3458	-	-	-	X
56	MG	1A	3509	-	-	-	X
56	MG	1A	3552	-	-	-	X
56	MG	1A	3559	-	-	-	X
56	MG	1A	3576	-	-	-	X
56	MG	1A	3578	-	-	-	X
56	MG	1A	3603	-	-	-	X
56	MG	1A	3628	-	-	-	X
56	MG	1A	3658	-	-	-	X
56	MG	1A	3704	-	-	-	X
56	MG	1A	3744	-	-	-	X
56	MG	1A	3753	-	-	-	X
56	MG	1A	3803	-	-	-	X
56	MG	1A	3809	-	-	-	X
56	MG	1A	3842	-	-	-	X
56	MG	1A	3857	-	-	-	X
56	MG	1A	3865	-	-	-	X
56	MG	1A	3871	-	-	-	X
56	MG	1A	3971	-	-	-	X
56	MG	1A	4047	-	-	-	X
56	MG	1A	4072	-	-	-	X
56	MG	1A	4076	-	-	-	X
56	MG	1A	4078	-	-	-	X
56	MG	1A	4086	-	-	-	X
56	MG	1A	4090	-	-	-	X
56	MG	1A	4093	-	-	-	X
56	MG	1A	4115	-	-	-	X
56	MG	1A	4124	-	-	-	X
56	MG	1A	4141	-	-	-	X
56	MG	1B	3010	-	-	-	X
56	MG	1B	3019	-	-	-	X
56	MG	1D	301	-	-	-	X
56	MG	1D	302	-	-	-	X
56	MG	1D	310	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1D	312	-	-	-	X
56	MG	1E	304	-	-	-	X
56	MG	1N	201	-	-	-	X
56	MG	1N	204	-	-	-	X
56	MG	1O	202	-	-	-	X
56	MG	1O	203	-	-	-	X
56	MG	1S	3001	-	-	-	X
56	MG	1U	202	-	-	-	X
56	MG	1Y	504	-	-	-	X
56	MG	1a	1657	-	-	-	X
56	MG	1a	1659	-	-	-	X
56	MG	1a	1699	-	-	-	X
56	MG	2A	3003	-	-	-	X
56	MG	2A	3014	-	-	-	X
56	MG	2A	3025	-	-	-	X
56	MG	2A	3070	-	-	-	X
56	MG	2A	3083	-	-	-	X
56	MG	2A	3092	-	-	-	X
56	MG	2A	3093	-	-	-	X
56	MG	2A	3096	-	-	-	X
56	MG	2A	3108	-	-	-	X
56	MG	2A	3160	-	-	-	X
56	MG	2A	3165	-	-	-	X
56	MG	2A	3167	-	-	-	X
56	MG	2A	3181	-	-	-	X
56	MG	2A	3191	-	-	-	X
56	MG	2A	3347	-	-	-	X
56	MG	2A	3364	-	-	-	X
56	MG	2A	3409	-	-	-	X
56	MG	2A	3444	-	-	-	X
56	MG	2A	3445	-	-	-	X
56	MG	2A	3448	-	-	-	X
56	MG	2A	3449	-	-	-	X
56	MG	2A	3455	-	-	-	X
56	MG	2A	3461	-	-	-	X
56	MG	2A	3468	-	-	-	X
56	MG	2A	3472	-	-	-	X
56	MG	2A	3486	-	-	-	X
56	MG	2A	3493	-	-	-	X
56	MG	2A	3579	-	-	-	X
56	MG	2A	3633	-	-	-	X
56	MG	2A	3673	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3677	-	-	-	X
56	MG	2A	3687	-	-	-	X
56	MG	2A	3745	-	-	-	X
56	MG	2A	3814	-	-	-	X
56	MG	2A	3856	-	-	-	X
56	MG	2A	3876	-	-	-	X
56	MG	2A	3883	-	-	-	X
56	MG	2A	3886	-	-	-	X
56	MG	2A	3897	-	-	-	X
56	MG	2A	3900	-	-	-	X
56	MG	2A	3906	-	-	-	X
56	MG	2B	3008	-	-	-	X
56	MG	2D	304	-	-	-	X
56	MG	2F	304	-	-	-	X
56	MG	2U	201	-	-	-	X
56	MG	2a	3010	-	-	-	X
56	MG	2a	3041	-	-	-	X
56	MG	2a	3091	-	-	-	X
56	MG	2a	3165	-	-	-	X
56	MG	2a	3208	-	-	-	X
58	ZN	15	101	-	-	-	X
58	ZN	25	102	-	-	-	X

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 300910 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	9	Total	Mg	0	0
			9	9		
56	17	1	Total	Mg	0	0
			1	1		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	2	Total	Mg	0	0
			2	2		
56	1N	6	Total	Mg	0	0
			6	6		
56	20	3	Total	Mg	0	0
			3	3		
56	18	3	Total	Mg	0	0
			3	3		
56	2W	3	Total	Mg	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	3	Total 3	Mg 3	0	0
56	13	3	Total 3	Mg 3	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1P	4	Total 4	Mg 4	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2a	244	Total 244	Mg 244	0	0
56	1E	11	Total 11	Mg 11	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2F	4	Total 4	Mg 4	0	0
56	16	3	Total 3	Mg 3	0	0
56	28	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1A	1141	Total 1141	Mg 1141	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	0	0
56	2P	1	Total 1	Mg 1	0	0
56	1X	6	Total 6	Mg 6	0	0
56	12	1	Total 1	Mg 1	0	0
56	1y	4	Total 4	Mg 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2i	1	Total 1	Mg 1	0	0
56	1S	3	Total 3	Mg 3	0	0
56	25	4	Total 4	Mg 4	0	0
56	2T	3	Total 3	Mg 3	0	0
56	1D	12	Total 12	Mg 12	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	0	0
56	2G	1	Total 1	Mg 1	0	0
56	1I	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	1V	3	Total 3	Mg 3	0	0
56	2X	3	Total 3	Mg 3	0	0
56	1w	11	Total 11	Mg 11	0	0
56	1a	229	Total 229	Mg 229	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	15	2	Total 2	Mg 2	0	0
56	1x	16	Total 16	Mg 16	0	0
56	2j	2	Total 2	Mg 2	0	0
56	1R	3	Total 3	Mg 3	0	0
56	1s	1	Total 1	Mg 1	0	0
56	2v	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2U	4	Total 4	Mg 4	0	0
56	1G	5	Total 5	Mg 5	0	0
56	2O	1	Total 1	Mg 1	0	0
56	11	3	Total 3	Mg 3	0	0
56	1d	1	Total 1	Mg 1	0	0
56	2n	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2x	5	Total 5	Mg 5	0	0
56	2R	1	Total 1	Mg 1	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	2D	5	Total 5	Mg 5	0	0
56	2q	2	Total 2	Mg 2	0	0
56	1U	8	Total 8	Mg 8	0	0
56	2r	2	Total 2	Mg 2	0	0
56	1O	7	Total 7	Mg 7	0	0
56	27	1	Total 1	Mg 1	0	0
56	19	2	Total 2	Mg 2	0	0
56	1l	3	Total 3	Mg 3	0	0
56	2V	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1F	8	Total Mg 8 8	0	0
56	10	6	Total Mg 6 6	0	0
56	2t	1	Total Mg 1 1	0	0
56	1Q	6	Total Mg 6 6	0	0
56	2A	909	Total Mg 909 909	0	0
56	23	2	Total Mg 2 2	0	0
56	2Z	1	Total Mg 1 1	0	0
56	1B	37	Total Mg 37 37	0	0
56	2y	7	Total Mg 7 7	0	0
56	2w	8	Total Mg 8 8	0	0

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total K 1 1	0	0
57	2A	1	Total K 1 1	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

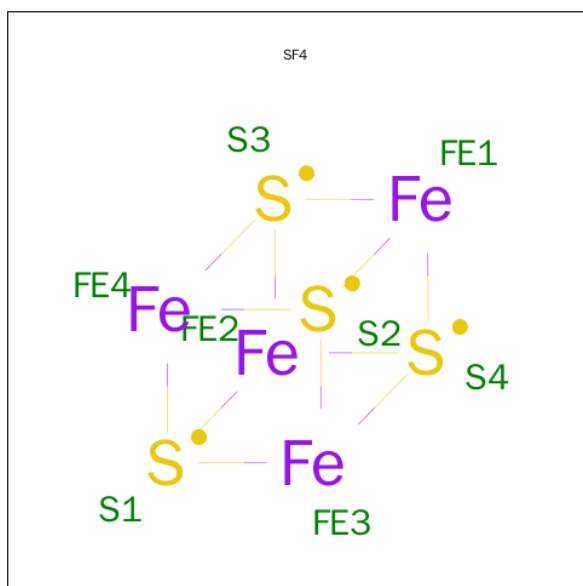
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1Y	1	Total Zn 1 1	0	0
58	14	1	Total Zn 1 1	0	0
58	1n	1	Total Zn 1 1	0	0
58	15	1	Total Zn 1 1	0	0
58	29	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2238	Total 2238	O 2238	0	0
60	1B	68	Total 68	O 68	0	0
60	1D	28	Total 28	O 28	0	0
60	1E	28	Total 28	O 28	0	0
60	1F	13	Total 13	O 13	0	0
60	1G	7	Total 7	O 7	0	0
60	1H	2	Total 2	O 2	0	0
60	1I	3	Total 3	O 3	0	0
60	1N	7	Total 7	O 7	0	0
60	1O	8	Total 8	O 8	0	0
60	1P	23	Total 23	O 23	0	0
60	1Q	14	Total 14	O 14	0	0
60	1R	14	Total 14	O 14	0	0
60	1S	5	Total 5	O 5	0	0
60	1T	8	Total 8	O 8	0	0
60	1U	11	Total 11	O 11	0	0
60	1V	9	Total 9	O 9	0	0
60	1W	6	Total 6	O 6	0	0
60	1X	8	Total 8	O 8	0	0
60	1Y	4	Total 4	O 4	0	0
60	1Z	1	Total 1	O 1	0	0
60	10	12	Total 12	O 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	11	10	Total 10	O 10	0	0
60	12	4	Total 4	O 4	0	0
60	13	6	Total 6	O 6	0	0
60	14	1	Total 1	O 1	0	0
60	15	6	Total 6	O 6	0	0
60	16	3	Total 3	O 3	0	0
60	17	9	Total 9	O 9	0	0
60	18	13	Total 13	O 13	0	0
60	1a	438	Total 438	O 438	0	0
60	1b	1	Total 1	O 1	0	0
60	1d	1	Total 1	O 1	0	0
60	1e	1	Total 1	O 1	0	0
60	1f	1	Total 1	O 1	0	0
60	1g	1	Total 1	O 1	0	0
60	1i	1	Total 1	O 1	0	0
60	1l	8	Total 8	O 8	0	0
60	1m	2	Total 2	O 2	0	0
60	1o	1	Total 1	O 1	0	0
60	1p	1	Total 1	O 1	0	0
60	1q	4	Total 4	O 4	0	0
60	1u	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1v	5	Total 5	O 5	0	0
60	1w	21	Total 21	O 21	0	0
60	1x	15	Total 15	O 15	0	0
60	1y	1	Total 1	O 1	0	0
60	2A	1389	Total 1389	O 1389	0	0
60	2B	26	Total 26	O 26	0	0
60	2D	28	Total 28	O 28	0	0
60	2E	16	Total 16	O 16	0	0
60	2F	16	Total 16	O 16	0	0
60	2H	1	Total 1	O 1	0	0
60	2I	4	Total 4	O 4	0	0
60	2N	1	Total 1	O 1	0	0
60	2P	14	Total 14	O 14	0	0
60	2Q	2	Total 2	O 2	0	0
60	2R	2	Total 2	O 2	0	0
60	2T	6	Total 6	O 6	0	0
60	2U	2	Total 2	O 2	0	0
60	2V	2	Total 2	O 2	0	0
60	2W	2	Total 2	O 2	0	0
60	2X	5	Total 5	O 5	0	0
60	2Y	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

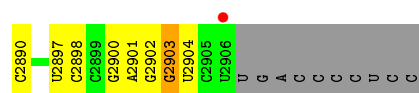
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2Z	2	Total 2	O 2	0	0
60	20	7	Total 7	O 7	0	0
60	21	12	Total 12	O 12	0	0
60	22	1	Total 1	O 1	0	0
60	23	1	Total 1	O 1	0	0
60	25	4	Total 4	O 4	0	0
60	26	1	Total 1	O 1	0	0
60	27	4	Total 4	O 4	0	0
60	28	6	Total 6	O 6	0	0
60	29	1	Total 1	O 1	0	0
60	2a	377	Total 377	O 377	0	0
60	2d	1	Total 1	O 1	0	0
60	2e	2	Total 2	O 2	0	0
60	2g	1	Total 1	O 1	0	0
60	2i	1	Total 1	O 1	0	0
60	2j	4	Total 4	O 4	0	0
60	2l	5	Total 5	O 5	0	0
60	2o	1	Total 1	O 1	0	0
60	2p	2	Total 2	O 2	0	0
60	2q	1	Total 1	O 1	0	0
60	2r	1	Total 1	O 1	0	0

Continued on next page...

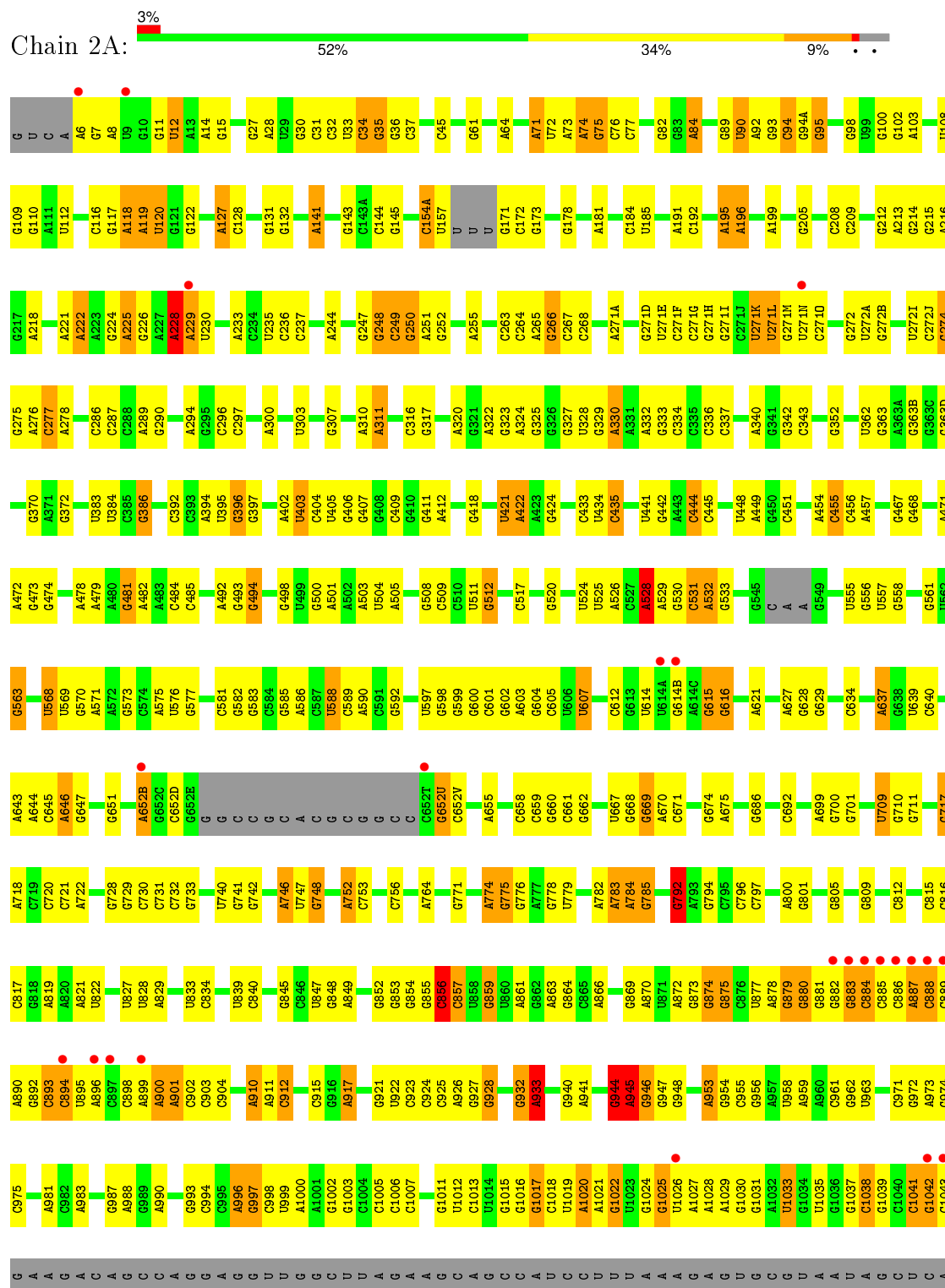
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2t	4	Total 4	O 4	0	0
60	2u	1	Total 1	O 1	0	0
60	2v	1	Total 1	O 1	0	0
60	2w	2	Total 2	O 2	0	0
60	2x	7	Total 7	O 7	0	0
60	2y	19	Total 19	O 19	0	0

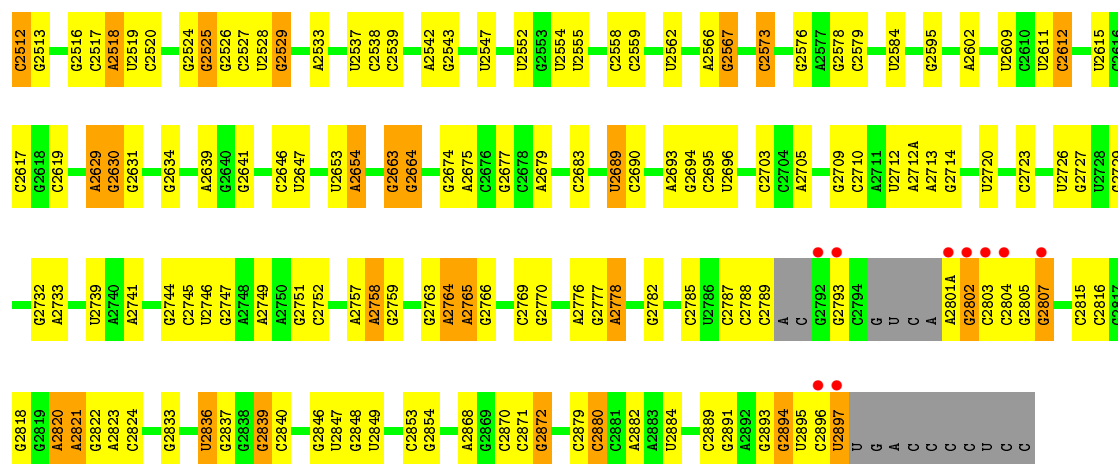
U2799	C2678	C2570	A2430	G2316	G2209	G2147	U2044	C1915	G1807	A1584	U1560	G1431	G1305	C1180
C2800	C2679	A2576	U2431	A2317	C2210	A2143	G2045	G1921	U1808	C1585	C1561	G1436	G1312	G1181
C2801	G2680	A2577	C2436	G2320	G2211	C2150	G2051	A1922	U1809	U1686	U1562	U1436	U1313	A1188
C2804	U2694	A2578	A2437	A2321	G2213	C2151	A2052	A1923	U1810	G1687	U1566	A1441	A1314	G1195
C2805	U2695	G2579	A2438	G2324	G2214	U2152	G2053	C1924	A1811	G1688	U1567	U1442	G1317	
G2806	G2697	C2580	C2439	U2327	A2220	G2153	G2054	G1928	G1812	G1689	G1568	U1451	A1318	A1201
G2807	G2698	C2585	G2440	G2327	A2221	U2154	A2055	U2056	C1813	G1694	G1569	U1452	U1319	A1202
G	U2699	C2586	G2441	C2328	G2227	A2155	U2056	A1934	A1814	C1695	U1569	U1452	A1320	
U	U2700	C2587	U2442	G2328	G2228	A2156	G2057	A1935	A1815	C1700	G1572	C1453	A1321	G1206
C	U2701	G2588	U2443	G2331	A2229	C2158	C2061	A1936	A1816	A1701	G1573	G1462	G1323	G1210
A	C2702	G2589	A2447	A2332	U2330	C2159	C2061		A1817			C1463	A1324	U1211
A2812	C2703	G2590		G2337	G2231	C2160	C2065	U1939	C1821		G1579	C1463		
G2813	U2714	C2598	A2451	G2338	A2237	C2161	G2071	U1945	A1822	C1709	G	A1464	G1331	U1212
G2814	U2715	C2603	C2452	C2339	A2237	G2162	G2072	U1946	G1823	C1710	U	A1465		U1213
A2819	U2724	G2604	C2453	A2340	U2245	G2163	C2073	A1946	G1824	A1711	A	U1466		
A2820	A2725	U2604	G2457	G2341	G2246	C2164	A2073	G1951	U1825		C	U1467	U1338	G1217
C2825	G2735	C2613	A2460	G2346	G2250	U2165	C2077	G1952	C1826	A1716	G1584	U1477	U1339	G1218
C2826	G2736	A2614	G2467	A2347	G2251	U2166	G2078	A1958	U1827	G1717	G1585	A1473		A1219
G2827	C2736	G2615	G2470	A2348	G2252	C2167	G2078	A1959	C1828	U1718	U1586	C1474	G1342	U1220
G2828	U2736	U2616	C2473	G2349	U2255	C2168	A2082	A1960	U1829	C1719	U1587	C1475	C1343	G1221
G2829	U2737	G2619	U2474	C2359	U2256	G2171	G2083	U1961	G1830	U1720	U1588	C1476	U1346	C1223
A2830	U2738	G2620	C2475	U2359	U2257	U2172	A2084	U1977	G1831	G1721	A1589	U1477	U1347	
A2831	U2739	U2621	G2476	C2362	U2258	G2173			G1832			U1479	A1348	G1228
G2832	U2741	G2622	C2477	U2362	A2259	G2174	G2091	U1985	G1833	U1739	C1593		U1349	G1229
G2833	G2742	U2623	C2486	C2367	U2260	G2175	U2108	G1989	A1846	C1740	C1594	A1491	C1352	U1233
C2838	C2743	C2624	C2487	C2368	U2261	G2176	G2109	C1990	G1847	G1742	A1605	G1494	U1358	
G2843	A2746	U2627	A2488	U2369	G2262	U2177	C2109	A1991	G1848	G1743	A1613	A1495	U1361	A1239
G2844	U2759	C2628	A2500	G2370	G2264	A2180	G2115	G1992	G1857	A1747	A1616	G1497	C1361	
A2845	G2760	U2629	C2472	C2371	A2280	G2181	G2116	A1993	G1858	G1750	U1625	G1502	C1366	U1243
U2846	C2761	C2629	A2504	A2373	A2281	C2182	U2121	A1994	G1859	U1756	A1626	G1502	C1246	
G2849	G2764	C2638	C2511	C2376	G2282	G2183	G2122	G1995	A1860	C1757	A1627	G1513	G1371	
C2850	U2765	G2639	G2514	G2377	G2283	C2185	G2123	C1996	C1861	G1758	G1628	C1514	U1378	A1255
G2854	A2766	C2640	G2514	G2377	U2284	U2186	U2124	G1997	C1874	C1759		G1525		U1256
G2855	U2767	A2641	G2514	G2377	A2285	G2187	C2125	U1998	A1878	U1760	C1631	G1529	C1391	C1263
G2856	G2768	G2642	G2517	G2384	A2286	U2188	G2126	G2007	U1882	U1765	A1632	G1529	G1391	
U2857	U2769	G2643	G2517	G2384	C2287	U2189	C2127	A2008	C1883	A1766	C1634	G1530	U1398	G1273
G2858	A2770	U2618	U2518	A2388	G2288	G2190	G2128		U1883	U1768	C1635	G1537	G1402	G1277
U2859	C2771	C2647	A2530	A2389	G2289	A2191	C2129	G2011	C1889			G1538	G1405	G1278
	G2772		G2530	A2389	A2290	A2192	C2130		G1891	C1775	G1639	A1540	A1406	G1281
	G2776	G2653	G2541	G2395	G2291	A2193	U2131	G2014	G1889	C1776	G1640	G1546	G1410	A1288
G2863	A2777	C2658	A2542	G2397	G2292	U2194	G2132	U2015	A1890	G1785	A1654	G1546	A1411	
G2864	A2778	U2659	A2542	C2397	A2295	A2195	U2135		G1891	G1786		G1547	A1411	A1289
		C2660	A2545	U2402	G2296	C2197	G2137	C2018	G1897	A1788		G1548	A1411	G1290
G2874	C2782	U2661	A2546		C2297	A2198	G2137	G2019	A1898	U1789	C1657	G1549	U1418	G1291
A2878	G2783	U2662	G2546	G2411	A2298	C2200	G2138	A2023	A1899	G1789		C1550	G1423	G1296
G2879	C2784	U2665	G2561	U2418	A2299	G2203	U2140	G2024	C1904	A1793	G1668	C1551	A1424	
C2880	C2785	U2666	G2562	G2419	U2303	G2204	G2141	A2035	C1908	G1794	G1676	C1552	A1424	
C2881	G2785	A2666	C2563	U2420	C2304	G2205	A2142		G1908	G1795	C1677	A1553	A1425	A1299
G2882	U2791	A2672	G2564	G2421	C2305	G2206	G2143	A2041				A1554	G1426	
G2883	G2796	G2573	G2566	G2422	G2314	C2207	U2144	A2042	A1911			C1555		G1302
C2884	C2797	U2677	G2569	C2429	G2315	G2208	G2146	C2043		A1904	C1683	A1556		



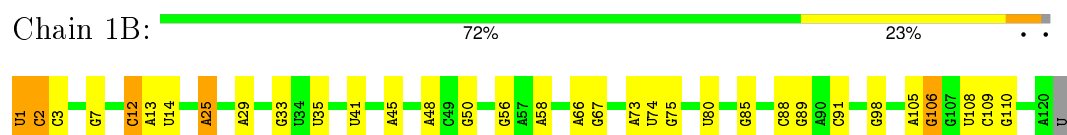
● Molecule 1: 23S Ribosomal RNA



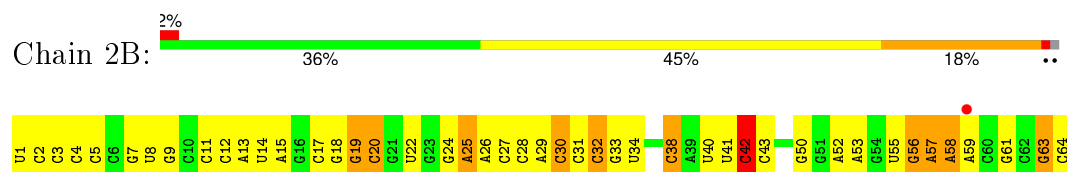
G2430	G2431	G2432	G2433	G2434	G2435	G2436	G2437	G2341	G2342	A2273	G2166	G2106	G2018	A1900	A1786	A1664	C1546	G1368	A1262	C
U2431	A2432	A2433	U2434	A2435	A2436	C2437	C2350	G2341	C2342	A2274	U2167	C2107	G2019	G1906	C1790	A1665	C1547	G1369	U1263	U
A2433	U2434	A2435	A2436	A2437	A2438	A2439	C2351	G2342	C2343	A2275	A2169	U2109	A2020	A2020	A1791	A1666	C1557	C1370	G1264	G
A2434	A2435	A2436	A2437	A2438	A2439	A2440	C2352	G2343	C2344	A2276	A2171	G2110	U2021	A1910	U1794	C1670	A1558	U1371	C1180	C
A2435	A2436	A2437	A2438	A2439	A2440	A2441	C2353	G2344	C2345	A2277	A2172	G2111	U2022	A1911	U1795	C1671	A1559	U1372	G1186	G
U2438	A2439	C2440	A2441	A2442	A2443	A2444	C2354	G2345	C2346	A2278	A2173	G2112	G2023	A1912	U1796	C1672	A1560	U1373	U1187	A
A2439	C2440	A2441	A2442	A2443	A2444	A2445	C2355	G2346	C2347	G2279	A2174	G2113	G2024	A1913	U1797	C1673	A1561	G1374	U1188	G
C2441	A2442	A2443	A2444	A2445	A2446	A2447	C2356	G2347	C2348	A2280	A2175	G2114	C2025	A1914	C1797	C1674	A1562	G1375	U1189	G
G2445	G2446	A2447	A2448	A2449	A2450	G2451	C2357	G2348	C2349	C2283	C2177	G2115	C2026	U1915	U1798	C1675	A1563	G1376	G1191	G
G2446	A2447	A2448	A2449	A2450	G2451	G2452	C2358	G2349	C2350	C2284	C2178	G2116	G2027	U1916	U1799	C1676	A1564	G1377	G1192	G
A2447	A2448	A2449	A2450	G2451	G2452	G2453	C2359	G2350	C2351	C2285	C2179	G2117	G2028	U1917	U1800	C1677	A1565	G1378	G1193	G
G2448	A2449	A2450	G2451	G2452	G2453	G2454	C2360	G2351	C2352	C2286	C2180	G2118	G2029	U1918	U1801	C1678	A1566	A1379	G1194	G
A2449	A2450	G2451	G2452	G2453	G2454	G2455	C2361	G2352	C2353	A2287	G2181	G2119	A2030	A1919	A1471	C1473	A1278	G1195	G1195	G
G2450	G2451	G2452	G2453	G2454	G2455	G2456	C2362	G2353	C2354	C2287	G2182	G2120	A2031	A1920	A1472	C1474	G1279	A1204	G1196	G
G2451	G2452	G2453	G2454	G2455	G2456	G2457	C2363	G2354	C2355	C2288	G2183	G2121	A2032	G1921	C1804	G1475	A1279	U1205	G1206	G
G2452	G2453	G2454	G2455	G2456	G2457	G2458	C2364	G2355	C2356	U2296	G2184	G2122	A2033	G1922	U1805	U1693	A1278	A1206	G1207	G
G2453	G2454	G2455	G2456	G2457	G2458	G2459	C2365	G2356	C2357	U2297	G2185	G2123	C2040	G1923	G1811	G1696	G1389	A1210	G1210	G
G2454	G2455	G2456	G2457	G2458	G2459	G2460	C2366	G2357	C2358	C2297	G2186	G2124	U2041	C1924	A1812	G1697	G1390	U1211	G1211	G
G2455	G2456	G2457	G2458	G2459	G2460	G2461	C2367	G2358	C2359	C2298	G2187	G2125	A2042	A1927	G1815	G1698	A1385	U1212	G1212	G
C2465	G2466	G2467	G2468	G2469	G2470	G2471	C2368	G2359	C2360	A2299	U2189	G2126	G2043	A1928	G1816	G1699	U1590	A1213	A1214	G
G2466	A2467	A2468	A2469	G2470	G2471	G2472	C2369	G2360	C2361	G2300	G2190	G2127	G2046	G1929	G1817	G1699	G1591	C1298	U1330	G
A2467	A2468	A2469	A2470	G2471	G2472	G2473	C2370	G2361	C2362	G2301	G2191	G2128	G2047	G1930	G1818	G1699	G1592	C1299	G1131	G
G2468	A2469	A2470	A2471	G2472	G2473	G2474	C2371	G2362	C2363	G2302	G2192	G2129	G2048	U1931	U1819	G1703	G1593	G1303	C1218	G
A2469	A2470	A2471	A2472	G2473	G2474	G2475	C2372	G2363	C2364	G2303	G2193	G2130	G2049	U1932	G1820	G1704	G1594	C1302	G1219	G
U2473	A2474	A2475	A2476	A2477	A2478	G2479	C2373	G2364	C2365	A2305	G2194	G2131	G2050	A1933	G1821	G1705	A1609	C1303	C1224	G
A2474	A2475	A2476	A2477	A2478	G2479	G2480	C2374	G2365	C2366	G2306	G2195	G2132	C2055	A1937	G1822	G1706	A1610	C1304	G1225	G
G2475	A2476	A2477	A2478	G2479	G2480	G2481	C2375	G2366	C2367	G2307	G2196	G2133	C2056	A1938	G1823	G1707	A1611	C1305	G1226	G
A2476	A2477	A2478	G2479	G2480	G2481	G2482	C2376	G2367	C2368	A2308	G2197	G2134	C2057	A1939	G1824	G1708	A1612	C1306	G1227	G
A2477	A2478	G2479	G2480	G2481	G2482	G2483	C2377	G2368	C2369	G2309	G2198	G2135	C2058	G2061	G1825	G1709	A1613	C1307	G1228	G
G2478	G2479	G2480	G2481	G2482	G2483	G2484	C2378	G2369	C2370	A2310	G2199	G2136	C2059	A2062	G1826	G1710	A1614	C1308	G1229	G
G2481	G2482	G2483	G2484	G2485	G2486	G2487	C2379	G2370	C2371	G2311	G2200	G2137	C2060	A2063	G1827	G1711	A1615	C1309	G1230	G
A2482	G2483	G2484	G2485	G2486	G2487	G2488	C2380	G2371	C2372	A2312	G2201	G2138	C2061	A2064	G1828	G1712	A1616	C1310	G1231	G
G2483	G2484	G2485	G2486	G2487	G2488	G2489	C2381	G2372	C2373	G2313	G2202	G2139	C2062	A2065	G1829	G1713	A1617	C1311	G1232	G
G2484	G2485	G2486	G2487	G2488	G2489	G2490	C2382	G2373	C2374	G2314	G2203	G2140	C2063	A2066	G1830	G1714	A1618	C1312	G1233	G
G2485	G2486	G2487	G2488	G2489	G2490	G2491	C2383	G2374	C2375	G2315	G2204	G2141	C2064	A2067	G1831	G1715	A1619	C1313	G1234	G
G2486	G2487	G2488	G2489	G2490	G2491	G2492	C2384	G2375	C2376	G2316	G2205	G2142	C2065	A2068	G1832	G1716	A1620	C1314	G1235	G
G2487	G2488	G2489	G2490	G2491	G2492	G2493	C2385	G2376	C2377	G2317	G2206	G2143	C2066	A2069	G1833	G1717	A1621	C1315	G1236	G
G2488	G2489	G2490	G2491	G2492	G2493	G2494	C2386	G2377	C2378	G2318	G2207	G2144	C2067	A2070	G1834	G1718	A1622	C1316	G1237	G
G2489	G2490	G2491	G2492	G2493	G2494	G2495	C2387	G2378	C2379	G2319	G2208	G2145	C2068	A2071	G1835	G1719	A1623	C1317	G1238	G
G2490	G2491	G2492	G2493	G2494	G2495	G2496	C2388	G2379	C2380	G2320	G2209	G2146	C2069	A2072	G1836	G1720	A1624	C1318	G1239	G
G2491	G2492	G2493	G2494	G2495	G2496	G2497	C2389	G2380	C2381	A2320	G2210	G2147	C2070	A2073	G1837	G1721	A1625	C1319	G1240	G
G2492	G2493	G2494	G2495	G2496	G2497	G2498	C2390	G2381	C2382	G2321	G2211	G2148	C2071	A2074	G1838	G1722	A1626	C1320	G1241	G
G2493	G2494	G2495	G2496	G2497	G2498	G2499	C2391	G2382	C2383	G2322	G2212	G2149	C2072	A2075	G1839	G1723	A1627	C1321	G1242	G
G2494	G2495	G2496	G2497	G2498	G2499	G2500	C2392	G2383	C2384	G2323	G2213	G2150	C2073	A2076	G1840	G1724	A1628	C1322	G1243	G
G2495	G2496	G2497	G2498	G2499	G2500	G2501	C2393	G2384	C2385	G2324	G2214	G2151	C2074	A2077	G1841	G1725	A1629	C1323	G1244	G
G2496	G2497	G2498	G2499	G2500	G2501	G2502	C2394	G2385	C2386	G2325	G2215	G2152	C2075	A2078	G1842	G1726	A1630	C1324	G1245	G
G2497	G2498	G2499	G2500	G2501	G2502	G2503	C2395	G2386	C2387	G2326	G2216	G2153	C2076	A2079	G1843	G1727	A1631	C1325	G1246	G
G2498	G2499	G2500	G2501	G2502	G2503	G2504	C2396	G2387	C2388	G2327	G2217	G2154	C2077	A2080	G1844	G1728	A1632	C1326	G1247	G
G2499	G2500	G2501	G2502	G2503	G2504	G2505	C2397	G2388	C2389	G2328	G2218	G2155	C2078	A2081	G1845	G1729	A1633	C1327	G1248	G
G2500	G2501	G2502	G2503	G2504	G2505	G2506	C2398	G2389	C2390	G2329	G2219	G2156	C2079	A2082	G1846	G1730	A1634	C1328	G1249	G
G2501	G2502	G2503	G2504	G2505	G2506	G2507	C2399	G2390	C2391	G2330	G2220	G2157	C2080	A2083	G1847	G1731	A1635	C1329	G1250	G
G2502	G2503	G2504	G2505	G2506	G2507	G2508	C2400	G2391	C2392	G2331	G2221	G2158	C2081	A2084	G1848	G1732	A1636	C1330	G1251	G
G2503	G2504	G2505	G2506	G2507	G2508	G2509	C2401	G2392	C2393	G2332	G2222	G2159	C2082	A2085	G1849	G1733	A1637	C1331	G1252	G
G2504	G2505	G2506	G2507	G2508	G2509	G2510	C2402	G2393	C2394	G2333	G2223	G2160	C2083	A2086	G1850	G1734	A1638	C1332	G1253	G
G2505	G2506	G2507	G2508	G2509	G2510	G2511	C2403	G2394	C2395	G2334	G2224	G2161	C2084	A2087	G1851	G1735	A1639	C1333	G1254	G
G2506	G2507	G2508	G2509	G2510	G2511	G2512	C2404	G2395	C2396	G2335	G2225	G2162	C2085	A2088	G1852	G1736	A1640	C1334	G1255	G
G2507	G2508	G2509	G2510	G2511	G2512	G2513	C2405	G2396	C2397	G2336	G2226	G2163	C2086	A2089	G1853	G1737	A1641	C1335	G1256	G
G2508	G2509	G2510	G2511	G2512	G2513	G2514	C2406	G2397	C2398	G2337	G2227	G2164	C2087	A2090	G1854	G1738	A1642	C1336	G1257	G
G2509	G2510	G2511	G2512	G2513	G2514	G2515	C2407	G2398	C2399	G2338	G2228	G2165	C2088	A2091	G1855	G1739	A1643	C1337	G1258	G
G2510	G2511	G2512	G2513	G2514	G2515	G2516	C2408	G2399	C2400	G2339	G2229	G2166	C2089	A2092	G1856	G1740	A1644	C1338	G1259	G
G2511	G2512	G2513	G2514	G2515	G2516	G2517	C2409	G2400	C2401	G2340	G2230	G2167	C2090	A2093	G1857	G1741	A1645	C1339	G1260	G
G2512	G2513	G2514	G2515	G2516	G2517	G2518	C2410	G2401	C2402	G2341	G2231	G2168	C2091	A2094	G1858	G1742	A1646	C1340	G1261	G
G2513	G2514	G2515	G2516	G2517	G2518	G2519	C2411	G2402	C2403	G2342	G2232	G2169	C2092	A2095	G1859	G1743	A1647	C1341	G1262	G
G2514	G2515	G2516	G2517	G2518	G2519	G2520	C2412	G2403	C2404	G2343	G2233	G2170	C2093	A2096	G1860	G1744	A1648	C1342	G1263	G
G2515	G2516	G2517	G2518	G2519	G2520	G2521	C2413	G2404	C2405	G2344	G2234	G2171								



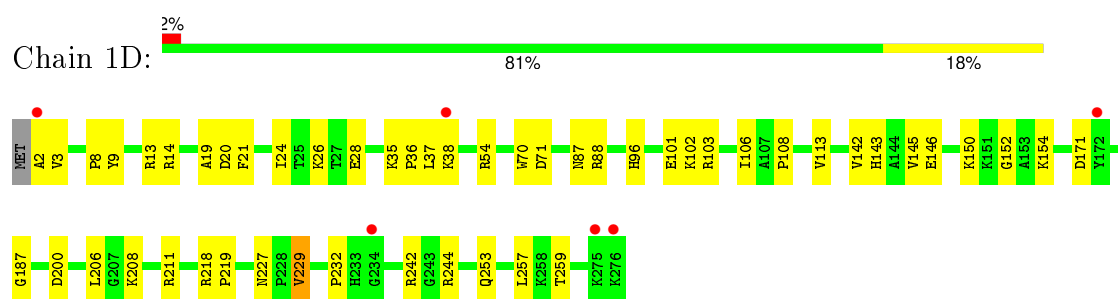
• Molecule 2: 5S Ribosomal RNA



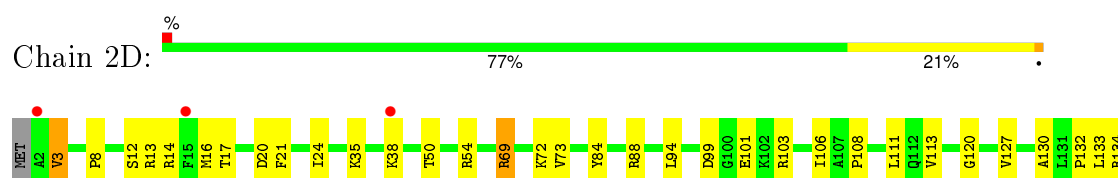
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

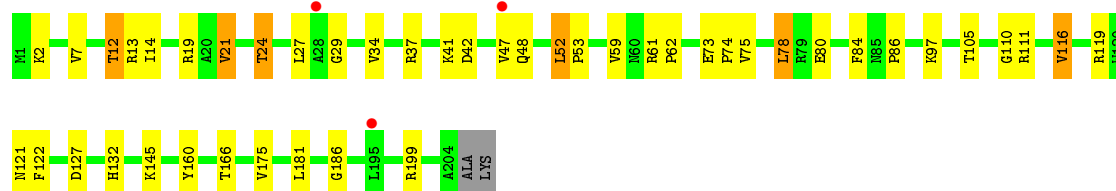
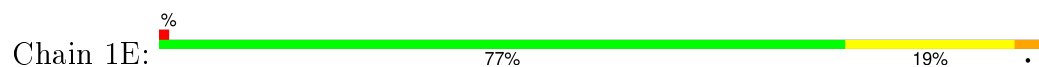


• Molecule 3: 50S ribosomal protein L2

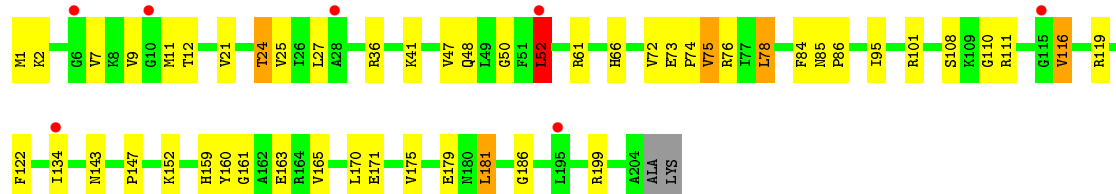
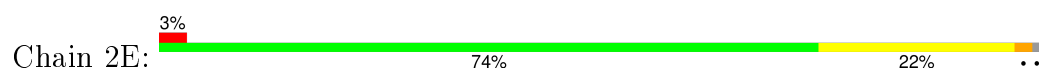




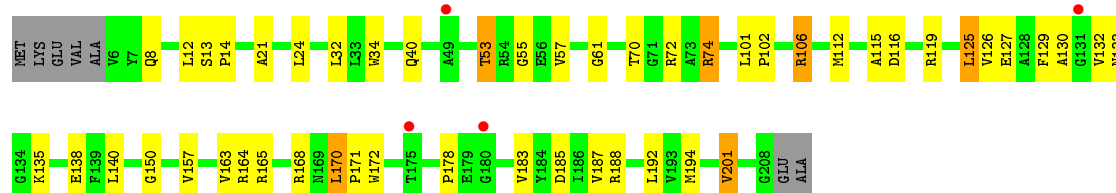
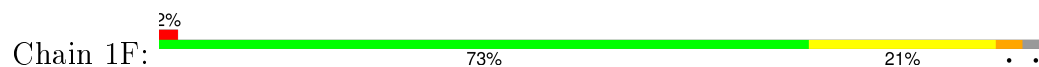
- Molecule 4: 50S ribosomal protein L3



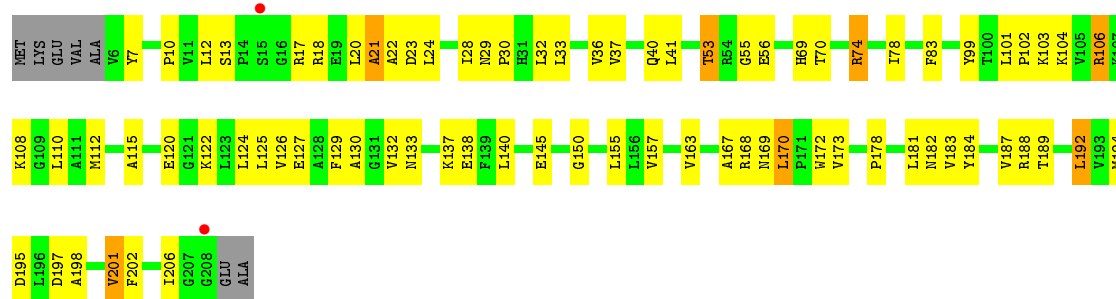
- Molecule 4: 50S ribosomal protein L3



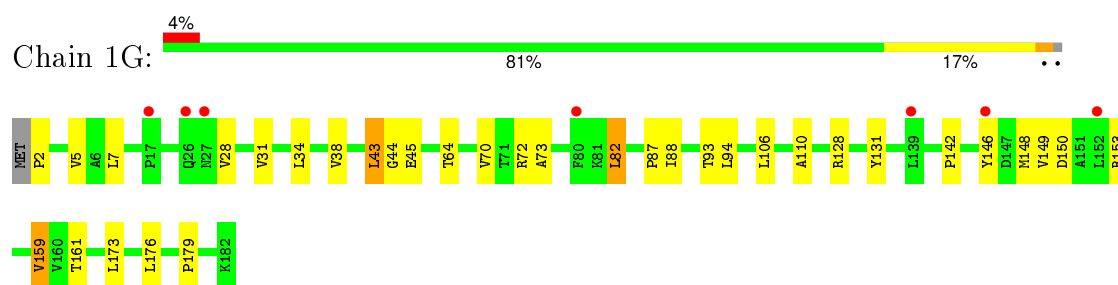
- Molecule 5: 50S ribosomal protein L4



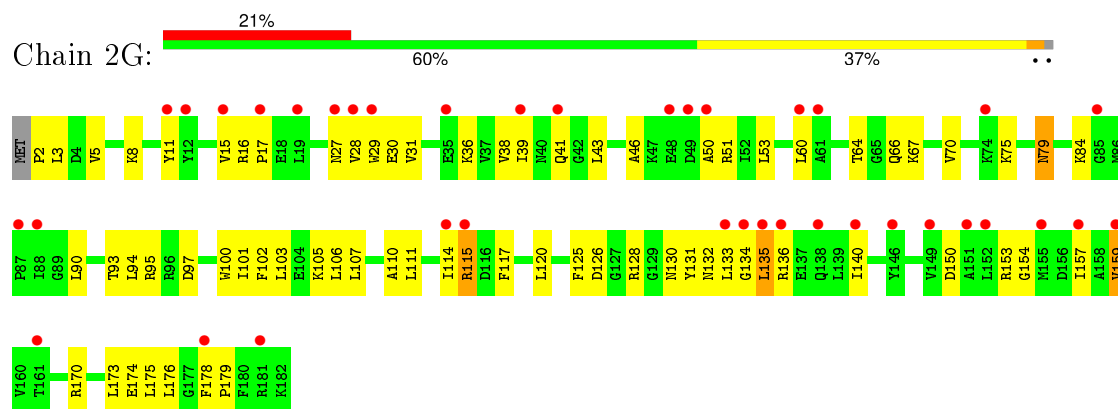
- Molecule 5: 50S ribosomal protein L4



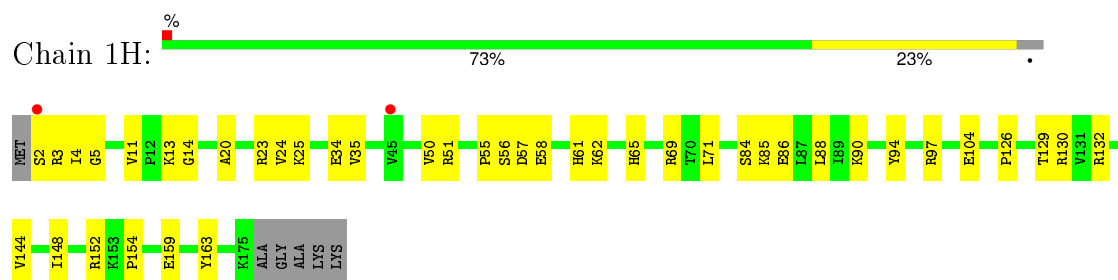
- Molecule 6: 50S ribosomal protein L5



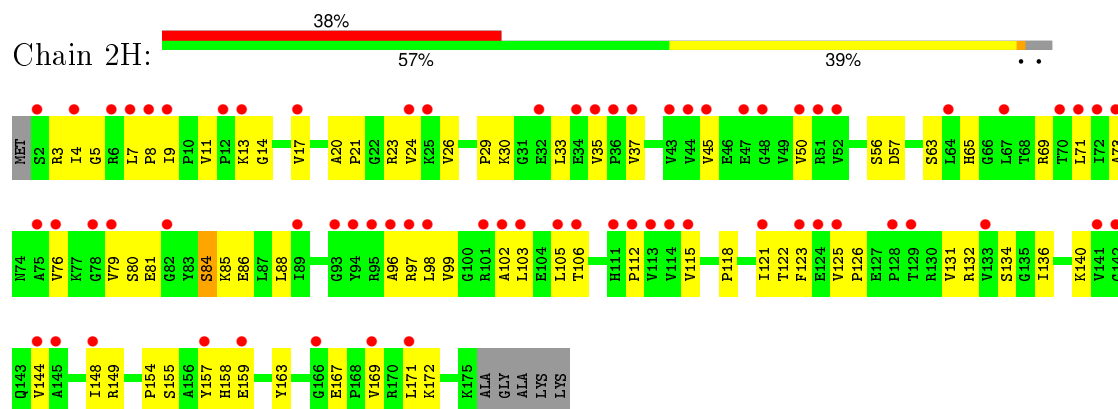
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

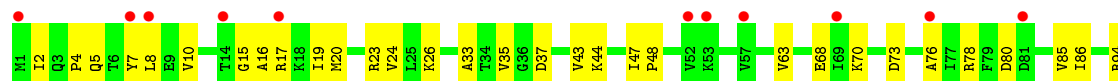


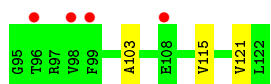
• Molecule 7: 50S ribosomal protein L6



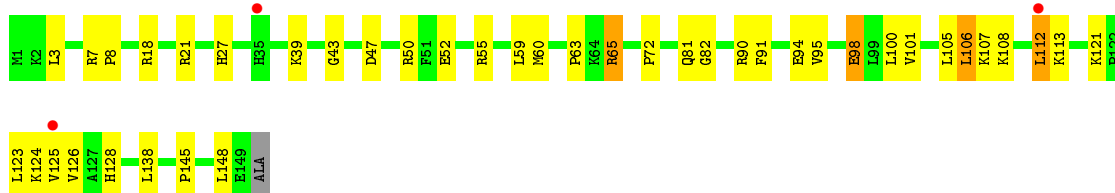
• Molecule 8: 50S ribosomal protein L9



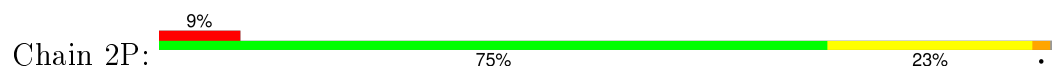




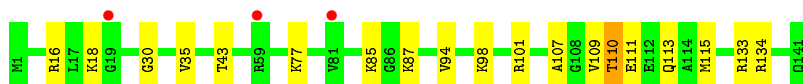
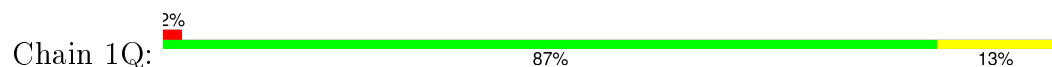
- Molecule 11: 50S ribosomal protein L15



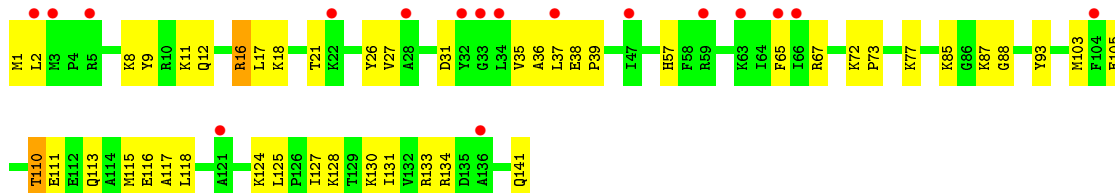
- Molecule 11: 50S ribosomal protein L15



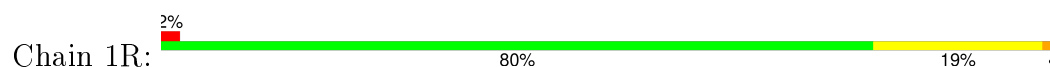
- Molecule 12: 50S ribosomal protein L16



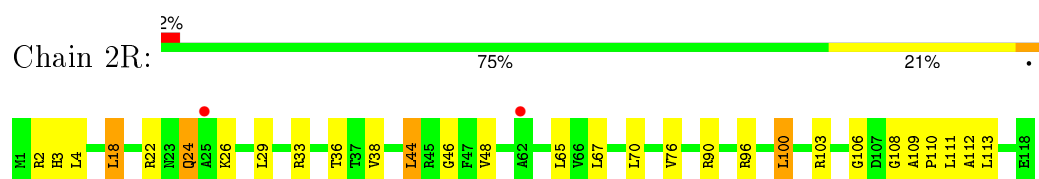
- Molecule 12: 50S ribosomal protein L16



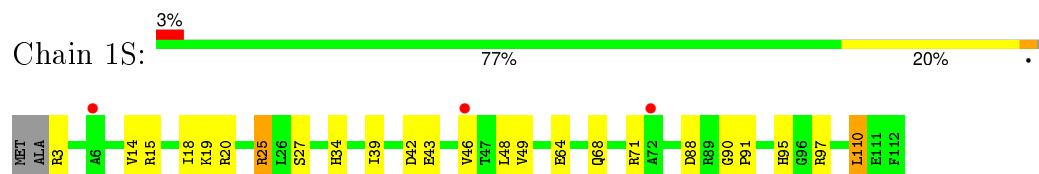
- Molecule 13: 50S ribosomal protein L17



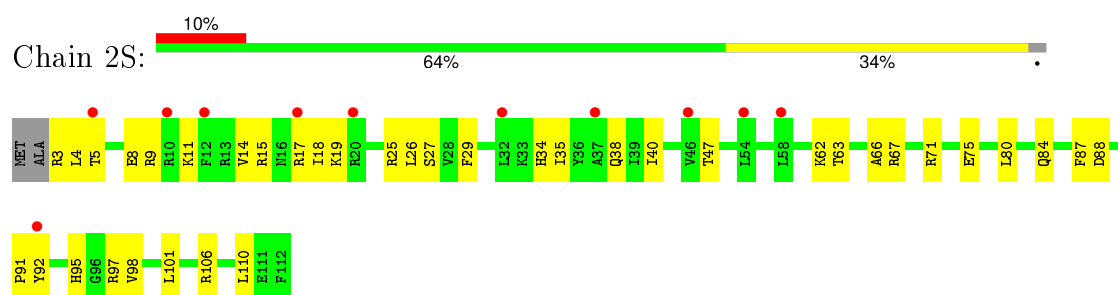
- Molecule 13: 50S ribosomal protein L17



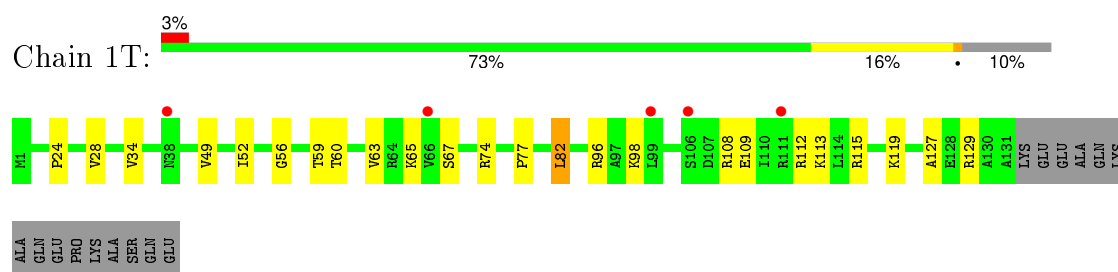
- Molecule 14: 50S ribosomal protein L18



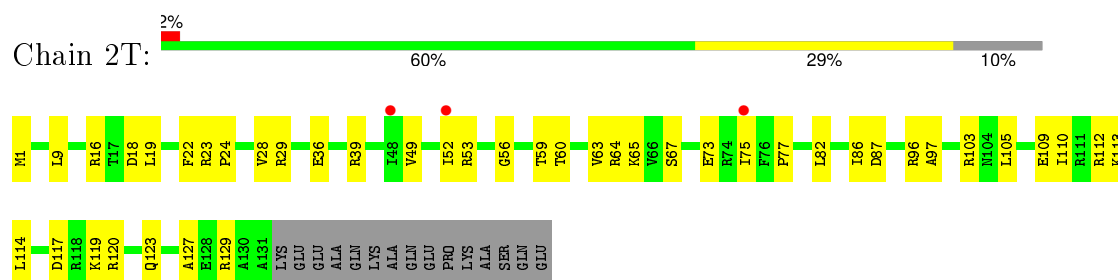
- Molecule 14: 50S ribosomal protein L18



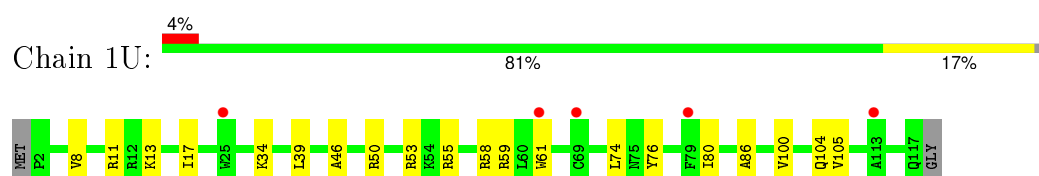
- Molecule 15: 50S ribosomal protein L19



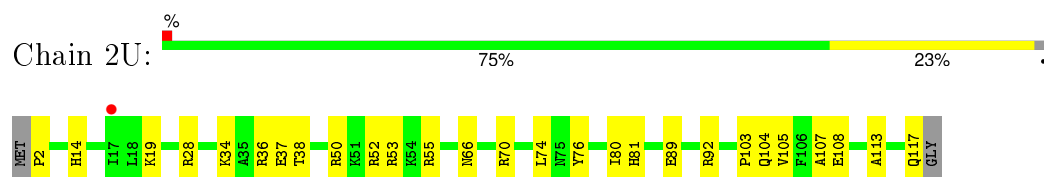
- Molecule 15: 50S ribosomal protein L19



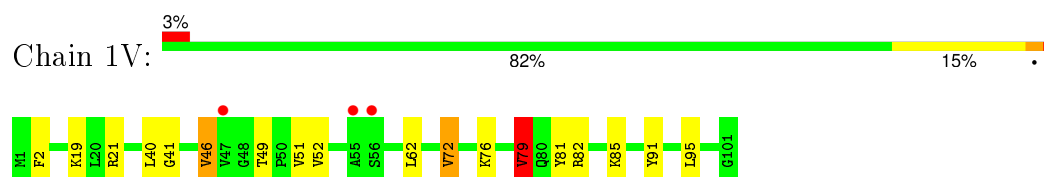
- Molecule 16: 50S ribosomal protein L20



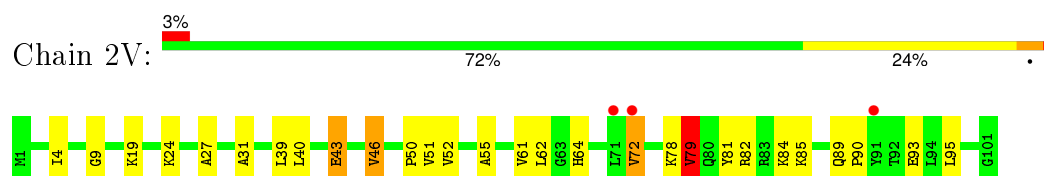
- Molecule 16: 50S ribosomal protein L20



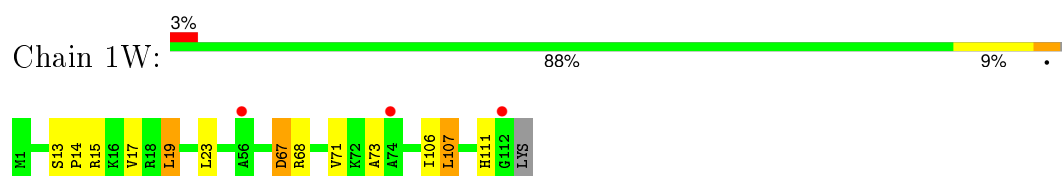
- Molecule 17: 50S ribosomal protein L21



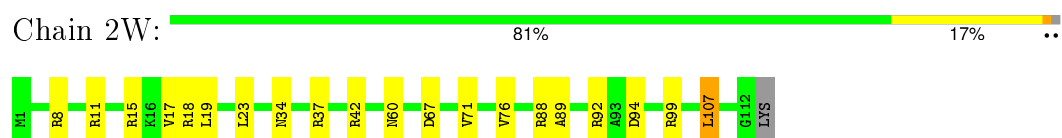
- Molecule 17: 50S ribosomal protein L21



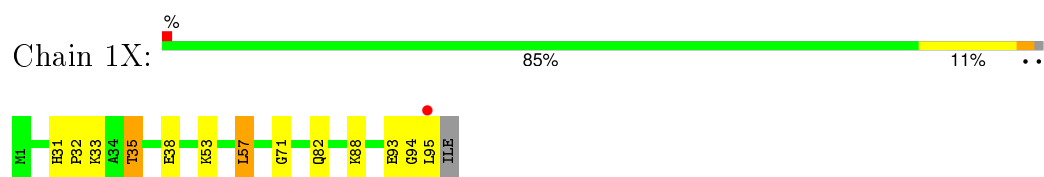
- Molecule 18: 50S ribosomal protein L22



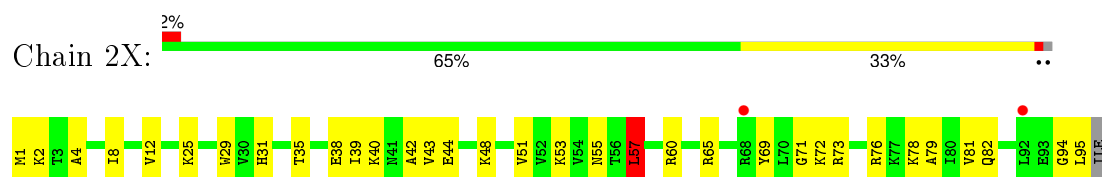
- Molecule 18: 50S ribosomal protein L22



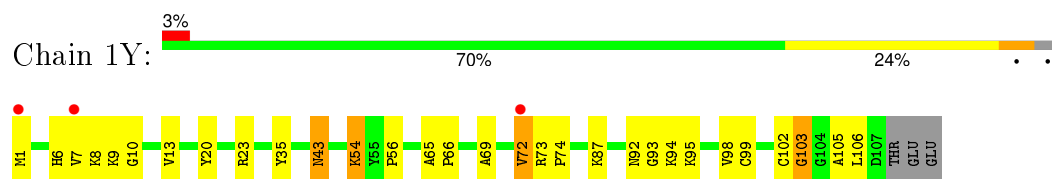
- Molecule 19: 50S ribosomal protein L23



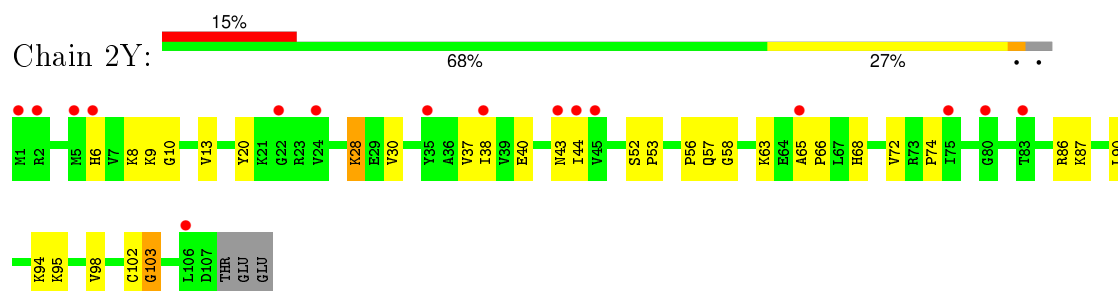
- Molecule 19: 50S ribosomal protein L23



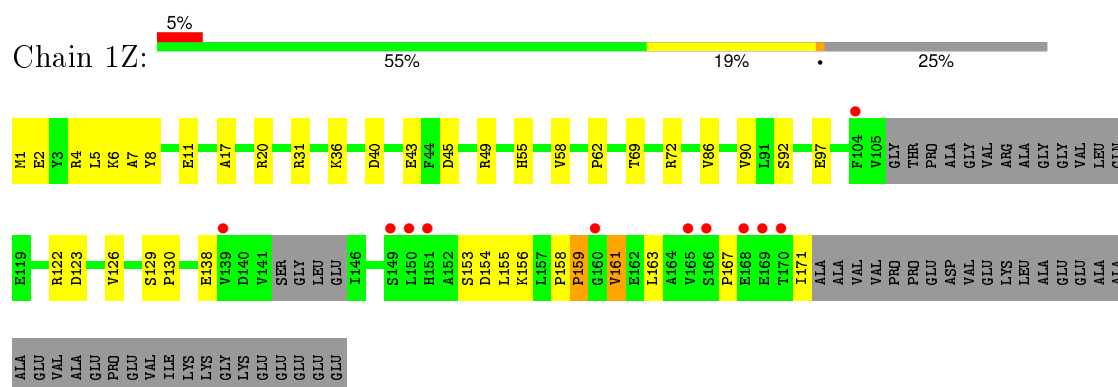
- Molecule 20: 50S ribosomal protein L24



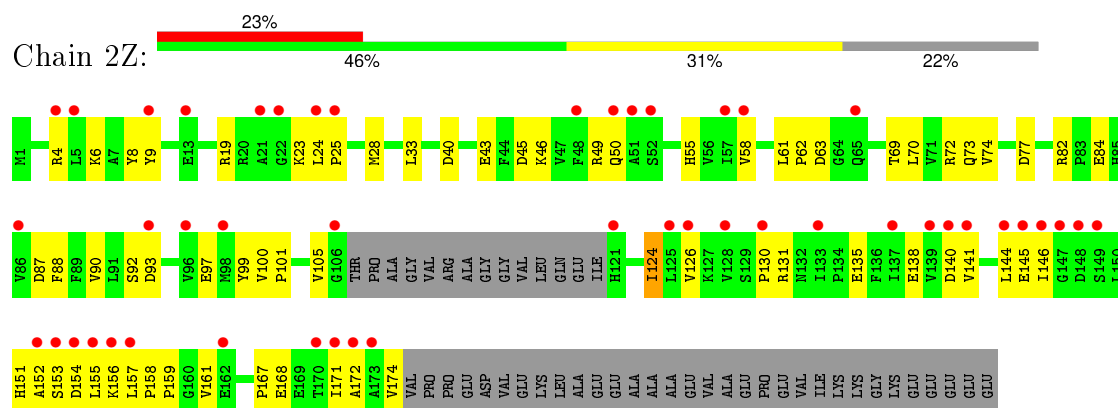
- Molecule 20: 50S ribosomal protein L24



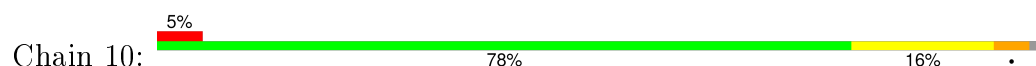
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

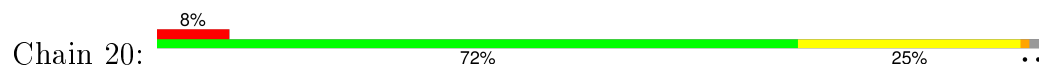


- Molecule 22: 50S ribosomal protein L27

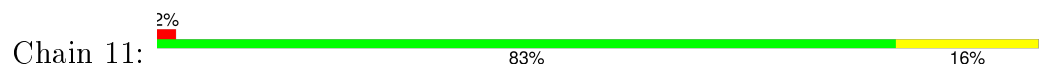




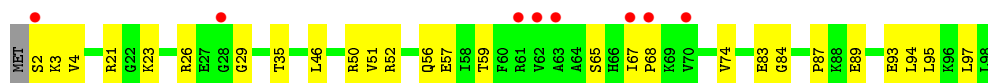
- Molecule 22: 50S ribosomal protein L27



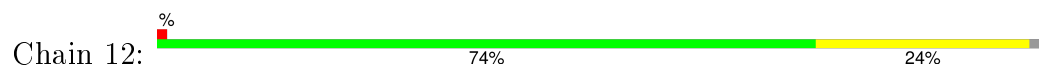
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



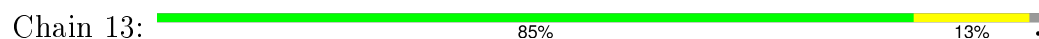
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29

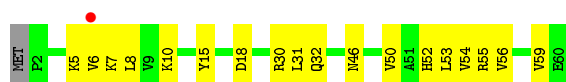


- Molecule 25: 50S ribosomal protein L30

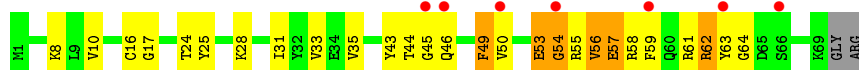


- Molecule 25: 50S ribosomal protein L30

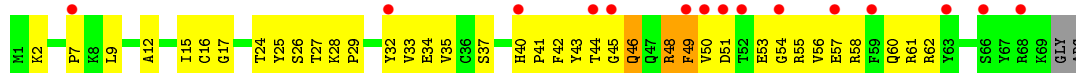
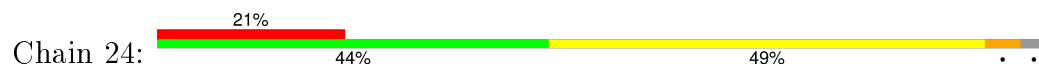




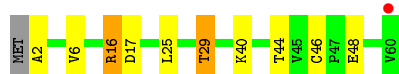
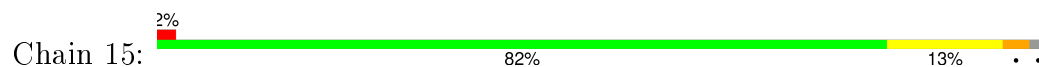
- Molecule 26: 50S ribosomal protein L31



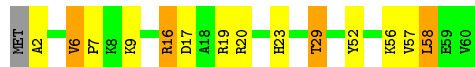
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



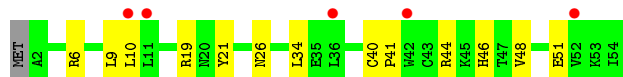
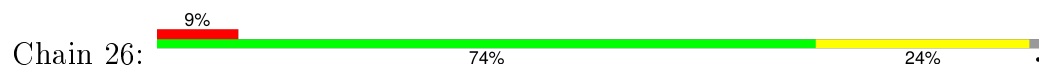
- Molecule 27: 50S ribosomal protein L32



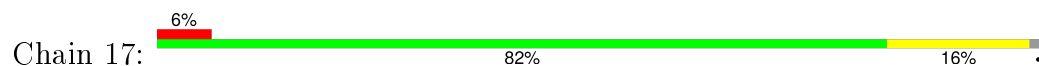
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33

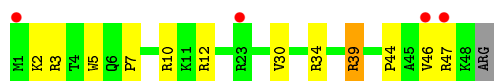
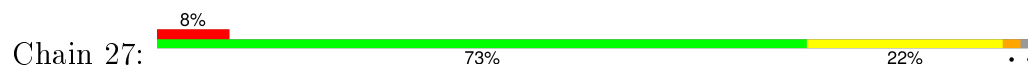


- Molecule 29: 50S ribosomal protein L34

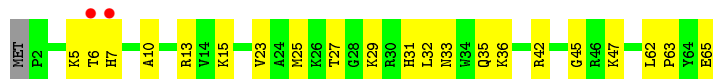




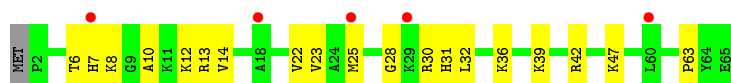
- Molecule 29: 50S ribosomal protein L34



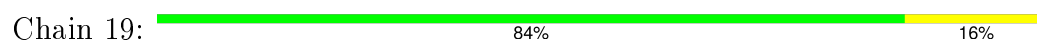
- Molecule 30: 50S ribosomal protein L35



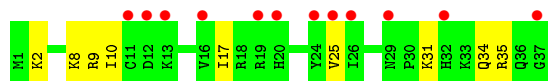
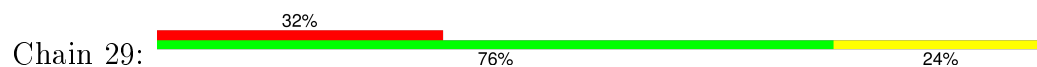
- Molecule 30: 50S ribosomal protein L35



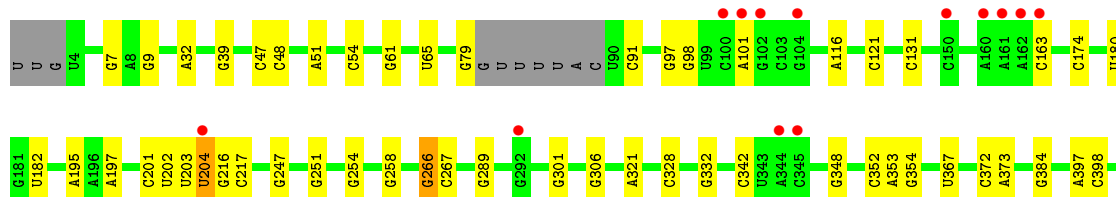
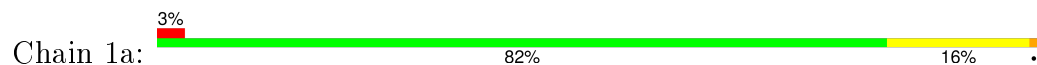
- Molecule 31: 50S ribosomal protein L36

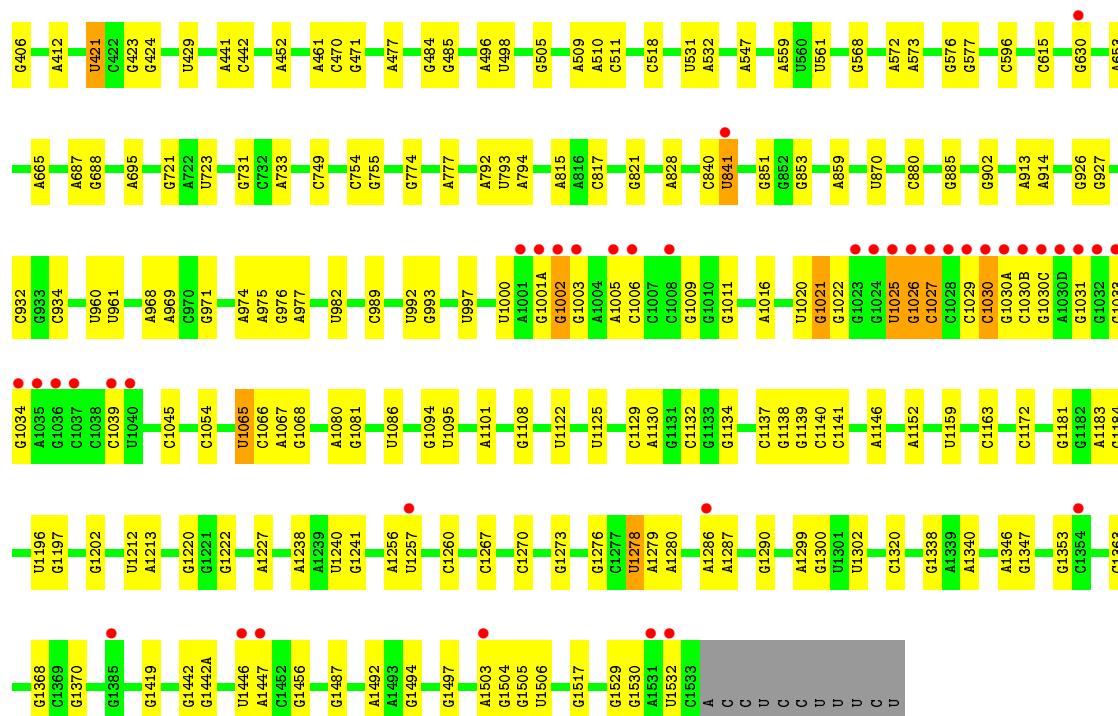


- Molecule 31: 50S ribosomal protein L36

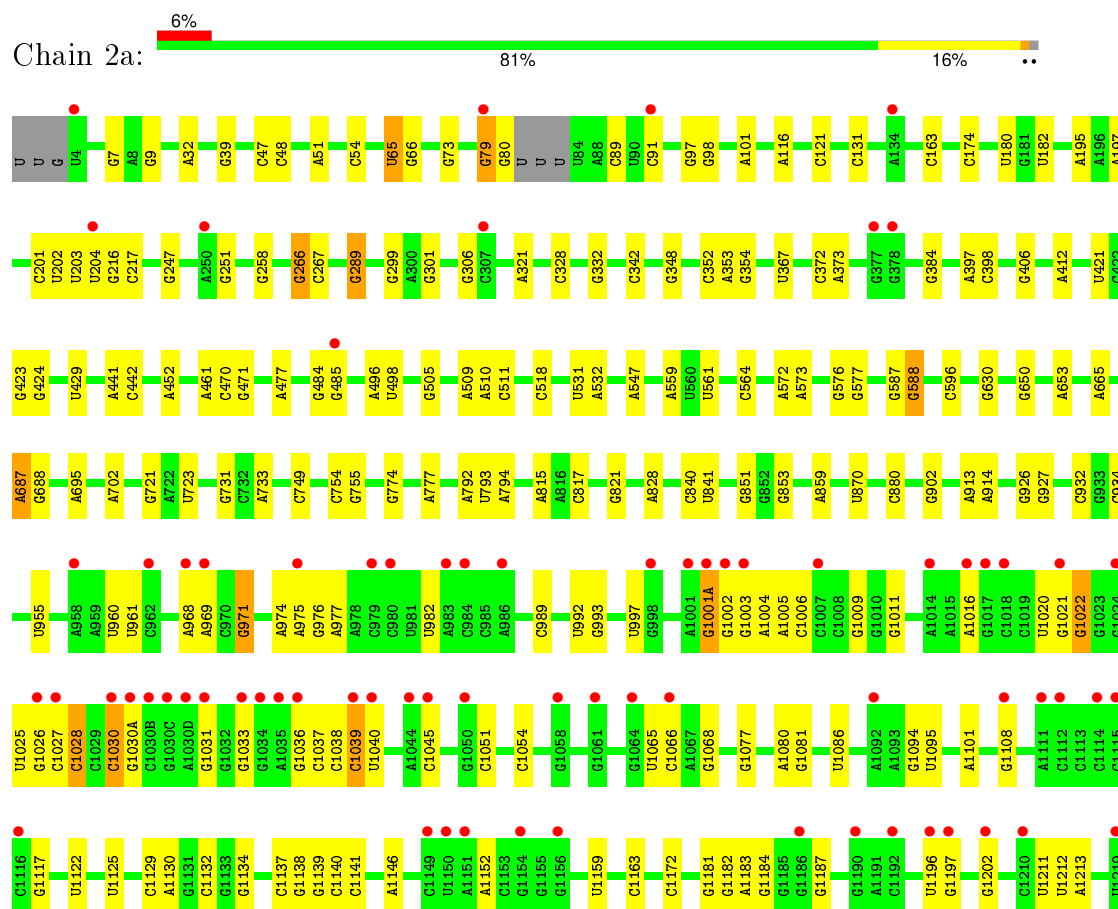


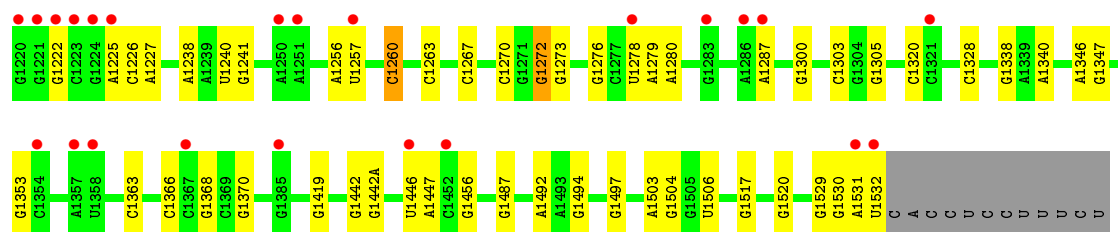
- Molecule 32: 16S Ribosomal RNA



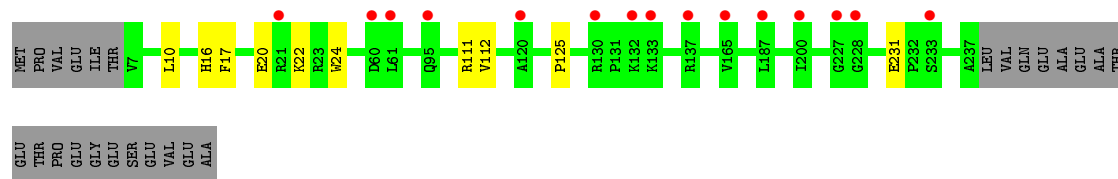
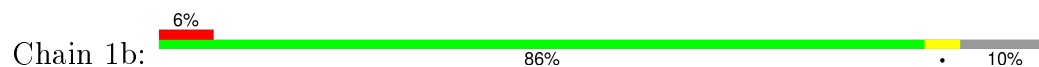


• Molecule 32: 16S Ribosomal RNA

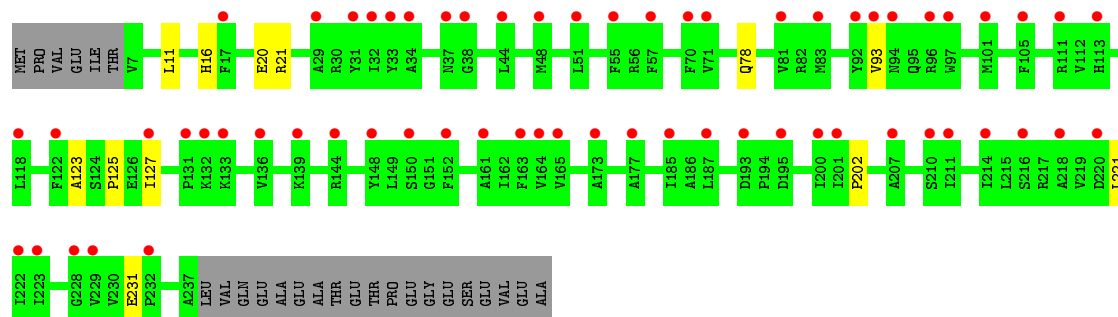
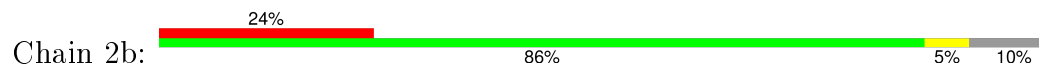




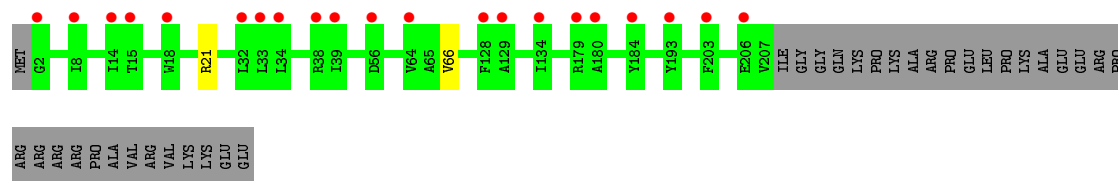
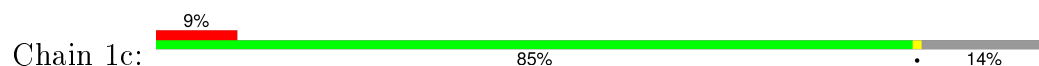
• Molecule 33: 30S ribosomal protein S2



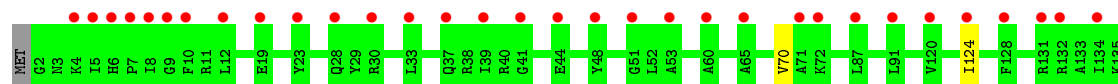
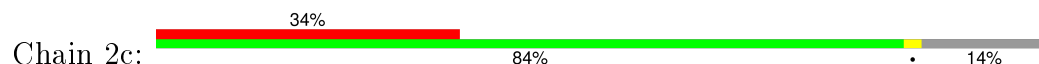
• Molecule 33: 30S ribosomal protein S2

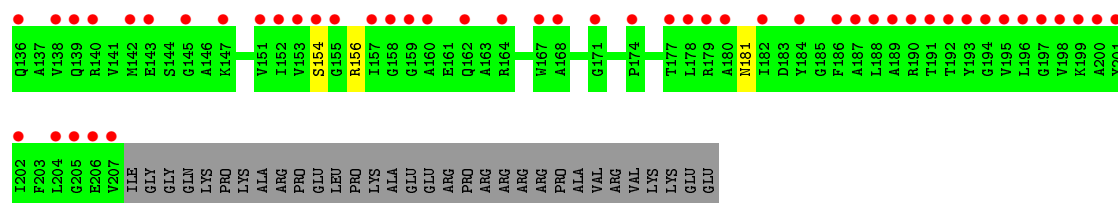


• Molecule 34: 30S ribosomal protein S3

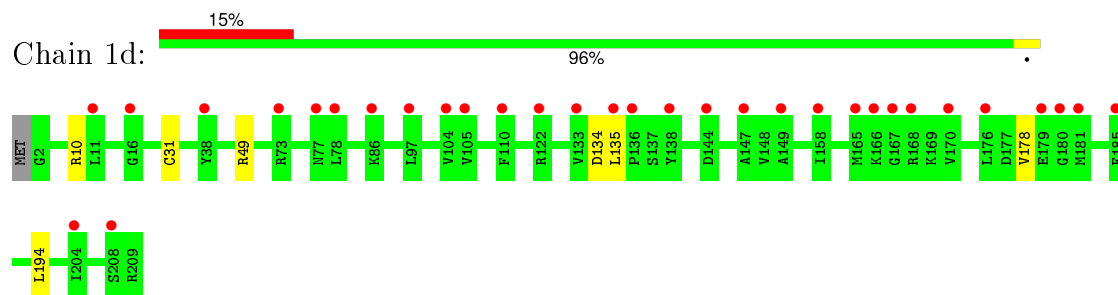


• Molecule 34: 30S ribosomal protein S3

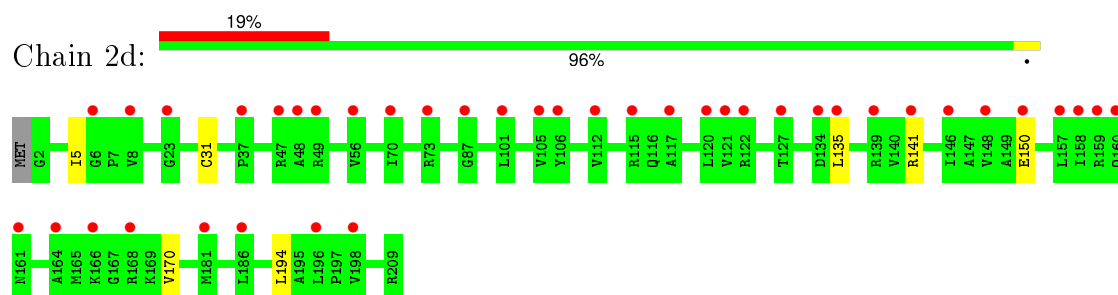




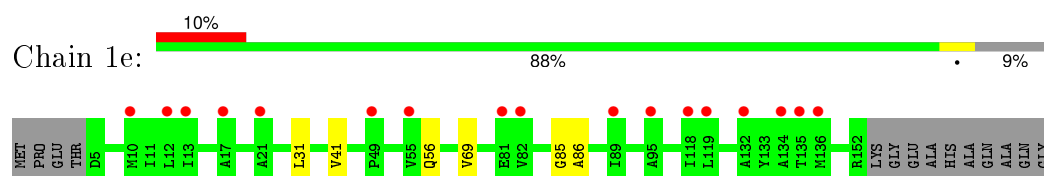
• Molecule 35: 30S ribosomal protein S4



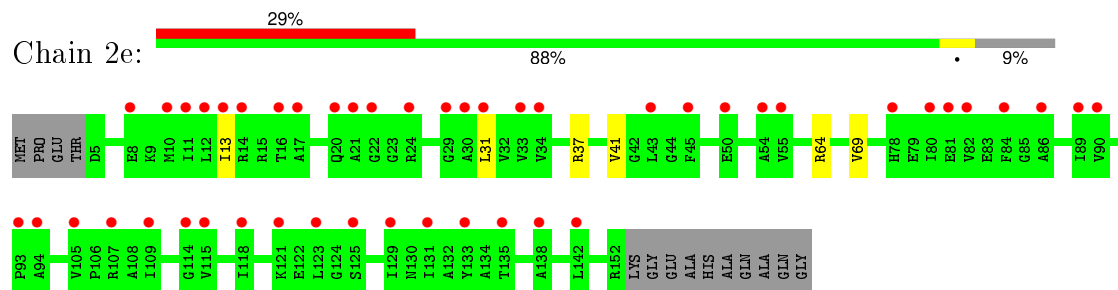
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5

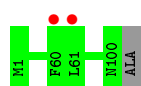


• Molecule 36: 30S ribosomal protein S5



• Molecule 37: 30S ribosomal protein S6

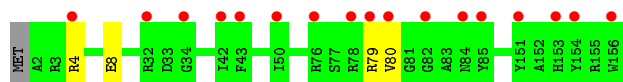




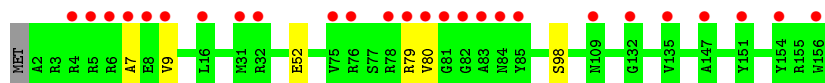
- Molecule 37: 30S ribosomal protein S6



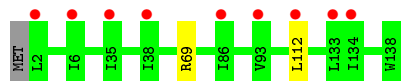
- Molecule 38: 30S ribosomal protein S7



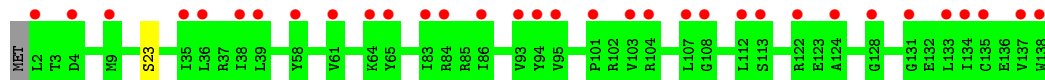
- Molecule 38: 30S ribosomal protein S7



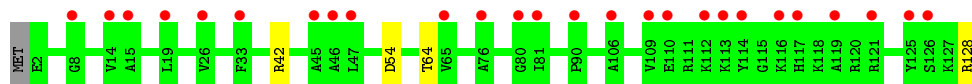
- Molecule 39: 30S ribosomal protein S8



- Molecule 39: 30S ribosomal protein S8

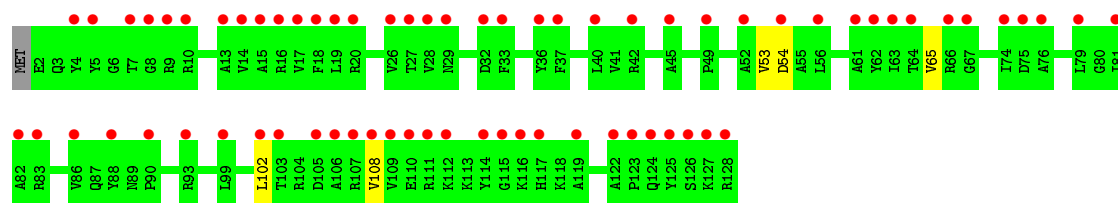


- Molecule 40: 30S ribosomal protein S9

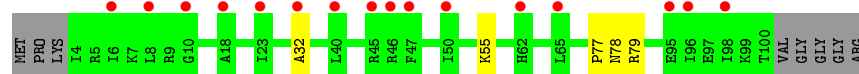
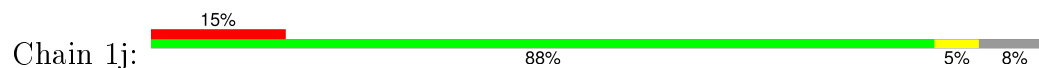


- Molecule 40: 30S ribosomal protein S9

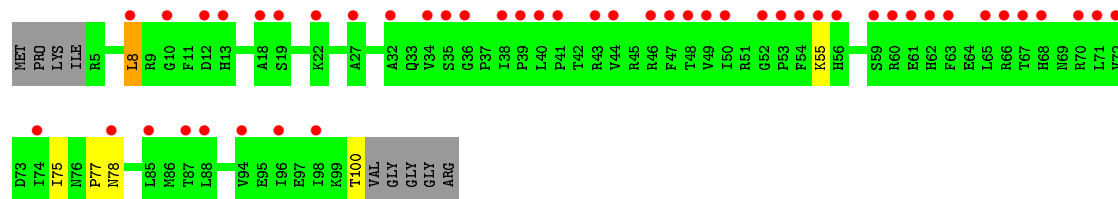
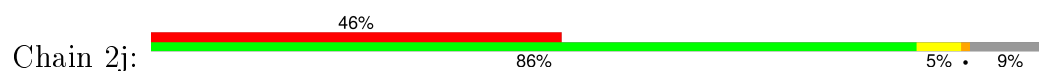




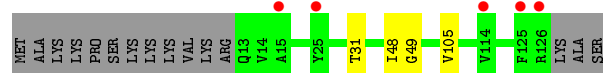
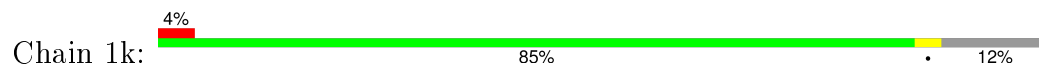
- Molecule 41: 30S ribosomal protein S10



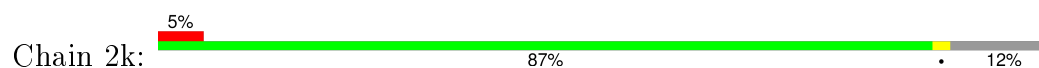
- Molecule 41: 30S ribosomal protein S10



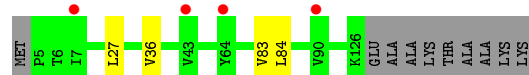
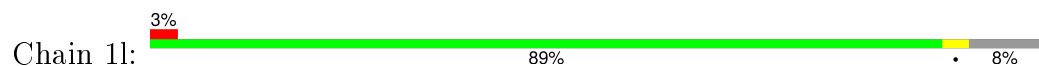
- Molecule 42: 30S ribosomal protein S11



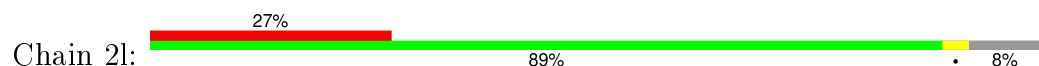
- Molecule 42: 30S ribosomal protein S11

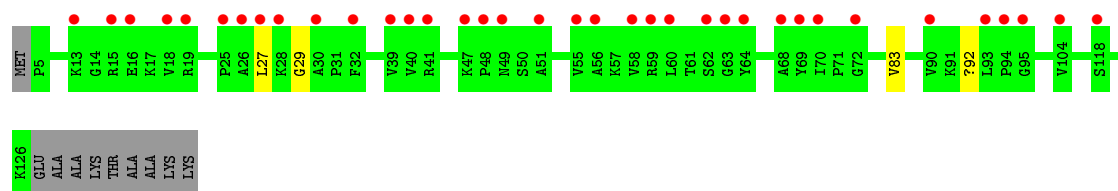


- Molecule 43: 30S ribosomal protein S12

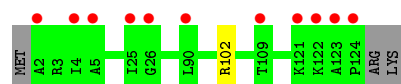


- Molecule 43: 30S ribosomal protein S12

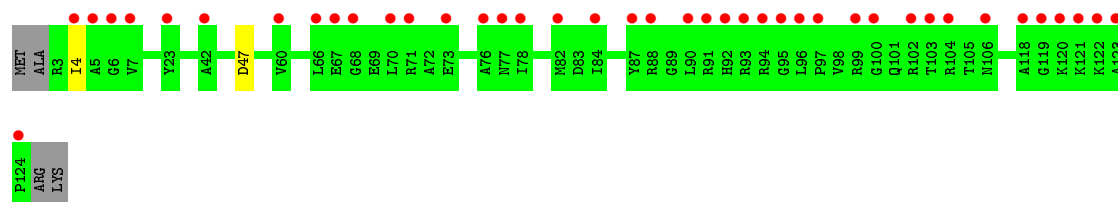




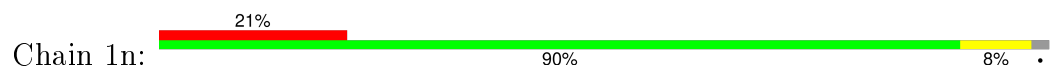
- Molecule 44: 30S ribosomal protein S13



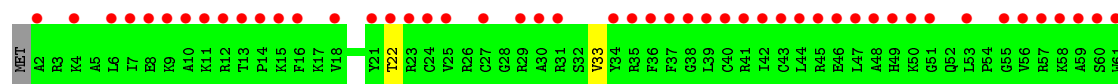
- Molecule 44: 30S ribosomal protein S13



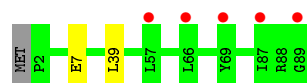
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z

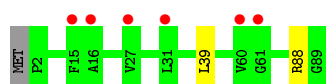


- Molecule 46: 30S ribosomal protein S15

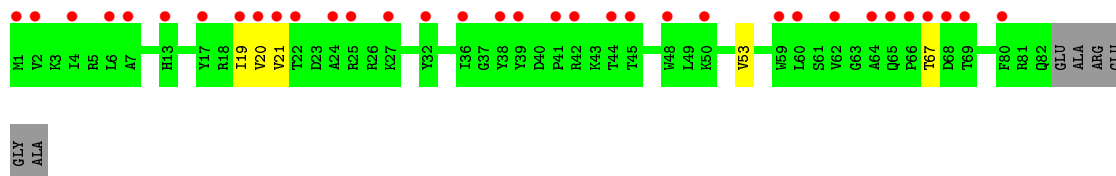
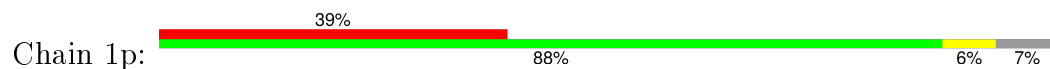


- Molecule 46: 30S ribosomal protein S15

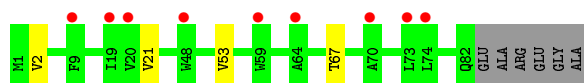
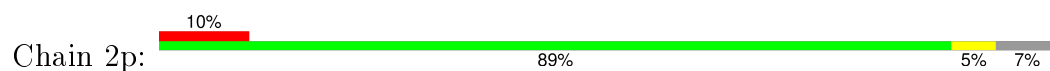




- Molecule 47: 30S ribosomal protein S16



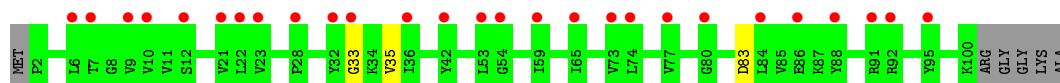
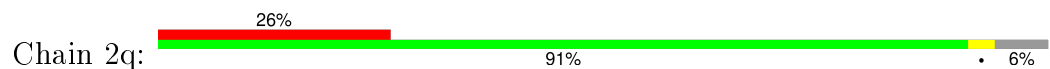
- Molecule 47: 30S ribosomal protein S16



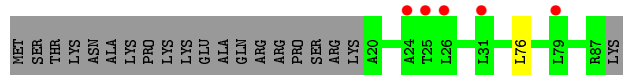
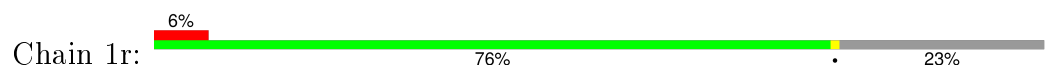
- Molecule 48: 30S ribosomal protein S17



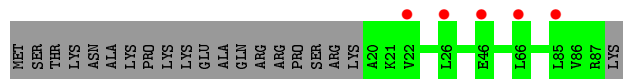
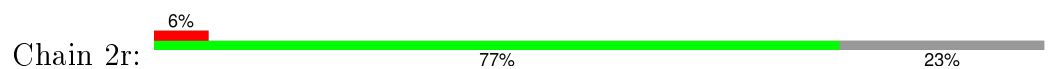
- Molecule 48: 30S ribosomal protein S17



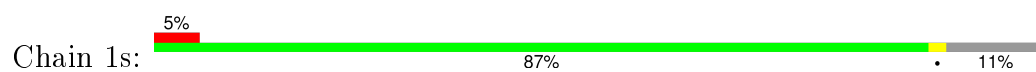
- Molecule 49: 30S ribosomal protein S18



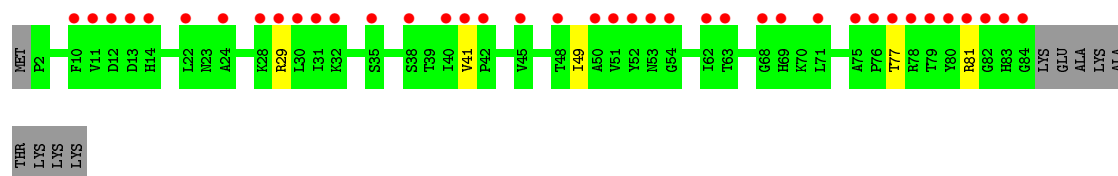
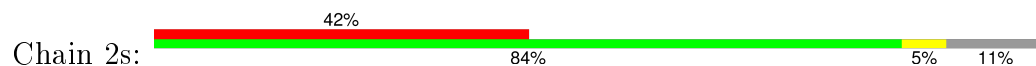
- Molecule 49: 30S ribosomal protein S18



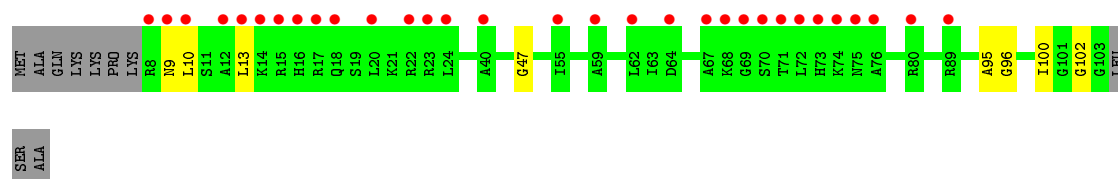
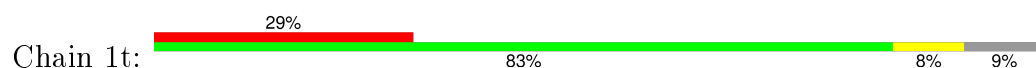
- Molecule 50: 30S ribosomal protein S19



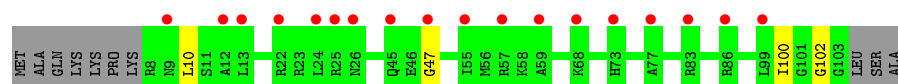
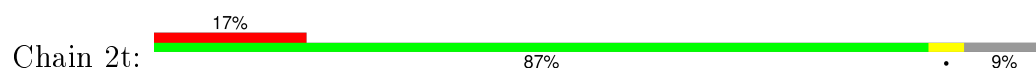
- Molecule 50: 30S ribosomal protein S19



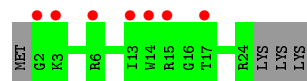
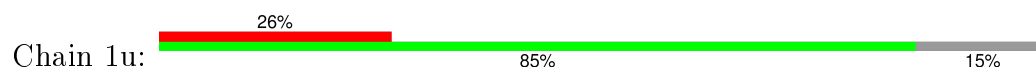
- Molecule 51: 30S ribosomal protein S20



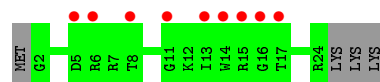
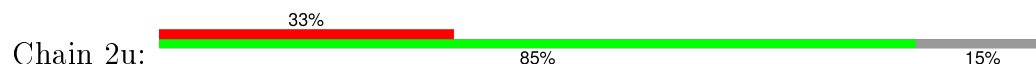
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx

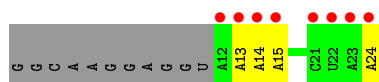


- Molecule 52: 30S ribosomal protein Thx

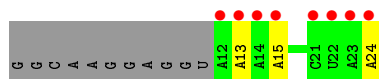
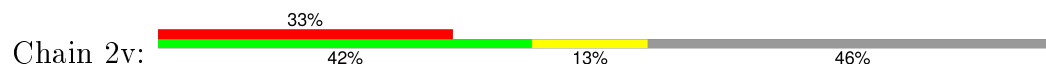


- Molecule 53: mRNA





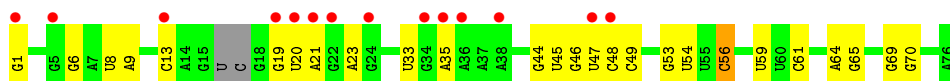
- Molecule 53: mRNA



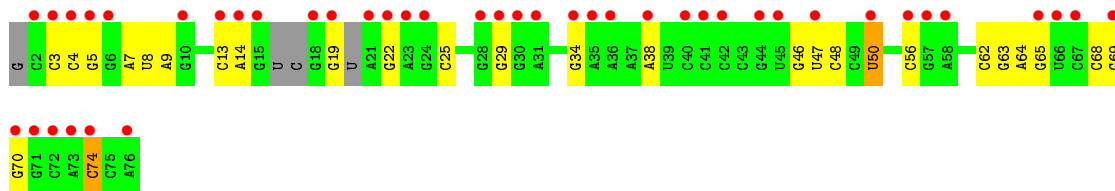
- Molecule 54: A-site and E-site tRNAs



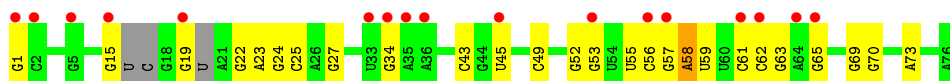
- Molecule 54: A-site and E-site tRNAs



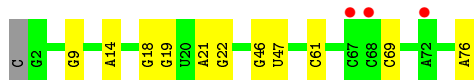
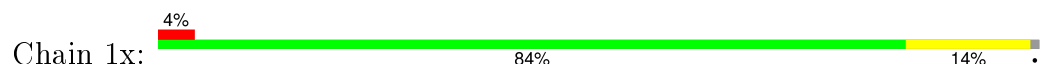
- Molecule 54: A-site and E-site tRNAs



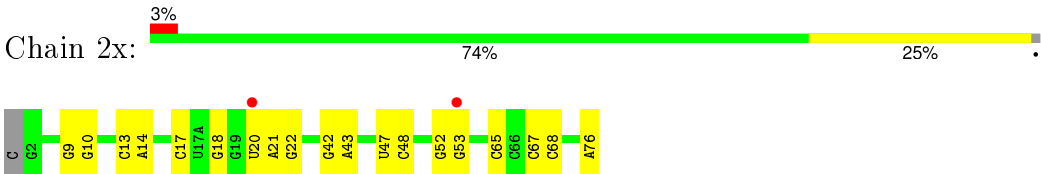
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.70Å 450.05Å 624.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.01 – 2.50 198.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (122.01-2.50) 97.8 (198.78-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.52Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.231 , 0.281 0.244 , 0.291	Depositor DCC
R_{free} test set	98495 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	0 of 1962083 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	300910	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.61	0/69009	1.05	129/107712 (0.1%)
1	2A	0.52	1/67293 (0.0%)	1.03	84/105034 (0.1%)
2	1B	0.51	1/2882 (0.0%)	0.87	0/4494
2	2B	0.59	1/2879 (0.0%)	1.01	4/4487 (0.1%)
3	1D	0.44	0/2186	0.61	0/2944
3	2D	0.38	0/2186	0.61	0/2944
4	1E	0.43	0/1592	0.61	0/2149
4	2E	0.37	0/1592	0.59	0/2149
5	1F	0.40	0/1619	0.58	0/2193
5	2F	0.37	0/1615	0.58	0/2188
6	1G	0.34	0/1448	0.54	0/1957
6	2G	0.36	0/1453	0.58	0/1963
7	1H	0.36	0/1356	0.55	0/1834
7	2H	0.33	0/1356	0.55	0/1834
8	1I	0.31	0/1112	0.55	0/1514
8	2I	0.30	0/1079	0.54	0/1475
9	1N	0.39	0/1144	0.57	0/1543
9	2N	0.36	0/1144	0.58	0/1543
10	1O	0.42	0/943	0.58	0/1269
10	2O	0.35	0/943	0.54	0/1269
11	1P	0.39	0/1152	0.60	0/1533
11	2P	0.36	0/1152	0.62	0/1533
12	1Q	0.41	0/1143	0.57	0/1527
12	2Q	0.37	0/1143	0.60	0/1527
13	1R	0.43	0/982	0.63	0/1312
13	2R	0.38	0/982	0.60	0/1312
14	1S	0.34	0/883	0.56	0/1176
14	2S	0.38	0/880	0.59	0/1172
15	1T	0.39	0/1105	0.61	1/1477 (0.1%)
15	2T	0.36	0/1097	0.59	0/1468
16	1U	0.46	0/977	0.62	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.39	0/977	0.60	0/1301
17	1V	0.45	0/782	0.62	0/1049
17	2V	0.35	0/782	0.59	0/1049
18	1W	0.45	0/897	0.66	0/1205
18	2W	0.39	0/897	0.58	0/1205
19	1X	0.44	0/764	0.61	0/1025
19	2X	0.40	0/764	0.63	1/1025 (0.1%)
20	1Y	0.39	0/819	0.57	0/1095
20	2Y	0.35	0/819	0.56	0/1095
21	1Z	0.35	0/1267	0.59	0/1717
21	2Z	0.31	0/1299	0.53	0/1763
22	10	0.43	0/662	0.66	1/881 (0.1%)
22	20	0.33	0/662	0.56	0/881
23	11	0.39	0/762	0.58	0/1014
23	21	0.35	0/762	0.57	0/1014
24	12	0.35	0/590	0.56	0/781
24	22	0.33	0/590	0.51	0/781
25	13	0.41	0/474	0.60	0/635
25	23	0.33	0/469	0.57	0/630
26	14	0.35	0/565	0.69	1/761 (0.1%)
26	24	0.37	0/545	0.64	0/737
27	15	0.42	0/469	0.64	0/635
27	25	0.38	0/469	0.60	1/635 (0.2%)
28	16	0.44	0/460	0.56	0/613
28	26	0.35	0/456	0.51	0/608
29	17	0.44	0/426	0.70	0/561
29	27	0.42	0/426	0.66	0/561
30	18	0.41	0/525	0.59	0/691
30	28	0.39	0/525	0.60	0/691
31	19	0.42	0/310	0.60	0/407
31	29	0.38	0/310	0.60	0/407
32	1a	0.43	0/35795	0.92	40/55864 (0.1%)
32	2a	0.45	3/35886 (0.0%)	0.98	62/56005 (0.1%)
33	1b	0.31	0/1881	0.59	0/2542
33	2b	0.34	0/1860	0.57	0/2518
34	1c	0.28	0/1572	0.49	0/2126
34	2c	0.34	0/1566	0.55	0/2119
35	1d	0.31	0/1685	0.54	0/2262
35	2d	0.31	0/1704	0.52	0/2284
36	1e	0.31	0/1145	0.55	0/1543
36	2e	0.34	0/1149	0.61	0/1548
37	1f	0.32	0/823	0.53	0/1115
37	2f	0.32	0/829	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1250	0.52	0/1679
38	2g	0.31	0/1254	0.54	0/1683
39	1h	0.30	0/1108	0.54	0/1494
39	2h	0.30	0/1108	0.55	0/1494
40	1i	0.31	0/1002	0.59	0/1346
40	2i	0.32	0/997	0.56	0/1343
41	1j	0.30	0/722	0.54	0/982
41	2j	0.34	0/727	0.59	1/988 (0.1%)
42	1k	0.30	0/844	0.55	0/1145
42	2k	0.31	0/848	0.52	0/1149
43	1l	0.34	0/937	0.54	0/1260
43	2l	0.32	0/937	0.59	1/1260 (0.1%)
44	1m	0.32	0/969	0.57	0/1302
44	2m	0.31	0/961	0.57	0/1291
45	1n	0.33	0/501	0.51	0/664
45	2n	0.31	0/501	0.53	0/664
46	1o	0.30	0/739	0.49	0/985
46	2o	0.30	0/739	0.51	0/985
47	1p	0.31	0/697	0.54	0/939
47	2p	0.31	0/693	0.53	0/935
48	1q	0.33	0/836	0.55	0/1117
48	2q	0.31	0/836	0.52	0/1117
49	1r	0.32	0/560	0.53	0/746
49	2r	0.30	0/560	0.51	0/746
50	1s	0.29	0/667	0.58	0/900
50	2s	0.38	0/661	0.66	0/893
51	1t	0.28	0/730	0.53	0/965
51	2t	0.30	0/729	0.54	0/965
52	1u	0.27	0/203	0.46	0/266
52	2u	0.34	0/203	0.50	0/266
53	1v	0.46	0/310	0.93	0/480
53	2v	0.60	0/310	0.91	0/480
54	1w	0.57	1/1606 (0.1%)	1.10	3/2497 (0.1%)
54	1y	0.56	1/1606 (0.1%)	1.13	9/2497 (0.4%)
54	2w	0.53	0/1556	1.12	2/2418 (0.1%)
54	2y	0.59	1/1583 (0.1%)	1.17	4/2459 (0.2%)
55	1x	0.57	3/1725 (0.2%)	1.16	16/2689 (0.6%)
55	2x	0.49	0/1725	1.06	8/2689 (0.3%)
All	All	0.49	12/316686 (0.0%)	0.92	368/474113 (0.1%)

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
43	2l	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	1	G	OP3-P	-10.21	1.48	1.61
2	1B	1	U	OP3-P	-10.20	1.49	1.61
54	1y	1	G	OP3-P	-10.20	1.49	1.61
2	2B	1	U	OP3-P	-9.87	1.49	1.61
54	1w	1	G	OP3-P	-9.63	1.49	1.61

The worst 5 of 368 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	22.29	132.27	118.90
32	2a	1272	G	N3-C2-N2	21.80	135.16	119.90
32	2a	1272	G	C5-C6-O6	20.59	140.96	128.60
32	2a	1272	G	N1-C2-N2	-18.95	99.14	116.20
32	2a	1263	C	C2-N3-C4	15.04	127.42	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	2l	92	0TD	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31193	648	0
1	2A	60322	0	30425	904	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	65	0
3	1D	2136	0	2218	45	0
3	2D	2136	0	2218	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	37	0
5	1F	1584	0	1625	34	0
5	2F	1580	0	1619	54	0
6	1G	1423	0	1436	22	0
6	2G	1428	0	1438	73	0
7	1H	1330	0	1407	26	0
7	2H	1330	0	1407	44	0
8	1I	1097	0	1140	31	0
8	2I	1064	0	1082	24	0
9	1N	1117	0	1184	21	0
9	2N	1117	0	1184	22	0
10	1O	933	0	996	17	0
10	2O	933	0	996	23	0
11	1P	1135	0	1212	36	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	14	0
12	2Q	1122	0	1179	33	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	21	0
14	1S	873	0	927	19	0
14	2S	870	0	923	31	0
15	1T	1091	0	1151	17	0
15	2T	1083	0	1136	31	0
16	1U	959	0	1019	18	0
16	2U	959	0	1019	25	0
17	1V	771	0	830	10	0
17	2V	771	0	830	22	0
18	1W	886	0	940	8	0
18	2W	886	0	940	13	0
19	1X	750	0	814	10	0
19	2X	750	0	814	28	0
20	1Y	806	0	881	21	0
20	2Y	806	0	881	23	0
21	1Z	1240	0	1240	24	0
21	2Z	1271	0	1273	46	0
22	10	653	0	674	14	0
22	20	653	0	674	19	0
23	11	755	0	826	11	0
23	21	755	0	826	20	0
24	12	588	0	643	11	0
24	22	588	0	643	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	469	0	518	5	0
25	23	464	0	514	12	0
26	14	552	0	533	20	0
26	24	532	0	503	31	0
27	15	455	0	465	7	0
27	25	455	0	465	11	0
28	16	453	0	473	12	0
28	26	449	0	469	11	0
29	17	418	0	467	7	0
29	27	418	0	467	17	0
30	18	517	0	582	19	0
30	28	517	0	582	17	0
31	19	307	0	335	4	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16339	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	277	0	140	0	0
53	2v	277	0	140	0	0
54	1w	1592	0	819	0	0
54	1y	1585	0	804	0	0
54	2w	1544	0	788	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	828	0	0
55	2x	1625	0	828	0	0
56	10	6	0	0	0	0
56	11	3	0	0	0	0
56	12	1	0	0	0	0
56	13	3	0	0	0	0
56	15	2	0	0	0	0
56	16	3	0	0	0	0
56	17	1	0	0	0	0
56	18	3	0	0	0	0
56	19	2	0	0	0	0
56	1A	1141	0	0	0	0
56	1B	37	0	0	0	0
56	1D	12	0	0	0	0
56	1E	11	0	0	0	0
56	1F	8	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	7	0	0	0	0
56	1P	4	0	0	0	0
56	1Q	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	8	0	0	0	0
56	1V	3	0	0	0	0
56	1W	5	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	229	0	0	0	0
56	1b	2	0	0	0	0
56	1d	1	0	0	0	0
56	1e	1	0	0	0	0
56	1f	2	0	0	0	0
56	1l	3	0	0	0	0
56	1n	2	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	11	0	0	0	0
56	1x	16	0	0	0	0
56	1y	4	0	0	0	0
56	20	3	0	0	0	0
56	23	2	0	0	0	0
56	25	4	0	0	0	0
56	27	1	0	0	0	0
56	28	2	0	0	0	0
56	2A	909	0	0	0	0
56	2B	21	0	0	0	0
56	2D	5	0	0	0	0
56	2E	9	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	1	0	0	0	0
56	2T	3	0	0	0	0
56	2U	4	0	0	0	0
56	2V	1	0	0	0	0
56	2W	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2X	3	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	244	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0
56	2i	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	2	0	0	0	0
56	2n	1	0	0	0	0
56	2q	2	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	2	0	0	0	0
56	2w	8	0	0	0	0
56	2x	5	0	0	0	0
56	2y	7	0	0	0	0
57	1A	1	0	0	0	0
57	2A	1	0	0	0	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	0	0
60	10	12	0	0	0	0
60	11	10	0	0	0	0
60	12	4	0	0	0	0
60	13	6	0	0	0	0
60	14	1	0	0	0	0
60	15	6	0	0	0	0
60	16	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	17	9	0	0	0	0
60	18	13	0	0	1	0
60	1A	2238	0	0	95	0
60	1B	68	0	0	3	0
60	1D	28	0	0	1	0
60	1E	28	0	0	3	0
60	1F	13	0	0	1	0
60	1G	7	0	0	1	0
60	1H	2	0	0	0	0
60	1I	3	0	0	0	0
60	1N	7	0	0	1	0
60	1O	8	0	0	0	0
60	1P	23	0	0	3	0
60	1Q	14	0	0	0	0
60	1R	14	0	0	0	0
60	1S	5	0	0	0	0
60	1T	8	0	0	1	0
60	1U	11	0	0	1	0
60	1V	9	0	0	0	0
60	1W	6	0	0	0	0
60	1X	8	0	0	2	0
60	1Y	4	0	0	0	0
60	1Z	1	0	0	0	0
60	1a	438	0	0	0	0
60	1b	1	0	0	0	0
60	1d	1	0	0	0	0
60	1e	1	0	0	0	0
60	1f	1	0	0	0	0
60	1g	1	0	0	0	0
60	1i	1	0	0	0	0
60	1l	8	0	0	0	0
60	1m	2	0	0	0	0
60	1o	1	0	0	0	0
60	1p	1	0	0	0	0
60	1q	4	0	0	0	0
60	1u	1	0	0	0	0
60	1v	5	0	0	0	0
60	1w	21	0	0	0	0
60	1x	15	0	0	0	0
60	1y	1	0	0	0	0
60	20	7	0	0	0	0
60	21	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	22	1	0	0	0	0
60	23	1	0	0	0	0
60	25	4	0	0	1	0
60	26	1	0	0	0	0
60	27	4	0	0	1	0
60	28	6	0	0	2	0
60	29	1	0	0	0	0
60	2A	1389	0	0	90	0
60	2B	26	0	0	1	0
60	2D	28	0	0	2	0
60	2E	16	0	0	0	0
60	2F	16	0	0	0	0
60	2H	1	0	0	0	0
60	2I	4	0	0	0	0
60	2N	1	0	0	0	0
60	2P	14	0	0	1	0
60	2Q	2	0	0	0	0
60	2R	2	0	0	0	0
60	2T	6	0	0	0	0
60	2U	2	0	0	0	0
60	2V	2	0	0	0	0
60	2W	2	0	0	0	0
60	2X	5	0	0	0	0
60	2Y	1	0	0	1	0
60	2Z	2	0	0	0	0
60	2a	377	0	0	0	0
60	2d	1	0	0	0	0
60	2e	2	0	0	0	0
60	2g	1	0	0	0	0
60	2i	1	0	0	0	0
60	2j	4	0	0	0	0
60	2l	5	0	0	0	0
60	2o	1	0	0	0	0
60	2p	2	0	0	0	0
60	2q	1	0	0	0	0
60	2r	1	0	0	0	0
60	2t	4	0	0	0	0
60	2u	1	0	0	0	0
60	2v	1	0	0	0	0
60	2w	2	0	0	0	0
60	2x	7	0	0	0	0
60	2y	19	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	300910	0	196690	2580	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 2580 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1128:U:H3	1:1A:1132:A:N6	1.34	1.25
1:2A:2136:C:N4	1:2A:2155:G:H1	1.44	1.15
1:1A:1128:U:O4	1:1A:1132:A:N1	1.85	1.09
1:2A:2138:C:N4	1:2A:2153:G:H1	1.48	1.09
1:1A:1740:U:H1'	3:1D:14:ARG:HH22	1.22	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	11 (4%)	2 (1%)	26	46
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	34	55
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	34	55
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	34	55
5	2F	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	19	34
6	1G	179/182 (98%)	170 (95%)	9 (5%)	0	100	100
6	2G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	30	50
7	1H	172/180 (96%)	164 (95%)	7 (4%)	1 (1%)	30	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	2H	172/180 (96%)	158 (92%)	12 (7%)	2 (1%)	16	29
8	1I	144/148 (97%)	132 (92%)	12 (8%)	0	100	100
8	2I	144/148 (97%)	128 (89%)	14 (10%)	2 (1%)	14	24
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	26	46
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	26	46
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
14	2S	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	21	37
15	1T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
15	2T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	19	34
17	2V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	19	34
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	17	31
20	1Y	105/110 (96%)	98 (93%)	5 (5%)	2 (2%)	10	16
20	2Y	105/110 (96%)	99 (94%)	4 (4%)	2 (2%)	10	16
21	1Z	148/206 (72%)	136 (92%)	11 (7%)	1 (1%)	26	46
21	2Z	156/206 (76%)	141 (90%)	15 (10%)	0	100	100
22	10	81/85 (95%)	80 (99%)	0	1 (1%)	16	29
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	16	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	11	18
26	14	67/71 (94%)	58 (87%)	4 (6%)	5 (8%)	1	1
26	24	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	2	2
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	8	13
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	200 (87%)	22 (10%)	7 (3%)	5	7
33	2b	229/256 (90%)	202 (88%)	19 (8%)	8 (4%)	4	6
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	34	55
34	2c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	19	34
35	1d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	34	55
35	2d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	34	55
36	1e	146/162 (90%)	137 (94%)	6 (4%)	3 (2%)	9	14
36	2e	146/162 (90%)	139 (95%)	5 (3%)	2 (1%)	14	24
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	144 (94%)	6 (4%)	3 (2%)	9	15
38	2g	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	9	15
39	1h	135/138 (98%)	133 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	1i	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	24	41
40	2i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	24	41
41	1j	95/105 (90%)	86 (90%)	4 (4%)	5 (5%)	2	2
41	2j	94/105 (90%)	85 (90%)	5 (5%)	4 (4%)	3	4
42	1k	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	11	18
42	2k	112/129 (87%)	107 (96%)	3 (3%)	2 (2%)	11	18
43	1l	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	114 (94%)	7 (6%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	9 (8%)	1 (1%)	24	41
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	16	29
47	1p	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	15	26
47	2p	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	15	26
48	1q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	19	34
48	2q	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	19	34
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	75 (93%)	5 (6%)	1 (1%)	16	29
50	2s	81/93 (87%)	74 (91%)	5 (6%)	2 (2%)	7	10
51	1t	94/106 (89%)	87 (93%)	0	7 (7%)	1	1
51	2t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	3	4
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	21 (100%)	0	0	100	100
All	All	11370/12128 (94%)	10779 (95%)	488 (4%)	103 (1%)	21	37

5 of 103 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	1H	126	PRO
21	1Z	159	PRO
26	14	62	ARG
33	1b	10	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	209 (97%)	6 (3%)	51	78
3	2D	215/218 (99%)	208 (97%)	7 (3%)	45	73
4	1E	164/166 (99%)	154 (94%)	10 (6%)	23	42
4	2E	164/166 (99%)	154 (94%)	10 (6%)	23	42
5	1F	160/166 (96%)	150 (94%)	10 (6%)	22	40
5	2F	159/166 (96%)	150 (94%)	9 (6%)	25	46
6	1G	143/156 (92%)	139 (97%)	4 (3%)	51	78
6	2G	143/156 (92%)	135 (94%)	8 (6%)	26	47
7	1H	144/148 (97%)	141 (98%)	3 (2%)	61	85
7	2H	144/148 (97%)	142 (99%)	2 (1%)	74	91
8	1I	113/124 (91%)	108 (96%)	5 (4%)	35	60
8	2I	105/124 (85%)	99 (94%)	6 (6%)	25	46
9	1N	118/119 (99%)	110 (93%)	8 (7%)	20	36
9	2N	118/119 (99%)	109 (92%)	9 (8%)	16	30
10	1O	100/100 (100%)	98 (98%)	2 (2%)	63	86
10	2O	100/100 (100%)	99 (99%)	1 (1%)	82	95
11	1P	115/116 (99%)	109 (95%)	6 (5%)	29	51
11	2P	115/116 (99%)	112 (97%)	3 (3%)	54	81
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	52	79
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	27	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1R	101/101 (100%)	90 (89%)	11 (11%)	8	15
13	2R	101/101 (100%)	94 (93%)	7 (7%)	19	35
14	1S	86/88 (98%)	84 (98%)	2 (2%)	58	83
14	2S	85/88 (97%)	83 (98%)	2 (2%)	57	82
15	1T	115/127 (91%)	113 (98%)	2 (2%)	68	89
15	2T	113/127 (89%)	113 (100%)	0	100	100
16	1U	93/94 (99%)	92 (99%)	1 (1%)	80	94
16	2U	93/94 (99%)	91 (98%)	2 (2%)	60	84
17	1V	80/82 (98%)	74 (92%)	6 (8%)	17	31
17	2V	80/82 (98%)	74 (92%)	6 (8%)	17	31
18	1W	90/92 (98%)	85 (94%)	5 (6%)	26	47
18	2W	90/92 (98%)	85 (94%)	5 (6%)	26	47
19	1X	77/78 (99%)	75 (97%)	2 (3%)	54	81
19	2X	77/78 (99%)	76 (99%)	1 (1%)	76	92
20	1Y	85/91 (93%)	82 (96%)	3 (4%)	43	70
20	2Y	85/91 (93%)	82 (96%)	3 (4%)	43	70
21	1Z	135/179 (75%)	129 (96%)	6 (4%)	35	60
21	2Z	137/179 (76%)	136 (99%)	1 (1%)	88	97
22	10	65/67 (97%)	63 (97%)	2 (3%)	47	75
22	20	65/67 (97%)	64 (98%)	1 (2%)	72	91
23	11	80/83 (96%)	79 (99%)	1 (1%)	76	92
23	21	80/83 (96%)	78 (98%)	2 (2%)	55	82
24	12	65/67 (97%)	64 (98%)	1 (2%)	72	91
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	49 (96%)	2 (4%)	39	66
25	23	50/52 (96%)	48 (96%)	2 (4%)	38	64
26	14	59/63 (94%)	58 (98%)	1 (2%)	68	89
26	24	53/63 (84%)	49 (92%)	4 (8%)	17	31
27	15	50/52 (96%)	47 (94%)	3 (6%)	24	43
27	25	50/52 (96%)	47 (94%)	3 (6%)	24	43
28	16	51/52 (98%)	49 (96%)	2 (4%)	39	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	26	50/52 (96%)	49 (98%)	1 (2%)	63	86
29	17	41/42 (98%)	40 (98%)	1 (2%)	57	82
29	27	41/42 (98%)	40 (98%)	1 (2%)	57	82
30	18	54/55 (98%)	52 (96%)	2 (4%)	41	68
30	28	54/55 (98%)	52 (96%)	2 (4%)	41	68
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	50	77
33	1b	192/220 (87%)	189 (98%)	3 (2%)	70	90
33	2b	187/220 (85%)	183 (98%)	4 (2%)	61	85
34	1c	142/188 (76%)	141 (99%)	1 (1%)	88	97
34	2c	140/188 (74%)	137 (98%)	3 (2%)	61	85
35	1d	169/181 (93%)	163 (96%)	6 (4%)	42	69
35	2d	173/181 (96%)	167 (96%)	6 (4%)	43	70
36	1e	113/123 (92%)	110 (97%)	3 (3%)	52	79
36	2e	114/123 (93%)	110 (96%)	4 (4%)	43	70
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	83 (98%)	2 (2%)	57	82
38	1g	119/127 (94%)	118 (99%)	1 (1%)	86	96
38	2g	120/127 (94%)	117 (98%)	3 (2%)	55	82
39	1h	114/119 (96%)	112 (98%)	2 (2%)	66	88
39	2h	114/119 (96%)	113 (99%)	1 (1%)	84	95
40	1i	90/99 (91%)	87 (97%)	3 (3%)	45	73
40	2i	89/99 (90%)	85 (96%)	4 (4%)	34	59
41	1j	66/92 (72%)	66 (100%)	0	100	100
41	2j	69/92 (75%)	67 (97%)	2 (3%)	50	77
42	1k	82/99 (83%)	80 (98%)	2 (2%)	57	82
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	92 (96%)	4 (4%)	36	62
43	2l	96/108 (89%)	94 (98%)	2 (2%)	61	85
44	1m	93/101 (92%)	92 (99%)	1 (1%)	80	94
44	2m	92/101 (91%)	91 (99%)	1 (1%)	80	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1n	49/50 (98%)	44 (90%)	5 (10%)	9	17
45	2n	49/50 (98%)	47 (96%)	2 (4%)	37	63
46	1o	78/80 (98%)	76 (97%)	2 (3%)	54	81
46	2o	78/80 (98%)	77 (99%)	1 (1%)	76	92
47	1p	69/74 (93%)	65 (94%)	4 (6%)	25	45
47	2p	68/74 (92%)	65 (96%)	3 (4%)	35	60
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	92 (98%)	2 (2%)	61	85
49	1r	59/77 (77%)	58 (98%)	1 (2%)	68	89
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	68 (99%)	1 (1%)	74	91
50	2s	67/80 (84%)	64 (96%)	3 (4%)	34	59
51	1t	70/82 (85%)	69 (99%)	1 (1%)	74	91
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	9005 (97%)	298 (3%)	46	74

5 of 298 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	1l	84	LEU
4	2E	181	LEU
38	2g	52	GLU
45	1n	22	THR
3	2D	106	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
12	2Q	12	GLN
19	2X	82	GLN
42	2k	78	GLN
12	2Q	57	HIS
15	2T	79	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	414 (14%)	43 (1%)
1	2A	2788/2915 (95%)	510 (18%)	28 (1%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	35 (29%)	0
32	1a	1494/1521 (98%)	241 (16%)	0
32	2a	1498/1521 (98%)	253 (16%)	0
53	1v	12/24 (50%)	4 (33%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	22 (30%)	0
54	1y	71/76 (93%)	23 (32%)	0
54	2w	68/76 (89%)	27 (39%)	0
54	2y	69/76 (90%)	23 (33%)	0
55	1x	75/77 (97%)	8 (10%)	0
55	2x	75/77 (97%)	16 (21%)	0
All	All	9332/9620 (97%)	1590 (17%)	72 (0%)

5 of 1590 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	60	G

5 of 72 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	2156	A
1	1A	2641	A
1	2A	1992	G
1	1A	2180	A
1	1A	2205	C

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	1933	1	13,21,22	1.16	1 (7%)	18,30,33	3.28	5 (27%)
1	5MU	1A	1937	1	12,22,23	0.35	0	14,32,35	2.15	2 (14%)
1	PSU	1A	1939	1	13,21,22	1.47	1 (7%)	18,30,33	3.33	6 (33%)
1	4OC	1A	1942	1	13,22,24	0.43	0	20,31,35	1.15	1 (5%)
1	5MU	1A	1961	1,56	12,22,23	0.38	0	14,32,35	1.78	2 (14%)
1	5MC	1A	1964	1,56	13,22,23	1.29	1 (7%)	15,32,35	1.12	1 (6%)
1	5MC	1A	1984	1,56	13,22,23	1.33	1 (7%)	15,32,35	0.91	1 (6%)
1	OMG	1A	2263	1,55,56	17,26,27	1.17	2 (11%)	21,38,41	1.95	5 (23%)
1	2MA	1A	2515	1,56	16,25,26	1.65	3 (18%)	18,37,40	2.68	2 (11%)
1	2MU	1A	2564	1,56	12,22,24	0.65	0	19,31,36	1.57	1 (5%)
1	PSU	1A	2617	1,56	13,21,22	1.67	1 (7%)	18,30,33	3.28	6 (33%)
32	2MG	1a	1207	32	17,26,27	1.28	2 (11%)	21,38,41	2.34	9 (42%)
32	5MC	1a	1400	32	13,22,23	1.34	1 (7%)	15,32,35	1.06	1 (6%)
32	4OC	1a	1402	32	13,23,24	0.54	0	18,32,35	1.54	1 (5%)
32	5MC	1a	1404	32	13,22,23	1.34	1 (7%)	15,32,35	0.90	1 (6%)
32	5MC	1a	1407	32	13,22,23	1.39	1 (7%)	15,32,35	1.04	1 (6%)
32	UR3	1a	1498	32	12,22,23	0.79	1 (8%)	16,32,35	0.90	2 (12%)
32	MA6	1a	1518	32	16,26,27	0.91	1 (6%)	18,38,41	2.74	7 (38%)
32	MA6	1a	1519	32	16,26,27	1.10	1 (6%)	18,38,41	2.39	6 (33%)
32	PSU	1a	516	32	13,21,22	1.03	1 (7%)	18,30,33	3.48	5 (27%)
32	7MG	1a	527	32,56	19,26,27	1.02	1 (5%)	24,39,42	2.86	6 (25%)
32	M2G	1a	966	32	17,27,28	1.48	3 (17%)	22,40,43	1.89	7 (31%)
32	5MC	1a	967	32	13,22,23	1.36	1 (7%)	15,32,35	0.90	1 (6%)
43	0TD	1l	92	43	4,9,10	3.94	3 (75%)	4,11,13	5.11	3 (75%)
54	PSU	1w	32	54,56	13,21,22	1.18	1 (7%)	18,30,33	3.39	6 (33%)
54	MIA	1w	37	54	21,31,32	1.77	2 (9%)	26,44,47	1.62	5 (19%)
54	PSU	1w	39	54	13,21,22	1.26	1 (7%)	18,30,33	3.36	6 (33%)
54	7MG	1w	46	54	19,26,27	1.11	1 (5%)	24,39,42	3.08	7 (29%)
54	5MU	1w	54	54	12,22,23	0.32	0	14,32,35	2.30	2 (14%)
54	PSU	1w	55	54	13,21,22	1.11	1 (7%)	18,30,33	3.66	6 (33%)
54	4SU	1w	8	54	11,21,22	1.19	1 (9%)	13,30,33	1.24	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MC	1x	32	55	13,22,23	1.38	1 (7%)	15,32,35	1.17	1 (6%)
55	5MU	1x	54	55,56	12,22,23	0.36	0	14,32,35	2.54	2 (14%)
55	PSU	1x	55	55,56	13,21,22	1.44	1 (7%)	18,30,33	3.38	6 (33%)
55	4SU	1x	8	55	11,21,22	0.99	1 (9%)	13,30,33	2.05	1 (7%)
54	PSU	1y	32	54	13,21,22	0.98	1 (7%)	18,30,33	3.48	6 (33%)
54	MIA	1y	37	54	15,24,32	1.21	2 (13%)	16,35,47	2.20	2 (12%)
54	PSU	1y	39	54	13,21,22	1.16	1 (7%)	18,30,33	3.45	5 (27%)
54	7MG	1y	46	54	19,26,27	1.15	1 (5%)	24,39,42	3.16	7 (29%)
54	5MU	1y	54	54	12,22,23	0.33	0	14,32,35	2.40	2 (14%)
54	PSU	1y	55	54	13,21,22	1.45	1 (7%)	18,30,33	3.20	6 (33%)
54	4SU	1y	8	54	11,21,22	1.15	1 (9%)	13,30,33	1.59	1 (7%)
1	PSU	2A	1911	1	13,21,22	1.20	1 (7%)	18,30,33	3.57	6 (33%)
1	5MU	2A	1915	1	12,22,23	0.28	0	14,32,35	2.04	2 (14%)
1	PSU	2A	1917	1	13,21,22	1.34	1 (7%)	18,30,33	3.41	6 (33%)
1	4OC	2A	1920	1	13,22,24	0.49	0	20,31,35	1.21	1 (5%)
1	5MU	2A	1939	1,56	12,22,23	0.36	0	14,32,35	1.78	2 (14%)
1	5MC	2A	1942	1	13,22,23	1.23	1 (7%)	15,32,35	1.16	1 (6%)
1	5MC	2A	1962	1,56	13,22,23	1.30	1 (7%)	15,32,35	1.36	2 (13%)
1	OMG	2A	2251	1,55,56	17,26,27	1.22	2 (11%)	21,38,41	1.79	5 (23%)
1	2MA	2A	2503	1,56	16,25,26	1.41	3 (18%)	18,37,40	2.34	2 (11%)
1	2MU	2A	2552	1,56	12,22,24	0.79	0	19,31,36	1.80	1 (5%)
1	PSU	2A	2605	1	13,21,22	1.02	1 (7%)	18,30,33	3.24	6 (33%)
32	2MG	2a	1207	32	17,26,27	1.29	2 (11%)	21,38,41	2.34	7 (33%)
32	5MC	2a	1400	32	13,22,23	1.40	1 (7%)	15,32,35	0.98	1 (6%)
32	4OC	2a	1402	32,56	13,23,24	0.50	0	18,32,35	1.34	1 (5%)
32	5MC	2a	1404	32	13,22,23	1.38	1 (7%)	15,32,35	1.01	1 (6%)
32	5MC	2a	1407	32	13,22,23	1.32	1 (7%)	15,32,35	0.89	1 (6%)
32	UR3	2a	1498	32	12,22,23	0.68	0	16,32,35	0.87	0
32	MA6	2a	1518	32	16,26,27	1.03	1 (6%)	18,38,41	2.69	6 (33%)
32	MA6	2a	1519	32	16,26,27	1.07	1 (6%)	18,38,41	2.73	6 (33%)
32	PSU	2a	516	32	13,21,22	1.09	1 (7%)	18,30,33	3.53	6 (33%)
32	7MG	2a	527	32,56	19,26,27	1.03	1 (5%)	24,39,42	2.93	6 (25%)
32	M2G	2a	966	32	17,27,28	1.46	3 (17%)	22,40,43	1.89	5 (22%)
32	5MC	2a	967	32	13,22,23	1.54	1 (7%)	15,32,35	0.73	0
43	0TD	2l	92	43	4,9,10	3.49	1 (25%)	4,11,13	2.78	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	2w	32	54	13,21,22	1.30	1 (7%)	18,30,33	3.29	6 (33%)
54	MIA	2w	37	54	18,27,32	1.85	3 (16%)	21,39,47	1.65	6 (28%)
54	PSU	2w	39	54	13,21,22	1.18	1 (7%)	18,30,33	3.59	6 (33%)
54	7MG	2w	46	54	19,26,27	1.03	1 (5%)	24,39,42	2.75	6 (25%)
54	5MU	2w	54	54	12,22,23	0.44	0	14,32,35	2.65	2 (14%)
54	PSU	2w	55	54,56	13,21,22	1.00	1 (7%)	18,30,33	3.62	6 (33%)
54	4SU	2w	8	54	11,21,22	1.28	1 (9%)	13,30,33	1.01	1 (7%)
55	5MC	2x	32	55	13,22,23	1.27	1 (7%)	15,32,35	1.10	1 (6%)
55	5MU	2x	54	55	12,22,23	0.44	0	14,32,35	2.23	2 (14%)
55	PSU	2x	55	55	13,21,22	1.27	1 (7%)	18,30,33	3.34	6 (33%)
55	4SU	2x	8	55	11,21,22	1.08	1 (9%)	13,30,33	1.74	1 (7%)
54	PSU	2y	32	54	13,21,22	1.09	1 (7%)	18,30,33	3.38	5 (27%)
54	MIA	2y	37	54	15,24,32	1.18	2 (13%)	16,35,47	2.20	2 (12%)
54	PSU	2y	39	54	13,21,22	1.37	1 (7%)	18,30,33	3.58	6 (33%)
54	7MG	2y	46	54	19,26,27	1.37	2 (10%)	24,39,42	3.57	10 (41%)
54	5MU	2y	54	54	12,22,23	0.38	0	14,32,35	2.48	2 (14%)
54	PSU	2y	55	54	13,21,22	1.14	1 (7%)	18,30,33	3.68	6 (33%)
54	4SU	2y	8	54	11,21,22	1.33	1 (9%)	13,30,33	1.17	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/3/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	0/5/27/30	0/2/2/2
1	5MU	1A	1961	1,56	-	0/3/25/26	0/2/2/2
1	5MC	1A	1964	1,56	-	0/3/25/26	0/2/2/2
1	5MC	1A	1984	1,56	-	0/3/25/26	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	1A	2515	1,56	-	0/3/25/26	0/3/3/3
1	2MU	1A	2564	1,56	-	0/5/27/28	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	0/3/25/26	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	-	0/7/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	0/7/37/38	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	1l	92	43	-	0/2/12/14	0/0/0/0
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	0/11/33/34	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	0/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/3/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/3/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/3/25/26	0/2/2/2
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/3/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	0/7/37/38	0/3/3/3
54	5MU	1y	54	54	-	0/3/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	0/3/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/3/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/5/27/30	0/2/2/2
1	5MU	2A	1939	1,56	-	0/3/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/3/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/3/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	2MA	2A	2503	1,56	-	0/3/25/26	0/3/3/3
1	2MU	2A	2552	1,56	-	0/5/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/3/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	2a	1402	32,56	-	0/7/29/30	0/2/2/2
32	5MC	2a	1404	32	-	0/3/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/3/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/3/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	2a	1519	32	-	0/7/29/30	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	0/7/37/38	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/3/25/26	0/2/2/2
43	0TD	2l	92	43	-	0/2/12/14	0/0/0/0
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	0/7/37/38	0/3/3/3
54	5MU	2w	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2w	55	54,56	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/3/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/3/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/3/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/3/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/3/25/34	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	0/7/37/38	0/3/3/3
54	5MU	2y	54	54	-	0/3/25/26	0/2/2/2
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/3/25/26	0/2/2/2

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C2-S10	-6.84	1.70	1.75
43	2l	92	0TD	CB-SB	-6.73	1.67	1.84
43	1l	92	0TD	CB-SB	-6.69	1.67	1.84
54	2w	37	MIA	C2-S10	-6.07	1.70	1.75
1	1A	2617	PSU	C5-C1'	-5.44	1.47	1.52

The worst 5 of 304 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	55	PSU	N1-C2-N3	-11.77	120.82	128.33
54	2w	39	PSU	N1-C2-N3	-11.50	121.00	128.33
32	2a	516	PSU	N1-C2-N3	-11.26	121.15	128.33
32	1a	516	PSU	N1-C2-N3	-11.19	121.19	128.33
1	2A	1911	PSU	N1-C2-N3	-11.12	121.24	128.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1939	PSU	1	0
1	1A	1961	5MU	1	0
1	1A	2564	2MU	2	0
1	2A	1911	PSU	1	0
1	2A	1915	5MU	1	0
1	2A	1917	PSU	1	0
1	2A	1920	4OC	2	0
1	2A	2251	OMG	1	0
1	2A	2503	2MA	2	0
1	2A	2552	2MU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2853 ligands modelled in this entry, 2851 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	SF4	1d	501	35	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	SF4	2d	501	35	0,12,12	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	1d	501	35	-	0/0/48/48	0/6/5/5
59	SF4	2d	501	35	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.87	84 (2%)	55	60	24, 43, 91, 103	0
1	2A	2789/2915 (95%)	0.27	88 (3%)	51	56	28, 48, 89, 106	0
2	1B	120/121 (99%)	0.80	0	100	100	39, 61, 72, 90	0
2	2B	120/121 (99%)	0.14	2 (1%)	73	76	45, 68, 77, 91	0
3	1D	275/276 (99%)	0.71	6 (2%)	65	69	25, 42, 58, 80	0
3	2D	275/276 (99%)	0.51	4 (1%)	76	79	28, 45, 61, 78	0
4	1E	204/206 (99%)	0.76	3 (1%)	76	79	23, 46, 66, 80	0
4	2E	204/206 (99%)	0.67	7 (3%)	49	54	26, 50, 67, 80	0
5	1F	203/210 (96%)	0.92	4 (1%)	68	72	22, 51, 76, 91	0
5	2F	203/210 (96%)	0.34	2 (0%)	84	86	27, 56, 76, 91	0
6	1G	181/182 (99%)	0.73	7 (3%)	43	48	48, 69, 80, 92	0
6	2G	181/182 (99%)	1.30	38 (20%)	1	1	54, 73, 81, 93	0
7	1H	174/180 (96%)	0.73	2 (1%)	82	84	47, 64, 74, 83	0
7	2H	174/180 (96%)	1.96	69 (39%)	0	0	54, 70, 78, 83	0
8	1I	146/148 (98%)	0.57	8 (5%)	29	32	49, 73, 82, 85	0
8	2I	146/148 (98%)	0.95	25 (17%)	2	2	50, 73, 82, 86	0
9	1N	140/140 (100%)	1.00	4 (2%)	55	60	31, 48, 67, 77	0
9	2N	140/140 (100%)	0.69	7 (5%)	32	37	37, 53, 71, 80	0
10	1O	122/122 (100%)	0.53	2 (1%)	74	78	23, 40, 60, 74	0
10	2O	122/122 (100%)	0.98	15 (12%)	5	5	45, 59, 72, 81	0
11	1P	149/150 (99%)	0.94	3 (2%)	68	72	24, 53, 75, 81	0
11	2P	149/150 (99%)	0.67	13 (8%)	13	13	29, 58, 76, 85	0
12	1Q	141/141 (100%)	0.87	3 (2%)	67	71	33, 51, 68, 77	0
12	2Q	141/141 (100%)	1.10	17 (12%)	6	5	37, 56, 73, 79	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%)	0.75	2 (1%) 73 76	29, 40, 55, 62	0
13	2R	118/118 (100%)	0.44	2 (1%) 73 76	31, 43, 58, 65	0
14	1S	110/112 (98%)	0.84	3 (2%) 58 62	49, 62, 72, 77	0
14	2S	110/112 (98%)	0.96	11 (10%) 9 10	55, 66, 75, 79	0
15	1T	131/146 (89%)	0.66	5 (3%) 44 49	38, 51, 72, 77	0
15	2T	131/146 (89%)	0.59	3 (2%) 64 67	43, 53, 74, 78	0
16	1U	116/118 (98%)	1.13	5 (4%) 39 44	26, 39, 55, 73	0
16	2U	116/118 (98%)	0.33	1 (0%) 85 88	33, 46, 61, 73	0
17	1V	101/101 (100%)	1.02	3 (2%) 54 59	28, 51, 67, 76	0
17	2V	101/101 (100%)	0.35	3 (2%) 54 59	33, 57, 70, 76	0
18	1W	112/113 (99%)	1.00	3 (2%) 58 62	26, 37, 55, 88	0
18	2W	112/113 (99%)	0.41	0 100 100	30, 41, 57, 88	0
19	1X	95/96 (98%)	0.89	1 (1%) 82 84	30, 44, 63, 75	0
19	2X	95/96 (98%)	0.35	2 (2%) 67 71	34, 49, 65, 76	0
20	1Y	107/110 (97%)	0.88	3 (2%) 56 61	45, 57, 74, 83	0
20	2Y	107/110 (97%)	1.03	16 (14%) 3 3	48, 61, 76, 86	0
21	1Z	154/206 (74%)	0.70	11 (7%) 19 21	38, 64, 86, 96	0
21	2Z	160/206 (77%)	1.63	47 (29%) 1 0	72, 83, 93, 99	0
22	10	83/85 (97%)	0.85	4 (4%) 34 39	25, 38, 59, 71	0
22	20	83/85 (97%)	0.99	7 (8%) 14 14	41, 66, 78, 82	0
23	11	97/98 (98%)	0.60	2 (2%) 67 71	23, 44, 71, 77	0
23	21	97/98 (98%)	0.87	8 (8%) 14 15	38, 58, 74, 82	0
24	12	70/72 (97%)	0.90	1 (1%) 78 80	40, 57, 66, 79	0
24	22	70/72 (97%)	0.25	1 (1%) 78 80	46, 61, 69, 78	0
25	13	59/60 (98%)	0.97	0 100 100	29, 45, 69, 83	0
25	23	59/60 (98%)	0.59	1 (1%) 73 76	36, 51, 72, 87	0
26	14	69/71 (97%)	0.76	7 (10%) 9 9	64, 79, 89, 97	0
26	24	69/71 (97%)	1.26	15 (21%) 1 1	70, 80, 89, 97	0
27	15	59/60 (98%)	1.06	1 (1%) 73 76	25, 36, 57, 72	0
27	25	59/60 (98%)	0.27	0 100 100	30, 40, 60, 71	0
28	16	53/54 (98%)	0.79	0 100 100	38, 51, 64, 74	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%)	0.74	5 (9%) 11 11	42, 54, 65, 71	0
29	17	48/49 (97%)	1.01	3 (6%) 23 26	24, 31, 58, 69	0
29	27	48/49 (97%)	0.78	4 (8%) 14 15	28, 35, 58, 70	0
30	18	64/65 (98%)	0.92	2 (3%) 52 57	33, 42, 50, 66	0
30	28	64/65 (98%)	0.93	5 (7%) 16 17	38, 46, 53, 67	0
31	19	37/37 (100%)	0.96	0 100 100	37, 50, 67, 68	0
31	29	37/37 (100%)	1.69	12 (32%) 1 0	46, 54, 71, 72	0
32	1a	1488/1521 (97%)	0.55	52 (3%) 48 53	42, 72, 92, 103	0
32	2a	1491/1521 (98%)	0.60	96 (6%) 23 25	44, 74, 93, 103	0
33	1b	231/256 (90%)	0.57	15 (6%) 22 25	69, 82, 89, 94	0
33	2b	231/256 (90%)	1.37	62 (26%) 1 1	72, 83, 89, 94	0
34	1c	206/239 (86%)	0.91	21 (10%) 9 9	67, 80, 86, 92	0
34	2c	206/239 (86%)	1.93	82 (39%) 0 0	69, 82, 88, 93	0
35	1d	208/209 (99%)	1.01	32 (15%) 3 3	56, 72, 80, 87	0
35	2d	208/209 (99%)	1.22	40 (19%) 2 1	58, 71, 80, 88	0
36	1e	148/162 (91%)	0.97	17 (11%) 6 6	56, 72, 80, 86	0
36	2e	148/162 (91%)	1.77	47 (31%) 1 0	59, 74, 83, 87	0
37	1f	100/101 (99%)	0.37	2 (2%) 68 72	50, 66, 76, 78	0
37	2f	100/101 (99%)	0.28	1 (1%) 84 86	60, 72, 80, 86	0
38	1g	155/156 (99%)	0.96	17 (10%) 7 7	62, 74, 83, 100	0
38	2g	155/156 (99%)	1.11	26 (16%) 2 2	65, 76, 84, 102	0
39	1h	137/138 (99%)	0.72	9 (6%) 22 24	60, 72, 78, 83	0
39	2h	137/138 (99%)	1.24	33 (24%) 1 1	64, 74, 80, 84	0
40	1i	127/128 (99%)	1.18	26 (20%) 1 1	51, 75, 83, 87	0
40	2i	127/128 (99%)	2.51	69 (54%) 0 0	71, 85, 91, 92	0
41	1j	97/105 (92%)	0.97	16 (16%) 2 2	59, 78, 90, 95	0
41	2j	96/105 (91%)	2.28	48 (50%) 0 0	74, 87, 94, 98	0
42	1k	114/129 (88%)	0.73	5 (4%) 38 43	52, 69, 80, 83	0
42	2k	114/129 (88%)	0.64	6 (5%) 30 34	55, 71, 81, 87	0
43	1l	121/132 (91%)	0.70	4 (3%) 50 55	53, 64, 74, 77	0
43	2l	121/132 (91%)	1.44	36 (29%) 1 0	55, 67, 75, 80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.67	11 (8%) 12 13	54, 69, 78, 82	0
44	2m	122/126 (96%)	1.76	41 (33%) 0 0	73, 84, 90, 94	0
45	1n	60/61 (98%)	1.23	13 (21%) 1 1	57, 69, 78, 82	0
45	2n	60/61 (98%)	3.52	49 (81%) 0 0	78, 85, 93, 95	0
46	1o	88/89 (98%)	0.68	5 (5%) 27 31	56, 69, 78, 83	0
46	2o	88/89 (98%)	0.67	6 (6%) 20 23	57, 70, 80, 83	0
47	1p	82/88 (93%)	1.86	34 (41%) 0 0	58, 70, 80, 83	0
47	2p	82/88 (93%)	1.09	9 (10%) 7 7	59, 69, 81, 82	0
48	1q	99/105 (94%)	0.86	8 (8%) 15 16	57, 70, 79, 82	0
48	2q	99/105 (94%)	1.31	27 (27%) 1 1	60, 70, 79, 82	0
49	1r	68/88 (77%)	0.63	5 (7%) 17 19	60, 68, 79, 82	0
49	2r	68/88 (77%)	0.57	5 (7%) 17 19	60, 70, 80, 82	0
50	1s	83/93 (89%)	0.82	5 (6%) 25 28	70, 79, 86, 91	0
50	2s	83/93 (89%)	2.29	39 (46%) 0 0	74, 81, 88, 94	0
51	1t	96/106 (90%)	1.47	31 (32%) 1 0	58, 71, 80, 86	0
51	2t	96/106 (90%)	1.12	18 (18%) 2 1	59, 71, 81, 85	0
52	1u	23/27 (85%)	1.52	7 (30%) 1 0	65, 74, 78, 80	0
52	2u	23/27 (85%)	2.10	9 (39%) 0 0	68, 75, 80, 83	0
53	1v	13/24 (54%)	2.81	8 (61%) 0 0	60, 74, 92, 98	0
53	2v	13/24 (54%)	3.50	8 (61%) 0 0	65, 78, 95, 98	0
54	1w	67/76 (88%)	2.01	21 (31%) 1 0	44, 89, 97, 101	0
54	1y	67/76 (88%)	1.15	14 (20%) 1 1	37, 91, 97, 101	0
54	2w	65/76 (85%)	2.83	43 (66%) 0 0	56, 96, 101, 104	0
54	2y	66/76 (86%)	1.37	17 (25%) 1 1	51, 95, 99, 100	0
55	1x	72/77 (93%)	0.48	3 (4%) 40 45	33, 66, 84, 87	0
55	2x	72/77 (93%)	0.41	2 (2%) 56 61	52, 81, 90, 95	0
All	All	20875/21748 (95%)	0.81	1812 (8%) 13 13	22, 63, 89, 106	0

The worst 5 of 1812 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	25	VAL	13.2
38	2g	82	GLY	11.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	10.6
44	2m	124	PRO	10.4
54	2w	71	G	9.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
54	7MG	1w	46	24/25	0.78	0.20	-	76,90,101,124	0
32	5MC	2a	1404	21/22	0.92	0.21	-	47,59,74,77	0
1	2MU	2A	2552	21/23	0.97	0.20	-	28,38,46,52	0
1	4OC	1A	1942	21/23	0.96	0.20	-	42,55,61,65	0
1	2MA	1A	2515	23/24	0.98	0.24	-	20,26,31,34	0
1	5MU	2A	1915	21/22	0.91	0.18	-	64,72,79,93	0
43	0TD	1l	92	10/11	0.87	0.23	-	61,64,70,74	0
32	2MG	2a	1207	24/25	0.85	0.17	-	74,85,90,98	0
54	PSU	2w	32	20/21	0.90	0.32	-	69,85,94,103	0
1	2MA	2A	2503	23/24	0.98	0.20	-	25,30,35,37	0
54	PSU	1w	39	20/21	0.93	0.23	-	50,70,80,83	0
1	PSU	2A	2605	20/21	0.97	0.18	-	25,33,40,42	0
32	PSU	2a	516	20/21	0.92	0.15	-	65,72,79,83	0
54	PSU	2w	39	20/21	0.91	0.33	-	80,88,96,102	0
1	PSU	1A	2617	20/21	0.98	0.20	-	24,31,37,39	0
32	MA6	1a	1519	24/25	0.97	0.21	-	39,48,57,71	0
54	MIA	1y	37	22/30	0.87	0.23	-	76,83,93,94	0
32	5MC	1a	1404	21/22	0.97	0.19	-	32,43,50,53	0
1	5MC	1A	1964	21/22	0.97	0.21	-	38,47,52,60	0
32	7MG	1a	527	24/25	0.96	0.19	-	40,50,60,67	0
1	5MU	1A	1937	21/22	0.95	0.18	-	56,67,75,82	0
32	4OC	1a	1402	22/23	0.97	0.18	-	37,47,55,61	0
1	OMG	1A	2263	24/25	0.97	0.22	-	22,32,39,44	0
54	5MU	1w	54	21/22	0.94	0.16	-	55,67,78,79	0
1	2MU	1A	2564	21/23	0.98	0.22	-	26,36,40,46	0
54	MIA	2y	37	22/30	0.76	0.27	-	72,86,94,120	0
54	PSU	2w	55	20/21	0.76	0.29	-	80,94,98,113	0
54	5MU	2y	54	21/22	0.71	0.31	-	79,93,108,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	7MG	2a	527	24/25	0.94	0.19	-	61,70,77,88	0
54	4SU	2w	8	20/21	0.75	0.30	-	81,98,120,128	0
1	5MC	1A	1984	21/22	0.98	0.18	-	31,38,48,57	0
32	5MC	1a	1400	21/22	0.98	0.19	-	39,53,61,67	0
1	5MC	2A	1962	21/22	0.96	0.18	-	28,43,52,59	0
54	5MU	2w	54	21/22	0.86	0.21	-	66,85,93,101	0
1	5MU	1A	1961	21/22	0.98	0.19	-	21,33,38,44	0
54	PSU	2y	39	20/21	0.85	0.23	-	78,84,100,112	0
54	PSU	1y	55	20/21	0.72	0.20	-	72,89,99,120	0
32	MA6	2a	1519	24/25	0.95	0.26	-	47,65,74,81	0
54	PSU	1y	39	20/21	0.91	0.18	-	71,81,89,95	0
1	5MU	2A	1939	21/22	0.97	0.17	-	24,34,41,46	0
32	5MC	2a	967	21/22	0.90	0.19	-	62,71,79,86	0
32	UR3	1a	1498	21/22	0.98	0.18	-	38,43,50,54	0
55	5MU	1x	54	21/22	0.95	0.14	-	57,71,79,83	0
32	5MC	2a	1400	21/22	0.96	0.23	-	70,74,80,93	0
32	5MC	1a	967	21/22	0.96	0.21	-	51,58,67,70	0
32	5MC	1a	1407	21/22	0.97	0.19	-	34,42,56,62	0
1	5MC	2A	1942	21/22	0.97	0.16	-	45,50,58,61	0
54	4SU	1y	8	20/21	0.79	0.23	-	80,98,105,114	0
54	PSU	1w	32	20/21	0.93	0.20	-	59,72,79,83	0
55	5MC	1x	32	21/22	0.96	0.21	-	44,54,67,73	0
54	7MG	2y	46	24/25	0.65	0.20	-	68,95,99,128	0
54	7MG	1y	46	24/25	0.83	0.24	-	76,95,106,115	0
32	2MG	1a	1207	24/25	0.93	0.14	-	62,72,76,80	0
54	MIA	2w	37	25/30	0.88	0.29	-	70,82,91,110	0
1	PSU	2A	1917	20/21	0.94	0.21	-	56,65,75,76	0
54	5MU	1y	54	21/22	0.79	0.20	-	76,87,95,116	0
54	4SU	1w	8	20/21	0.83	0.20	-	75,86,105,114	0
54	PSU	2y	55	20/21	0.77	0.28	-	80,96,115,118	0
32	PSU	1a	516	20/21	0.94	0.16	-	63,70,78,78	0
32	MA6	1a	1518	24/25	0.97	0.21	-	31,47,51,57	0
55	PSU	2x	55	20/21	0.88	0.18	-	69,84,106,107	0
54	PSU	1y	32	20/21	0.84	0.23	-	69,87,94,95	0
1	PSU	1A	1933	20/21	0.97	0.21	-	49,59,62,66	0
1	OMG	2A	2251	24/25	0.97	0.17	-	27,36,44,46	0
1	PSU	2A	1911	20/21	0.93	0.17	-	56,60,66,70	0
32	M2G	2a	966	25/26	0.87	0.22	-	52,69,95,99	0
54	4SU	2y	8	20/21	0.83	0.12	-	87,94,106,113	0
55	4SU	2x	8	20/21	0.84	0.16	-	74,85,90,96	0
32	4OC	2a	1402	22/23	0.92	0.17	-	45,63,71,90	0
54	7MG	2w	46	24/25	0.77	0.24	-	83,96,107,134	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	UR3	2a	1498	21/22	0.95	0.20	-	48,58,62,68	0
43	0TD	2l	92	10/11	0.93	0.23	-	65,68,73,79	0
54	PSU	2y	32	20/21	0.77	0.21	-	73,89,97,108	0
55	PSU	1x	55	20/21	0.94	0.16	-	56,67,81,87	0
55	5MC	2x	32	21/22	0.92	0.19	-	65,78,87,88	0
54	PSU	1w	55	20/21	0.80	0.22	-	72,81,90,98	0
55	4SU	1x	8	20/21	0.96	0.17	-	46,60,69,73	0
32	MA6	2a	1518	24/25	0.95	0.20	-	41,63,74,82	0
1	PSU	1A	1939	20/21	0.95	0.23	-	53,60,71,72	0
54	MIA	1w	37	29/30	0.93	0.22	-	43,62,74,78	0
55	5MU	2x	54	21/22	0.86	0.24	-	71,87,95,100	0
32	5MC	2a	1407	21/22	0.95	0.20	-	48,57,69,76	0
32	M2G	1a	966	25/26	0.96	0.20	-	41,55,61,77	0
1	4OC	2A	1920	21/23	0.95	0.23	-	46,57,62,72	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1B	3010	1/1	0.88	0.82	35.83	73,73,73,73	0
56	MG	1A	3016	1/1	0.86	0.33	26.20	51,51,51,51	0
56	MG	2A	3165	1/1	0.93	0.35	22.86	49,49,49,49	0
56	MG	2F	304	1/1	0.97	0.50	22.20	53,53,53,53	0
56	MG	1A	3162	1/1	0.96	0.43	21.27	44,44,44,44	0
56	MG	1A	3354	1/1	0.96	0.38	20.12	68,68,68,68	0
56	MG	2A	3906	1/1	0.87	0.66	18.72	62,62,62,62	0
56	MG	1A	3306	1/1	0.97	0.47	18.44	38,38,38,38	0
56	MG	1A	3189	1/1	0.88	0.41	18.38	43,43,43,43	0
56	MG	1A	3857	1/1	0.91	0.36	16.91	48,48,48,48	0
56	MG	2A	3468	1/1	0.88	0.30	16.35	59,59,59,59	0
56	MG	1A	4141	1/1	0.98	0.36	16.01	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3687	1/1	0.90	0.37	15.51	63,63,63,63	0
56	MG	2A	3493	1/1	0.86	0.38	14.78	53,53,53,53	0
56	MG	1N	201	1/1	0.87	0.61	12.72	59,59,59,59	0
56	MG	2a	3091	1/1	0.93	0.42	12.65	76,76,76,76	0
56	MG	1a	1699	1/1	0.95	0.28	11.93	40,40,40,40	0
56	MG	2A	3167	1/1	0.90	0.27	11.53	52,52,52,52	0
56	MG	2A	3444	1/1	0.95	0.29	11.26	49,49,49,49	0
56	MG	2A	3886	1/1	0.92	0.29	11.20	45,45,45,45	0
56	MG	1A	3803	1/1	0.97	0.39	11.14	44,44,44,44	0
56	MG	1A	3309	1/1	0.97	0.29	10.80	33,33,33,33	0
56	MG	2A	3677	1/1	0.98	0.32	10.71	35,35,35,35	0
56	MG	2a	3208	1/1	0.96	0.30	10.69	75,75,75,75	0
56	MG	1N	204	1/1	0.96	0.51	10.49	64,64,64,64	0
56	MG	2A	3486	1/1	0.98	0.36	10.10	55,55,55,55	0
56	MG	1U	202	1/1	0.73	0.49	9.97	73,73,73,73	0
56	MG	1A	4078	1/1	0.97	0.33	9.70	41,41,41,41	0
56	MG	1A	3865	1/1	0.96	0.36	9.57	43,43,43,43	0
56	MG	2A	3449	1/1	0.95	0.38	9.47	47,47,47,47	0
56	MG	2A	3096	1/1	0.84	0.26	9.43	59,59,59,59	0
56	MG	1A	3809	1/1	0.98	0.31	9.16	51,51,51,51	0
56	MG	2A	3455	1/1	0.91	0.30	8.94	54,54,54,54	0
56	MG	1A	3509	1/1	0.96	0.30	8.86	45,45,45,45	0
56	MG	1A	3307	1/1	0.89	0.32	8.86	45,45,45,45	0
56	MG	1Y	504	1/1	0.97	0.41	8.84	48,48,48,48	0
56	MG	1A	4124	1/1	0.95	0.36	8.55	46,46,46,46	0
56	MG	1A	4076	1/1	0.61	0.29	8.47	75,75,75,75	0
56	MG	2A	3003	1/1	0.95	0.28	8.38	43,43,43,43	0
56	MG	1A	3578	1/1	0.97	0.28	8.32	33,33,33,33	0
56	MG	2A	3092	1/1	0.98	0.27	8.24	43,43,43,43	0
56	MG	2A	3191	1/1	0.92	0.21	8.14	50,50,50,50	0
56	MG	1A	3013	1/1	0.95	0.33	7.84	35,35,35,35	0
56	MG	2A	3856	1/1	0.93	0.32	7.82	41,41,41,41	0
56	MG	2A	3083	1/1	0.98	0.43	7.77	49,49,49,49	0
56	MG	1A	3311	1/1	0.97	0.25	7.41	48,48,48,48	0
56	MG	1A	3603	1/1	0.95	0.28	7.35	39,39,39,39	0
56	MG	1A	3200	1/1	0.98	0.27	6.91	23,23,23,23	0
56	MG	2A	3409	1/1	0.98	0.23	6.78	47,47,47,47	0
56	MG	1A	3842	1/1	0.97	0.27	6.75	26,26,26,26	0
56	MG	2D	304	1/1	0.87	0.36	6.71	45,45,45,45	0
58	ZN	25	102	1/1	0.97	0.31	6.63	68,68,68,68	0
56	MG	1A	3194	1/1	0.97	0.27	6.57	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3900	1/1	0.96	0.34	6.52	44,44,44,44	0
56	MG	1A	3056	1/1	0.99	0.27	6.51	28,28,28,28	0
56	MG	2A	3445	1/1	0.90	0.24	6.50	55,55,55,55	0
56	MG	2A	3160	1/1	0.93	0.25	6.49	44,44,44,44	0
56	MG	1A	3458	1/1	0.75	0.29	6.40	54,54,54,54	0
56	MG	1A	3177	1/1	0.97	0.27	6.38	38,38,38,38	0
56	MG	1A	3628	1/1	0.98	0.27	6.19	28,28,28,28	0
56	MG	2A	3461	1/1	0.98	0.26	5.92	52,52,52,52	0
56	MG	1A	3338	1/1	0.98	0.20	5.87	49,49,49,49	0
56	MG	1A	3351	1/1	0.94	0.29	5.49	49,49,49,49	0
56	MG	1a	1659	1/1	0.97	0.26	5.27	62,62,62,62	0
56	MG	1A	3559	1/1	0.97	0.27	5.08	34,34,34,34	0
56	MG	1D	302	1/1	0.94	0.44	5.01	55,55,55,55	0
56	MG	1A	3055	1/1	0.95	0.27	5.01	43,43,43,43	0
56	MG	2A	3633	1/1	0.97	0.24	4.98	55,55,55,55	0
56	MG	2A	3070	1/1	0.98	0.24	4.86	42,42,42,42	0
56	MG	2A	3897	1/1	0.94	0.32	4.80	57,57,57,57	0
56	MG	1A	3280	1/1	0.93	0.26	4.77	50,50,50,50	0
56	MG	2U	201	1/1	0.97	0.24	4.73	40,40,40,40	0
56	MG	1A	4086	1/1	0.98	0.33	4.71	43,43,43,43	0
56	MG	2A	3347	1/1	0.94	0.24	4.69	51,51,51,51	0
56	MG	2A	3814	1/1	0.88	0.29	4.51	55,55,55,55	0
56	MG	1O	203	1/1	0.93	0.31	4.50	63,63,63,63	0
56	MG	1A	3104	1/1	0.91	0.27	4.49	40,40,40,40	0
56	MG	1A	3753	1/1	0.93	0.27	4.49	34,34,34,34	0
56	MG	2a	3041	1/1	0.97	0.26	4.49	50,50,50,50	0
56	MG	1a	1657	1/1	0.95	0.24	4.32	57,57,57,57	0
56	MG	1A	4115	1/1	0.96	0.35	4.30	51,51,51,51	0
56	MG	1O	202	1/1	0.89	0.50	4.30	67,67,67,67	0
56	MG	1A	4072	1/1	0.70	0.37	4.22	62,62,62,62	0
56	MG	2A	3108	1/1	0.97	0.23	4.11	44,44,44,44	0
56	MG	1A	3744	1/1	0.90	0.28	4.07	74,74,74,74	0
56	MG	1A	4090	1/1	0.98	0.29	4.06	37,37,37,37	0
56	MG	1A	3068	1/1	0.98	0.24	4.04	38,38,38,38	0
56	MG	2A	3364	1/1	0.58	0.17	3.98	77,77,77,77	0
56	MG	1D	310	1/1	0.95	0.34	3.97	39,39,39,39	0
56	MG	1A	3171	1/1	0.94	0.33	3.86	53,53,53,53	0
56	MG	2A	3883	1/1	0.87	0.34	3.84	56,56,56,56	0
56	MG	2B	3008	1/1	0.81	0.18	3.82	58,58,58,58	0
56	MG	1A	3576	1/1	0.84	0.25	3.71	57,57,57,57	0
56	MG	1A	4047	1/1	0.95	0.27	3.70	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	ZN	15	101	1/1	1.00	0.27	3.60	37,37,37,37	0
56	MG	2A	3025	1/1	0.98	0.27	3.51	42,42,42,42	0
56	MG	1A	3971	1/1	0.79	0.24	3.51	44,44,44,44	0
56	MG	1D	301	1/1	0.97	0.27	3.51	46,46,46,46	0
56	MG	2A	3448	1/1	0.99	0.20	3.47	49,49,49,49	0
56	MG	2A	3093	1/1	0.88	0.25	3.43	54,54,54,54	0
56	MG	2A	3673	1/1	0.92	0.24	3.43	64,64,64,64	0
56	MG	1A	3185	1/1	0.90	0.24	3.43	47,47,47,47	0
56	MG	16	101	1/1	0.90	0.25	3.42	45,45,45,45	0
56	MG	1E	304	1/1	0.82	0.24	3.41	55,55,55,55	0
56	MG	2A	3745	1/1	0.71	0.20	3.39	56,56,56,56	0
56	MG	2a	3010	1/1	0.74	0.18	3.38	76,76,76,76	0
56	MG	2A	3876	1/1	0.72	0.30	3.14	66,66,66,66	0
56	MG	1A	3347	1/1	0.97	0.24	3.13	44,44,44,44	0
56	MG	1A	3063	1/1	0.92	0.20	3.07	38,38,38,38	0
56	MG	1A	3313	1/1	0.90	0.25	3.03	49,49,49,49	0
56	MG	1A	3165	1/1	0.92	0.24	2.97	48,48,48,48	0
56	MG	1S	3001	1/1	0.85	0.30	2.94	51,51,51,51	0
56	MG	1D	312	1/1	0.96	0.27	2.80	42,42,42,42	0
56	MG	1A	3658	1/1	0.96	0.24	2.75	37,37,37,37	0
56	MG	2A	3014	1/1	0.92	0.26	2.73	43,43,43,43	0
56	MG	1A	3552	1/1	0.88	0.22	2.64	60,60,60,60	0
56	MG	1A	4093	1/1	0.95	0.27	2.62	35,35,35,35	0
56	MG	2A	3579	1/1	0.87	0.18	2.59	60,60,60,60	0
56	MG	1A	3248	1/1	0.83	0.26	2.51	47,47,47,47	0
56	MG	1A	3704	1/1	0.88	0.24	2.50	49,49,49,49	0
56	MG	2A	3181	1/1	0.98	0.22	2.44	40,40,40,40	0
56	MG	1A	3095	1/1	0.85	0.20	2.43	55,55,55,55	0
56	MG	1A	3252	1/1	0.89	0.23	2.36	52,52,52,52	0
56	MG	1A	3125	1/1	0.95	0.26	2.29	41,41,41,41	0
56	MG	1A	3151	1/1	0.87	0.23	2.29	47,47,47,47	0
56	MG	1B	3019	1/1	0.93	0.23	2.22	56,56,56,56	0
56	MG	1A	3871	1/1	0.90	0.26	2.18	49,49,49,49	0
56	MG	2A	3472	1/1	0.94	0.18	2.13	60,60,60,60	0
56	MG	2a	3165	1/1	0.93	0.26	2.10	54,54,54,54	0
56	MG	2A	3192	1/1	0.96	0.19	1.97	44,44,44,44	0
56	MG	2A	3714	1/1	0.98	0.23	1.91	39,39,39,39	0
56	MG	2A	3899	1/1	0.94	0.21	1.84	45,45,45,45	0
56	MG	1A	3751	1/1	0.87	0.27	1.82	48,48,48,48	0
56	MG	1A	3728	1/1	0.86	0.24	1.82	26,26,26,26	0
56	MG	19	101	1/1	0.88	0.26	1.81	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3644	1/1	0.99	0.22	1.77	33,33,33,33	0
56	MG	1A	3748	1/1	0.97	0.23	1.75	25,25,25,25	0
56	MG	2A	3013	1/1	0.99	0.19	1.73	44,44,44,44	0
56	MG	1A	4107	1/1	0.96	0.26	1.73	42,42,42,42	0
56	MG	2A	3635	1/1	0.92	0.18	1.72	43,43,43,43	0
56	MG	1A	3605	1/1	0.98	0.20	1.58	32,32,32,32	0
56	MG	2A	3552	1/1	0.93	0.18	1.56	59,59,59,59	0
56	MG	2A	3112	1/1	0.83	0.17	1.51	42,42,42,42	0
56	MG	1A	3887	1/1	0.97	0.23	1.51	31,31,31,31	0
56	MG	1n	103	1/1	0.99	0.23	1.49	48,48,48,48	0
56	MG	2A	3538	1/1	0.97	0.19	1.48	35,35,35,35	0
56	MG	1A	3745	1/1	0.88	0.23	1.42	19,19,19,19	0
56	MG	1a	1701	1/1	0.92	0.22	1.38	51,51,51,51	0
56	MG	1A	3729	1/1	0.93	0.26	1.35	42,42,42,42	0
56	MG	2A	3910	1/1	0.95	0.27	1.27	57,57,57,57	0
56	MG	1A	4079	1/1	0.88	0.25	1.25	46,46,46,46	0
56	MG	1a	1607	1/1	0.90	0.20	1.23	67,67,67,67	0
56	MG	1P	203	1/1	0.99	0.27	1.21	30,30,30,30	0
56	MG	2F	303	1/1	0.97	0.21	1.20	48,48,48,48	0
56	MG	1a	1652	1/1	0.94	0.20	1.20	63,63,63,63	0
56	MG	2A	3484	1/1	0.88	0.21	1.19	53,53,53,53	0
56	MG	1X	103	1/1	0.98	0.25	1.19	40,40,40,40	0
56	MG	1A	3035	1/1	0.98	0.23	1.18	20,20,20,20	0
56	MG	2U	204	1/1	0.81	0.21	1.10	45,45,45,45	0
56	MG	2a	3192	1/1	0.72	0.20	1.08	63,63,63,63	0
56	MG	2B	3009	1/1	0.87	0.16	1.08	61,61,61,61	0
56	MG	1A	3757	1/1	0.91	0.23	1.07	27,27,27,27	0
56	MG	2A	3095	1/1	0.93	0.19	1.05	39,39,39,39	0
56	MG	1A	3811	1/1	0.98	0.22	1.04	45,45,45,45	0
56	MG	1W	203	1/1	0.99	0.24	1.04	30,30,30,30	0
56	MG	2A	3761	1/1	0.97	0.23	1.01	46,46,46,46	0
56	MG	1A	3355	1/1	0.97	0.26	0.94	47,47,47,47	0
56	MG	1A	4080	1/1	0.96	0.24	0.93	23,23,23,23	0
56	MG	1A	3041	1/1	0.96	0.23	0.87	38,38,38,38	0
58	ZN	16	102	1/1	1.00	0.22	0.84	44,44,44,44	0
56	MG	1B	3027	1/1	0.96	0.22	0.82	35,35,35,35	0
56	MG	1n	102	1/1	0.88	0.24	0.81	66,66,66,66	0
56	MG	2A	3756	1/1	0.88	0.18	0.78	42,42,42,42	0
56	MG	2A	3697	1/1	0.95	0.18	0.73	34,34,34,34	0
56	MG	1A	3793	1/1	0.99	0.24	0.72	37,37,37,37	0
56	MG	2A	3098	1/1	0.91	0.17	0.71	49,49,49,49	0
56	MG	2w	105	1/1	0.95	0.31	0.64	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3026	1/1	0.97	0.19	0.61	36,36,36,36	0
56	MG	2a	3244	1/1	0.96	0.18	0.60	43,43,43,43	0
56	MG	1A	4118	1/1	0.98	0.25	0.60	36,36,36,36	0
56	MG	2A	3235	1/1	0.94	0.18	0.58	50,50,50,50	0
56	MG	2A	3144	1/1	0.94	0.19	0.55	45,45,45,45	0
56	MG	18	101	1/1	0.84	0.24	0.54	47,47,47,47	0
56	MG	2A	3905	1/1	0.96	0.23	0.54	38,38,38,38	0
56	MG	1E	302	1/1	0.82	0.24	0.53	58,58,58,58	0
56	MG	1A	3285	1/1	0.96	0.22	0.50	39,39,39,39	0
58	ZN	1Y	501	1/1	0.99	0.19	0.47	60,60,60,60	0
56	MG	2A	3040	1/1	0.89	0.18	0.46	52,52,52,52	0
56	MG	1A	3054	1/1	0.97	0.23	0.46	39,39,39,39	0
56	MG	1A	3855	1/1	0.93	0.22	0.46	53,53,53,53	0
56	MG	1A	3654	1/1	0.88	0.24	0.44	36,36,36,36	0
56	MG	1F	304	1/1	0.98	0.25	0.42	40,40,40,40	0
56	MG	1A	4108	1/1	0.95	0.23	0.42	48,48,48,48	0
56	MG	1A	3606	1/1	0.98	0.23	0.39	36,36,36,36	0
56	MG	1D	306	1/1	0.98	0.21	0.39	32,32,32,32	0
56	MG	1A	3532	1/1	0.95	0.23	0.39	36,36,36,36	0
56	MG	1A	3376	1/1	0.92	0.21	0.38	51,51,51,51	0
56	MG	2r	101	1/1	0.92	0.15	0.33	68,68,68,68	0
56	MG	1a	1603	1/1	0.89	0.18	0.32	59,59,59,59	0
56	MG	1A	3608	1/1	0.95	0.20	0.31	51,51,51,51	0
56	MG	1a	1823	1/1	0.78	0.21	0.31	68,68,68,68	0
56	MG	1A	3963	1/1	0.90	0.23	0.30	60,60,60,60	0
56	MG	1A	4081	1/1	0.95	0.22	0.30	44,44,44,44	0
56	MG	2U	203	1/1	0.94	0.25	0.29	46,46,46,46	0
56	MG	1A	4051	1/1	0.92	0.23	0.27	38,38,38,38	0
56	MG	1A	3229	1/1	0.91	0.23	0.26	33,33,33,33	0
56	MG	2A	3001	1/1	0.91	0.19	0.24	47,47,47,47	0
56	MG	2A	3151	1/1	0.97	0.18	0.23	40,40,40,40	0
56	MG	1A	3526	1/1	0.95	0.24	0.21	53,53,53,53	0
56	MG	1U	204	1/1	0.95	0.22	0.20	38,38,38,38	0
56	MG	1a	1829	1/1	0.77	0.20	0.20	73,73,73,73	0
56	MG	1A	4098	1/1	0.92	0.21	0.16	45,45,45,45	0
56	MG	2A	3534	1/1	0.93	0.19	0.12	40,40,40,40	0
56	MG	1A	3130	1/1	0.92	0.23	0.12	41,41,41,41	0
56	MG	2B	3006	1/1	0.92	0.23	0.11	59,59,59,59	0
56	MG	2A	3884	1/1	0.74	0.19	0.08	42,42,42,42	0
56	MG	2f	3001	1/1	0.98	0.19	0.08	41,41,41,41	0
56	MG	1A	3193	1/1	0.95	0.21	0.03	34,34,34,34	0
56	MG	2A	3888	1/1	0.88	0.20	-0.01	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	1614	1/1	0.96	0.17	-0.03	45,45,45,45	0
56	MG	2A	3187	1/1	0.91	0.17	-0.07	50,50,50,50	0
56	MG	2A	3626	1/1	0.92	0.19	-0.08	53,53,53,53	0
56	MG	1A	4101	1/1	0.96	0.20	-0.11	39,39,39,39	0
56	MG	1x	103	1/1	0.58	0.16	-0.11	71,71,71,71	0
56	MG	1A	4117	1/1	0.98	0.22	-0.13	39,39,39,39	0
56	MG	1A	3078	1/1	0.97	0.22	-0.13	31,31,31,31	0
56	MG	2a	3238	1/1	0.81	0.17	-0.14	62,62,62,62	0
56	MG	1A	3358	1/1	0.94	0.23	-0.15	33,33,33,33	0
56	MG	2a	3161	1/1	0.93	0.21	-0.18	91,91,91,91	0
56	MG	1A	3172	1/1	0.94	0.22	-0.20	43,43,43,43	0
56	MG	2A	3904	1/1	0.98	0.19	-0.23	41,41,41,41	0
56	MG	2A	3560	1/1	0.92	0.19	-0.24	63,63,63,63	0
56	MG	2A	3162	1/1	0.95	0.17	-0.25	53,53,53,53	0
56	MG	1A	3135	1/1	0.97	0.23	-0.26	32,32,32,32	0
56	MG	1D	304	1/1	0.93	0.19	-0.27	30,30,30,30	0
56	MG	2A	3832	1/1	0.81	0.16	-0.27	54,54,54,54	0
56	MG	1A	4059	1/1	0.98	0.20	-0.28	21,21,21,21	0
56	MG	1A	3562	1/1	0.95	0.21	-0.28	24,24,24,24	0
56	MG	2A	3542	1/1	0.97	0.16	-0.28	39,39,39,39	0
56	MG	1A	4099	1/1	0.95	0.21	-0.28	41,41,41,41	0
56	MG	1Q	201	1/1	0.96	0.20	-0.29	36,36,36,36	0
56	MG	2A	3121	1/1	0.87	0.18	-0.29	42,42,42,42	0
56	MG	1A	4132	1/1	0.99	0.23	-0.29	39,39,39,39	0
56	MG	1A	3707	1/1	0.94	0.21	-0.31	29,29,29,29	0
56	MG	2A	3126	1/1	0.87	0.18	-0.32	58,58,58,58	0
56	MG	2a	3232	1/1	0.87	0.23	-0.36	77,77,77,77	0
56	MG	1A	3379	1/1	0.97	0.21	-0.39	37,37,37,37	0
56	MG	1A	3650	1/1	0.98	0.20	-0.39	35,35,35,35	0
56	MG	1A	3863	1/1	0.82	0.23	-0.42	50,50,50,50	0
56	MG	1B	3022	1/1	0.97	0.19	-0.44	60,60,60,60	0
56	MG	2A	3849	1/1	0.87	0.18	-0.44	44,44,44,44	0
56	MG	2A	3410	1/1	0.88	0.16	-0.45	55,55,55,55	0
56	MG	2A	3692	1/1	0.97	0.17	-0.47	56,56,56,56	0
56	MG	1A	4129	1/1	0.93	0.23	-0.49	42,42,42,42	0
56	MG	2A	3452	1/1	0.86	0.19	-0.50	42,42,42,42	0
56	MG	2A	3643	1/1	0.86	0.15	-0.52	34,34,34,34	0
56	MG	1b	3001	1/1	0.89	0.15	-0.53	83,83,83,83	0
56	MG	1A	3686	1/1	0.92	0.20	-0.54	35,35,35,35	0
56	MG	1A	3781	1/1	0.74	0.21	-0.55	32,32,32,32	0
56	MG	1A	3205	1/1	0.97	0.20	-0.57	42,42,42,42	0
56	MG	1A	3668	1/1	0.85	0.20	-0.59	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1B	3023	1/1	0.95	0.18	-0.60	54,54,54,54	0
56	MG	1A	4114	1/1	0.97	0.21	-0.63	34,34,34,34	0
56	MG	2A	3877	1/1	0.97	0.19	-0.64	28,28,28,28	0
56	MG	1A	3693	1/1	0.88	0.19	-0.64	40,40,40,40	0
56	MG	1A	3010	1/1	0.97	0.20	-0.64	39,39,39,39	0
56	MG	2A	3694	1/1	0.92	0.15	-0.65	51,51,51,51	0
56	MG	2w	107	1/1	0.66	0.22	-0.66	75,75,75,75	0
56	MG	2A	3638	1/1	0.94	0.18	-0.66	43,43,43,43	0
56	MG	1a	1617	1/1	0.72	0.18	-0.66	63,63,63,63	0
56	MG	2a	3103	1/1	0.64	0.16	-0.69	76,76,76,76	0
56	MG	2A	3127	1/1	0.93	0.13	-0.71	50,50,50,50	0
56	MG	1A	3414	1/1	0.96	0.19	-0.71	39,39,39,39	0
56	MG	1A	4012	1/1	0.86	0.20	-0.72	34,34,34,34	0
56	MG	1A	4109	1/1	0.94	0.21	-0.74	49,49,49,49	0
56	MG	1D	305	1/1	0.88	0.18	-0.74	42,42,42,42	0
56	MG	1a	1825	1/1	0.98	0.18	-0.75	37,37,37,37	0
56	MG	1A	3921	1/1	0.91	0.17	-0.77	50,50,50,50	0
56	MG	2A	3441	1/1	0.90	0.15	-0.78	51,51,51,51	0
56	MG	1a	1730	1/1	0.93	0.16	-0.80	80,80,80,80	0
56	MG	1A	4097	1/1	0.97	0.15	-0.80	47,47,47,47	0
56	MG	1A	3700	1/1	0.98	0.20	-0.80	16,16,16,16	0
56	MG	16	104	1/1	0.97	0.21	-0.81	53,53,53,53	0
58	ZN	19	103	1/1	0.99	0.19	-0.82	44,44,44,44	0
56	MG	2a	3076	1/1	0.79	0.15	-0.82	73,73,73,73	0
56	MG	2A	3080	1/1	0.80	0.16	-0.83	58,58,58,58	0
58	ZN	26	501	1/1	0.96	0.14	-0.83	60,60,60,60	0
56	MG	2A	3634	1/1	0.95	0.17	-0.83	34,34,34,34	0
56	MG	1A	3652	1/1	0.96	0.20	-0.87	31,31,31,31	0
56	MG	1E	311	1/1	0.85	0.20	-0.87	42,42,42,42	0
56	MG	2a	3145	1/1	0.86	0.20	-0.87	76,76,76,76	0
56	MG	1D	309	1/1	0.94	0.18	-0.88	46,46,46,46	0
56	MG	1A	3691	1/1	0.90	0.20	-0.89	41,41,41,41	0
56	MG	2a	3096	1/1	0.78	0.14	-0.91	65,65,65,65	0
56	MG	1A	3619	1/1	0.98	0.20	-0.93	31,31,31,31	0
56	MG	1l	201	1/1	0.98	0.16	-0.95	43,43,43,43	0
56	MG	2Q	3003	1/1	0.98	0.17	-0.95	51,51,51,51	0
56	MG	1a	1745	1/1	0.87	0.16	-0.95	55,55,55,55	0
56	MG	1N	202	1/1	0.85	0.22	-0.95	48,48,48,48	0
56	MG	1A	3074	1/1	0.93	0.21	-0.97	27,27,27,27	0
56	MG	1A	3122	1/1	0.96	0.22	-0.97	44,44,44,44	0
56	MG	2A	3840	1/1	0.98	0.18	-0.97	43,43,43,43	0
56	MG	1A	4116	1/1	0.90	0.22	-1.00	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3142	1/1	0.96	0.17	-1.00	41,41,41,41	0
56	MG	2A	3903	1/1	0.93	0.14	-1.01	58,58,58,58	0
56	MG	1U	207	1/1	0.96	0.20	-1.01	31,31,31,31	0
56	MG	1F	308	1/1	0.93	0.20	-1.01	53,53,53,53	0
56	MG	2A	3907	1/1	0.93	0.16	-1.01	57,57,57,57	0
56	MG	2a	3046	1/1	0.72	0.17	-1.02	64,64,64,64	0
56	MG	2T	3002	1/1	0.85	0.15	-1.02	58,58,58,58	0
56	MG	2A	3548	1/1	0.97	0.17	-1.04	38,38,38,38	0
56	MG	2A	3619	1/1	0.95	0.16	-1.04	37,37,37,37	0
56	MG	2A	3513	1/1	0.98	0.15	-1.06	34,34,34,34	0
56	MG	2A	3615	1/1	0.79	0.13	-1.06	51,51,51,51	0
56	MG	1A	3460	1/1	0.93	0.22	-1.07	48,48,48,48	0
56	MG	2A	3841	1/1	0.97	0.16	-1.08	30,30,30,30	0
56	MG	2a	3229	1/1	0.90	0.15	-1.11	69,69,69,69	0
56	MG	2a	3105	1/1	0.82	0.17	-1.14	45,45,45,45	0
56	MG	1A	3680	1/1	0.92	0.19	-1.16	44,44,44,44	0
56	MG	1A	3741	1/1	0.80	0.18	-1.18	45,45,45,45	0
56	MG	1U	203	1/1	0.91	0.23	-1.19	42,42,42,42	0
56	MG	2a	3128	1/1	0.87	0.12	-1.19	87,87,87,87	0
56	MG	2a	3189	1/1	0.94	0.16	-1.20	48,48,48,48	0
58	ZN	24	501	1/1	0.72	0.10	-1.21	128,128,128,128	0
56	MG	2A	3890	1/1	0.86	0.16	-1.21	61,61,61,61	0
56	MG	1A	3843	1/1	0.99	0.21	-1.22	31,31,31,31	0
56	MG	2D	301	1/1	0.95	0.15	-1.22	57,57,57,57	0
56	MG	2a	3157	1/1	0.93	0.12	-1.23	64,64,64,64	0
56	MG	2j	8002	1/1	0.90	0.16	-1.25	66,66,66,66	0
56	MG	2A	3140	1/1	0.93	0.18	-1.27	50,50,50,50	0
56	MG	2a	3047	1/1	0.83	0.12	-1.31	52,52,52,52	0
56	MG	1G	3003	1/1	0.88	0.11	-1.31	66,66,66,66	0
58	ZN	14	501	1/1	0.92	0.11	-1.32	99,99,99,99	0
58	ZN	2Y	501	1/1	0.96	0.13	-1.36	81,81,81,81	0
56	MG	1A	4119	1/1	0.98	0.23	-1.37	34,34,34,34	0
56	MG	1x	107	1/1	0.76	0.12	-1.38	61,61,61,61	0
56	MG	2t	3001	1/1	0.52	0.15	-1.39	60,60,60,60	0
59	SF4	1d	501	8/8	0.98	0.13	-1.39	59,71,76,86	0
56	MG	2A	3737	1/1	0.94	0.13	-1.40	72,72,72,72	0
56	MG	1A	3105	1/1	0.98	0.17	-1.40	40,40,40,40	0
56	MG	2D	303	1/1	0.95	0.15	-1.40	35,35,35,35	0
56	MG	1a	1654	1/1	0.80	0.17	-1.42	49,49,49,49	0
56	MG	2U	202	1/1	0.89	0.13	-1.43	54,54,54,54	0
56	MG	1A	3166	1/1	0.87	0.22	-1.44	38,38,38,38	0
56	MG	1a	1740	1/1	0.99	0.17	-1.45	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3666	1/1	0.87	0.16	-1.46	34,34,34,34	0
56	MG	2A	3645	1/1	0.93	0.16	-1.48	40,40,40,40	0
56	MG	2A	3034	1/1	0.90	0.15	-1.49	45,45,45,45	0
56	MG	2A	3674	1/1	0.96	0.17	-1.50	55,55,55,55	0
56	MG	1A	3195	1/1	0.93	0.21	-1.51	40,40,40,40	0
56	MG	1A	3800	1/1	0.88	0.15	-1.51	65,65,65,65	0
56	MG	1A	3042	1/1	0.98	0.18	-1.52	40,40,40,40	0
56	MG	1R	202	1/1	0.92	0.18	-1.54	38,38,38,38	0
56	MG	2A	3726	1/1	0.84	0.13	-1.55	56,56,56,56	0
56	MG	2T	3001	1/1	0.91	0.13	-1.55	53,53,53,53	0
56	MG	1A	3764	1/1	0.89	0.18	-1.57	31,31,31,31	0
56	MG	1A	3514	1/1	0.96	0.20	-1.57	53,53,53,53	0
56	MG	1A	3873	1/1	0.98	0.21	-1.58	35,35,35,35	0
56	MG	1A	3961	1/1	0.98	0.18	-1.59	38,38,38,38	0
56	MG	1A	3919	1/1	0.95	0.18	-1.59	38,38,38,38	0
56	MG	1Q	202	1/1	0.96	0.20	-1.61	46,46,46,46	0
56	MG	1A	3730	1/1	0.75	0.18	-1.62	43,43,43,43	0
56	MG	1A	3405	1/1	0.91	0.21	-1.63	42,42,42,42	0
58	ZN	29	101	1/1	0.97	0.08	-1.64	73,73,73,73	0
56	MG	1A	3909	1/1	0.97	0.20	-1.64	40,40,40,40	0
56	MG	2A	3475	1/1	0.86	0.16	-1.66	44,44,44,44	0
56	MG	1A	3752	1/1	0.82	0.19	-1.66	41,41,41,41	0
56	MG	1A	3040	1/1	0.95	0.20	-1.66	36,36,36,36	0
58	ZN	1n	101	1/1	0.98	0.12	-1.68	71,71,71,71	0
56	MG	1A	3775	1/1	0.98	0.21	-1.68	27,27,27,27	0
56	MG	1A	3535	1/1	0.93	0.20	-1.70	45,45,45,45	0
56	MG	2A	3037	1/1	0.97	0.14	-1.70	35,35,35,35	0
56	MG	2X	101	1/1	0.96	0.10	-1.71	37,37,37,37	0
56	MG	1A	3190	1/1	0.90	0.21	-1.72	39,39,39,39	0
56	MG	2a	3173	1/1	0.87	0.12	-1.72	62,62,62,62	0
56	MG	1A	3187	1/1	0.91	0.21	-1.74	47,47,47,47	0
56	MG	1A	3641	1/1	0.82	0.17	-1.75	65,65,65,65	0
56	MG	1A	3595	1/1	0.92	0.21	-1.76	59,59,59,59	0
56	MG	1A	4104	1/1	0.94	0.15	-1.77	30,30,30,30	0
56	MG	1a	1608	1/1	0.95	0.18	-1.77	60,60,60,60	0
56	MG	2A	3163	1/1	0.94	0.13	-1.78	56,56,56,56	0
56	MG	2e	3001	1/1	0.95	0.08	-1.79	79,79,79,79	0
56	MG	2Q	3001	1/1	0.97	0.15	-1.80	50,50,50,50	0
56	MG	2l	201	1/1	0.96	0.14	-1.81	66,66,66,66	0
56	MG	1a	1747	1/1	0.94	0.14	-1.82	49,49,49,49	0
56	MG	2A	3158	1/1	0.98	0.17	-1.84	41,41,41,41	0
56	MG	2n	502	1/1	0.95	0.06	-1.84	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3750	1/1	0.97	0.21	-1.85	29,29,29,29	0
56	MG	1A	3066	1/1	0.93	0.17	-1.89	35,35,35,35	0
56	MG	1a	1634	1/1	0.95	0.17	-1.91	27,27,27,27	0
56	MG	2a	3097	1/1	0.83	0.13	-1.91	72,72,72,72	0
56	MG	2a	3241	1/1	0.94	0.10	-1.92	41,41,41,41	0
56	MG	1A	4140	1/1	0.96	0.18	-1.92	31,31,31,31	0
56	MG	2A	3889	1/1	0.97	0.11	-1.94	49,49,49,49	0
56	MG	13	101	1/1	0.88	0.22	-1.95	55,55,55,55	0
56	MG	1a	1827	1/1	0.86	0.14	-1.95	58,58,58,58	0
56	MG	1A	3790	1/1	0.96	0.18	-1.99	25,25,25,25	0
56	MG	2A	3530	1/1	0.97	0.15	-1.99	37,37,37,37	0
56	MG	2A	3565	1/1	0.94	0.16	-2.00	36,36,36,36	0
56	MG	2W	201	1/1	0.96	0.14	-2.00	57,57,57,57	0
56	MG	1D	303	1/1	0.94	0.14	-2.00	37,37,37,37	0
56	MG	1A	3653	1/1	0.94	0.19	-2.00	27,27,27,27	0
56	MG	1A	3109	1/1	0.99	0.20	-2.00	35,35,35,35	0
56	MG	1A	3902	1/1	0.95	0.21	-2.01	33,33,33,33	0
56	MG	2A	3690	1/1	0.96	0.12	-2.02	61,61,61,61	0
56	MG	1A	4077	1/1	0.98	0.19	-2.04	11,11,11,11	0
56	MG	1a	1618	1/1	0.96	0.17	-2.04	48,48,48,48	0
56	MG	2A	3581	1/1	0.98	0.17	-2.05	25,25,25,25	0
56	MG	2A	3516	1/1	0.97	0.14	-2.05	56,56,56,56	0
56	MG	2A	3103	1/1	0.96	0.15	-2.06	42,42,42,42	0
56	MG	2a	3113	1/1	0.97	0.14	-2.08	46,46,46,46	0
56	MG	1A	4002	1/1	0.94	0.20	-2.08	33,33,33,33	0
56	MG	2A	3812	1/1	0.79	0.13	-2.09	47,47,47,47	0
56	MG	1E	309	1/1	0.94	0.15	-2.10	50,50,50,50	0
56	MG	2a	3200	1/1	0.96	0.14	-2.12	76,76,76,76	0
56	MG	2A	3207	1/1	0.92	0.14	-2.13	44,44,44,44	0
56	MG	1A	3657	1/1	0.95	0.18	-2.15	27,27,27,27	0
56	MG	28	102	1/1	0.76	0.18	-2.17	52,52,52,52	0
56	MG	1A	3184	1/1	0.84	0.15	-2.17	62,62,62,62	0
56	MG	1a	1806	1/1	0.90	0.13	-2.19	66,66,66,66	0
56	MG	2A	3570	1/1	0.95	0.13	-2.19	53,53,53,53	0
56	MG	2G	3001	1/1	0.83	0.16	-2.19	51,51,51,51	0
56	MG	1A	3241	1/1	0.96	0.18	-2.19	44,44,44,44	0
56	MG	2A	3514	1/1	0.96	0.13	-2.20	32,32,32,32	0
56	MG	2X	103	1/1	0.95	0.11	-2.20	46,46,46,46	0
56	MG	1A	3663	1/1	0.98	0.18	-2.21	28,28,28,28	0
56	MG	1A	4130	1/1	0.97	0.18	-2.21	38,38,38,38	0
56	MG	2a	3195	1/1	0.93	0.13	-2.22	41,41,41,41	0
56	MG	2a	3149	1/1	0.86	0.12	-2.22	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1X	101	1/1	0.84	0.17	-2.23	40,40,40,40	0
56	MG	1A	3735	1/1	0.97	0.18	-2.24	41,41,41,41	0
56	MG	1a	1751	1/1	0.84	0.14	-2.25	70,70,70,70	0
56	MG	2A	3564	1/1	0.94	0.15	-2.25	31,31,31,31	0
56	MG	1A	3746	1/1	0.87	0.20	-2.26	55,55,55,55	0
56	MG	2A	3122	1/1	0.94	0.13	-2.27	39,39,39,39	0
56	MG	2a	3098	1/1	0.97	0.14	-2.27	46,46,46,46	0
56	MG	2A	3016	1/1	0.91	0.14	-2.28	61,61,61,61	0
56	MG	1A	3596	1/1	0.93	0.20	-2.31	51,51,51,51	0
56	MG	1A	3228	1/1	0.96	0.20	-2.33	41,41,41,41	0
56	MG	2A	3650	1/1	0.97	0.14	-2.34	41,41,41,41	0
56	MG	1A	4096	1/1	0.94	0.14	-2.35	30,30,30,30	0
56	MG	1a	1737	1/1	0.94	0.11	-2.35	66,66,66,66	0
56	MG	2A	3577	1/1	0.77	0.12	-2.37	56,56,56,56	0
56	MG	1A	3880	1/1	0.95	0.17	-2.39	30,30,30,30	0
59	SF4	2d	501	8/8	0.97	0.11	-2.41	61,71,85,99	0
56	MG	1A	3626	1/1	0.94	0.14	-2.42	44,44,44,44	0
56	MG	2a	3082	1/1	0.94	0.14	-2.43	54,54,54,54	0
56	MG	2a	3175	1/1	0.95	0.13	-2.45	46,46,46,46	0
58	ZN	2n	501	1/1	0.96	0.09	-2.46	107,107,107,107	0
56	MG	1A	3756	1/1	0.92	0.20	-2.46	39,39,39,39	0
56	MG	1a	1629	1/1	0.81	0.16	-2.46	57,57,57,57	0
56	MG	2A	3601	1/1	0.97	0.15	-2.48	39,39,39,39	0
56	MG	2A	3606	1/1	0.92	0.15	-2.49	61,61,61,61	0
56	MG	2A	3902	1/1	0.97	0.14	-2.51	43,43,43,43	0
56	MG	1a	1826	1/1	0.89	0.06	-2.54	58,58,58,58	0
56	MG	1A	3328	1/1	0.88	0.17	-2.57	64,64,64,64	0
56	MG	2A	3881	1/1	0.89	0.14	-2.57	48,48,48,48	0
56	MG	2a	3154	1/1	0.96	0.11	-2.58	68,68,68,68	0
56	MG	2a	3217	1/1	0.96	0.07	-2.59	61,61,61,61	0
56	MG	1A	3237	1/1	0.96	0.19	-2.60	38,38,38,38	0
56	MG	1E	308	1/1	0.95	0.11	-2.60	34,34,34,34	0
56	MG	1A	3120	1/1	0.94	0.18	-2.61	42,42,42,42	0
56	MG	2A	3145	1/1	0.97	0.15	-2.63	36,36,36,36	0
56	MG	1A	3859	1/1	0.90	0.19	-2.64	44,44,44,44	0
56	MG	1A	3034	1/1	0.87	0.16	-2.65	45,45,45,45	0
56	MG	1a	1822	1/1	0.96	0.11	-2.66	54,54,54,54	0
56	MG	1a	1667	1/1	0.91	0.12	-2.66	65,65,65,65	0
56	MG	2a	3092	1/1	0.93	0.13	-2.67	51,51,51,51	0
56	MG	1A	3210	1/1	0.90	0.16	-2.67	42,42,42,42	0
56	MG	2E	304	1/1	0.89	0.12	-2.68	46,46,46,46	0
56	MG	2a	3070	1/1	0.80	0.15	-2.69	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3144	1/1	0.81	0.19	-2.69	52,52,52,52	0
56	MG	1A	3861	1/1	0.94	0.17	-2.70	33,33,33,33	0
56	MG	2A	3709	1/1	0.97	0.14	-2.72	33,33,33,33	0
56	MG	1A	3904	1/1	0.93	0.17	-2.72	36,36,36,36	0
56	MG	1A	3984	1/1	0.98	0.16	-2.74	34,34,34,34	0
56	MG	2A	3613	1/1	0.91	0.16	-2.75	33,33,33,33	0
56	MG	2A	3576	1/1	0.96	0.15	-2.79	39,39,39,39	0
56	MG	2A	3562	1/1	0.89	0.11	-2.81	37,37,37,37	0
56	MG	1a	1778	1/1	0.94	0.17	-2.82	64,64,64,64	0
56	MG	1Q	205	1/1	0.96	0.17	-2.84	39,39,39,39	0
56	MG	2d	502	1/1	0.91	0.09	-2.84	68,68,68,68	0
56	MG	2A	3879	1/1	0.86	0.10	-2.84	37,37,37,37	0
56	MG	2A	3515	1/1	0.81	0.11	-2.84	55,55,55,55	0
56	MG	1A	3607	1/1	0.86	0.17	-2.85	35,35,35,35	0
56	MG	1A	3021	1/1	0.94	0.17	-2.85	45,45,45,45	0
56	MG	1U	205	1/1	0.95	0.16	-2.85	35,35,35,35	0
56	MG	2A	3550	1/1	0.95	0.15	-2.86	44,44,44,44	0
56	MG	1A	3046	1/1	0.99	0.17	-2.87	32,32,32,32	0
56	MG	1a	1776	1/1	0.91	0.12	-2.88	91,91,91,91	0
56	MG	1A	4142	1/1	0.97	0.17	-2.90	42,42,42,42	0
56	MG	1w	105	1/1	0.75	0.10	-2.94	87,87,87,87	0
56	MG	2A	3019	1/1	0.95	0.15	-2.96	38,38,38,38	0
56	MG	2A	3616	1/1	0.95	0.15	-2.98	46,46,46,46	0
56	MG	2A	3748	1/1	0.77	0.10	-2.99	57,57,57,57	0
56	MG	2A	3242	1/1	0.96	0.16	-3.00	52,52,52,52	0
56	MG	1a	1670	1/1	0.94	0.11	-3.01	59,59,59,59	0
56	MG	2a	3199	1/1	0.93	0.11	-3.02	72,72,72,72	0
56	MG	2A	3819	1/1	0.89	0.13	-3.02	64,64,64,64	0
56	MG	2A	3233	1/1	0.94	0.14	-3.04	32,32,32,32	0
56	MG	2A	3067	1/1	0.82	0.11	-3.07	57,57,57,57	0
56	MG	1A	4106	1/1	0.96	0.17	-3.08	29,29,29,29	0
56	MG	2A	3882	1/1	0.99	0.13	-3.08	44,44,44,44	0
56	MG	1N	203	1/1	0.96	0.19	-3.10	48,48,48,48	0
56	MG	1A	3481	1/1	0.96	0.14	-3.10	39,39,39,39	0
56	MG	2a	3090	1/1	0.66	0.11	-3.12	68,68,68,68	0
56	MG	1F	303	1/1	0.93	0.17	-3.12	38,38,38,38	0
56	MG	2A	3211	1/1	0.92	0.10	-3.13	43,43,43,43	0
56	MG	2A	3568	1/1	0.71	0.14	-3.14	46,46,46,46	0
56	MG	1A	4111	1/1	0.94	0.17	-3.15	34,34,34,34	0
56	MG	1A	3772	1/1	0.92	0.16	-3.16	36,36,36,36	0
56	MG	2A	3895	1/1	0.90	0.15	-3.20	46,46,46,46	0
56	MG	1a	1724	1/1	0.97	0.10	-3.20	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3574	1/1	0.94	0.18	-3.21	43,43,43,43	0
56	MG	1A	3243	1/1	0.95	0.15	-3.21	53,53,53,53	0
56	MG	1A	3731	1/1	0.99	0.18	-3.21	17,17,17,17	0
56	MG	1a	1620	1/1	0.81	0.15	-3.22	66,66,66,66	0
56	MG	1t	3001	1/1	0.93	0.13	-3.24	58,58,58,58	0
56	MG	1A	4127	1/1	0.97	0.18	-3.26	34,34,34,34	0
56	MG	1B	3005	1/1	0.94	0.16	-3.29	55,55,55,55	0
56	MG	2a	3203	1/1	0.95	0.14	-3.30	62,62,62,62	0
56	MG	2A	3898	1/1	0.99	0.13	-3.32	28,28,28,28	0
56	MG	1A	3221	1/1	0.83	0.17	-3.32	55,55,55,55	0
56	MG	1A	3008	1/1	0.99	0.18	-3.33	26,26,26,26	0
56	MG	1A	3533	1/1	0.92	0.18	-3.34	36,36,36,36	0
56	MG	2A	3722	1/1	0.87	0.10	-3.34	58,58,58,58	0
56	MG	1A	3038	1/1	0.98	0.13	-3.37	50,50,50,50	0
56	MG	2A	3051	1/1	0.80	0.15	-3.38	43,43,43,43	0
56	MG	1a	1653	1/1	0.99	0.13	-3.38	54,54,54,54	0
56	MG	1A	4137	1/1	0.97	0.18	-3.41	44,44,44,44	0
56	MG	2A	3776	1/1	0.95	0.13	-3.42	44,44,44,44	0
56	MG	2A	3046	1/1	0.96	0.11	-3.42	48,48,48,48	0
56	MG	1A	3893	1/1	0.98	0.18	-3.42	17,17,17,17	0
56	MG	1a	1752	1/1	0.90	0.13	-3.43	68,68,68,68	0
56	MG	2a	3151	1/1	0.88	0.09	-3.43	78,78,78,78	0
56	MG	2a	3114	1/1	0.92	0.13	-3.44	51,51,51,51	0
56	MG	2q	202	1/1	0.93	0.06	-3.45	78,78,78,78	0
56	MG	2A	3742	1/1	0.97	0.09	-3.46	49,49,49,49	0
56	MG	1a	1800	1/1	0.95	0.12	-3.46	70,70,70,70	0
56	MG	2A	3908	1/1	0.97	0.14	-3.49	44,44,44,44	0
56	MG	2A	3299	1/1	0.91	0.12	-3.51	51,51,51,51	0
56	MG	2A	3668	1/1	0.99	0.12	-3.52	45,45,45,45	0
56	MG	1A	3780	1/1	0.95	0.16	-3.53	21,21,21,21	0
56	MG	1X	104	1/1	0.91	0.18	-3.54	52,52,52,52	0
56	MG	2A	3735	1/1	0.96	0.10	-3.55	55,55,55,55	0
56	MG	1A	4112	1/1	0.94	0.17	-3.56	42,42,42,42	0
56	MG	1A	3508	1/1	0.95	0.14	-3.56	36,36,36,36	0
56	MG	1a	1611	1/1	0.96	0.16	-3.56	22,22,22,22	0
56	MG	1B	3006	1/1	0.91	0.15	-3.57	45,45,45,45	0
56	MG	2A	3837	1/1	0.81	0.14	-3.61	37,37,37,37	0
56	MG	1F	302	1/1	0.85	0.16	-3.62	47,47,47,47	0
56	MG	1A	3482	1/1	0.92	0.16	-3.65	50,50,50,50	0
56	MG	1A	4010	1/1	0.80	0.20	-3.66	26,26,26,26	0
56	MG	2A	3476	1/1	0.94	0.13	-3.67	41,41,41,41	0
56	MG	1E	303	1/1	0.99	0.16	-3.68	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3685	1/1	0.94	0.09	-3.69	53,53,53,53	0
56	MG	1A	3524	1/1	0.96	0.16	-3.70	47,47,47,47	0
56	MG	2a	3094	1/1	0.97	0.12	-3.73	68,68,68,68	0
56	MG	1A	3905	1/1	0.97	0.16	-3.74	46,46,46,46	0
56	MG	2A	3131	1/1	0.96	0.11	-3.74	42,42,42,42	0
56	MG	1A	3649	1/1	0.70	0.16	-3.75	54,54,54,54	0
56	MG	2A	3614	1/1	0.94	0.14	-3.78	36,36,36,36	0
56	MG	1a	1649	1/1	0.97	0.12	-3.79	45,45,45,45	0
56	MG	1A	3303	1/1	0.94	0.17	-3.81	33,33,33,33	0
56	MG	1a	1615	1/1	0.90	0.11	-3.81	67,67,67,67	0
56	MG	1A	3001	1/1	0.95	0.17	-3.83	42,42,42,42	0
56	MG	1A	3620	1/1	0.99	0.19	-3.85	25,25,25,25	0
56	MG	1B	3031	1/1	0.87	0.12	-3.89	67,67,67,67	0
56	MG	1x	116	1/1	0.95	0.12	-3.90	59,59,59,59	0
56	MG	2A	3057	1/1	0.88	0.07	-3.94	46,46,46,46	0
56	MG	1A	3646	1/1	0.96	0.18	-3.94	32,32,32,32	0
56	MG	2A	3857	1/1	0.84	0.13	-3.95	47,47,47,47	0
56	MG	1A	3903	1/1	0.92	0.17	-3.95	40,40,40,40	0
56	MG	2A	3011	1/1	0.88	0.07	-4.00	48,48,48,48	0
56	MG	1A	4091	1/1	0.95	0.16	-4.02	49,49,49,49	0
56	MG	1A	3923	1/1	0.96	0.14	-4.03	47,47,47,47	0
56	MG	1A	3960	1/1	0.96	0.18	-4.03	23,23,23,23	0
56	MG	1A	3806	1/1	0.97	0.17	-4.05	34,34,34,34	0
56	MG	2A	3099	1/1	0.89	0.13	-4.05	42,42,42,42	0
56	MG	2A	3620	1/1	0.95	0.10	-4.05	65,65,65,65	0
56	MG	2a	3119	1/1	0.85	0.15	-4.05	71,71,71,71	0
56	MG	1A	3240	1/1	0.91	0.15	-4.08	35,35,35,35	0
56	MG	2A	3545	1/1	0.95	0.14	-4.11	52,52,52,52	0
56	MG	2A	3637	1/1	0.95	0.11	-4.11	42,42,42,42	0
56	MG	1A	4133	1/1	0.92	0.15	-4.14	45,45,45,45	0
56	MG	1A	4068	1/1	0.70	0.18	-4.15	48,48,48,48	0
56	MG	1A	3076	1/1	0.92	0.15	-4.16	53,53,53,53	0
56	MG	1a	1819	1/1	0.84	0.10	-4.17	48,48,48,48	0
56	MG	2A	3499	1/1	0.93	0.11	-4.17	46,46,46,46	0
56	MG	1A	3634	1/1	0.92	0.18	-4.19	44,44,44,44	0
56	MG	1A	3640	1/1	0.94	0.17	-4.22	53,53,53,53	0
56	MG	2a	3187	1/1	0.92	0.13	-4.29	72,72,72,72	0
56	MG	1A	3360	1/1	0.96	0.16	-4.29	31,31,31,31	0
56	MG	2A	3541	1/1	0.94	0.14	-4.30	30,30,30,30	0
56	MG	1a	1795	1/1	0.81	0.12	-4.31	70,70,70,70	0
56	MG	1A	3449	1/1	0.97	0.12	-4.33	41,41,41,41	0
56	MG	1A	3015	1/1	0.94	0.16	-4.33	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1T	8002	1/1	0.97	0.14	-4.34	58,58,58,58	0
56	MG	2a	3118	1/1	0.91	0.12	-4.35	65,65,65,65	0
56	MG	1N	205	1/1	0.92	0.14	-4.35	57,57,57,57	0
56	MG	1A	4024	1/1	0.72	0.12	-4.35	71,71,71,71	0
56	MG	1A	3359	1/1	0.98	0.14	-4.36	38,38,38,38	0
56	MG	2A	3551	1/1	0.97	0.14	-4.37	39,39,39,39	0
56	MG	1A	3012	1/1	0.95	0.16	-4.37	30,30,30,30	0
56	MG	1A	3845	1/1	0.97	0.17	-4.39	38,38,38,38	0
56	MG	1A	4120	1/1	0.96	0.16	-4.42	44,44,44,44	0
56	MG	1A	3673	1/1	0.98	0.15	-4.45	29,29,29,29	0
56	MG	2a	3084	1/1	0.96	0.10	-4.49	44,44,44,44	0
56	MG	1A	3774	1/1	0.74	0.17	-4.56	55,55,55,55	0
56	MG	1A	3203	1/1	0.83	0.16	-4.59	50,50,50,50	0
56	MG	1A	3128	1/1	0.90	0.17	-4.62	41,41,41,41	0
56	MG	1A	3624	1/1	0.97	0.17	-4.64	28,28,28,28	0
56	MG	1A	3765	1/1	0.95	0.13	-4.66	25,25,25,25	0
56	MG	1A	4139	1/1	0.98	0.15	-4.68	35,35,35,35	0
56	MG	2a	3159	1/1	0.95	0.09	-4.70	71,71,71,71	0
56	MG	16	103	1/1	0.94	0.12	-4.70	54,54,54,54	0
56	MG	1A	3812	1/1	0.95	0.17	-4.74	45,45,45,45	0
56	MG	1a	1789	1/1	0.81	0.15	-4.74	72,72,72,72	0
56	MG	1A	4085	1/1	0.98	0.22	-4.75	21,21,21,21	0
56	MG	2A	3407	1/1	0.89	0.12	-4.76	61,61,61,61	0
56	MG	2A	3869	1/1	0.88	0.07	-4.77	56,56,56,56	0
56	MG	1A	3575	1/1	0.93	0.14	-4.80	33,33,33,33	0
56	MG	1U	206	1/1	0.94	0.12	-4.83	32,32,32,32	0
56	MG	2A	3007	1/1	0.95	0.10	-4.93	43,43,43,43	0
56	MG	2A	3061	1/1	0.94	0.12	-4.96	49,49,49,49	0
56	MG	1A	3043	1/1	0.94	0.19	-4.97	39,39,39,39	0
56	MG	1A	3208	1/1	0.85	0.16	-4.99	55,55,55,55	0
56	MG	1A	3885	1/1	0.96	0.15	-4.99	37,37,37,37	0
56	MG	2A	3660	1/1	0.95	0.08	-5.01	45,45,45,45	0
56	MG	1A	3675	1/1	0.95	0.16	-5.04	32,32,32,32	0
56	MG	2A	3715	1/1	0.87	0.13	-5.06	46,46,46,46	0
56	MG	1A	4074	1/1	0.70	0.15	-5.07	64,64,64,64	0
56	MG	2A	3248	1/1	0.93	0.13	-5.08	42,42,42,42	0
56	MG	1P	202	1/1	0.94	0.11	-5.16	31,31,31,31	0
56	MG	1A	3852	1/1	0.94	0.14	-5.16	33,33,33,33	0
56	MG	2A	3094	1/1	0.95	0.17	-5.17	44,44,44,44	0
56	MG	20	3003	1/1	0.92	0.09	-5.22	58,58,58,58	0
56	MG	2A	3693	1/1	0.92	0.11	-5.25	35,35,35,35	0
56	MG	2a	3071	1/1	0.89	0.08	-5.27	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3310	1/1	0.92	0.18	-5.28	40,40,40,40	0
56	MG	2A	3808	1/1	0.83	0.12	-5.29	60,60,60,60	0
56	MG	1D	308	1/1	0.95	0.11	-5.29	48,48,48,48	0
56	MG	1A	3196	1/1	0.93	0.10	-5.30	59,59,59,59	0
56	MG	1A	3356	1/1	0.96	0.14	-5.32	39,39,39,39	0
56	MG	1A	4039	1/1	0.98	0.15	-5.33	21,21,21,21	0
56	MG	1A	3115	1/1	0.92	0.14	-5.34	57,57,57,57	0
56	MG	1a	1742	1/1	0.94	0.08	-5.35	51,51,51,51	0
56	MG	1a	1626	1/1	0.96	0.13	-5.38	61,61,61,61	0
56	MG	1l	102	1/1	0.98	0.10	-5.43	36,36,36,36	0
56	MG	2A	3404	1/1	0.96	0.10	-5.44	53,53,53,53	0
56	MG	1a	1791	1/1	0.94	0.09	-5.44	54,54,54,54	0
56	MG	1a	1613	1/1	0.92	0.08	-5.47	74,74,74,74	0
56	MG	1A	4121	1/1	0.98	0.17	-5.50	34,34,34,34	0
56	MG	1A	3439	1/1	0.98	0.14	-5.53	40,40,40,40	0
56	MG	1A	3670	1/1	0.96	0.16	-5.53	32,32,32,32	0
56	MG	1G	3001	1/1	0.95	0.15	-5.55	41,41,41,41	0
56	MG	1A	3612	1/1	0.96	0.12	-5.58	41,41,41,41	0
56	MG	1A	3230	1/1	0.89	0.18	-5.63	60,60,60,60	0
56	MG	2a	3080	1/1	0.86	0.11	-5.63	50,50,50,50	0
56	MG	1A	3892	1/1	0.95	0.13	-5.66	39,39,39,39	0
56	MG	1A	3810	1/1	0.92	0.15	-5.66	45,45,45,45	0
56	MG	2A	3020	1/1	0.96	0.08	-5.68	49,49,49,49	0
56	MG	1A	3366	1/1	0.98	0.17	-5.73	38,38,38,38	0
56	MG	1A	3174	1/1	0.98	0.14	-5.73	38,38,38,38	0
56	MG	1a	1668	1/1	0.92	0.13	-5.76	67,67,67,67	0
56	MG	1a	1754	1/1	0.94	0.09	-5.77	51,51,51,51	0
56	MG	2A	3768	1/1	0.93	0.10	-5.79	62,62,62,62	0
56	MG	1W	205	1/1	0.97	0.15	-5.82	39,39,39,39	0
56	MG	1A	3022	1/1	0.99	0.14	-5.83	21,21,21,21	0
56	MG	2A	3021	1/1	0.98	0.11	-5.85	28,28,28,28	0
56	MG	1A	3998	1/1	0.80	0.16	-5.99	65,65,65,65	0
56	MG	1A	3314	1/1	0.98	0.16	-6.03	33,33,33,33	0
56	MG	1A	3112	1/1	0.84	0.17	-6.04	49,49,49,49	0
56	MG	2A	3786	1/1	0.95	0.09	-6.07	48,48,48,48	0
56	MG	1A	3717	1/1	0.95	0.17	-6.08	22,22,22,22	0
56	MG	2A	3555	1/1	0.92	0.10	-6.09	43,43,43,43	0
56	MG	1A	4071	1/1	0.85	0.15	-6.13	26,26,26,26	0
56	MG	1A	3688	1/1	0.99	0.15	-6.16	15,15,15,15	0
56	MG	1A	3070	1/1	0.90	0.15	-6.17	41,41,41,41	0
56	MG	1B	3018	1/1	0.94	0.15	-6.18	37,37,37,37	0
56	MG	1A	4001	1/1	0.98	0.19	-6.20	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3524	1/1	0.97	0.11	-6.30	48,48,48,48	0
56	MG	2A	3846	1/1	0.87	0.09	-6.33	47,47,47,47	0
56	MG	2A	3631	1/1	0.95	0.11	-6.36	39,39,39,39	0
56	MG	1a	1638	1/1	0.95	0.14	-6.39	58,58,58,58	0
56	MG	1A	3097	1/1	0.99	0.11	-6.41	35,35,35,35	0
56	MG	2A	3666	1/1	0.93	0.10	-6.43	34,34,34,34	0
56	MG	2A	3834	1/1	0.97	0.10	-6.43	40,40,40,40	0
56	MG	1A	3159	1/1	0.95	0.15	-6.43	39,39,39,39	0
56	MG	1A	3047	1/1	0.96	0.15	-6.46	21,21,21,21	0
56	MG	1A	3020	1/1	0.97	0.15	-6.49	25,25,25,25	0
56	MG	2A	3032	1/1	0.92	0.10	-6.49	38,38,38,38	0
56	MG	1A	3767	1/1	0.96	0.14	-6.50	41,41,41,41	0
56	MG	1R	201	1/1	0.99	0.13	-6.51	30,30,30,30	0
56	MG	1A	3103	1/1	0.93	0.15	-6.55	38,38,38,38	0
56	MG	1A	4016	1/1	0.92	0.13	-6.56	46,46,46,46	0
56	MG	10	101	1/1	0.92	0.12	-6.57	63,63,63,63	0
56	MG	1A	3866	1/1	0.93	0.17	-6.63	46,46,46,46	0
56	MG	1A	3616	1/1	0.73	0.17	-6.64	40,40,40,40	0
56	MG	2A	3152	1/1	0.81	0.11	-6.64	62,62,62,62	0
56	MG	1A	3032	1/1	0.97	0.18	-6.65	31,31,31,31	0
56	MG	1A	4136	1/1	0.98	0.16	-6.65	40,40,40,40	0
56	MG	1A	4003	1/1	0.93	0.18	-6.67	20,20,20,20	0
56	MG	1E	310	1/1	0.82	0.09	-6.70	42,42,42,42	0
56	MG	1A	4062	1/1	0.97	0.12	-6.72	14,14,14,14	0
56	MG	1A	3598	1/1	0.93	0.13	-6.77	51,51,51,51	0
56	MG	2A	3618	1/1	0.98	0.08	-6.78	39,39,39,39	0
56	MG	2A	3848	1/1	0.93	0.10	-6.82	36,36,36,36	0
56	MG	2A	3624	1/1	0.97	0.10	-6.91	32,32,32,32	0
56	MG	1A	3395	1/1	0.83	0.16	-6.93	42,42,42,42	0
56	MG	2A	3855	1/1	0.85	0.11	-7.00	69,69,69,69	0
56	MG	2A	3547	1/1	0.94	0.09	-7.04	37,37,37,37	0
56	MG	1A	4122	1/1	0.95	0.13	-7.11	41,41,41,41	0
56	MG	1A	3033	1/1	0.96	0.17	-7.14	36,36,36,36	0
56	MG	2A	3594	1/1	0.91	0.09	-7.14	38,38,38,38	0
56	MG	1A	3659	1/1	0.96	0.15	-7.23	23,23,23,23	0
56	MG	1a	1771	1/1	0.93	0.08	-7.27	70,70,70,70	0
56	MG	1A	3926	1/1	0.62	0.10	-7.27	53,53,53,53	0
56	MG	2A	3629	1/1	0.87	0.13	-7.32	43,43,43,43	0
56	MG	1a	1817	1/1	0.88	0.04	-7.39	79,79,79,79	0
56	MG	2A	3557	1/1	0.87	0.08	-7.47	45,45,45,45	0
56	MG	1a	1805	1/1	0.95	0.08	-7.48	47,47,47,47	0
56	MG	1A	3630	1/1	0.88	0.17	-7.52	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	1779	1/1	0.81	0.08	-7.54	65,65,65,65	0
56	MG	1A	3881	1/1	0.94	0.19	-7.55	37,37,37,37	0
56	MG	1A	3403	1/1	0.96	0.17	-7.61	27,27,27,27	0
56	MG	1A	3176	1/1	0.96	0.16	-7.63	37,37,37,37	0
56	MG	1A	3202	1/1	0.92	0.15	-7.72	32,32,32,32	0
56	MG	2A	3623	1/1	0.97	0.10	-7.91	48,48,48,48	0
56	MG	1A	4032	1/1	0.94	0.07	-8.00	68,68,68,68	0
56	MG	1a	1655	1/1	0.97	0.07	-8.19	43,43,43,43	0
56	MG	2A	3023	1/1	0.94	0.05	-8.23	48,48,48,48	0
56	MG	1A	4110	1/1	0.93	0.13	-8.24	56,56,56,56	0
56	MG	2a	3182	1/1	0.82	0.09	-8.26	71,71,71,71	0
56	MG	1A	3807	1/1	0.97	0.15	-8.26	38,38,38,38	0
56	MG	1A	3275	1/1	0.96	0.13	-8.31	44,44,44,44	0
56	MG	2A	3188	1/1	0.94	0.07	-8.42	36,36,36,36	0
56	MG	2A	3561	1/1	0.95	0.09	-8.51	62,62,62,62	0
56	MG	2A	3035	1/1	0.96	0.10	-8.61	31,31,31,31	0
56	MG	2A	3844	1/1	0.78	0.08	-8.65	50,50,50,50	0
56	MG	2A	3720	1/1	0.97	0.11	-8.66	41,41,41,41	0
56	MG	1A	3820	1/1	0.96	0.11	-8.67	41,41,41,41	0
56	MG	2A	3648	1/1	0.80	0.08	-8.88	51,51,51,51	0
56	MG	1A	3213	1/1	0.92	0.12	-9.01	42,42,42,42	0
56	MG	2A	3571	1/1	0.90	0.08	-9.04	35,35,35,35	0
56	MG	1A	3930	1/1	0.96	0.15	-9.08	30,30,30,30	0
56	MG	2A	3529	1/1	0.90	0.07	-9.24	43,43,43,43	0
56	MG	2A	3522	1/1	0.95	0.08	-9.26	59,59,59,59	0
56	MG	1A	3784	1/1	0.91	0.10	-9.28	39,39,39,39	0
56	MG	2A	3587	1/1	0.95	0.11	-9.32	37,37,37,37	0
56	MG	1A	3948	1/1	0.84	0.12	-9.56	60,60,60,60	0
56	MG	1a	1818	1/1	0.90	0.08	-9.74	54,54,54,54	0
56	MG	1A	3738	1/1	0.94	0.12	-9.98	43,43,43,43	0
56	MG	1a	1619	1/1	0.98	0.13	-10.01	62,62,62,62	0
56	MG	1A	3661	1/1	0.91	0.13	-10.15	32,32,32,32	0
56	MG	1A	4055	1/1	0.94	0.09	-10.28	33,33,33,33	0
56	MG	2A	3500	1/1	0.87	0.10	-10.53	55,55,55,55	0
56	MG	1A	3789	1/1	0.98	0.11	-10.67	29,29,29,29	0
56	MG	1A	3597	1/1	0.94	0.18	-10.91	50,50,50,50	0
56	MG	1a	1709	1/1	0.80	0.07	-10.94	59,59,59,59	0
56	MG	2a	3222	1/1	0.92	0.09	-11.11	63,63,63,63	0
56	MG	1a	1741	1/1	0.95	0.08	-11.27	34,34,34,34	0
56	MG	2A	3504	1/1	0.95	0.09	-11.50	36,36,36,36	0
56	MG	1A	3906	1/1	0.89	0.12	-11.74	51,51,51,51	0
56	MG	1A	3594	1/1	0.93	0.13	-11.80	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3669	1/1	0.93	0.10	-11.94	34,34,34,34	0
56	MG	1A	3007	1/1	0.92	0.14	-12.00	38,38,38,38	0
56	MG	1A	3947	1/1	0.81	0.12	-12.26	44,44,44,44	0
56	MG	1A	3914	1/1	0.98	0.10	-12.46	53,53,53,53	0
56	MG	1a	1758	1/1	0.97	0.06	-12.51	56,56,56,56	0
56	MG	2A	3521	1/1	0.93	0.11	-12.58	51,51,51,51	0
56	MG	1A	3577	1/1	0.99	0.17	-13.30	27,27,27,27	0
56	MG	1A	4013	1/1	0.96	0.13	-15.40	33,33,33,33	0
56	MG	1A	3882	1/1	0.96	0.17	-15.40	36,36,36,36	0
56	MG	1A	3938	1/1	0.94	0.08	-16.03	55,55,55,55	0
56	MG	1A	4063	1/1	0.95	0.08	-17.29	57,57,57,57	0
56	MG	1A	3939	1/1	0.91	0.14	-17.95	53,53,53,53	0
56	MG	1A	4011	1/1	0.93	0.10	-18.74	43,43,43,43	0
56	MG	1A	3621	1/1	0.97	0.11	-19.16	48,48,48,48	0
56	MG	1A	3635	1/1	0.98	0.11	-19.87	32,32,32,32	0
56	MG	2A	3792	1/1	0.86	0.10	-	51,51,51,51	0
56	MG	1A	3318	1/1	0.90	0.12	-	46,46,46,46	0
56	MG	1A	3315	1/1	0.90	0.35	-	61,61,61,61	0
56	MG	1A	3002	1/1	0.82	0.24	-	59,59,59,59	0
56	MG	2A	3312	1/1	0.93	0.12	-	51,51,51,51	0
56	MG	1A	4042	1/1	0.90	0.10	-	46,46,46,46	0
56	MG	2a	3155	1/1	0.64	0.12	-	81,81,81,81	0
56	MG	1A	3545	1/1	0.88	0.16	-	67,67,67,67	0
56	MG	1A	3636	1/1	0.96	0.07	-	38,38,38,38	0
56	MG	1A	3722	1/1	0.85	0.12	-	39,39,39,39	0
56	MG	1A	3821	1/1	0.91	0.16	-	47,47,47,47	0
56	MG	2A	3711	1/1	0.95	0.17	-	56,56,56,56	0
56	MG	1A	3273	1/1	0.92	0.28	-	53,53,53,53	0
56	MG	2A	3370	1/1	0.90	0.23	-	50,50,50,50	0
56	MG	2A	3465	1/1	0.88	0.22	-	55,55,55,55	0
56	MG	1A	3014	1/1	0.97	0.20	-	31,31,31,31	0
56	MG	2A	3443	1/1	0.98	0.28	-	50,50,50,50	0
56	MG	2A	3251	1/1	0.95	0.10	-	42,42,42,42	0
56	MG	1a	1660	1/1	0.91	0.12	-	74,74,74,74	0
56	MG	2A	3657	1/1	0.95	0.13	-	39,39,39,39	0
56	MG	2A	3760	1/1	0.97	0.56	-	58,58,58,58	0
56	MG	1a	1672	1/1	0.65	0.17	-	73,73,73,73	0
56	MG	1A	3695	1/1	0.94	0.09	-	57,57,57,57	0
56	MG	2A	3492	1/1	0.90	0.17	-	54,54,54,54	0
56	MG	2A	3746	1/1	0.86	0.08	-	68,68,68,68	0
56	MG	1V	202	1/1	0.92	0.15	-	53,53,53,53	0
56	MG	2a	3153	1/1	0.79	0.17	-	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3036	1/1	0.94	0.19	-	31,31,31,31	0
56	MG	2A	3428	1/1	0.94	0.15	-	52,52,52,52	0
56	MG	1A	3955	1/1	0.95	0.14	-	30,30,30,30	0
56	MG	2A	3419	1/1	0.88	0.14	-	51,51,51,51	0
56	MG	2a	3017	1/1	0.86	0.09	-	66,66,66,66	0
56	MG	2a	3234	1/1	0.82	0.13	-	66,66,66,66	0
56	MG	1A	3877	1/1	0.93	0.15	-	39,39,39,39	0
56	MG	1a	1744	1/1	0.80	0.25	-	73,73,73,73	0
56	MG	1G	3002	1/1	0.89	0.17	-	56,56,56,56	0
56	MG	2D	302	1/1	0.90	0.16	-	51,51,51,51	0
56	MG	1A	3263	1/1	0.96	0.18	-	52,52,52,52	0
56	MG	2a	3049	1/1	0.90	0.12	-	55,55,55,55	0
56	MG	1A	3797	1/1	0.95	0.14	-	53,53,53,53	0
56	MG	2a	3028	1/1	0.38	0.23	-	84,84,84,84	0
56	MG	1A	3805	1/1	0.93	0.23	-	54,54,54,54	0
56	MG	2A	3214	1/1	0.96	0.11	-	56,56,56,56	0
56	MG	2A	3420	1/1	0.95	0.37	-	43,43,43,43	0
56	MG	1a	1774	1/1	0.95	0.11	-	60,60,60,60	0
56	MG	1A	3415	1/1	0.94	0.30	-	59,59,59,59	0
56	MG	2A	3206	1/1	0.97	0.17	-	56,56,56,56	0
56	MG	2A	3089	1/1	0.90	0.12	-	46,46,46,46	0
56	MG	2A	3153	1/1	0.89	0.20	-	52,52,52,52	0
56	MG	1A	3107	1/1	0.97	0.18	-	35,35,35,35	0
56	MG	2B	3014	1/1	0.79	0.17	-	77,77,77,77	0
56	MG	2A	3185	1/1	0.94	0.08	-	45,45,45,45	0
56	MG	1a	1807	1/1	0.90	0.06	-	67,67,67,67	0
56	MG	2A	3437	1/1	0.93	0.13	-	67,67,67,67	0
56	MG	1A	3101	1/1	0.92	0.12	-	44,44,44,44	0
56	MG	1a	1761	1/1	0.91	0.11	-	64,64,64,64	0
56	MG	2A	3481	1/1	0.91	0.20	-	56,56,56,56	0
56	MG	2q	201	1/1	0.85	0.17	-	76,76,76,76	0
56	MG	2A	3520	1/1	0.77	0.11	-	65,65,65,65	0
56	MG	2a	3131	1/1	0.69	0.11	-	80,80,80,80	0
56	MG	1A	3412	1/1	0.96	0.21	-	52,52,52,52	0
56	MG	1A	3437	1/1	0.87	0.15	-	52,52,52,52	0
56	MG	2A	3325	1/1	0.91	0.10	-	63,63,63,63	0
56	MG	1A	3350	1/1	0.88	0.25	-	59,59,59,59	0
56	MG	1A	3242	1/1	0.85	0.24	-	43,43,43,43	0
56	MG	1a	1632	1/1	0.95	0.18	-	52,52,52,52	0
56	MG	2A	3721	1/1	0.95	0.18	-	46,46,46,46	0
56	MG	2A	3688	1/1	0.93	0.09	-	38,38,38,38	0
56	MG	2a	3147	1/1	0.97	0.13	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	1765	1/1	0.93	0.11	-	49,49,49,49	0
56	MG	1A	3916	1/1	0.91	0.14	-	53,53,53,53	0
56	MG	2A	3183	1/1	0.93	0.17	-	56,56,56,56	0
56	MG	1A	3991	1/1	0.91	0.10	-	48,48,48,48	0
56	MG	2a	3202	1/1	0.90	0.17	-	64,64,64,64	0
56	MG	1A	3147	1/1	0.82	0.28	-	54,54,54,54	0
56	MG	2A	3172	1/1	0.94	0.09	-	47,47,47,47	0
56	MG	2B	3013	1/1	0.89	0.20	-	61,61,61,61	0
56	MG	1A	3459	1/1	0.86	0.23	-	47,47,47,47	0
56	MG	2A	3389	1/1	0.94	0.11	-	58,58,58,58	0
56	MG	2A	3362	1/1	0.85	0.12	-	68,68,68,68	0
56	MG	1A	3637	1/1	0.89	0.19	-	50,50,50,50	0
56	MG	2A	3580	1/1	0.94	0.23	-	49,49,49,49	0
56	MG	2A	3079	1/1	0.88	0.11	-	41,41,41,41	0
56	MG	1A	3874	1/1	0.89	0.12	-	40,40,40,40	0
56	MG	2w	102	1/1	0.88	0.17	-	62,62,62,62	0
56	MG	2A	3590	1/1	0.89	0.08	-	64,64,64,64	0
56	MG	1A	3030	1/1	0.98	0.18	-	34,34,34,34	0
56	MG	1a	1673	1/1	0.94	0.13	-	67,67,67,67	0
56	MG	1A	3849	1/1	0.96	0.26	-	44,44,44,44	0
56	MG	1A	4089	1/1	0.97	0.15	-	36,36,36,36	0
56	MG	1B	3001	1/1	0.98	0.30	-	48,48,48,48	0
56	MG	1A	3436	1/1	0.90	0.14	-	45,45,45,45	0
56	MG	2A	3044	1/1	0.92	0.10	-	48,48,48,48	0
56	MG	1B	3003	1/1	0.92	0.23	-	56,56,56,56	0
56	MG	1a	1728	1/1	0.91	0.24	-	48,48,48,48	0
56	MG	1A	3952	1/1	0.96	0.18	-	46,46,46,46	0
56	MG	1A	3501	1/1	0.90	0.25	-	51,51,51,51	0
56	MG	2A	3377	1/1	0.98	0.15	-	57,57,57,57	0
56	MG	2a	3050	1/1	0.89	0.20	-	61,61,61,61	0
56	MG	2A	3723	1/1	0.88	0.10	-	50,50,50,50	0
56	MG	1A	3672	1/1	0.91	0.16	-	31,31,31,31	0
56	MG	2B	3011	1/1	0.96	0.31	-	67,67,67,67	0
56	MG	1A	3733	1/1	0.92	0.12	-	52,52,52,52	0
56	MG	25	101	1/1	0.94	0.15	-	55,55,55,55	0
56	MG	2a	3107	1/1	0.94	0.14	-	57,57,57,57	0
56	MG	1A	3927	1/1	0.94	0.10	-	47,47,47,47	0
56	MG	1A	3727	1/1	0.91	0.15	-	36,36,36,36	0
56	MG	2a	3139	1/1	0.94	0.11	-	73,73,73,73	0
56	MG	2A	3533	1/1	0.99	0.12	-	48,48,48,48	0
56	MG	1O	207	1/1	0.77	0.12	-	65,65,65,65	0
56	MG	1A	3418	1/1	0.86	0.11	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3532	1/1	0.94	0.14	-	65,65,65,65	0
56	MG	2a	3193	1/1	0.93	0.12	-	73,73,73,73	0
56	MG	1A	3610	1/1	0.95	0.23	-	54,54,54,54	0
56	MG	1A	3541	1/1	0.85	0.13	-	73,73,73,73	0
56	MG	1x	110	1/1	0.87	0.14	-	52,52,52,52	0
56	MG	1A	3681	1/1	0.96	0.07	-	34,34,34,34	0
56	MG	1a	1658	1/1	0.96	0.13	-	57,57,57,57	0
56	MG	1A	3933	1/1	0.78	0.10	-	47,47,47,47	0
56	MG	2A	3339	1/1	0.94	0.20	-	51,51,51,51	0
56	MG	1A	3602	1/1	0.97	0.25	-	25,25,25,25	0
56	MG	1A	4075	1/1	0.92	0.13	-	42,42,42,42	0
56	MG	2B	3004	1/1	0.89	0.13	-	69,69,69,69	0
56	MG	2A	3416	1/1	0.92	0.15	-	59,59,59,59	0
56	MG	1a	1628	1/1	0.87	0.11	-	58,58,58,58	0
56	MG	1A	3152	1/1	0.84	0.21	-	55,55,55,55	0
56	MG	1A	3126	1/1	0.97	0.20	-	41,41,41,41	0
56	MG	1A	3287	1/1	0.95	0.18	-	30,30,30,30	0
56	MG	2A	3287	1/1	0.91	0.09	-	55,55,55,55	0
56	MG	1A	3139	1/1	0.96	0.14	-	48,48,48,48	0
56	MG	1a	1639	1/1	0.89	0.10	-	62,62,62,62	0
56	MG	1A	3519	1/1	0.90	0.16	-	49,49,49,49	0
56	MG	2A	3036	1/1	0.94	0.14	-	54,54,54,54	0
56	MG	1A	3276	1/1	0.98	0.14	-	49,49,49,49	0
56	MG	1A	3264	1/1	0.66	0.18	-	63,63,63,63	0
56	MG	2P	201	1/1	0.94	0.13	-	45,45,45,45	0
56	MG	1A	3326	1/1	0.86	0.18	-	41,41,41,41	0
56	MG	1A	3265	1/1	0.97	0.10	-	63,63,63,63	0
56	MG	2A	3332	1/1	0.77	0.34	-	62,62,62,62	0
56	MG	1E	305	1/1	0.93	0.22	-	57,57,57,57	0
56	MG	2a	3079	1/1	0.96	0.11	-	59,59,59,59	0
56	MG	1a	1625	1/1	0.81	0.26	-	63,63,63,63	0
56	MG	1A	4083	1/1	0.94	0.15	-	44,44,44,44	0
56	MG	1A	3831	1/1	0.95	0.15	-	70,70,70,70	0
56	MG	1a	1756	1/1	0.97	0.14	-	72,72,72,72	0
56	MG	2A	3279	1/1	0.96	0.28	-	53,53,53,53	0
56	MG	1A	3999	1/1	0.86	0.20	-	55,55,55,55	0
56	MG	2A	3290	1/1	0.90	0.19	-	50,50,50,50	0
56	MG	1A	3951	1/1	0.89	0.20	-	72,72,72,72	0
56	MG	1A	3051	1/1	0.93	0.28	-	50,50,50,50	0
56	MG	2A	3038	1/1	0.97	0.16	-	31,31,31,31	0
56	MG	1A	3225	1/1	0.94	0.22	-	52,52,52,52	0
56	MG	1A	3170	1/1	0.94	0.15	-	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	3146	1/1	0.73	0.32	-	84,84,84,84	0
56	MG	2A	3062	1/1	0.95	0.20	-	61,61,61,61	0
56	MG	1A	3698	1/1	0.61	0.11	-	73,73,73,73	0
56	MG	1A	3890	1/1	0.90	0.16	-	57,57,57,57	0
56	MG	2A	3880	1/1	0.80	0.13	-	65,65,65,65	0
56	MG	1A	3278	1/1	0.93	0.20	-	51,51,51,51	0
56	MG	2A	3652	1/1	0.94	0.12	-	41,41,41,41	0
56	MG	1A	3037	1/1	0.95	0.42	-	40,40,40,40	0
56	MG	2A	3359	1/1	0.95	0.05	-	56,56,56,56	0
56	MG	2A	3769	1/1	0.76	0.10	-	62,62,62,62	0
56	MG	2A	3559	1/1	0.95	0.14	-	39,39,39,39	0
56	MG	2A	3508	1/1	0.95	0.10	-	60,60,60,60	0
56	MG	2A	3433	1/1	0.87	0.13	-	64,64,64,64	0
56	MG	2a	3212	1/1	0.99	0.12	-	51,51,51,51	0
56	MG	1A	3941	1/1	0.92	0.15	-	46,46,46,46	0
56	MG	1A	3083	1/1	0.85	0.26	-	44,44,44,44	0
56	MG	1a	1769	1/1	0.93	0.11	-	55,55,55,55	0
56	MG	1A	3791	1/1	0.93	0.17	-	43,43,43,43	0
56	MG	2A	3193	1/1	0.95	0.06	-	55,55,55,55	0
56	MG	2A	3892	1/1	0.48	0.31	-	78,78,78,78	0
56	MG	1w	101	1/1	0.88	0.14	-	64,64,64,64	0
56	MG	1A	3900	1/1	0.84	0.19	-	44,44,44,44	0
56	MG	2A	3213	1/1	0.95	0.23	-	45,45,45,45	0
56	MG	1a	1707	1/1	0.91	0.14	-	63,63,63,63	0
56	MG	1y	3001	1/1	0.88	0.09	-	64,64,64,64	0
56	MG	1e	201	1/1	0.80	0.12	-	79,79,79,79	0
56	MG	1A	3888	1/1	0.86	0.24	-	70,70,70,70	0
56	MG	2A	3874	1/1	0.88	0.17	-	53,53,53,53	0
56	MG	2w	101	1/1	0.86	0.20	-	73,73,73,73	0
56	MG	1A	3471	1/1	0.96	0.18	-	57,57,57,57	0
56	MG	1A	3965	1/1	0.98	0.14	-	67,67,67,67	0
56	MG	1A	3931	1/1	0.90	0.17	-	55,55,55,55	0
56	MG	2A	3426	1/1	0.88	0.23	-	63,63,63,63	0
56	MG	2a	3130	1/1	0.89	0.08	-	72,72,72,72	0
56	MG	1l	103	1/1	0.93	0.09	-	65,65,65,65	0
56	MG	1A	3754	1/1	0.88	0.20	-	48,48,48,48	0
56	MG	1A	3029	1/1	0.95	0.24	-	38,38,38,38	0
56	MG	1A	3966	1/1	0.91	0.20	-	59,59,59,59	0
56	MG	1A	4084	1/1	0.75	0.12	-	50,50,50,50	0
56	MG	1A	4123	1/1	0.95	0.22	-	35,35,35,35	0
56	MG	2A	3136	1/1	0.93	0.18	-	45,45,45,45	0
56	MG	2A	3180	1/1	0.79	0.19	-	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3981	1/1	0.91	0.09	-	52,52,52,52	0
56	MG	1A	3281	1/1	0.85	0.26	-	50,50,50,50	0
56	MG	2a	3204	1/1	0.67	0.44	-	86,86,86,86	0
56	MG	1a	1767	1/1	0.93	0.12	-	66,66,66,66	0
56	MG	2A	3458	1/1	0.87	0.11	-	65,65,65,65	0
56	MG	1A	3516	1/1	0.96	0.11	-	25,25,25,25	0
56	MG	1A	3292	1/1	0.96	0.17	-	56,56,56,56	0
56	MG	2A	3804	1/1	0.96	0.06	-	31,31,31,31	0
56	MG	2A	3479	1/1	0.89	0.17	-	54,54,54,54	0
56	MG	1A	4037	1/1	0.68	0.12	-	62,62,62,62	0
56	MG	1A	3896	1/1	0.94	0.22	-	47,47,47,47	0
56	MG	2A	3607	1/1	0.72	0.18	-	55,55,55,55	0
56	MG	1A	3956	1/1	0.83	0.17	-	61,61,61,61	0
56	MG	1A	3488	1/1	0.88	0.30	-	59,59,59,59	0
56	MG	2A	3585	1/1	0.96	0.10	-	43,43,43,43	0
56	MG	1A	3525	1/1	0.90	0.18	-	58,58,58,58	0
56	MG	2A	3005	1/1	0.91	0.22	-	48,48,48,48	0
56	MG	2A	3055	1/1	0.92	0.15	-	46,46,46,46	0
56	MG	1A	3011	1/1	0.98	0.13	-	46,46,46,46	0
56	MG	2A	3518	1/1	0.86	0.09	-	52,52,52,52	0
56	MG	1A	3494	1/1	0.96	0.21	-	39,39,39,39	0
56	MG	2A	3490	1/1	0.83	0.14	-	61,61,61,61	0
56	MG	1A	3555	1/1	0.66	0.26	-	60,60,60,60	0
56	MG	1A	3915	1/1	0.91	0.14	-	39,39,39,39	0
56	MG	1x	115	1/1	0.92	0.15	-	75,75,75,75	0
56	MG	1A	3496	1/1	0.95	0.16	-	38,38,38,38	0
56	MG	2A	3381	1/1	0.88	0.13	-	53,53,53,53	0
56	MG	2A	3265	1/1	0.81	0.17	-	59,59,59,59	0
56	MG	2A	3699	1/1	0.84	0.09	-	76,76,76,76	0
56	MG	1a	1692	1/1	0.91	0.09	-	69,69,69,69	0
56	MG	1a	1662	1/1	0.94	0.12	-	67,67,67,67	0
56	MG	1a	1650	1/1	0.90	0.12	-	53,53,53,53	0
56	MG	2A	3597	1/1	0.92	0.16	-	61,61,61,61	0
56	MG	2A	3762	1/1	0.93	0.09	-	52,52,52,52	0
56	MG	1a	1717	1/1	0.95	0.16	-	64,64,64,64	0
56	MG	2a	3032	1/1	0.96	0.10	-	60,60,60,60	0
56	MG	2A	3527	1/1	0.93	0.12	-	31,31,31,31	0
56	MG	1A	3343	1/1	0.86	0.34	-	59,59,59,59	0
56	MG	1A	3836	1/1	0.91	0.23	-	54,54,54,54	0
56	MG	1A	3891	1/1	0.93	0.18	-	41,41,41,41	0
56	MG	1A	4105	1/1	0.87	0.13	-	44,44,44,44	0
56	MG	2A	3117	1/1	0.88	0.28	-	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	3177	1/1	0.93	0.07	-	67,67,67,67	0
56	MG	2A	3743	1/1	0.96	0.16	-	75,75,75,75	0
56	MG	1A	3817	1/1	0.96	0.19	-	45,45,45,45	0
56	MG	1a	1651	1/1	0.82	0.11	-	56,56,56,56	0
56	MG	1A	3913	1/1	0.78	0.24	-	80,80,80,80	0
56	MG	2A	3203	1/1	0.92	0.22	-	46,46,46,46	0
56	MG	2E	306	1/1	0.84	0.09	-	67,67,67,67	0
56	MG	2a	3044	1/1	0.96	0.19	-	57,57,57,57	0
56	MG	2A	3610	1/1	0.51	0.14	-	67,67,67,67	0
56	MG	1A	3158	1/1	0.93	0.19	-	56,56,56,56	0
56	MG	1A	3167	1/1	0.94	0.15	-	41,41,41,41	0
56	MG	1A	3699	1/1	0.85	0.25	-	64,64,64,64	0
56	MG	1A	3288	1/1	0.92	0.12	-	43,43,43,43	0
56	MG	2A	3408	1/1	0.90	0.10	-	51,51,51,51	0
56	MG	2A	3128	1/1	0.94	0.19	-	48,48,48,48	0
56	MG	1a	1612	1/1	0.76	0.09	-	74,74,74,74	0
56	MG	2A	3173	1/1	0.95	0.09	-	51,51,51,51	0
56	MG	1A	3627	1/1	0.84	0.13	-	62,62,62,62	0
56	MG	2a	3210	1/1	0.83	0.10	-	70,70,70,70	0
56	MG	1A	4043	1/1	0.85	0.10	-	50,50,50,50	0
56	MG	2a	3136	1/1	0.91	0.28	-	73,73,73,73	0
56	MG	1B	3034	1/1	0.91	0.19	-	58,58,58,58	0
56	MG	1A	3997	1/1	0.89	0.14	-	39,39,39,39	0
56	MG	1y	3002	1/1	0.91	0.16	-	75,75,75,75	0
56	MG	1W	202	1/1	0.96	0.24	-	50,50,50,50	0
56	MG	1A	4033	1/1	0.83	0.10	-	76,76,76,76	0
56	MG	1a	1691	1/1	0.90	0.21	-	69,69,69,69	0
56	MG	1T	8001	1/1	0.88	0.10	-	63,63,63,63	0
56	MG	2A	3707	1/1	0.87	0.06	-	61,61,61,61	0
56	MG	1a	1792	1/1	0.95	0.05	-	59,59,59,59	0
56	MG	1a	1777	1/1	0.90	0.16	-	55,55,55,55	0
56	MG	2A	3210	1/1	0.91	0.14	-	47,47,47,47	0
57	K	2A	3496	1/1	0.93	0.09	-	73,73,73,73	0
56	MG	1A	3638	1/1	0.95	0.06	-	53,53,53,53	0
56	MG	2A	3253	1/1	0.89	0.12	-	47,47,47,47	0
56	MG	1A	3236	1/1	0.93	0.35	-	37,37,37,37	0
56	MG	1A	3466	1/1	0.83	0.15	-	64,64,64,64	0
56	MG	1A	3053	1/1	0.94	0.17	-	52,52,52,52	0
56	MG	1A	3065	1/1	0.94	0.22	-	33,33,33,33	0
56	MG	2A	3090	1/1	0.93	0.07	-	60,60,60,60	0
56	MG	1A	3062	1/1	0.95	0.23	-	59,59,59,59	0
56	MG	2A	3853	1/1	0.94	0.12	-	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	1790	1/1	0.65	0.20	-	73,73,73,73	0
56	MG	2A	3554	1/1	0.97	0.10	-	39,39,39,39	0
56	MG	2A	3823	1/1	0.84	0.15	-	73,73,73,73	0
56	MG	1A	3378	1/1	0.78	0.14	-	53,53,53,53	0
56	MG	2A	3651	1/1	0.92	0.14	-	44,44,44,44	0
56	MG	2a	3216	1/1	0.98	0.12	-	65,65,65,65	0
56	MG	1A	3703	1/1	0.89	0.11	-	56,56,56,56	0
56	MG	2a	3099	1/1	0.76	0.14	-	74,74,74,74	0
56	MG	1A	3647	1/1	0.92	0.22	-	29,29,29,29	0
56	MG	1A	3912	1/1	0.49	0.30	-	80,80,80,80	0
56	MG	2r	102	1/1	0.88	0.10	-	73,73,73,73	0
56	MG	1A	3548	1/1	0.87	0.12	-	49,49,49,49	0
56	MG	2A	3280	1/1	0.92	0.17	-	54,54,54,54	0
56	MG	2A	3401	1/1	0.96	0.16	-	52,52,52,52	0
56	MG	1A	3121	1/1	0.97	0.20	-	43,43,43,43	0
56	MG	1A	4015	1/1	0.97	0.14	-	37,37,37,37	0
56	MG	1a	1718	1/1	0.85	0.11	-	70,70,70,70	0
56	MG	2A	3868	1/1	0.63	0.16	-	69,69,69,69	0
56	MG	1W	204	1/1	0.92	0.14	-	40,40,40,40	0
56	MG	1A	3934	1/1	0.74	0.11	-	44,44,44,44	0
56	MG	1a	1799	1/1	0.95	0.08	-	49,49,49,49	0
56	MG	2a	3027	1/1	0.87	0.18	-	61,61,61,61	0
56	MG	1x	109	1/1	0.93	0.10	-	82,82,82,82	0
56	MG	1A	3082	1/1	0.95	0.27	-	49,49,49,49	0
56	MG	1A	3150	1/1	0.96	0.22	-	50,50,50,50	0
56	MG	1A	4028	1/1	0.92	0.12	-	69,69,69,69	0
56	MG	1A	3801	1/1	0.94	0.17	-	28,28,28,28	0
56	MG	2A	3772	1/1	0.93	0.14	-	53,53,53,53	0
56	MG	1A	3593	1/1	0.97	0.18	-	56,56,56,56	0
56	MG	2A	3166	1/1	0.96	0.29	-	47,47,47,47	0
56	MG	2A	3578	1/1	0.98	0.09	-	39,39,39,39	0
56	MG	1a	1816	1/1	0.98	0.13	-	48,48,48,48	0
56	MG	2A	3861	1/1	0.91	0.13	-	36,36,36,36	0
56	MG	1N	206	1/1	0.97	0.29	-	42,42,42,42	0
56	MG	2a	3143	1/1	0.82	0.07	-	73,73,73,73	0
56	MG	2a	3167	1/1	0.96	0.09	-	69,69,69,69	0
56	MG	1a	1746	1/1	0.85	0.08	-	84,84,84,84	0
56	MG	1a	1768	1/1	0.97	0.06	-	53,53,53,53	0
56	MG	2F	302	1/1	0.89	0.16	-	53,53,53,53	0
56	MG	1A	3851	1/1	0.86	0.14	-	62,62,62,62	0
56	MG	1A	3829	1/1	0.85	0.13	-	59,59,59,59	0
56	MG	1A	4060	1/1	0.87	0.10	-	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	1645	1/1	0.83	0.22	-	80,80,80,80	0
56	MG	1a	1794	1/1	0.87	0.14	-	52,52,52,52	0
56	MG	2A	3031	1/1	0.96	0.06	-	45,45,45,45	0
56	MG	2A	3818	1/1	0.75	0.31	-	66,66,66,66	0
56	MG	1A	4066	1/1	0.88	0.11	-	71,71,71,71	0
56	MG	1A	3692	1/1	0.83	0.29	-	64,64,64,64	0
56	MG	1A	3413	1/1	0.98	0.21	-	36,36,36,36	0
56	MG	1x	108	1/1	0.92	0.15	-	63,63,63,63	0
56	MG	2A	3134	1/1	0.78	0.26	-	72,72,72,72	0
56	MG	1A	3026	1/1	0.84	0.10	-	60,60,60,60	0
56	MG	2A	3110	1/1	0.85	0.16	-	58,58,58,58	0
56	MG	2A	3159	1/1	0.96	0.16	-	53,53,53,53	0
56	MG	1A	3417	1/1	0.81	0.17	-	51,51,51,51	0
56	MG	1A	3994	1/1	0.56	0.33	-	76,76,76,76	0
56	MG	2a	3170	1/1	0.86	0.10	-	80,80,80,80	0
56	MG	2A	3771	1/1	0.92	0.13	-	39,39,39,39	0
56	MG	2A	3186	1/1	0.91	0.14	-	54,54,54,54	0
56	MG	1x	101	1/1	0.59	0.09	-	56,56,56,56	0
56	MG	1A	3507	1/1	0.83	0.21	-	51,51,51,51	0
56	MG	2a	3069	1/1	0.85	0.10	-	62,62,62,62	0
56	MG	1a	1803	1/1	0.76	0.22	-	73,73,73,73	0
56	MG	1a	1780	1/1	0.90	0.11	-	74,74,74,74	0
56	MG	1V	201	1/1	0.96	0.25	-	49,49,49,49	0
56	MG	1A	4006	1/1	0.83	0.11	-	76,76,76,76	0
56	MG	1a	1804	1/1	0.89	0.17	-	77,77,77,77	0
56	MG	2A	3511	1/1	0.97	0.17	-	24,24,24,24	0
56	MG	1A	4126	1/1	0.98	0.18	-	45,45,45,45	0
56	MG	1A	3089	1/1	0.90	0.26	-	48,48,48,48	0
56	MG	10	102	1/1	0.94	0.12	-	44,44,44,44	0
56	MG	2A	3738	1/1	0.86	0.19	-	59,59,59,59	0
56	MG	2a	3191	1/1	0.93	0.15	-	63,63,63,63	0
56	MG	1A	3908	1/1	0.96	0.09	-	65,65,65,65	0
56	MG	2A	3535	1/1	0.70	0.17	-	59,59,59,59	0
56	MG	2A	3789	1/1	0.88	0.10	-	49,49,49,49	0
56	MG	1A	3451	1/1	0.87	0.16	-	47,47,47,47	0
56	MG	1A	4053	1/1	0.91	0.37	-	37,37,37,37	0
56	MG	2A	3066	1/1	0.92	0.10	-	41,41,41,41	0
56	MG	1a	1684	1/1	0.90	0.14	-	60,60,60,60	0
56	MG	1a	1802	1/1	0.97	0.07	-	52,52,52,52	0
56	MG	1A	3419	1/1	0.90	0.15	-	60,60,60,60	0
56	MG	2A	3807	1/1	0.92	0.07	-	61,61,61,61	0
56	MG	1A	3059	1/1	0.95	0.15	-	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	4138	1/1	0.97	0.26	-	43,43,43,43	0
56	MG	1A	3705	1/1	0.91	0.09	-	42,42,42,42	0
56	MG	2A	3575	1/1	0.94	0.11	-	39,39,39,39	0
56	MG	1A	3388	1/1	0.96	0.20	-	42,42,42,42	0
56	MG	1A	3254	1/1	0.96	0.22	-	53,53,53,53	0
56	MG	1A	3725	1/1	0.95	0.14	-	52,52,52,52	0
56	MG	2A	3675	1/1	0.92	0.17	-	55,55,55,55	0
56	MG	2a	3031	1/1	0.94	0.19	-	49,49,49,49	0
56	MG	1U	208	1/1	0.94	0.23	-	38,38,38,38	0
56	MG	2A	3706	1/1	0.98	0.12	-	47,47,47,47	0
56	MG	1A	3060	1/1	0.92	0.10	-	45,45,45,45	0
56	MG	1A	4041	1/1	0.93	0.14	-	36,36,36,36	0
56	MG	2A	3179	1/1	0.97	0.17	-	59,59,59,59	0
56	MG	2A	3608	1/1	0.80	0.09	-	61,61,61,61	0
56	MG	2A	3334	1/1	0.95	0.08	-	64,64,64,64	0
56	MG	1w	110	1/1	0.90	0.11	-	66,66,66,66	0
56	MG	2A	3348	1/1	0.94	0.20	-	48,48,48,48	0
56	MG	1A	3539	1/1	0.89	0.16	-	49,49,49,49	0
56	MG	2x	105	1/1	0.97	0.15	-	57,57,57,57	0
56	MG	1A	3530	1/1	0.86	0.21	-	63,63,63,63	0
56	MG	1A	3145	1/1	0.92	0.23	-	32,32,32,32	0
56	MG	1A	3678	1/1	0.94	0.12	-	61,61,61,61	0
56	MG	1B	3024	1/1	0.77	0.10	-	50,50,50,50	0
56	MG	2A	3716	1/1	0.72	0.63	-	55,55,55,55	0
56	MG	2a	3168	1/1	0.51	0.10	-	78,78,78,78	0
56	MG	1x	105	1/1	0.91	0.11	-	62,62,62,62	0
56	MG	2a	3169	1/1	0.97	0.08	-	51,51,51,51	0
56	MG	2A	3730	1/1	0.91	0.18	-	43,43,43,43	0
56	MG	1a	1687	1/1	0.91	0.18	-	50,50,50,50	0
56	MG	2a	3043	1/1	0.97	0.08	-	64,64,64,64	0
56	MG	2A	3526	1/1	0.86	0.09	-	41,41,41,41	0
56	MG	1O	204	1/1	0.75	0.12	-	58,58,58,58	0
56	MG	1O	205	1/1	0.96	0.08	-	44,44,44,44	0
56	MG	2A	3111	1/1	0.88	0.16	-	54,54,54,54	0
56	MG	2A	3540	1/1	0.61	0.13	-	47,47,47,47	0
56	MG	19	102	1/1	0.76	0.21	-	51,51,51,51	0
56	MG	1A	3219	1/1	0.93	0.16	-	37,37,37,37	0
56	MG	1B	3028	1/1	0.94	0.08	-	61,61,61,61	0
56	MG	2A	3295	1/1	0.81	0.14	-	63,63,63,63	0
56	MG	2a	3095	1/1	0.94	0.11	-	71,71,71,71	0
56	MG	1A	3039	1/1	0.98	0.17	-	36,36,36,36	0
56	MG	2A	3584	1/1	0.96	0.24	-	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	4004	1/1	0.96	0.15	-	29,29,29,29	0
56	MG	2A	3054	1/1	0.93	0.19	-	54,54,54,54	0
56	MG	1A	3498	1/1	0.94	0.14	-	46,46,46,46	0
56	MG	1A	3950	1/1	0.92	0.09	-	41,41,41,41	0
56	MG	2O	8001	1/1	0.75	0.10	-	65,65,65,65	0
56	MG	1A	3075	1/1	0.90	0.11	-	28,28,28,28	0
56	MG	2A	3627	1/1	0.85	0.17	-	50,50,50,50	0
56	MG	2A	3843	1/1	0.81	0.17	-	58,58,58,58	0
56	MG	2W	202	1/1	0.78	0.22	-	58,58,58,58	0
56	MG	1I	202	1/1	0.86	0.13	-	69,69,69,69	0
56	MG	2a	3040	1/1	0.79	0.09	-	57,57,57,57	0
56	MG	1A	3173	1/1	0.97	0.17	-	42,42,42,42	0
56	MG	2A	3817	1/1	0.92	0.08	-	56,56,56,56	0
56	MG	1A	3478	1/1	0.88	0.23	-	65,65,65,65	0
56	MG	2a	3144	1/1	0.79	0.08	-	83,83,83,83	0
56	MG	1A	3808	1/1	0.89	0.16	-	36,36,36,36	0
56	MG	1A	3411	1/1	0.99	0.18	-	43,43,43,43	0
56	MG	2A	3800	1/1	0.95	0.08	-	67,67,67,67	0
56	MG	1O	206	1/1	0.87	0.24	-	84,84,84,84	0
56	MG	1a	1810	1/1	0.97	0.07	-	51,51,51,51	0
56	MG	1A	3269	1/1	0.95	0.12	-	52,52,52,52	0
56	MG	1A	3925	1/1	0.97	0.17	-	14,14,14,14	0
56	MG	1A	3426	1/1	0.96	0.14	-	50,50,50,50	0
56	MG	1A	3476	1/1	0.93	0.16	-	52,52,52,52	0
56	MG	2A	3281	1/1	0.93	0.16	-	63,63,63,63	0
56	MG	1A	3833	1/1	0.89	0.09	-	60,60,60,60	0
56	MG	1A	4027	1/1	0.87	0.09	-	50,50,50,50	0
56	MG	2a	3230	1/1	0.75	0.12	-	63,63,63,63	0
56	MG	1A	3274	1/1	0.91	0.17	-	36,36,36,36	0
56	MG	1A	4061	1/1	0.76	0.17	-	72,72,72,72	0
56	MG	2a	3106	1/1	0.87	0.16	-	62,62,62,62	0
56	MG	1A	3234	1/1	0.90	0.42	-	54,54,54,54	0
56	MG	2A	3434	1/1	0.82	0.14	-	59,59,59,59	0
56	MG	1A	4029	1/1	0.81	0.08	-	53,53,53,53	0
56	MG	2A	3736	1/1	0.98	0.13	-	67,67,67,67	0
56	MG	1A	3968	1/1	0.89	0.09	-	62,62,62,62	0
56	MG	1A	3323	1/1	0.90	0.17	-	50,50,50,50	0
56	MG	2E	309	1/1	0.95	0.09	-	60,60,60,60	0
56	MG	2A	3268	1/1	0.90	0.18	-	63,63,63,63	0
56	MG	1Q	203	1/1	0.90	0.19	-	64,64,64,64	0
56	MG	1A	3181	1/1	0.96	0.14	-	54,54,54,54	0
56	MG	2A	3391	1/1	0.90	0.18	-	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3495	1/1	0.93	0.26	-	42,42,42,42	0
56	MG	1a	1697	1/1	0.81	0.22	-	63,63,63,63	0
56	MG	1A	3475	1/1	0.95	0.11	-	42,42,42,42	0
56	MG	1A	3453	1/1	0.96	0.17	-	57,57,57,57	0
56	MG	2a	3150	1/1	0.91	0.05	-	78,78,78,78	0
56	MG	1A	3935	1/1	0.97	0.08	-	50,50,50,50	0
56	MG	1A	3123	1/1	0.88	0.24	-	54,54,54,54	0
56	MG	2A	3397	1/1	0.92	0.17	-	54,54,54,54	0
56	MG	2a	3006	1/1	0.89	0.17	-	74,74,74,74	0
56	MG	1Z	301	1/1	0.91	0.27	-	56,56,56,56	0
56	MG	1a	1734	1/1	0.98	0.08	-	67,67,67,67	0
56	MG	1A	3188	1/1	0.96	0.17	-	49,49,49,49	0
56	MG	1A	3322	1/1	0.72	0.17	-	59,59,59,59	0
56	MG	2A	3572	1/1	0.90	0.11	-	44,44,44,44	0
56	MG	1A	3381	1/1	0.92	0.14	-	43,43,43,43	0
56	MG	2A	3851	1/1	0.96	0.08	-	46,46,46,46	0
56	MG	1A	3206	1/1	0.88	0.14	-	55,55,55,55	0
56	MG	2A	3765	1/1	0.94	0.13	-	53,53,53,53	0
56	MG	1A	3694	1/1	0.89	0.17	-	61,61,61,61	0
56	MG	2A	3372	1/1	0.96	0.24	-	41,41,41,41	0
56	MG	1A	3942	1/1	0.83	0.10	-	56,56,56,56	0
56	MG	2A	3249	1/1	0.88	0.13	-	57,57,57,57	0
56	MG	1a	1689	1/1	0.85	0.12	-	73,73,73,73	0
56	MG	1A	4056	1/1	0.91	0.12	-	47,47,47,47	0
56	MG	1A	3483	1/1	0.92	0.17	-	46,46,46,46	0
56	MG	1a	1783	1/1	0.86	0.23	-	83,83,83,83	0
56	MG	1A	3277	1/1	0.95	0.20	-	38,38,38,38	0
56	MG	2A	3454	1/1	0.96	0.21	-	58,58,58,58	0
56	MG	2a	3014	1/1	0.86	0.11	-	64,64,64,64	0
56	MG	1A	3794	1/1	0.83	0.28	-	61,61,61,61	0
56	MG	2a	3152	1/1	0.89	0.17	-	67,67,67,67	0
56	MG	1A	3983	1/1	0.86	0.13	-	48,48,48,48	0
56	MG	1x	112	1/1	0.93	0.14	-	71,71,71,71	0
56	MG	1A	3467	1/1	0.98	0.16	-	45,45,45,45	0
56	MG	2a	3184	1/1	0.97	0.16	-	54,54,54,54	0
56	MG	1A	3796	1/1	0.96	0.18	-	34,34,34,34	0
56	MG	2A	3501	1/1	0.85	0.12	-	59,59,59,59	0
56	MG	1A	3631	1/1	0.94	0.20	-	32,32,32,32	0
56	MG	1A	3696	1/1	0.84	0.21	-	61,61,61,61	0
56	MG	1A	3284	1/1	0.89	0.39	-	56,56,56,56	0
56	MG	1A	3689	1/1	0.97	0.23	-	51,51,51,51	0
56	MG	2a	3033	1/1	0.89	0.14	-	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3153	1/1	0.92	0.14	-	37,37,37,37	0
56	MG	1w	103	1/1	0.85	0.14	-	57,57,57,57	0
56	MG	1A	3091	1/1	0.96	0.22	-	43,43,43,43	0
56	MG	1a	1775	1/1	0.67	0.19	-	76,76,76,76	0
56	MG	1A	3677	1/1	0.96	0.15	-	29,29,29,29	0
56	MG	2A	3747	1/1	0.83	0.11	-	51,51,51,51	0
56	MG	2A	3825	1/1	0.94	0.12	-	58,58,58,58	0
56	MG	2a	3016	1/1	0.87	0.14	-	66,66,66,66	0
56	MG	1A	3771	1/1	0.96	0.18	-	49,49,49,49	0
56	MG	1a	1723	1/1	0.91	0.10	-	61,61,61,61	0
56	MG	2l	202	1/1	0.84	0.09	-	70,70,70,70	0
56	MG	2B	3017	1/1	0.90	0.11	-	65,65,65,65	0
56	MG	1A	3683	1/1	0.93	0.19	-	40,40,40,40	0
56	MG	2A	3774	1/1	0.91	0.11	-	51,51,51,51	0
56	MG	1A	3100	1/1	0.94	0.18	-	60,60,60,60	0
56	MG	1A	3268	1/1	0.91	0.18	-	59,59,59,59	0
56	MG	2A	3718	1/1	0.90	0.36	-	64,64,64,64	0
56	MG	2A	3320	1/1	0.83	0.15	-	54,54,54,54	0
56	MG	1A	3614	1/1	0.80	0.13	-	39,39,39,39	0
56	MG	1A	3622	1/1	0.96	0.16	-	36,36,36,36	0
56	MG	1A	3400	1/1	0.96	0.16	-	54,54,54,54	0
56	MG	2A	3078	1/1	0.95	0.20	-	25,25,25,25	0
56	MG	1A	3506	1/1	0.97	0.19	-	42,42,42,42	0
56	MG	1P	204	1/1	0.95	0.21	-	47,47,47,47	0
56	MG	2A	3470	1/1	0.74	0.15	-	56,56,56,56	0
56	MG	1A	3140	1/1	0.95	0.14	-	43,43,43,43	0
56	MG	1A	3017	1/1	0.93	0.14	-	54,54,54,54	0
56	MG	2A	3778	1/1	0.94	0.18	-	52,52,52,52	0
56	MG	2A	3732	1/1	0.91	0.13	-	42,42,42,42	0
56	MG	1A	3198	1/1	0.97	0.20	-	41,41,41,41	0
56	MG	1a	1764	1/1	0.94	0.06	-	59,59,59,59	0
56	MG	2A	3862	1/1	0.91	0.11	-	71,71,71,71	0
56	MG	2a	3171	1/1	0.77	0.09	-	73,73,73,73	0
56	MG	2A	3231	1/1	0.99	0.15	-	49,49,49,49	0
56	MG	1A	3404	1/1	0.85	0.23	-	59,59,59,59	0
56	MG	1A	3832	1/1	0.86	0.10	-	62,62,62,62	0
56	MG	1a	1738	1/1	0.58	0.21	-	66,66,66,66	0
56	MG	1A	3247	1/1	0.90	0.26	-	58,58,58,58	0
56	MG	2A	3277	1/1	0.96	0.17	-	50,50,50,50	0
56	MG	1A	3816	1/1	0.92	0.22	-	49,49,49,49	0
56	MG	1F	306	1/1	0.91	0.28	-	53,53,53,53	0
56	MG	1A	3398	1/1	0.94	0.31	-	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2B	3001	1/1	0.93	0.16	-	62,62,62,62	0
56	MG	2A	3058	1/1	0.73	0.18	-	66,66,66,66	0
56	MG	2A	3815	1/1	0.90	0.14	-	48,48,48,48	0
56	MG	1l	203	1/1	0.94	0.14	-	63,63,63,63	0
56	MG	2a	3163	1/1	0.96	0.10	-	72,72,72,72	0
56	MG	2A	3698	1/1	0.84	0.12	-	51,51,51,51	0
56	MG	1w	108	1/1	0.95	0.07	-	63,63,63,63	0
56	MG	1A	3632	1/1	0.93	0.12	-	34,34,34,34	0
56	MG	1A	3377	1/1	0.84	0.21	-	54,54,54,54	0
56	MG	1A	3260	1/1	0.93	0.12	-	39,39,39,39	0
56	MG	1A	3389	1/1	0.98	0.20	-	53,53,53,53	0
56	MG	1Q	204	1/1	0.88	0.15	-	51,51,51,51	0
56	MG	1A	3839	1/1	0.90	0.08	-	66,66,66,66	0
56	MG	2A	3415	1/1	0.94	0.10	-	50,50,50,50	0
56	MG	2a	3142	1/1	0.69	0.15	-	74,74,74,74	0
56	MG	1A	3116	1/1	0.91	0.22	-	47,47,47,47	0
56	MG	1A	3569	1/1	0.89	0.25	-	54,54,54,54	0
56	MG	1A	3346	1/1	0.96	0.19	-	48,48,48,48	0
56	MG	1A	3443	1/1	0.94	0.27	-	54,54,54,54	0
56	MG	1A	3824	1/1	0.72	0.16	-	70,70,70,70	0
56	MG	2a	3062	1/1	0.85	0.20	-	70,70,70,70	0
56	MG	1A	3550	1/1	0.92	0.19	-	38,38,38,38	0
56	MG	1A	3472	1/1	0.97	0.24	-	56,56,56,56	0
56	MG	2A	3194	1/1	0.89	0.24	-	67,67,67,67	0
56	MG	2A	3105	1/1	0.85	0.09	-	51,51,51,51	0
56	MG	1A	3878	1/1	0.89	0.23	-	33,33,33,33	0
56	MG	1a	1759	1/1	0.92	0.13	-	64,64,64,64	0
56	MG	2A	3354	1/1	0.83	0.15	-	68,68,68,68	0
56	MG	1A	3365	1/1	0.91	0.31	-	53,53,53,53	0
56	MG	2A	3053	1/1	0.73	0.21	-	54,54,54,54	0
56	MG	2A	3573	1/1	0.89	0.11	-	42,42,42,42	0
56	MG	1A	3216	1/1	0.94	0.42	-	50,50,50,50	0
56	MG	2A	3639	1/1	0.99	0.17	-	34,34,34,34	0
56	MG	1a	1665	1/1	0.92	0.10	-	78,78,78,78	0
56	MG	2A	3266	1/1	0.84	0.12	-	59,59,59,59	0
56	MG	2a	3060	1/1	0.87	0.11	-	63,63,63,63	0
56	MG	1A	3295	1/1	0.94	0.14	-	48,48,48,48	0
56	MG	2B	3010	1/1	0.95	0.22	-	73,73,73,73	0
56	MG	2A	3676	1/1	0.92	0.09	-	48,48,48,48	0
56	MG	1A	3737	1/1	0.79	0.21	-	57,57,57,57	0
56	MG	2A	3425	1/1	0.93	0.16	-	58,58,58,58	0
56	MG	1a	1753	1/1	0.75	0.10	-	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3357	1/1	0.87	0.23	-	56,56,56,56	0
56	MG	2A	3065	1/1	0.91	0.20	-	57,57,57,57	0
56	MG	2A	3803	1/1	0.89	0.10	-	42,42,42,42	0
56	MG	2A	3169	1/1	0.84	0.22	-	73,73,73,73	0
56	MG	2A	3678	1/1	0.90	0.09	-	49,49,49,49	0
56	MG	1A	3160	1/1	0.93	0.23	-	41,41,41,41	0
56	MG	1B	3030	1/1	0.96	0.15	-	59,59,59,59	0
56	MG	1A	3922	1/1	0.89	0.10	-	57,57,57,57	0
56	MG	2A	3267	1/1	0.91	0.11	-	58,58,58,58	0
56	MG	2a	3088	1/1	0.76	0.20	-	62,62,62,62	0
56	MG	2A	3891	1/1	0.68	0.15	-	71,71,71,71	0
56	MG	1A	3161	1/1	0.98	0.27	-	38,38,38,38	0
56	MG	1A	3024	1/1	0.88	0.17	-	43,43,43,43	0
56	MG	1A	3776	1/1	0.86	0.20	-	75,75,75,75	0
56	MG	1A	3073	1/1	0.77	0.35	-	69,69,69,69	0
56	MG	2A	3852	1/1	0.91	0.12	-	49,49,49,49	0
56	MG	1A	3294	1/1	0.96	0.19	-	52,52,52,52	0
56	MG	2A	3328	1/1	0.94	0.20	-	39,39,39,39	0
56	MG	1A	3546	1/1	0.87	0.19	-	45,45,45,45	0
56	MG	1A	3613	1/1	0.91	0.13	-	33,33,33,33	0
56	MG	1A	4064	1/1	0.82	0.13	-	66,66,66,66	0
56	MG	1A	3570	1/1	0.94	0.22	-	54,54,54,54	0
56	MG	1a	1731	1/1	0.95	0.16	-	50,50,50,50	0
56	MG	2A	3863	1/1	0.92	0.05	-	58,58,58,58	0
56	MG	2a	3009	1/1	0.98	0.07	-	60,60,60,60	0
56	MG	2A	3680	1/1	0.95	0.05	-	62,62,62,62	0
56	MG	2A	3870	1/1	0.98	0.18	-	33,33,33,33	0
56	MG	2A	3865	1/1	0.59	0.17	-	71,71,71,71	0
56	MG	2A	3071	1/1	0.93	0.06	-	52,52,52,52	0
56	MG	2A	3418	1/1	0.92	0.09	-	61,61,61,61	0
56	MG	2A	3893	1/1	0.81	0.08	-	66,66,66,66	0
56	MG	1A	3656	1/1	0.93	0.10	-	46,46,46,46	0
56	MG	2a	3039	1/1	0.91	0.21	-	73,73,73,73	0
56	MG	1A	3538	1/1	0.97	0.13	-	54,54,54,54	0
56	MG	2A	3082	1/1	0.84	0.12	-	50,50,50,50	0
56	MG	1A	3573	1/1	0.90	0.09	-	60,60,60,60	0
56	MG	1A	3018	1/1	0.94	0.14	-	33,33,33,33	0
56	MG	2A	3873	1/1	0.98	0.12	-	40,40,40,40	0
56	MG	1A	3995	1/1	0.91	0.21	-	73,73,73,73	0
56	MG	2A	3322	1/1	0.88	0.11	-	60,60,60,60	0
56	MG	2A	3039	1/1	0.76	0.16	-	55,55,55,55	0
56	MG	2A	3556	1/1	0.82	0.16	-	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	1814	1/1	0.96	0.26	-	55,55,55,55	0
56	MG	2A	3184	1/1	0.98	0.25	-	48,48,48,48	0
56	MG	2v	3002	1/1	0.94	0.09	-	77,77,77,77	0
56	MG	2A	3440	1/1	0.95	0.20	-	43,43,43,43	0
56	MG	2a	3115	1/1	0.92	0.09	-	57,57,57,57	0
56	MG	2A	3024	1/1	0.93	0.13	-	49,49,49,49	0
56	MG	2A	3335	1/1	0.76	0.17	-	59,59,59,59	0
56	MG	1A	3813	1/1	0.95	0.21	-	56,56,56,56	0
56	MG	1A	3058	1/1	0.71	0.19	-	54,54,54,54	0
56	MG	2y	3005	1/1	0.75	0.30	-	82,82,82,82	0
56	MG	1a	1784	1/1	0.78	0.25	-	74,74,74,74	0
56	MG	1A	3421	1/1	0.79	0.15	-	46,46,46,46	0
56	MG	2A	3775	1/1	0.96	0.12	-	38,38,38,38	0
56	MG	1A	3245	1/1	0.90	0.26	-	64,64,64,64	0
56	MG	1a	1624	1/1	0.93	0.15	-	50,50,50,50	0
56	MG	2A	3665	1/1	0.97	0.09	-	52,52,52,52	0
56	MG	2A	3246	1/1	0.93	0.12	-	65,65,65,65	0
56	MG	1A	3072	1/1	0.98	0.26	-	19,19,19,19	0
56	MG	1A	3489	1/1	0.88	0.19	-	44,44,44,44	0
56	MG	1A	3929	1/1	0.88	0.15	-	42,42,42,42	0
56	MG	1A	3579	1/1	0.90	0.17	-	44,44,44,44	0
56	MG	1A	3231	1/1	0.89	0.23	-	51,51,51,51	0
56	MG	2A	3148	1/1	0.92	0.16	-	52,52,52,52	0
56	MG	1A	3718	1/1	0.66	0.13	-	67,67,67,67	0
56	MG	2A	3218	1/1	0.95	0.19	-	61,61,61,61	0
56	MG	2a	3059	1/1	0.95	0.13	-	74,74,74,74	0
56	MG	1A	4000	1/1	0.95	0.18	-	34,34,34,34	0
56	MG	2a	3074	1/1	0.82	0.09	-	63,63,63,63	0
56	MG	2a	3007	1/1	0.88	0.11	-	71,71,71,71	0
56	MG	1F	301	1/1	0.92	0.16	-	40,40,40,40	0
56	MG	1A	3937	1/1	0.89	0.24	-	31,31,31,31	0
56	MG	2A	3672	1/1	0.94	0.23	-	45,45,45,45	0
56	MG	1A	3515	1/1	0.95	0.10	-	29,29,29,29	0
56	MG	1A	3837	1/1	0.97	0.23	-	21,21,21,21	0
56	MG	1A	3769	1/1	0.94	0.24	-	29,29,29,29	0
56	MG	1A	3979	1/1	0.94	0.09	-	73,73,73,73	0
56	MG	2y	3007	1/1	0.94	0.15	-	68,68,68,68	0
56	MG	2A	3827	1/1	0.88	0.12	-	58,58,58,58	0
56	MG	1A	3448	1/1	0.90	0.16	-	59,59,59,59	0
56	MG	15	102	1/1	0.93	0.19	-	39,39,39,39	0
56	MG	2a	3042	1/1	0.84	0.24	-	58,58,58,58	0
56	MG	1a	1666	1/1	0.92	0.14	-	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	1664	1/1	0.90	0.25	-	62,62,62,62	0
56	MG	1A	3455	1/1	0.98	0.12	-	47,47,47,47	0
56	MG	2A	3909	1/1	0.96	0.15	-	43,43,43,43	0
56	MG	1A	3642	1/1	0.93	0.10	-	40,40,40,40	0
56	MG	1A	3136	1/1	0.93	0.08	-	52,52,52,52	0
56	MG	1a	1763	1/1	0.96	0.10	-	55,55,55,55	0
56	MG	2a	3220	1/1	0.91	0.12	-	66,66,66,66	0
56	MG	1A	3114	1/1	0.94	0.17	-	57,57,57,57	0
56	MG	1A	3599	1/1	0.97	0.16	-	21,21,21,21	0
56	MG	1B	3014	1/1	0.90	0.13	-	63,63,63,63	0
56	MG	1a	1633	1/1	0.93	0.21	-	60,60,60,60	0
56	MG	1A	4054	1/1	0.58	0.13	-	81,81,81,81	0
56	MG	1A	3587	1/1	0.90	0.21	-	38,38,38,38	0
56	MG	1a	1696	1/1	0.88	0.14	-	71,71,71,71	0
56	MG	2A	3321	1/1	0.93	0.13	-	54,54,54,54	0
56	MG	2A	3345	1/1	0.82	0.19	-	59,59,59,59	0
56	MG	1y	3003	1/1	0.92	0.23	-	71,71,71,71	0
56	MG	1A	3057	1/1	0.85	0.22	-	54,54,54,54	0
56	MG	1A	3710	1/1	0.91	0.12	-	68,68,68,68	0
56	MG	1A	3222	1/1	0.94	0.16	-	56,56,56,56	0
56	MG	1A	3325	1/1	0.88	0.21	-	64,64,64,64	0
56	MG	2A	3829	1/1	0.75	0.12	-	59,59,59,59	0
56	MG	1A	3894	1/1	0.83	0.10	-	73,73,73,73	0
56	MG	1A	3327	1/1	0.89	0.16	-	28,28,28,28	0
56	MG	2A	3256	1/1	0.94	0.31	-	53,53,53,53	0
56	MG	2A	3754	1/1	0.76	0.13	-	45,45,45,45	0
56	MG	25	103	1/1	0.94	0.21	-	52,52,52,52	0
56	MG	2A	3305	1/1	0.86	0.13	-	56,56,56,56	0
56	MG	1A	3452	1/1	0.94	0.23	-	58,58,58,58	0
56	MG	2A	3901	1/1	0.93	0.31	-	59,59,59,59	0
56	MG	2V	201	1/1	0.98	0.16	-	53,53,53,53	0
56	MG	2A	3788	1/1	0.91	0.10	-	53,53,53,53	0
56	MG	1A	3701	1/1	0.95	0.09	-	48,48,48,48	0
56	MG	1A	3087	1/1	0.84	0.22	-	32,32,32,32	0
56	MG	2A	3734	1/1	0.85	0.14	-	57,57,57,57	0
56	MG	2A	3512	1/1	0.89	0.12	-	53,53,53,53	0
56	MG	1B	3036	1/1	0.99	0.10	-	36,36,36,36	0
56	MG	2A	3361	1/1	0.93	0.15	-	51,51,51,51	0
56	MG	2a	3135	1/1	0.82	0.19	-	62,62,62,62	0
56	MG	2B	3005	1/1	0.79	0.13	-	53,53,53,53	0
56	MG	2A	3701	1/1	0.93	0.19	-	64,64,64,64	0
56	MG	2A	3417	1/1	0.89	0.10	-	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3740	1/1	0.81	0.17	-	53,53,53,53	0
56	MG	2y	3002	1/1	0.80	0.13	-	64,64,64,64	0
56	MG	2A	3753	1/1	0.91	0.13	-	45,45,45,45	0
56	MG	2A	3138	1/1	0.91	0.15	-	59,59,59,59	0
56	MG	2A	3289	1/1	0.87	0.13	-	47,47,47,47	0
56	MG	1a	1760	1/1	0.86	0.17	-	74,74,74,74	0
56	MG	2A	3027	1/1	0.98	0.32	-	48,48,48,48	0
56	MG	2a	3183	1/1	0.81	0.10	-	76,76,76,76	0
56	MG	1a	1606	1/1	0.94	0.17	-	65,65,65,65	0
56	MG	2A	3866	1/1	0.95	0.11	-	42,42,42,42	0
56	MG	1A	3080	1/1	0.89	0.26	-	42,42,42,42	0
56	MG	1A	3954	1/1	0.58	0.16	-	58,58,58,58	0
56	MG	1A	3702	1/1	0.99	0.15	-	34,34,34,34	0
56	MG	1A	3209	1/1	0.89	0.26	-	68,68,68,68	0
56	MG	1a	1766	1/1	0.67	0.17	-	76,76,76,76	0
56	MG	2A	3269	1/1	0.89	0.17	-	53,53,53,53	0
56	MG	2E	308	1/1	0.76	0.14	-	38,38,38,38	0
56	MG	2a	3226	1/1	0.97	0.07	-	64,64,64,64	0
56	MG	2a	3117	1/1	0.89	0.85	-	81,81,81,81	0
56	MG	2A	3682	1/1	0.93	0.15	-	70,70,70,70	0
56	MG	2x	101	1/1	0.93	0.10	-	42,42,42,42	0
56	MG	1f	3001	1/1	0.95	0.20	-	34,34,34,34	0
56	MG	2A	3398	1/1	0.94	0.30	-	55,55,55,55	0
56	MG	2a	3111	1/1	0.95	0.14	-	76,76,76,76	0
56	MG	1a	1781	1/1	0.83	0.11	-	71,71,71,71	0
56	MG	1x	113	1/1	0.93	0.19	-	62,62,62,62	0
56	MG	1a	1671	1/1	0.79	0.15	-	66,66,66,66	0
56	MG	2a	3225	1/1	0.88	0.10	-	57,57,57,57	0
56	MG	1A	3585	1/1	0.94	0.08	-	66,66,66,66	0
56	MG	2A	3549	1/1	0.86	0.15	-	58,58,58,58	0
56	MG	2A	3796	1/1	0.87	0.10	-	49,49,49,49	0
56	MG	1A	3108	1/1	0.87	0.45	-	43,43,43,43	0
56	MG	2a	3156	1/1	0.89	0.13	-	69,69,69,69	0
56	MG	1A	3432	1/1	0.75	0.14	-	54,54,54,54	0
56	MG	1A	3565	1/1	0.93	0.32	-	71,71,71,71	0
56	MG	1a	1801	1/1	0.95	0.07	-	53,53,53,53	0
56	MG	1A	3272	1/1	0.58	0.30	-	60,60,60,60	0
56	MG	2A	3196	1/1	0.90	0.14	-	56,56,56,56	0
56	MG	27	101	1/1	0.92	0.20	-	51,51,51,51	0
56	MG	1A	4005	1/1	0.95	0.11	-	50,50,50,50	0
56	MG	2A	3298	1/1	0.96	0.12	-	41,41,41,41	0
56	MG	1A	3407	1/1	0.87	0.36	-	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3402	1/1	0.86	0.17	-	50,50,50,50	0
56	MG	1A	3782	1/1	0.96	0.19	-	25,25,25,25	0
56	MG	1A	3527	1/1	0.88	0.30	-	40,40,40,40	0
56	MG	1a	1787	1/1	0.92	0.07	-	72,72,72,72	0
56	MG	1a	1798	1/1	0.94	0.14	-	56,56,56,56	0
56	MG	2A	3363	1/1	0.92	0.22	-	65,65,65,65	0
56	MG	2A	3779	1/1	0.95	0.08	-	56,56,56,56	0
56	MG	2A	3358	1/1	0.76	0.12	-	65,65,65,65	0
56	MG	2A	3451	1/1	0.93	0.19	-	56,56,56,56	0
56	MG	1a	1704	1/1	0.78	0.20	-	63,63,63,63	0
56	MG	1a	1715	1/1	0.98	0.11	-	49,49,49,49	0
56	MG	1A	3023	1/1	0.91	0.17	-	59,59,59,59	0
56	MG	2A	3283	1/1	0.94	0.24	-	61,61,61,61	0
56	MG	2A	3097	1/1	0.97	0.13	-	56,56,56,56	0
56	MG	2A	3824	1/1	0.57	0.14	-	78,78,78,78	0
56	MG	2A	3600	1/1	0.97	0.15	-	40,40,40,40	0
56	MG	2A	3878	1/1	0.88	0.10	-	49,49,49,49	0
56	MG	2A	3860	1/1	0.87	0.12	-	59,59,59,59	0
56	MG	1A	3560	1/1	0.86	0.22	-	55,55,55,55	0
56	MG	1A	3917	1/1	0.84	0.17	-	80,80,80,80	0
56	MG	1A	3499	1/1	0.90	0.11	-	49,49,49,49	0
56	MG	2A	3385	1/1	0.96	0.24	-	52,52,52,52	0
56	MG	2A	3724	1/1	0.95	0.06	-	57,57,57,57	0
56	MG	2A	3797	1/1	0.95	0.15	-	52,52,52,52	0
56	MG	2A	3388	1/1	0.93	0.18	-	56,56,56,56	0
56	MG	25	105	1/1	0.90	0.09	-	58,58,58,58	0
56	MG	2A	3376	1/1	0.94	0.13	-	58,58,58,58	0
56	MG	1A	3623	1/1	0.82	0.21	-	59,59,59,59	0
56	MG	1A	3009	1/1	0.95	0.12	-	24,24,24,24	0
56	MG	2A	3896	1/1	0.89	0.18	-	39,39,39,39	0
56	MG	1X	102	1/1	0.91	0.22	-	46,46,46,46	0
56	MG	1A	3768	1/1	0.87	0.17	-	61,61,61,61	0
56	MG	1A	3492	1/1	0.80	0.29	-	52,52,52,52	0
56	MG	2A	3307	1/1	0.73	0.16	-	68,68,68,68	0
56	MG	1A	4094	1/1	0.90	0.09	-	37,37,37,37	0
56	MG	2A	3292	1/1	0.91	0.11	-	54,54,54,54	0
56	MG	2A	3741	1/1	0.77	0.12	-	61,61,61,61	0
56	MG	1A	3651	1/1	0.94	0.22	-	32,32,32,32	0
56	MG	1A	3267	1/1	0.94	0.15	-	57,57,57,57	0
56	MG	2B	3020	1/1	0.91	0.20	-	78,78,78,78	0
56	MG	1A	3920	1/1	0.96	0.14	-	44,44,44,44	0
56	MG	1B	3011	1/1	0.85	0.16	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	3024	1/1	0.86	0.11	-	72,72,72,72	0
56	MG	2a	3021	1/1	0.98	0.14	-	65,65,65,65	0
56	MG	2A	3679	1/1	0.98	0.11	-	41,41,41,41	0
56	MG	1A	3709	1/1	0.88	0.31	-	52,52,52,52	0
56	MG	1A	3218	1/1	0.78	0.22	-	62,62,62,62	0
56	MG	1A	3178	1/1	0.97	0.26	-	21,21,21,21	0
56	MG	1A	3823	1/1	0.90	0.18	-	65,65,65,65	0
56	MG	2a	3081	1/1	0.83	0.18	-	49,49,49,49	0
56	MG	1A	3779	1/1	0.94	0.10	-	56,56,56,56	0
56	MG	2A	3205	1/1	0.89	0.22	-	52,52,52,52	0
56	MG	2A	3583	1/1	0.93	0.16	-	69,69,69,69	0
56	MG	1A	3868	1/1	0.96	0.15	-	47,47,47,47	0
56	MG	1A	3052	1/1	0.93	0.15	-	56,56,56,56	0
56	MG	1a	1773	1/1	0.78	0.14	-	90,90,90,90	0
56	MG	1A	3049	1/1	0.97	0.23	-	26,26,26,26	0
56	MG	2a	3214	1/1	0.69	0.16	-	91,91,91,91	0
56	MG	2A	3847	1/1	0.98	0.06	-	42,42,42,42	0
56	MG	2A	3161	1/1	0.93	0.18	-	44,44,44,44	0
56	MG	2A	3830	1/1	0.81	0.19	-	48,48,48,48	0
56	MG	1A	3940	1/1	0.63	0.12	-	48,48,48,48	0
56	MG	2A	3805	1/1	0.84	0.26	-	77,77,77,77	0
56	MG	1A	3886	1/1	0.91	0.13	-	57,57,57,57	0
56	MG	2A	3177	1/1	0.94	0.15	-	63,63,63,63	0
56	MG	2a	3224	1/1	0.88	0.20	-	74,74,74,74	0
56	MG	2A	3149	1/1	0.89	0.22	-	54,54,54,54	0
56	MG	2A	3085	1/1	0.87	0.12	-	44,44,44,44	0
56	MG	1A	3349	1/1	0.81	0.20	-	44,44,44,44	0
56	MG	2A	3244	1/1	0.88	0.09	-	54,54,54,54	0
56	MG	25	104	1/1	0.94	0.11	-	43,43,43,43	0
56	MG	1A	3304	1/1	0.94	0.29	-	55,55,55,55	0
56	MG	1A	3301	1/1	0.97	0.05	-	54,54,54,54	0
56	MG	1A	3957	1/1	0.97	0.11	-	55,55,55,55	0
56	MG	2A	3073	1/1	0.88	0.11	-	36,36,36,36	0
56	MG	2A	3602	1/1	0.95	0.14	-	42,42,42,42	0
56	MG	1a	1674	1/1	0.85	0.17	-	72,72,72,72	0
56	MG	1B	3013	1/1	0.95	0.09	-	55,55,55,55	0
56	MG	1A	3391	1/1	0.92	0.20	-	41,41,41,41	0
56	MG	2A	3135	1/1	0.93	0.20	-	43,43,43,43	0
56	MG	1A	3830	1/1	0.24	0.16	-	66,66,66,66	0
56	MG	1d	502	1/1	0.90	0.23	-	67,67,67,67	0
56	MG	2Y	502	1/1	0.93	0.25	-	54,54,54,54	0
56	MG	2A	3238	1/1	0.90	0.39	-	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2B	3016	1/1	0.83	0.13	-	81,81,81,81	0
56	MG	1a	1811	1/1	0.75	0.08	-	77,77,77,77	0
56	MG	2a	3121	1/1	0.80	0.24	-	75,75,75,75	0
56	MG	1A	3257	1/1	0.74	0.24	-	68,68,68,68	0
56	MG	1w	104	1/1	0.95	0.13	-	69,69,69,69	0
56	MG	2A	3240	1/1	0.95	0.13	-	40,40,40,40	0
56	MG	2A	3075	1/1	0.92	0.19	-	37,37,37,37	0
56	MG	2a	3002	1/1	0.87	0.10	-	50,50,50,50	0
56	MG	2w	104	1/1	0.86	0.14	-	69,69,69,69	0
56	MG	1A	3402	1/1	0.95	0.23	-	54,54,54,54	0
56	MG	1a	1601	1/1	0.85	0.11	-	53,53,53,53	0
56	MG	2A	3845	1/1	0.95	0.13	-	42,42,42,42	0
56	MG	2A	3293	1/1	0.93	0.13	-	50,50,50,50	0
56	MG	1A	3169	1/1	0.79	0.23	-	55,55,55,55	0
56	MG	2a	3086	1/1	0.93	0.11	-	57,57,57,57	0
56	MG	2A	3605	1/1	0.90	0.15	-	51,51,51,51	0
56	MG	2A	3429	1/1	0.92	0.11	-	65,65,65,65	0
56	MG	1A	3980	1/1	0.64	0.11	-	74,74,74,74	0
56	MG	1a	1729	1/1	0.93	0.20	-	61,61,61,61	0
56	MG	2A	3399	1/1	0.90	0.15	-	60,60,60,60	0
56	MG	1A	3643	1/1	0.86	0.17	-	34,34,34,34	0
56	MG	2A	3382	1/1	0.93	0.07	-	50,50,50,50	0
56	MG	1A	3815	1/1	0.93	0.27	-	44,44,44,44	0
56	MG	2A	3489	1/1	0.94	0.17	-	41,41,41,41	0
56	MG	2A	3182	1/1	0.89	0.13	-	42,42,42,42	0
56	MG	2A	3310	1/1	0.95	0.15	-	62,62,62,62	0
56	MG	2A	3731	1/1	0.87	0.14	-	57,57,57,57	0
56	MG	1a	1714	1/1	0.88	0.14	-	66,66,66,66	0
56	MG	2A	3641	1/1	0.91	0.25	-	57,57,57,57	0
56	MG	1A	3580	1/1	0.91	0.27	-	39,39,39,39	0
56	MG	1A	3456	1/1	0.97	0.22	-	48,48,48,48	0
56	MG	2A	3130	1/1	0.91	0.19	-	53,53,53,53	0
56	MG	2A	3603	1/1	0.91	0.14	-	50,50,50,50	0
56	MG	1A	3742	1/1	0.94	0.13	-	64,64,64,64	0
56	MG	1A	3785	1/1	0.85	0.14	-	47,47,47,47	0
56	MG	1A	3766	1/1	0.90	0.08	-	47,47,47,47	0
56	MG	2A	3478	1/1	0.90	0.15	-	50,50,50,50	0
56	MG	1A	4102	1/1	0.93	0.10	-	45,45,45,45	0
56	MG	2a	3122	1/1	0.79	0.16	-	73,73,73,73	0
56	MG	2A	3671	1/1	0.92	0.10	-	46,46,46,46	0
56	MG	2N	8001	1/1	0.92	0.17	-	47,47,47,47	0
56	MG	2A	3393	1/1	0.95	0.09	-	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	3019	1/1	0.93	0.11	-	57,57,57,57	0
56	MG	1a	1726	1/1	0.84	0.18	-	67,67,67,67	0
56	MG	1A	3799	1/1	0.93	0.18	-	57,57,57,57	0
56	MG	1A	3755	1/1	0.94	0.20	-	36,36,36,36	0
56	MG	1A	3463	1/1	0.96	0.16	-	53,53,53,53	0
56	MG	1A	3464	1/1	0.79	0.21	-	45,45,45,45	0
56	MG	2a	3196	1/1	0.93	0.11	-	64,64,64,64	0
56	MG	1A	4058	1/1	0.82	0.07	-	47,47,47,47	0
56	MG	1A	3235	1/1	0.90	0.25	-	66,66,66,66	0
56	MG	1A	3484	1/1	0.93	0.13	-	54,54,54,54	0
56	MG	2A	3859	1/1	0.87	0.10	-	53,53,53,53	0
57	K	1A	3584	1/1	0.95	0.13	-	58,58,58,58	0
56	MG	1A	3079	1/1	0.95	0.17	-	57,57,57,57	0
56	MG	2A	3052	1/1	0.83	0.16	-	58,58,58,58	0
56	MG	2A	3713	1/1	0.97	0.45	-	67,67,67,67	0
56	MG	1A	3371	1/1	0.91	0.14	-	45,45,45,45	0
56	MG	1A	3770	1/1	0.72	0.09	-	74,74,74,74	0
56	MG	1A	3217	1/1	0.93	0.29	-	47,47,47,47	0
56	MG	2a	3015	1/1	0.91	0.11	-	62,62,62,62	0
56	MG	2A	3421	1/1	0.93	0.16	-	61,61,61,61	0
56	MG	1A	3856	1/1	0.85	0.20	-	47,47,47,47	0
56	MG	1A	3440	1/1	0.82	0.17	-	50,50,50,50	0
56	MG	1A	3380	1/1	0.96	0.27	-	48,48,48,48	0
56	MG	1A	3528	1/1	0.95	0.17	-	45,45,45,45	0
56	MG	2A	3704	1/1	0.92	0.07	-	56,56,56,56	0
56	MG	1A	3331	1/1	0.93	0.23	-	54,54,54,54	0
56	MG	1A	3183	1/1	0.83	0.17	-	54,54,54,54	0
56	MG	1a	1815	1/1	0.85	0.07	-	64,64,64,64	0
56	MG	2A	3459	1/1	0.91	0.13	-	62,62,62,62	0
56	MG	1A	3758	1/1	0.88	0.10	-	71,71,71,71	0
56	MG	2B	3021	1/1	0.71	0.09	-	75,75,75,75	0
56	MG	2A	3810	1/1	0.71	0.20	-	51,51,51,51	0
56	MG	2A	3423	1/1	0.90	0.18	-	58,58,58,58	0
56	MG	1A	4128	1/1	0.92	0.32	-	43,43,43,43	0
56	MG	2a	3038	1/1	0.89	0.13	-	68,68,68,68	0
56	MG	2A	3291	1/1	0.72	0.15	-	56,56,56,56	0
56	MG	2A	3438	1/1	0.89	0.19	-	68,68,68,68	0
56	MG	1A	3373	1/1	0.93	0.24	-	52,52,52,52	0
56	MG	2A	3488	1/1	0.74	0.21	-	65,65,65,65	0
56	MG	1A	3090	1/1	0.90	0.16	-	54,54,54,54	0
56	MG	1A	3521	1/1	0.76	0.18	-	65,65,65,65	0
56	MG	2A	3116	1/1	0.93	0.23	-	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3872	1/1	0.96	0.23	-	33,33,33,33	0
56	MG	2A	3088	1/1	0.85	0.11	-	49,49,49,49	0
56	MG	2A	3539	1/1	0.91	0.16	-	62,62,62,62	0
56	MG	1a	1681	1/1	0.89	0.25	-	54,54,54,54	0
56	MG	1A	3883	1/1	0.95	0.16	-	68,68,68,68	0
56	MG	1A	3975	1/1	0.75	0.25	-	93,93,93,93	0
56	MG	1A	4045	1/1	0.79	0.10	-	38,38,38,38	0
56	MG	2A	3274	1/1	0.87	0.11	-	53,53,53,53	0
56	MG	2A	3712	1/1	0.82	0.15	-	63,63,63,63	0
56	MG	1A	3086	1/1	0.94	0.42	-	50,50,50,50	0
56	MG	2a	3219	1/1	0.91	0.07	-	65,65,65,65	0
56	MG	2A	3261	1/1	0.88	0.20	-	59,59,59,59	0
56	MG	1A	3715	1/1	0.97	0.09	-	54,54,54,54	0
56	MG	1A	3239	1/1	0.97	0.18	-	30,30,30,30	0
56	MG	2a	3045	1/1	0.94	0.06	-	65,65,65,65	0
56	MG	2A	3378	1/1	0.92	0.15	-	62,62,62,62	0
56	MG	2A	3230	1/1	0.90	0.13	-	48,48,48,48	0
56	MG	2A	3864	1/1	0.77	0.17	-	63,63,63,63	0
56	MG	1A	3422	1/1	0.96	0.24	-	38,38,38,38	0
56	MG	2A	3241	1/1	0.89	0.38	-	56,56,56,56	0
56	MG	2A	3510	1/1	0.86	0.18	-	46,46,46,46	0
56	MG	1A	3522	1/1	0.97	0.16	-	49,49,49,49	0
56	MG	1a	1622	1/1	0.93	0.28	-	62,62,62,62	0
56	MG	2a	3211	1/1	0.95	0.13	-	61,61,61,61	0
56	MG	1A	3542	1/1	0.89	0.21	-	75,75,75,75	0
56	MG	2a	3198	1/1	0.78	0.18	-	83,83,83,83	0
56	MG	1A	3232	1/1	0.92	0.10	-	47,47,47,47	0
56	MG	28	101	1/1	0.89	0.12	-	53,53,53,53	0
56	MG	2A	3894	1/1	0.95	0.15	-	55,55,55,55	0
56	MG	2A	3473	1/1	0.91	0.13	-	57,57,57,57	0
56	MG	2A	3684	1/1	0.82	0.10	-	44,44,44,44	0
56	MG	1A	3910	1/1	0.91	0.07	-	76,76,76,76	0
56	MG	2a	3186	1/1	0.94	0.12	-	53,53,53,53	0
56	MG	2A	3471	1/1	0.86	0.21	-	54,54,54,54	0
56	MG	1A	3457	1/1	0.95	0.16	-	59,59,59,59	0
56	MG	1A	3394	1/1	0.96	0.16	-	35,35,35,35	0
56	MG	1a	1683	1/1	0.94	0.14	-	61,61,61,61	0
56	MG	2A	3254	1/1	0.93	0.51	-	53,53,53,53	0
56	MG	2A	3197	1/1	0.93	0.12	-	57,57,57,57	0
56	MG	1A	3468	1/1	0.80	0.32	-	68,68,68,68	0
56	MG	1A	3518	1/1	0.85	0.17	-	48,48,48,48	0
56	MG	2A	3226	1/1	0.97	0.11	-	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3298	1/1	0.92	0.15	-	43,43,43,43	0
56	MG	1a	1713	1/1	0.90	0.08	-	68,68,68,68	0
56	MG	1A	3996	1/1	0.78	0.12	-	43,43,43,43	0
56	MG	2A	3356	1/1	0.88	0.30	-	55,55,55,55	0
56	MG	2A	3346	1/1	0.89	0.20	-	54,54,54,54	0
56	MG	1A	3352	1/1	0.89	0.22	-	64,64,64,64	0
56	MG	1A	3433	1/1	0.97	0.16	-	47,47,47,47	0
56	MG	1A	3155	1/1	0.93	0.20	-	47,47,47,47	0
56	MG	2x	103	1/1	0.93	0.13	-	64,64,64,64	0
56	MG	1a	1677	1/1	0.82	0.12	-	68,68,68,68	0
56	MG	2A	3681	1/1	0.94	0.08	-	50,50,50,50	0
56	MG	1A	3435	1/1	0.94	0.11	-	53,53,53,53	0
56	MG	2A	3858	1/1	0.96	0.13	-	43,43,43,43	0
56	MG	1A	4052	1/1	0.94	0.18	-	31,31,31,31	0
56	MG	2A	3119	1/1	0.90	0.19	-	47,47,47,47	0
56	MG	2A	3204	1/1	0.98	0.17	-	48,48,48,48	0
56	MG	1A	4007	1/1	0.69	0.09	-	86,86,86,86	0
56	MG	2A	3004	1/1	0.94	0.24	-	48,48,48,48	0
56	MG	2a	3227	1/1	0.90	0.12	-	59,59,59,59	0
56	MG	1A	3713	1/1	0.96	0.18	-	62,62,62,62	0
56	MG	1A	3664	1/1	0.92	0.14	-	48,48,48,48	0
56	MG	2A	3816	1/1	0.96	0.25	-	57,57,57,57	0
56	MG	10	103	1/1	0.94	0.18	-	45,45,45,45	0
56	MG	2A	3727	1/1	0.93	0.15	-	51,51,51,51	0
56	MG	2E	305	1/1	0.95	0.11	-	40,40,40,40	0
56	MG	1A	3840	1/1	0.93	0.11	-	63,63,63,63	0
56	MG	2a	3066	1/1	0.92	0.14	-	54,54,54,54	0
56	MG	2A	3636	1/1	0.98	0.15	-	59,59,59,59	0
56	MG	1A	3031	1/1	0.98	0.17	-	31,31,31,31	0
56	MG	1a	1716	1/1	0.91	0.22	-	53,53,53,53	0
56	MG	1A	3988	1/1	0.98	0.07	-	68,68,68,68	0
56	MG	2A	3485	1/1	0.93	0.23	-	63,63,63,63	0
56	MG	2A	3798	1/1	0.92	0.28	-	52,52,52,52	0
56	MG	2a	3180	1/1	0.94	0.11	-	73,73,73,73	0
56	MG	2A	3656	1/1	0.75	0.17	-	77,77,77,77	0
56	MG	2A	3450	1/1	0.89	0.20	-	50,50,50,50	0
56	MG	1A	3382	1/1	0.84	0.17	-	54,54,54,54	0
56	MG	1a	1679	1/1	0.98	0.10	-	73,73,73,73	0
56	MG	1R	203	1/1	0.90	0.31	-	47,47,47,47	0
56	MG	1A	3582	1/1	0.97	0.20	-	54,54,54,54	0
56	MG	1G	3004	1/1	0.73	0.34	-	92,92,92,92	0
56	MG	1V	203	1/1	0.84	0.26	-	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1B	3008	1/1	0.95	0.15	-	57,57,57,57	0
56	MG	1A	3629	1/1	0.97	0.21	-	32,32,32,32	0
56	MG	2A	3854	1/1	0.50	0.09	-	77,77,77,77	0
56	MG	1A	3982	1/1	0.91	0.26	-	29,29,29,29	0
56	MG	1A	3655	1/1	0.91	0.12	-	39,39,39,39	0
56	MG	1A	3132	1/1	0.92	0.26	-	40,40,40,40	0
56	MG	2A	3821	1/1	0.84	0.18	-	79,79,79,79	0
56	MG	1a	1757	1/1	0.93	0.10	-	48,48,48,48	0
56	MG	1A	3362	1/1	0.89	0.24	-	54,54,54,54	0
56	MG	1A	3763	1/1	0.95	0.15	-	52,52,52,52	0
56	MG	1A	3581	1/1	0.83	0.16	-	58,58,58,58	0
56	MG	2A	3340	1/1	0.95	0.26	-	51,51,51,51	0
56	MG	1A	3255	1/1	0.95	0.24	-	47,47,47,47	0
56	MG	1A	3500	1/1	0.97	0.18	-	38,38,38,38	0
56	MG	2A	3329	1/1	0.91	0.41	-	56,56,56,56	0
56	MG	1A	3271	1/1	0.96	0.12	-	50,50,50,50	0
56	MG	2a	3190	1/1	0.98	0.07	-	66,66,66,66	0
56	MG	1A	3557	1/1	0.90	0.32	-	60,60,60,60	0
56	MG	2A	3324	1/1	0.94	0.09	-	41,41,41,41	0
56	MG	2A	3836	1/1	0.82	0.23	-	42,42,42,42	0
56	MG	1a	1725	1/1	0.96	0.20	-	55,55,55,55	0
56	MG	1A	3447	1/1	0.87	0.15	-	46,46,46,46	0
56	MG	2a	3205	1/1	0.99	0.22	-	70,70,70,70	0
56	MG	2A	3284	1/1	0.89	0.16	-	59,59,59,59	0
56	MG	2a	3243	1/1	0.95	0.13	-	64,64,64,64	0
56	MG	2A	3702	1/1	0.94	0.07	-	49,49,49,49	0
56	MG	1A	3441	1/1	0.87	0.10	-	56,56,56,56	0
56	MG	2A	3353	1/1	0.83	0.19	-	65,65,65,65	0
56	MG	2A	3221	1/1	0.98	0.10	-	48,48,48,48	0
56	MG	1A	3862	1/1	0.90	0.22	-	43,43,43,43	0
56	MG	2A	3195	1/1	0.86	0.21	-	56,56,56,56	0
56	MG	2A	3630	1/1	0.93	0.16	-	69,69,69,69	0
56	MG	1A	3901	1/1	0.90	0.21	-	43,43,43,43	0
56	MG	2a	3160	1/1	0.91	0.09	-	49,49,49,49	0
56	MG	2x	104	1/1	0.92	0.24	-	60,60,60,60	0
56	MG	2A	3806	1/1	0.93	0.11	-	66,66,66,66	0
56	MG	2a	3197	1/1	0.82	0.09	-	69,69,69,69	0
56	MG	1A	3847	1/1	0.93	0.09	-	48,48,48,48	0
56	MG	10	105	1/1	0.90	0.17	-	70,70,70,70	0
56	MG	2a	3058	1/1	0.83	0.20	-	73,73,73,73	0
56	MG	1f	3002	1/1	0.86	0.28	-	80,80,80,80	0
56	MG	2A	3286	1/1	0.88	0.20	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3077	1/1	0.86	0.15	-	45,45,45,45	0
56	MG	1A	3110	1/1	0.90	0.12	-	42,42,42,42	0
56	MG	2R	201	1/1	0.91	0.11	-	48,48,48,48	0
56	MG	1A	3554	1/1	0.92	0.28	-	47,47,47,47	0
56	MG	1a	1678	1/1	0.91	0.18	-	63,63,63,63	0
56	MG	1A	3543	1/1	0.97	0.17	-	73,73,73,73	0
56	MG	2A	3793	1/1	0.87	0.16	-	56,56,56,56	0
56	MG	2A	3250	1/1	0.96	0.11	-	41,41,41,41	0
56	MG	1w	111	1/1	0.93	0.17	-	41,41,41,41	0
56	MG	2A	3783	1/1	0.90	0.25	-	58,58,58,58	0
56	MG	2A	3384	1/1	0.90	0.17	-	62,62,62,62	0
56	MG	2A	3041	1/1	0.93	0.20	-	49,49,49,49	0
56	MG	1A	3401	1/1	0.92	0.21	-	35,35,35,35	0
56	MG	1A	3479	1/1	0.94	0.17	-	38,38,38,38	0
56	MG	1A	3461	1/1	0.89	0.31	-	44,44,44,44	0
56	MG	23	101	1/1	0.94	0.32	-	61,61,61,61	0
56	MG	1A	3300	1/1	0.94	0.18	-	61,61,61,61	0
56	MG	2A	3068	1/1	0.95	0.14	-	56,56,56,56	0
56	MG	1A	3353	1/1	0.83	0.32	-	64,64,64,64	0
56	MG	1A	3788	1/1	0.92	0.10	-	59,59,59,59	0
56	MG	2A	3045	1/1	0.92	0.15	-	58,58,58,58	0
56	MG	2A	3048	1/1	0.97	0.12	-	41,41,41,41	0
56	MG	2A	3412	1/1	0.91	0.30	-	59,59,59,59	0
56	MG	2A	3239	1/1	0.88	0.40	-	52,52,52,52	0
56	MG	2A	3076	1/1	0.96	0.27	-	35,35,35,35	0
56	MG	1a	1685	1/1	0.91	0.14	-	51,51,51,51	0
56	MG	1w	102	1/1	0.97	0.17	-	61,61,61,61	0
56	MG	2A	3757	1/1	0.90	0.12	-	52,52,52,52	0
56	MG	1A	3854	1/1	0.92	0.12	-	51,51,51,51	0
56	MG	1A	3536	1/1	0.96	0.17	-	37,37,37,37	0
56	MG	2A	3338	1/1	0.84	0.22	-	62,62,62,62	0
56	MG	2a	3108	1/1	0.81	0.21	-	78,78,78,78	0
56	MG	2A	3457	1/1	0.97	0.34	-	57,57,57,57	0
56	MG	2A	3033	1/1	0.85	0.18	-	42,42,42,42	0
56	MG	2A	3257	1/1	0.94	0.19	-	65,65,65,65	0
56	MG	2A	3799	1/1	0.92	0.41	-	68,68,68,68	0
56	MG	1D	307	1/1	0.87	0.16	-	45,45,45,45	0
56	MG	2A	3227	1/1	0.88	0.18	-	57,57,57,57	0
56	MG	1A	4070	1/1	0.95	0.13	-	56,56,56,56	0
56	MG	2g	8001	1/1	0.85	0.12	-	75,75,75,75	0
56	MG	1A	3098	1/1	0.97	0.18	-	25,25,25,25	0
56	MG	1A	4095	1/1	0.70	0.17	-	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3985	1/1	0.94	0.17	-	23,23,23,23	0
56	MG	1A	3976	1/1	0.72	0.14	-	72,72,72,72	0
56	MG	2A	3220	1/1	0.82	0.27	-	68,68,68,68	0
56	MG	2A	3234	1/1	0.88	0.14	-	52,52,52,52	0
56	MG	2A	3217	1/1	0.97	0.22	-	64,64,64,64	0
56	MG	2a	3223	1/1	0.97	0.16	-	52,52,52,52	0
56	MG	1a	1647	1/1	0.91	0.16	-	65,65,65,65	0
56	MG	2A	3744	1/1	0.93	0.15	-	55,55,55,55	0
56	MG	2A	3294	1/1	0.86	0.12	-	52,52,52,52	0
56	MG	1A	3586	1/1	0.91	0.22	-	49,49,49,49	0
56	MG	2a	3057	1/1	0.88	0.14	-	71,71,71,71	0
56	MG	1A	3679	1/1	0.86	0.25	-	39,39,39,39	0
56	MG	2a	3233	1/1	0.95	0.44	-	68,68,68,68	0
56	MG	2a	3055	1/1	0.92	0.07	-	51,51,51,51	0
56	MG	2A	3422	1/1	0.88	0.15	-	58,58,58,58	0
56	MG	1D	311	1/1	0.87	0.20	-	56,56,56,56	0
56	MG	2A	3306	1/1	0.94	0.12	-	58,58,58,58	0
56	MG	1A	3249	1/1	0.95	0.30	-	56,56,56,56	0
56	MG	1A	3712	1/1	0.97	0.08	-	40,40,40,40	0
56	MG	1A	3387	1/1	0.94	0.25	-	54,54,54,54	0
56	MG	1a	1770	1/1	0.96	0.10	-	60,60,60,60	0
56	MG	1x	111	1/1	0.96	0.12	-	66,66,66,66	0
56	MG	1A	3719	1/1	0.91	0.11	-	50,50,50,50	0
56	MG	1A	3335	1/1	0.88	0.36	-	62,62,62,62	0
56	MG	1A	3071	1/1	0.93	0.31	-	38,38,38,38	0
56	MG	1A	3568	1/1	0.92	0.26	-	50,50,50,50	0
56	MG	1A	3363	1/1	0.80	0.28	-	60,60,60,60	0
56	MG	2A	3155	1/1	0.91	0.12	-	59,59,59,59	0
56	MG	2A	3190	1/1	0.89	0.19	-	45,45,45,45	0
56	MG	2A	3106	1/1	0.97	0.09	-	59,59,59,59	0
56	MG	2a	3207	1/1	0.89	0.14	-	74,74,74,74	0
56	MG	2A	3006	1/1	0.90	0.23	-	56,56,56,56	0
56	MG	2A	3175	1/1	0.94	0.06	-	65,65,65,65	0
56	MG	1B	3004	1/1	0.91	0.29	-	50,50,50,50	0
56	MG	2A	3780	1/1	0.81	0.22	-	80,80,80,80	0
56	MG	1A	3409	1/1	0.96	0.23	-	60,60,60,60	0
56	MG	2A	3102	1/1	0.99	0.04	-	56,56,56,56	0
56	MG	1A	3283	1/1	0.95	0.17	-	40,40,40,40	0
56	MG	1A	4009	1/1	0.97	0.21	-	27,27,27,27	0
56	MG	1a	1642	1/1	0.81	0.10	-	67,67,67,67	0
56	MG	1A	3454	1/1	0.93	0.20	-	59,59,59,59	0
56	MG	1A	3962	1/1	0.78	0.17	-	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3228	1/1	0.96	0.18	-	65,65,65,65	0
56	MG	1A	3211	1/1	0.95	0.14	-	49,49,49,49	0
56	MG	1a	1782	1/1	0.71	0.17	-	79,79,79,79	0
56	MG	2a	3089	1/1	0.95	0.06	-	65,65,65,65	0
56	MG	2A	3212	1/1	0.87	0.13	-	52,52,52,52	0
56	MG	1A	4103	1/1	0.78	0.22	-	67,67,67,67	0
56	MG	1A	3490	1/1	0.93	0.11	-	50,50,50,50	0
56	MG	1a	1646	1/1	0.87	0.19	-	51,51,51,51	0
56	MG	2X	102	1/1	0.96	0.16	-	56,56,56,56	0
56	MG	1A	3611	1/1	0.98	0.23	-	25,25,25,25	0
56	MG	2A	3258	1/1	0.92	0.16	-	58,58,58,58	0
56	MG	1a	1705	1/1	0.92	0.18	-	63,63,63,63	0
56	MG	1A	3289	1/1	0.95	0.09	-	52,52,52,52	0
56	MG	1A	3736	1/1	0.96	0.15	-	46,46,46,46	0
56	MG	2a	3075	1/1	0.91	0.15	-	49,49,49,49	0
56	MG	2a	3162	1/1	0.96	0.08	-	62,62,62,62	0
56	MG	2A	3371	1/1	0.97	0.11	-	48,48,48,48	0
56	MG	2a	3134	1/1	0.96	0.15	-	64,64,64,64	0
56	MG	2a	3030	1/1	0.70	0.19	-	61,61,61,61	0
56	MG	2a	3026	1/1	0.66	0.17	-	64,64,64,64	0
56	MG	2A	3120	1/1	0.93	0.09	-	51,51,51,51	0
56	MG	2a	3166	1/1	0.58	0.13	-	84,84,84,84	0
56	MG	2A	3464	1/1	0.98	0.40	-	54,54,54,54	0
56	MG	1a	1694	1/1	0.88	0.11	-	58,58,58,58	0
56	MG	1A	3312	1/1	0.89	0.18	-	59,59,59,59	0
56	MG	1A	3827	1/1	0.95	0.25	-	50,50,50,50	0
56	MG	2A	3784	1/1	0.90	0.10	-	47,47,47,47	0
56	MG	1A	3786	1/1	0.18	0.32	-	81,81,81,81	0
56	MG	1A	3462	1/1	0.98	0.13	-	32,32,32,32	0
56	MG	1A	3502	1/1	0.94	0.26	-	49,49,49,49	0
56	MG	2a	3148	1/1	0.76	0.16	-	77,77,77,77	0
56	MG	2a	3126	1/1	0.90	0.09	-	69,69,69,69	0
56	MG	2A	3885	1/1	0.88	0.33	-	54,54,54,54	0
56	MG	2A	3875	1/1	0.88	0.50	-	76,76,76,76	0
56	MG	2A	3104	1/1	0.91	0.11	-	53,53,53,53	0
56	MG	2A	3275	1/1	0.83	0.19	-	58,58,58,58	0
56	MG	1A	3408	1/1	0.88	0.19	-	60,60,60,60	0
56	MG	2a	3093	1/1	0.82	0.15	-	64,64,64,64	0
56	MG	2a	3054	1/1	0.91	0.14	-	65,65,65,65	0
56	MG	1A	3258	1/1	0.90	0.17	-	33,33,33,33	0
56	MG	2E	307	1/1	0.78	0.13	-	54,54,54,54	0
56	MG	1A	3777	1/1	0.95	0.13	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3337	1/1	0.89	0.30	-	48,48,48,48	0
56	MG	20	3002	1/1	0.98	0.07	-	63,63,63,63	0
56	MG	1A	4046	1/1	0.95	0.13	-	30,30,30,30	0
56	MG	1S	3003	1/1	0.94	0.13	-	59,59,59,59	0
56	MG	2A	3357	1/1	0.98	0.10	-	39,39,39,39	0
56	MG	1A	3879	1/1	0.77	0.16	-	51,51,51,51	0
56	MG	2A	3751	1/1	0.94	0.12	-	61,61,61,61	0
56	MG	2A	3543	1/1	0.85	0.14	-	34,34,34,34	0
56	MG	2A	3337	1/1	0.90	0.09	-	47,47,47,47	0
56	MG	2A	3264	1/1	0.95	0.10	-	62,62,62,62	0
56	MG	2A	3318	1/1	0.93	0.15	-	48,48,48,48	0
56	MG	2A	3770	1/1	0.86	0.13	-	57,57,57,57	0
56	MG	2A	3247	1/1	0.84	0.12	-	51,51,51,51	0
56	MG	1a	1755	1/1	0.79	0.12	-	74,74,74,74	0
56	MG	1a	1750	1/1	0.94	0.10	-	85,85,85,85	0
56	MG	1A	3430	1/1	0.95	0.10	-	47,47,47,47	0
56	MG	1a	1640	1/1	0.95	0.05	-	58,58,58,58	0
56	MG	1A	3645	1/1	0.87	0.21	-	37,37,37,37	0
56	MG	1F	305	1/1	0.91	0.22	-	48,48,48,48	0
56	MG	2a	3109	1/1	0.92	0.20	-	67,67,67,67	0
56	MG	2A	3342	1/1	0.62	0.21	-	59,59,59,59	0
56	MG	2a	3242	1/1	0.95	0.20	-	55,55,55,55	0
56	MG	2A	3655	1/1	0.96	0.12	-	65,65,65,65	0
56	MG	2A	3272	1/1	0.89	0.18	-	51,51,51,51	0
56	MG	2A	3278	1/1	0.93	0.18	-	57,57,57,57	0
56	MG	2A	3431	1/1	0.92	0.14	-	62,62,62,62	0
56	MG	2A	3658	1/1	0.96	0.13	-	55,55,55,55	0
56	MG	2w	103	1/1	0.97	0.10	-	56,56,56,56	0
56	MG	1A	3520	1/1	0.97	0.25	-	41,41,41,41	0
56	MG	2a	3188	1/1	0.91	0.12	-	68,68,68,68	0
56	MG	1A	4030	1/1	0.93	0.12	-	44,44,44,44	0
56	MG	1A	4034	1/1	0.93	0.08	-	51,51,51,51	0
56	MG	2a	3078	1/1	0.91	0.27	-	74,74,74,74	0
56	MG	1a	1812	1/1	0.88	0.07	-	70,70,70,70	0
56	MG	1a	1748	1/1	0.97	0.11	-	43,43,43,43	0
56	MG	1A	3723	1/1	0.82	0.11	-	47,47,47,47	0
56	MG	1A	3330	1/1	0.88	0.28	-	50,50,50,50	0
56	MG	2w	106	1/1	0.93	0.12	-	60,60,60,60	0
56	MG	1A	3474	1/1	0.86	0.30	-	60,60,60,60	0
56	MG	2y	3004	1/1	0.93	0.19	-	59,59,59,59	0
56	MG	1A	3932	1/1	0.95	0.19	-	45,45,45,45	0
56	MG	2A	3394	1/1	0.89	0.32	-	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3192	1/1	0.90	0.19	-	52,52,52,52	0
56	MG	2A	3763	1/1	0.94	0.12	-	52,52,52,52	0
56	MG	2A	3794	1/1	0.93	0.09	-	67,67,67,67	0
56	MG	1A	3749	1/1	0.94	0.15	-	41,41,41,41	0
56	MG	2A	3018	1/1	0.90	0.24	-	44,44,44,44	0
56	MG	1A	3618	1/1	0.96	0.07	-	56,56,56,56	0
56	MG	1A	3798	1/1	0.86	0.09	-	63,63,63,63	0
56	MG	1A	3410	1/1	0.92	0.07	-	57,57,57,57	0
56	MG	1A	3368	1/1	0.93	0.29	-	47,47,47,47	0
56	MG	1A	3497	1/1	0.90	0.20	-	33,33,33,33	0
56	MG	2A	3400	1/1	0.92	0.25	-	56,56,56,56	0
56	MG	2A	3424	1/1	0.90	0.19	-	50,50,50,50	0
56	MG	1A	3324	1/1	0.89	0.25	-	55,55,55,55	0
56	MG	1A	3662	1/1	0.96	0.14	-	30,30,30,30	0
56	MG	1A	3297	1/1	0.98	0.29	-	32,32,32,32	0
56	MG	2A	3625	1/1	0.92	0.14	-	69,69,69,69	0
56	MG	1a	1686	1/1	0.88	0.09	-	54,54,54,54	0
56	MG	2A	3072	1/1	0.93	0.10	-	46,46,46,46	0
56	MG	2a	3138	1/1	0.76	0.24	-	79,79,79,79	0
56	MG	2A	3729	1/1	0.95	0.12	-	41,41,41,41	0
56	MG	1A	3344	1/1	0.81	0.27	-	64,64,64,64	0
56	MG	2a	3068	1/1	0.91	0.16	-	72,72,72,72	0
56	MG	2a	3178	1/1	0.84	0.22	-	75,75,75,75	0
56	MG	2A	3566	1/1	0.98	0.14	-	33,33,33,33	0
56	MG	10	106	1/1	0.87	0.16	-	65,65,65,65	0
56	MG	2A	3010	1/1	0.89	0.19	-	51,51,51,51	0
56	MG	1A	3556	1/1	0.97	0.33	-	42,42,42,42	0
56	MG	1A	3084	1/1	0.96	0.15	-	34,34,34,34	0
56	MG	1A	3227	1/1	0.88	0.29	-	42,42,42,42	0
56	MG	1a	1809	1/1	0.90	0.08	-	56,56,56,56	0
56	MG	1A	3392	1/1	0.87	0.27	-	56,56,56,56	0
56	MG	2A	3725	1/1	0.97	0.11	-	49,49,49,49	0
56	MG	1A	3092	1/1	0.94	0.21	-	50,50,50,50	0
56	MG	1A	3987	1/1	0.90	0.17	-	32,32,32,32	0
56	MG	2a	3064	1/1	0.90	0.10	-	81,81,81,81	0
56	MG	1A	3117	1/1	0.96	0.38	-	39,39,39,39	0
56	MG	2a	3206	1/1	0.92	0.17	-	69,69,69,69	0
56	MG	1A	3317	1/1	0.94	0.17	-	47,47,47,47	0
56	MG	2A	3311	1/1	0.92	0.12	-	63,63,63,63	0
56	MG	1A	4082	1/1	0.95	0.25	-	38,38,38,38	0
56	MG	2A	3124	1/1	0.94	0.10	-	48,48,48,48	0
56	MG	1A	3348	1/1	0.81	0.19	-	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3189	1/1	0.89	0.11	-	52,52,52,52	0
56	MG	1A	3372	1/1	0.87	0.24	-	58,58,58,58	0
56	MG	2A	3495	1/1	0.94	0.15	-	51,51,51,51	0
56	MG	1A	3734	1/1	0.85	0.13	-	59,59,59,59	0
56	MG	2A	3387	1/1	0.87	0.20	-	59,59,59,59	0
56	MG	2A	3069	1/1	0.93	0.15	-	40,40,40,40	0
56	MG	2A	3509	1/1	0.96	0.16	-	38,38,38,38	0
56	MG	2A	3750	1/1	0.96	0.26	-	47,47,47,47	0
56	MG	1A	3238	1/1	0.79	0.17	-	57,57,57,57	0
56	MG	2A	3667	1/1	0.81	0.12	-	49,49,49,49	0
56	MG	1a	1693	1/1	0.93	0.08	-	58,58,58,58	0
56	MG	2A	3208	1/1	0.83	0.14	-	57,57,57,57	0
56	MG	2A	3008	1/1	0.86	0.14	-	49,49,49,49	0
56	MG	2A	3413	1/1	0.80	0.17	-	56,56,56,56	0
56	MG	1A	3814	1/1	0.98	0.17	-	45,45,45,45	0
56	MG	1A	3511	1/1	0.86	0.16	-	45,45,45,45	0
56	MG	1A	3826	1/1	0.95	0.14	-	42,42,42,42	0
56	MG	1A	3027	1/1	0.99	0.20	-	33,33,33,33	0
56	MG	1A	3660	1/1	0.89	0.25	-	31,31,31,31	0
56	MG	2w	108	1/1	0.76	0.15	-	66,66,66,66	0
56	MG	1A	3424	1/1	0.92	0.33	-	70,70,70,70	0
56	MG	1A	3510	1/1	0.94	0.11	-	45,45,45,45	0
56	MG	1a	1702	1/1	0.67	0.28	-	73,73,73,73	0
56	MG	1A	3609	1/1	0.89	0.14	-	50,50,50,50	0
56	MG	1w	109	1/1	0.91	0.10	-	67,67,67,67	0
56	MG	1A	3600	1/1	0.90	0.13	-	46,46,46,46	0
56	MG	2B	3007	1/1	0.94	0.25	-	55,55,55,55	0
56	MG	1B	3009	1/1	0.91	0.16	-	43,43,43,43	0
56	MG	2A	3872	1/1	0.62	0.07	-	44,44,44,44	0
56	MG	2A	3612	1/1	0.93	0.07	-	39,39,39,39	0
56	MG	2a	3008	1/1	0.92	0.26	-	68,68,68,68	0
56	MG	1A	3445	1/1	0.77	0.18	-	62,62,62,62	0
56	MG	1A	3296	1/1	0.98	0.25	-	58,58,58,58	0
56	MG	1A	4049	1/1	0.80	0.13	-	55,55,55,55	0
56	MG	2a	3176	1/1	0.88	0.11	-	62,62,62,62	0
56	MG	2A	3700	1/1	0.83	0.19	-	65,65,65,65	0
56	MG	1a	1739	1/1	0.97	0.05	-	36,36,36,36	0
56	MG	1A	3732	1/1	0.94	0.23	-	64,64,64,64	0
56	MG	1A	3795	1/1	0.73	0.23	-	51,51,51,51	0
56	MG	13	102	1/1	0.90	0.24	-	53,53,53,53	0
56	MG	1A	3204	1/1	0.95	0.27	-	26,26,26,26	0
56	MG	1a	1676	1/1	0.74	0.18	-	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	18	102	1/1	0.95	0.30	-	50,50,50,50	0
56	MG	2B	3018	1/1	0.94	0.18	-	65,65,65,65	0
56	MG	1A	3835	1/1	0.91	0.18	-	59,59,59,59	0
56	MG	1A	4134	1/1	0.92	0.32	-	46,46,46,46	0
56	MG	1A	4021	1/1	0.79	0.23	-	66,66,66,66	0
56	MG	1A	4131	1/1	0.93	0.19	-	58,58,58,58	0
56	MG	1A	3503	1/1	0.94	0.17	-	32,32,32,32	0
56	MG	1A	3293	1/1	0.96	0.25	-	50,50,50,50	0
56	MG	1A	3928	1/1	0.95	0.20	-	31,31,31,31	0
56	MG	2y	3003	1/1	0.95	0.11	-	70,70,70,70	0
56	MG	1A	3220	1/1	0.97	0.23	-	41,41,41,41	0
56	MG	2A	3494	1/1	0.96	0.27	-	50,50,50,50	0
56	MG	2A	3352	1/1	0.99	0.14	-	53,53,53,53	0
56	MG	2A	3137	1/1	0.95	0.09	-	42,42,42,42	0
56	MG	1A	3369	1/1	0.98	0.19	-	57,57,57,57	0
56	MG	1A	3050	1/1	0.98	0.28	-	32,32,32,32	0
56	MG	2A	3453	1/1	0.65	0.15	-	45,45,45,45	0
56	MG	1A	3875	1/1	0.27	0.24	-	60,60,60,60	0
56	MG	1A	3282	1/1	0.94	0.17	-	30,30,30,30	0
56	MG	1A	3003	1/1	0.98	0.15	-	27,27,27,27	0
56	MG	1A	3048	1/1	0.96	0.20	-	48,48,48,48	0
56	MG	2A	3820	1/1	0.98	0.07	-	49,49,49,49	0
56	MG	2A	3133	1/1	0.95	0.11	-	49,49,49,49	0
56	MG	1a	1602	1/1	0.95	0.10	-	72,72,72,72	0
56	MG	1A	3431	1/1	0.91	0.13	-	52,52,52,52	0
56	MG	1a	1621	1/1	0.94	0.15	-	42,42,42,42	0
56	MG	2A	3491	1/1	0.95	0.30	-	55,55,55,55	0
56	MG	1A	3633	1/1	0.98	0.16	-	58,58,58,58	0
56	MG	2A	3537	1/1	0.96	0.12	-	35,35,35,35	0
56	MG	1A	3958	1/1	0.94	0.10	-	44,44,44,44	0
56	MG	1A	3513	1/1	0.73	0.16	-	62,62,62,62	0
56	MG	1A	3316	1/1	0.91	0.19	-	58,58,58,58	0
56	MG	1a	1663	1/1	0.81	0.15	-	76,76,76,76	0
56	MG	1x	114	1/1	0.87	0.10	-	82,82,82,82	0
56	MG	1A	3341	1/1	0.93	0.30	-	55,55,55,55	0
56	MG	1A	3802	1/1	0.90	0.13	-	57,57,57,57	0
56	MG	1A	3747	1/1	0.84	0.21	-	53,53,53,53	0
56	MG	1A	4125	1/1	0.92	0.34	-	54,54,54,54	0
56	MG	2a	3123	1/1	0.96	0.10	-	54,54,54,54	0
56	MG	2a	3239	1/1	0.92	0.14	-	65,65,65,65	0
56	MG	2a	3065	1/1	0.85	0.24	-	57,57,57,57	0
56	MG	2a	3104	1/1	0.74	0.19	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	4017	1/1	0.97	0.20	-	36,36,36,36	0
56	MG	2A	3285	1/1	0.93	0.12	-	49,49,49,49	0
56	MG	1A	3540	1/1	0.85	0.29	-	52,52,52,52	0
56	MG	2a	3235	1/1	0.93	0.06	-	71,71,71,71	0
56	MG	1A	4018	1/1	0.89	0.15	-	67,67,67,67	0
56	MG	1A	3197	1/1	0.98	0.19	-	52,52,52,52	0
56	MG	2A	3544	1/1	0.85	0.12	-	42,42,42,42	0
56	MG	1a	1636	1/1	0.81	0.21	-	67,67,67,67	0
56	MG	1A	3099	1/1	0.91	0.13	-	44,44,44,44	0
56	MG	1A	3259	1/1	0.90	0.16	-	40,40,40,40	0
56	MG	1P	201	1/1	0.96	0.13	-	26,26,26,26	0
56	MG	2A	3536	1/1	0.88	0.14	-	51,51,51,51	0
56	MG	1A	3674	1/1	0.90	0.16	-	39,39,39,39	0
56	MG	2a	3174	1/1	0.88	0.35	-	69,69,69,69	0
56	MG	1A	4135	1/1	0.90	0.23	-	44,44,44,44	0
56	MG	1A	3305	1/1	0.91	0.33	-	55,55,55,55	0
56	MG	2A	3317	1/1	0.88	0.13	-	55,55,55,55	0
56	MG	1I	3001	1/1	0.89	0.11	-	70,70,70,70	0
56	MG	1a	1623	1/1	0.92	0.14	-	60,60,60,60	0
56	MG	2a	3158	1/1	0.90	0.12	-	52,52,52,52	0
56	MG	1a	1732	1/1	0.96	0.16	-	48,48,48,48	0
56	MG	2A	3598	1/1	0.96	0.15	-	48,48,48,48	0
56	MG	1a	1610	1/1	0.84	0.46	-	79,79,79,79	0
56	MG	1A	3936	1/1	0.94	0.11	-	31,31,31,31	0
56	MG	1A	3067	1/1	0.98	0.18	-	51,51,51,51	0
56	MG	1A	3434	1/1	0.94	0.14	-	48,48,48,48	0
56	MG	1a	1695	1/1	0.95	0.15	-	68,68,68,68	0
56	MG	1A	3191	1/1	0.93	0.20	-	42,42,42,42	0
56	MG	1A	4036	1/1	0.91	0.08	-	43,43,43,43	0
56	MG	1A	4057	1/1	0.96	0.19	-	40,40,40,40	0
56	MG	1A	3853	1/1	0.79	0.10	-	52,52,52,52	0
56	MG	1A	3156	1/1	0.96	0.22	-	40,40,40,40	0
56	MG	1A	3564	1/1	0.90	0.19	-	40,40,40,40	0
56	MG	1A	3019	1/1	0.91	0.22	-	37,37,37,37	0
56	MG	2B	3012	1/1	0.96	0.23	-	55,55,55,55	0
56	MG	1A	3374	1/1	0.94	0.15	-	55,55,55,55	0
56	MG	2A	3773	1/1	0.93	0.05	-	63,63,63,63	0
56	MG	2A	3313	1/1	0.88	0.22	-	64,64,64,64	0
56	MG	2A	3101	1/1	0.79	0.15	-	59,59,59,59	0
56	MG	2A	3379	1/1	0.95	0.21	-	53,53,53,53	0
56	MG	2A	3589	1/1	0.91	0.09	-	45,45,45,45	0
56	MG	1A	3332	1/1	0.83	0.32	-	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3375	1/1	0.97	0.18	-	43,43,43,43	0
56	MG	1A	3085	1/1	0.99	0.26	-	30,30,30,30	0
56	MG	1a	1749	1/1	0.93	0.15	-	45,45,45,45	0
56	MG	1A	3993	1/1	0.95	0.14	-	37,37,37,37	0
56	MG	1Z	302	1/1	0.78	0.16	-	67,67,67,67	0
56	MG	2a	3036	1/1	0.85	0.18	-	83,83,83,83	0
56	MG	2A	3314	1/1	0.87	0.18	-	47,47,47,47	0
56	MG	1W	201	1/1	0.77	0.38	-	57,57,57,57	0
56	MG	2A	3323	1/1	0.90	0.13	-	56,56,56,56	0
56	MG	2A	3611	1/1	0.97	0.16	-	62,62,62,62	0
56	MG	1A	3973	1/1	0.90	0.10	-	85,85,85,85	0
56	MG	1A	3157	1/1	0.90	0.19	-	53,53,53,53	0
56	MG	1A	4092	1/1	0.94	0.22	-	37,37,37,37	0
56	MG	2A	3663	1/1	0.95	0.05	-	64,64,64,64	0
56	MG	2a	3127	1/1	0.66	0.15	-	85,85,85,85	0
56	MG	1A	3214	1/1	0.94	0.09	-	42,42,42,42	0
56	MG	2A	3154	1/1	0.98	0.14	-	48,48,48,48	0
56	MG	2A	3237	1/1	0.98	0.15	-	39,39,39,39	0
56	MG	1A	3625	1/1	0.97	0.17	-	19,19,19,19	0
56	MG	1A	3665	1/1	0.91	0.10	-	60,60,60,60	0
56	MG	1A	3138	1/1	0.96	0.23	-	36,36,36,36	0
56	MG	1A	4020	1/1	0.91	0.11	-	53,53,53,53	0
56	MG	2A	3531	1/1	0.86	0.23	-	51,51,51,51	0
56	MG	1A	3004	1/1	0.94	0.19	-	34,34,34,34	0
56	MG	2A	3644	1/1	0.86	0.21	-	64,64,64,64	0
56	MG	1A	4014	1/1	0.95	0.08	-	34,34,34,34	0
56	MG	2A	3336	1/1	0.97	0.18	-	53,53,53,53	0
56	MG	1a	1808	1/1	0.91	0.09	-	53,53,53,53	0
56	MG	2A	3270	1/1	0.94	0.10	-	53,53,53,53	0
56	MG	1Y	502	1/1	0.85	0.22	-	59,59,59,59	0
56	MG	2a	3137	1/1	0.71	0.18	-	79,79,79,79	0
56	MG	1A	3250	1/1	0.86	0.21	-	49,49,49,49	0
56	MG	2a	3085	1/1	0.94	0.11	-	65,65,65,65	0
56	MG	2a	3129	1/1	0.89	0.10	-	59,59,59,59	0
56	MG	1A	3491	1/1	0.88	0.15	-	59,59,59,59	0
56	MG	2A	3553	1/1	0.90	0.14	-	71,71,71,71	0
56	MG	1A	3102	1/1	0.94	0.17	-	54,54,54,54	0
56	MG	2F	301	1/1	0.88	0.18	-	58,58,58,58	0
56	MG	1a	1698	1/1	0.91	0.07	-	52,52,52,52	0
56	MG	2A	3777	1/1	0.89	0.15	-	41,41,41,41	0
56	MG	1A	3783	1/1	0.87	0.22	-	34,34,34,34	0
56	MG	1A	3291	1/1	0.92	0.13	-	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	1680	1/1	0.88	0.09	-	64,64,64,64	0
56	MG	2A	3132	1/1	0.94	0.22	-	56,56,56,56	0
56	MG	1a	1661	1/1	0.81	0.14	-	70,70,70,70	0
56	MG	2A	3107	1/1	0.94	0.10	-	46,46,46,46	0
56	MG	1a	1635	1/1	0.62	0.13	-	75,75,75,75	0
56	MG	1A	3262	1/1	0.91	0.14	-	49,49,49,49	0
56	MG	1A	3064	1/1	0.97	0.20	-	53,53,53,53	0
56	MG	2A	3586	1/1	0.97	0.09	-	53,53,53,53	0
56	MG	2A	3365	1/1	0.88	0.11	-	56,56,56,56	0
56	MG	2A	3466	1/1	0.71	0.37	-	65,65,65,65	0
56	MG	1A	3844	1/1	0.95	0.17	-	54,54,54,54	0
56	MG	1A	4073	1/1	0.86	0.10	-	42,42,42,42	0
56	MG	2E	302	1/1	0.96	0.09	-	52,52,52,52	0
56	MG	2A	3315	1/1	0.89	0.22	-	54,54,54,54	0
56	MG	2A	3115	1/1	0.97	0.10	-	51,51,51,51	0
56	MG	2A	3406	1/1	0.74	0.27	-	55,55,55,55	0
56	MG	2A	3050	1/1	0.84	0.10	-	51,51,51,51	0
56	MG	2A	3296	1/1	0.97	0.20	-	45,45,45,45	0
56	MG	2A	3150	1/1	0.98	0.35	-	39,39,39,39	0
56	MG	2a	3063	1/1	0.66	0.15	-	74,74,74,74	0
56	MG	1A	3270	1/1	0.93	0.25	-	59,59,59,59	0
56	MG	1A	3340	1/1	0.92	0.27	-	58,58,58,58	0
56	MG	2A	3582	1/1	0.97	0.11	-	51,51,51,51	0
56	MG	2a	3056	1/1	0.84	0.14	-	63,63,63,63	0
56	MG	2A	3330	1/1	0.82	0.14	-	63,63,63,63	0
56	MG	1A	4069	1/1	0.92	0.12	-	42,42,42,42	0
56	MG	2a	3215	1/1	0.77	0.19	-	71,71,71,71	0
56	MG	1a	1793	1/1	0.95	0.25	-	82,82,82,82	0
56	MG	2A	3081	1/1	0.91	0.22	-	45,45,45,45	0
56	MG	1A	3256	1/1	0.95	0.10	-	57,57,57,57	0
56	MG	2A	3223	1/1	0.96	0.19	-	44,44,44,44	0
56	MG	1A	3244	1/1	0.93	0.21	-	49,49,49,49	0
56	MG	1a	1637	1/1	0.93	0.19	-	68,68,68,68	0
56	MG	1A	3261	1/1	0.79	0.25	-	55,55,55,55	0
56	MG	1A	3180	1/1	0.92	0.21	-	36,36,36,36	0
56	MG	2A	3719	1/1	0.93	0.20	-	57,57,57,57	0
56	MG	1A	3567	1/1	0.85	0.08	-	54,54,54,54	0
56	MG	1F	307	1/1	0.95	0.13	-	50,50,50,50	0
56	MG	1A	3899	1/1	0.96	0.16	-	52,52,52,52	0
56	MG	1a	1735	1/1	0.91	0.18	-	57,57,57,57	0
56	MG	1A	3949	1/1	0.63	0.13	-	63,63,63,63	0
56	MG	1A	3523	1/1	0.92	0.26	-	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3781	1/1	0.87	0.10	-	55,55,55,55	0
56	MG	1A	3081	1/1	0.95	0.18	-	34,34,34,34	0
56	MG	1A	3869	1/1	0.77	0.20	-	56,56,56,56	0
56	MG	2A	3017	1/1	0.92	0.24	-	52,52,52,52	0
56	MG	1A	3320	1/1	0.91	0.23	-	60,60,60,60	0
56	MG	1A	3438	1/1	0.84	0.21	-	50,50,50,50	0
56	MG	1B	3029	1/1	0.70	0.28	-	66,66,66,66	0
56	MG	1a	1788	1/1	0.65	0.10	-	69,69,69,69	0
56	MG	2i	8001	1/1	0.97	0.12	-	51,51,51,51	0
56	MG	1A	3425	1/1	0.88	0.17	-	55,55,55,55	0
56	MG	1A	3590	1/1	0.88	0.21	-	37,37,37,37	0
56	MG	1A	3175	1/1	0.96	0.21	-	40,40,40,40	0
56	MG	1A	3804	1/1	0.97	0.10	-	40,40,40,40	0
56	MG	2A	3243	1/1	0.87	0.10	-	52,52,52,52	0
56	MG	2A	3375	1/1	0.74	0.25	-	52,52,52,52	0
56	MG	1A	3531	1/1	0.82	0.16	-	67,67,67,67	0
56	MG	2a	3218	1/1	0.92	0.20	-	61,61,61,61	0
56	MG	2A	3403	1/1	0.84	0.18	-	60,60,60,60	0
56	MG	2a	3011	1/1	0.80	0.11	-	64,64,64,64	0
56	MG	1A	3671	1/1	0.62	0.27	-	67,67,67,67	0
56	MG	2A	3304	1/1	0.89	0.17	-	60,60,60,60	0
56	MG	2T	3003	1/1	0.92	0.13	-	63,63,63,63	0
56	MG	1A	3077	1/1	0.94	0.09	-	35,35,35,35	0
56	MG	1A	3299	1/1	0.90	0.20	-	61,61,61,61	0
56	MG	2A	3042	1/1	0.93	0.22	-	42,42,42,42	0
56	MG	1A	4050	1/1	0.98	0.23	-	32,32,32,32	0
56	MG	1I	101	1/1	0.93	0.13	-	38,38,38,38	0
56	MG	1a	1706	1/1	0.85	0.20	-	60,60,60,60	0
56	MG	2A	3255	1/1	0.88	0.15	-	59,59,59,59	0
56	MG	1a	1828	1/1	0.88	0.08	-	59,59,59,59	0
56	MG	1A	3889	1/1	0.91	0.25	-	60,60,60,60	0
56	MG	1G	3005	1/1	0.96	0.10	-	66,66,66,66	0
56	MG	1B	3020	1/1	0.91	0.22	-	82,82,82,82	0
56	MG	2A	3593	1/1	0.94	0.16	-	30,30,30,30	0
56	MG	1A	3990	1/1	0.78	0.16	-	52,52,52,52	0
56	MG	1a	1727	1/1	0.95	0.16	-	49,49,49,49	0
56	MG	2A	3871	1/1	-0.25	0.20	-	70,70,70,70	0
56	MG	2a	3100	1/1	0.93	0.06	-	69,69,69,69	0
56	MG	1A	3119	1/1	0.95	0.25	-	51,51,51,51	0
56	MG	2A	3867	1/1	0.69	0.11	-	64,64,64,64	0
56	MG	1a	1630	1/1	0.89	0.13	-	60,60,60,60	0
56	MG	1A	3133	1/1	0.94	0.19	-	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3833	1/1	0.92	0.14	-	55,55,55,55	0
56	MG	2A	3835	1/1	0.96	0.09	-	43,43,43,43	0
56	MG	1A	3773	1/1	0.96	0.07	-	41,41,41,41	0
56	MG	2a	3213	1/1	0.92	0.18	-	69,69,69,69	0
56	MG	1a	1675	1/1	0.82	0.13	-	60,60,60,60	0
56	MG	2a	3018	1/1	0.93	0.18	-	65,65,65,65	0
56	MG	2A	3661	1/1	0.87	0.20	-	56,56,56,56	0
56	MG	1A	3473	1/1	0.92	0.26	-	50,50,50,50	0
56	MG	2A	3649	1/1	0.95	0.09	-	69,69,69,69	0
56	MG	1A	3399	1/1	0.90	0.22	-	52,52,52,52	0
56	MG	1A	3858	1/1	0.89	0.13	-	30,30,30,30	0
56	MG	1A	3697	1/1	0.91	0.14	-	51,51,51,51	0
56	MG	2A	3123	1/1	0.92	0.10	-	56,56,56,56	0
56	MG	1O	201	1/1	0.96	0.11	-	63,63,63,63	0
56	MG	2A	3367	1/1	0.87	0.18	-	61,61,61,61	0
56	MG	2a	3110	1/1	0.88	0.08	-	73,73,73,73	0
56	MG	2A	3752	1/1	0.90	0.14	-	61,61,61,61	0
56	MG	2A	3850	1/1	0.60	0.10	-	59,59,59,59	0
56	MG	2A	3170	1/1	0.98	0.14	-	54,54,54,54	0
56	MG	2A	3288	1/1	0.94	0.11	-	49,49,49,49	0
56	MG	1A	3726	1/1	0.95	0.06	-	48,48,48,48	0
56	MG	2A	3043	1/1	0.94	0.12	-	53,53,53,53	0
56	MG	1A	3025	1/1	0.98	0.17	-	41,41,41,41	0
56	MG	1A	3442	1/1	0.94	0.27	-	56,56,56,56	0
56	MG	1a	1643	1/1	0.82	0.17	-	61,61,61,61	0
56	MG	1A	3342	1/1	0.90	0.25	-	57,57,57,57	0
56	MG	1A	3199	1/1	0.93	0.19	-	45,45,45,45	0
56	MG	2A	3199	1/1	0.98	0.18	-	50,50,50,50	0
56	MG	1A	3427	1/1	0.95	0.14	-	44,44,44,44	0
56	MG	1a	1616	1/1	0.96	0.12	-	55,55,55,55	0
56	MG	2a	3201	1/1	0.72	0.13	-	79,79,79,79	0
56	MG	1a	1824	1/1	0.89	0.13	-	73,73,73,73	0
56	MG	2A	3831	1/1	0.95	0.10	-	45,45,45,45	0
56	MG	1A	3864	1/1	0.97	0.15	-	35,35,35,35	0
56	MG	2A	3143	1/1	0.94	0.12	-	56,56,56,56	0
56	MG	2A	3411	1/1	0.93	0.17	-	53,53,53,53	0
56	MG	2A	3574	1/1	0.87	0.12	-	44,44,44,44	0
56	MG	1A	3759	1/1	0.94	0.18	-	24,24,24,24	0
56	MG	1a	1669	1/1	0.88	0.23	-	73,73,73,73	0
56	MG	2A	3091	1/1	0.63	0.14	-	60,60,60,60	0
56	MG	1x	104	1/1	0.78	0.18	-	72,72,72,72	0
56	MG	2A	3028	1/1	0.87	0.14	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3561	1/1	0.91	0.31	-	48,48,48,48	0
56	MG	1A	3825	1/1	0.90	0.12	-	57,57,57,57	0
56	MG	2A	3436	1/1	0.96	0.17	-	49,49,49,49	0
56	MG	1A	3841	1/1	0.98	0.15	-	27,27,27,27	0
56	MG	2a	3048	1/1	0.85	0.13	-	67,67,67,67	0
56	MG	1y	3004	1/1	0.58	0.15	-	86,86,86,86	0
56	MG	1A	3386	1/1	0.87	0.21	-	54,54,54,54	0
56	MG	1A	3420	1/1	0.90	0.26	-	55,55,55,55	0
56	MG	2A	3139	1/1	0.93	0.14	-	32,32,32,32	0
56	MG	1A	3486	1/1	0.94	0.19	-	42,42,42,42	0
56	MG	1S	3002	1/1	0.93	0.17	-	49,49,49,49	0
56	MG	2A	3236	1/1	0.94	0.07	-	53,53,53,53	0
56	MG	1A	3450	1/1	0.90	0.19	-	57,57,57,57	0
56	MG	2A	3828	1/1	0.81	0.13	-	80,80,80,80	0
56	MG	2a	3053	1/1	0.90	0.09	-	66,66,66,66	0
56	MG	1A	3505	1/1	0.89	0.14	-	47,47,47,47	0
56	MG	1A	3708	1/1	0.79	0.16	-	76,76,76,76	0
56	MG	2a	3035	1/1	0.84	0.12	-	63,63,63,63	0
56	MG	1A	3549	1/1	0.97	0.13	-	38,38,38,38	0
56	MG	1Y	503	1/1	0.92	0.15	-	78,78,78,78	0
56	MG	2A	3609	1/1	0.98	0.16	-	42,42,42,42	0
56	MG	1A	3212	1/1	0.98	0.37	-	32,32,32,32	0
56	MG	2A	3390	1/1	0.93	0.14	-	57,57,57,57	0
56	MG	2A	3503	1/1	0.85	0.13	-	58,58,58,58	0
56	MG	2A	3308	1/1	0.85	0.11	-	49,49,49,49	0
56	MG	1A	3714	1/1	0.94	0.18	-	46,46,46,46	0
56	MG	1A	3164	1/1	0.85	0.18	-	73,73,73,73	0
56	MG	2B	3015	1/1	0.98	0.19	-	50,50,50,50	0
56	MG	2A	3405	1/1	0.96	0.24	-	33,33,33,33	0
56	MG	2A	3813	1/1	0.78	0.11	-	48,48,48,48	0
56	MG	1a	1711	1/1	0.95	0.17	-	65,65,65,65	0
56	MG	1A	3850	1/1	0.94	0.18	-	53,53,53,53	0
56	MG	1E	307	1/1	0.85	0.19	-	70,70,70,70	0
56	MG	2A	3456	1/1	0.96	0.36	-	60,60,60,60	0
56	MG	1A	3818	1/1	0.92	0.18	-	57,57,57,57	0
56	MG	1a	1688	1/1	0.60	0.16	-	74,74,74,74	0
56	MG	2A	3245	1/1	0.85	0.37	-	59,59,59,59	0
56	MG	2A	3059	1/1	0.98	0.17	-	46,46,46,46	0
56	MG	1A	3429	1/1	0.89	0.15	-	48,48,48,48	0
56	MG	1w	106	1/1	0.81	0.18	-	74,74,74,74	0
56	MG	1A	3867	1/1	0.89	0.13	-	69,69,69,69	0
56	MG	2A	3383	1/1	0.91	0.16	-	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3168	1/1	0.97	0.14	-	42,42,42,42	0
56	MG	2v	3001	1/1	0.95	0.09	-	69,69,69,69	0
56	MG	1A	3860	1/1	0.98	0.18	-	47,47,47,47	0
56	MG	2A	3480	1/1	0.90	0.21	-	65,65,65,65	0
56	MG	1A	3572	1/1	0.90	0.12	-	55,55,55,55	0
56	MG	1A	4113	1/1	0.83	0.24	-	56,56,56,56	0
56	MG	2A	3599	1/1	0.93	0.18	-	51,51,51,51	0
56	MG	2A	3487	1/1	0.93	0.23	-	62,62,62,62	0
56	MG	1A	3321	1/1	0.94	0.34	-	51,51,51,51	0
56	MG	1A	3591	1/1	0.88	0.13	-	52,52,52,52	0
56	MG	2A	3507	1/1	0.89	0.14	-	64,64,64,64	0
56	MG	2A	3467	1/1	0.97	0.09	-	60,60,60,60	0
56	MG	2y	3006	1/1	0.88	0.07	-	86,86,86,86	0
56	MG	2A	3303	1/1	0.89	0.16	-	60,60,60,60	0
56	MG	2A	3114	1/1	0.97	0.18	-	55,55,55,55	0
56	MG	2a	3001	1/1	0.91	0.22	-	57,57,57,57	0
56	MG	1a	1682	1/1	0.92	0.27	-	66,66,66,66	0
56	MG	2A	3301	1/1	0.88	0.11	-	60,60,60,60	0
56	MG	1A	3154	1/1	0.87	0.55	-	51,51,51,51	0
56	MG	1A	3897	1/1	0.79	0.24	-	62,62,62,62	0
56	MG	2A	3086	1/1	0.95	0.21	-	44,44,44,44	0
56	MG	1A	3141	1/1	0.94	0.16	-	35,35,35,35	0
56	MG	1A	3604	1/1	0.92	0.14	-	65,65,65,65	0
56	MG	2a	3020	1/1	0.84	0.13	-	71,71,71,71	0
56	MG	2A	3225	1/1	0.88	0.13	-	62,62,62,62	0
56	MG	1A	3838	1/1	0.95	0.25	-	45,45,45,45	0
56	MG	2A	3074	1/1	0.74	0.11	-	73,73,73,73	0
56	MG	1a	1821	1/1	0.86	0.09	-	62,62,62,62	0
56	MG	2A	3164	1/1	0.97	0.25	-	53,53,53,53	0
56	MG	1a	1700	1/1	0.99	0.26	-	50,50,50,50	0
56	MG	1A	3687	1/1	0.95	0.18	-	31,31,31,31	0
56	MG	1A	3308	1/1	0.90	0.26	-	51,51,51,51	0
56	MG	1A	3106	1/1	0.96	0.19	-	25,25,25,25	0
56	MG	2A	3705	1/1	0.97	0.32	-	57,57,57,57	0
56	MG	1A	3477	1/1	0.98	0.25	-	48,48,48,48	0
56	MG	1A	3512	1/1	0.91	0.17	-	50,50,50,50	0
56	MG	15	103	1/1	0.87	0.10	-	61,61,61,61	0
56	MG	1A	3667	1/1	0.94	0.20	-	61,61,61,61	0
56	MG	2A	3326	1/1	0.86	0.10	-	64,64,64,64	0
56	MG	1A	3974	1/1	0.88	0.06	-	45,45,45,45	0
56	MG	2A	3683	1/1	0.95	0.12	-	62,62,62,62	0
56	MG	1A	3504	1/1	0.92	0.19	-	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1Q	206	1/1	0.91	0.12	-	54,54,54,54	0
56	MG	1A	3367	1/1	0.93	0.23	-	57,57,57,57	0
56	MG	1A	3828	1/1	0.99	0.21	-	34,34,34,34	0
56	MG	1A	3302	1/1	0.85	0.21	-	56,56,56,56	0
56	MG	1A	4040	1/1	0.68	0.14	-	60,60,60,60	0
56	MG	1A	3319	1/1	0.94	0.14	-	63,63,63,63	0
56	MG	1a	1785	1/1	0.98	0.09	-	55,55,55,55	0
56	MG	2A	3622	1/1	0.97	0.25	-	63,63,63,63	0
56	MG	2a	3221	1/1	0.86	0.13	-	60,60,60,60	0
56	MG	2A	3588	1/1	0.92	0.10	-	47,47,47,47	0
56	MG	2A	3591	1/1	0.88	0.06	-	50,50,50,50	0
56	MG	1A	3953	1/1	0.91	0.10	-	46,46,46,46	0
56	MG	2A	3360	1/1	0.84	0.12	-	63,63,63,63	0
56	MG	2A	3156	1/1	0.96	0.15	-	48,48,48,48	0
56	MG	1B	3037	1/1	0.96	0.15	-	40,40,40,40	0
56	MG	1A	3972	1/1	0.96	0.16	-	60,60,60,60	0
56	MG	1A	3761	1/1	0.86	0.09	-	51,51,51,51	0
56	MG	1a	1743	1/1	0.85	0.12	-	73,73,73,73	0
56	MG	1A	3822	1/1	0.97	0.16	-	48,48,48,48	0
56	MG	1A	4008	1/1	0.83	0.14	-	56,56,56,56	0
56	MG	2a	3051	1/1	0.78	0.18	-	69,69,69,69	0
56	MG	2A	3647	1/1	0.85	0.22	-	51,51,51,51	0
56	MG	1A	3223	1/1	0.98	0.14	-	32,32,32,32	0
56	MG	2A	3344	1/1	0.88	0.19	-	55,55,55,55	0
56	MG	1A	3720	1/1	0.92	0.17	-	53,53,53,53	0
56	MG	2a	3240	1/1	0.77	0.36	-	63,63,63,63	0
56	MG	1A	3329	1/1	0.93	0.15	-	43,43,43,43	0
56	MG	2a	3034	1/1	0.76	0.17	-	72,72,72,72	0
56	MG	1B	3012	1/1	0.91	0.18	-	55,55,55,55	0
56	MG	2A	3670	1/1	0.89	0.12	-	70,70,70,70	0
56	MG	1A	3334	1/1	0.93	0.26	-	56,56,56,56	0
56	MG	2A	3030	1/1	0.94	0.13	-	51,51,51,51	0
56	MG	2A	3839	1/1	0.72	0.12	-	45,45,45,45	0
56	MG	2a	3237	1/1	0.96	0.07	-	66,66,66,66	0
56	MG	1A	3396	1/1	0.88	0.14	-	47,47,47,47	0
56	MG	2D	305	1/1	0.84	0.20	-	50,50,50,50	0
56	MG	1w	107	1/1	0.93	0.18	-	67,67,67,67	0
56	MG	1a	1712	1/1	0.92	0.19	-	67,67,67,67	0
56	MG	2A	3100	1/1	0.76	0.14	-	57,57,57,57	0
56	MG	2a	3077	1/1	0.90	0.21	-	61,61,61,61	0
56	MG	1A	3364	1/1	0.91	0.19	-	64,64,64,64	0
56	MG	2A	3252	1/1	0.96	0.30	-	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	4025	1/1	0.58	0.13	-	77,77,77,77	0
56	MG	2A	3446	1/1	0.96	0.27	-	45,45,45,45	0
56	MG	1A	3615	1/1	0.94	0.16	-	25,25,25,25	0
56	MG	2A	3200	1/1	0.93	0.15	-	42,42,42,42	0
56	MG	1A	4038	1/1	0.95	0.07	-	45,45,45,45	0
56	MG	1B	3021	1/1	0.92	0.26	-	46,46,46,46	0
56	MG	2A	3209	1/1	0.85	0.14	-	61,61,61,61	0
56	MG	1A	3465	1/1	0.90	0.18	-	60,60,60,60	0
56	MG	1a	1813	1/1	0.94	0.12	-	58,58,58,58	0
56	MG	2A	3759	1/1	0.89	0.12	-	46,46,46,46	0
56	MG	1A	3898	1/1	0.92	0.19	-	50,50,50,50	0
56	MG	2A	3271	1/1	0.84	0.13	-	49,49,49,49	0
56	MG	2A	3414	1/1	0.89	0.20	-	59,59,59,59	0
56	MG	2A	3567	1/1	0.97	0.08	-	50,50,50,50	0
56	MG	1A	3977	1/1	0.94	0.34	-	56,56,56,56	0
56	MG	1A	3944	1/1	0.90	0.15	-	60,60,60,60	0
56	MG	1A	3142	1/1	0.97	0.24	-	23,23,23,23	0
56	MG	2A	3659	1/1	0.94	0.07	-	59,59,59,59	0
56	MG	1a	1720	1/1	0.94	0.12	-	67,67,67,67	0
56	MG	2A	3282	1/1	0.89	0.24	-	63,63,63,63	0
56	MG	1A	3740	1/1	0.96	0.17	-	28,28,28,28	0
56	MG	2A	3669	1/1	0.95	0.12	-	42,42,42,42	0
56	MG	1A	3870	1/1	0.94	0.12	-	39,39,39,39	0
56	MG	2A	3276	1/1	0.95	0.18	-	55,55,55,55	0
56	MG	1B	3017	1/1	0.96	0.31	-	50,50,50,50	0
56	MG	2A	3056	1/1	0.78	0.17	-	60,60,60,60	0
56	MG	2A	3811	1/1	0.81	0.10	-	47,47,47,47	0
56	MG	1A	3907	1/1	0.95	0.23	-	54,54,54,54	0
56	MG	1A	3706	1/1	0.97	0.23	-	40,40,40,40	0
56	MG	2A	3063	1/1	0.90	0.12	-	67,67,67,67	0
56	MG	2A	3717	1/1	0.84	0.15	-	39,39,39,39	0
56	MG	2A	3569	1/1	0.93	0.09	-	49,49,49,49	0
56	MG	1B	3015	1/1	0.96	0.18	-	58,58,58,58	0
56	MG	1a	1721	1/1	0.88	0.11	-	58,58,58,58	0
56	MG	1A	3148	1/1	0.95	0.63	-	48,48,48,48	0
56	MG	2A	3432	1/1	0.86	0.19	-	60,60,60,60	0
56	MG	1A	3384	1/1	0.86	0.22	-	57,57,57,57	0
56	MG	1A	4026	1/1	0.62	0.15	-	51,51,51,51	0
56	MG	1A	3834	1/1	0.63	0.34	-	69,69,69,69	0
56	MG	2A	3733	1/1	0.88	0.13	-	50,50,50,50	0
56	MG	2A	3157	1/1	0.97	0.14	-	58,58,58,58	0
56	MG	2A	3708	1/1	0.94	0.11	-	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	3025	1/1	0.97	0.18	-	57,57,57,57	0
56	MG	2A	3260	1/1	0.89	0.17	-	53,53,53,53	0
56	MG	2A	3386	1/1	0.92	0.13	-	63,63,63,63	0
56	MG	2A	3168	1/1	0.87	0.20	-	52,52,52,52	0
56	MG	2A	3621	1/1	0.96	0.09	-	51,51,51,51	0
56	MG	2A	3460	1/1	0.95	0.36	-	64,64,64,64	0
56	MG	2a	3083	1/1	0.75	0.21	-	72,72,72,72	0
56	MG	2A	3366	1/1	0.92	0.10	-	54,54,54,54	0
56	MG	1A	3648	1/1	0.86	0.12	-	55,55,55,55	0
56	MG	2a	3101	1/1	0.96	0.15	-	56,56,56,56	0
56	MG	17	101	1/1	0.93	0.22	-	54,54,54,54	0
56	MG	2A	3297	1/1	0.95	0.20	-	51,51,51,51	0
56	MG	2A	3198	1/1	0.94	0.14	-	61,61,61,61	0
56	MG	2A	3505	1/1	0.90	0.11	-	59,59,59,59	0
56	MG	2A	3506	1/1	0.95	0.25	-	31,31,31,31	0
56	MG	1a	1656	1/1	0.81	0.22	-	75,75,75,75	0
56	MG	1a	1772	1/1	0.93	0.13	-	39,39,39,39	0
56	MG	1x	106	1/1	0.91	0.22	-	63,63,63,63	0
56	MG	2A	3060	1/1	0.98	0.10	-	53,53,53,53	0
56	MG	2A	3755	1/1	0.96	0.14	-	50,50,50,50	0
56	MG	1a	1708	1/1	0.85	0.16	-	68,68,68,68	0
56	MG	2Q	3002	1/1	0.95	0.16	-	44,44,44,44	0
56	MG	2a	3140	1/1	0.81	0.06	-	57,57,57,57	0
56	MG	2E	303	1/1	0.92	0.12	-	49,49,49,49	0
56	MG	1A	4035	1/1	0.96	0.11	-	46,46,46,46	0
56	MG	1A	3339	1/1	0.97	0.14	-	51,51,51,51	0
56	MG	1B	3026	1/1	0.87	0.21	-	42,42,42,42	0
56	MG	2a	3112	1/1	0.91	0.10	-	54,54,54,54	0
56	MG	1A	3226	1/1	0.97	0.31	-	47,47,47,47	0
56	MG	1A	3537	1/1	0.83	0.24	-	49,49,49,49	0
56	MG	1A	3716	1/1	0.94	0.20	-	28,28,28,28	0
56	MG	2A	3497	1/1	0.94	0.12	-	63,63,63,63	0
56	MG	1A	3967	1/1	0.93	0.15	-	65,65,65,65	0
56	MG	2A	3109	1/1	0.96	0.15	-	37,37,37,37	0
56	MG	1a	1719	1/1	0.92	0.22	-	63,63,63,63	0
56	MG	23	102	1/1	0.95	0.21	-	48,48,48,48	0
56	MG	1A	3946	1/1	0.87	0.13	-	49,49,49,49	0
56	MG	2a	3005	1/1	0.70	0.12	-	75,75,75,75	0
56	MG	1A	3778	1/1	0.90	0.08	-	57,57,57,57	0
56	MG	1A	4100	1/1	0.96	0.16	-	47,47,47,47	0
56	MG	1A	3945	1/1	0.85	0.21	-	41,41,41,41	0
56	MG	2A	3146	1/1	0.95	0.15	-	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	4022	1/1	0.93	0.11	-	72,72,72,72	0
56	MG	1x	102	1/1	0.80	0.21	-	63,63,63,63	0
56	MG	2A	3262	1/1	0.93	0.16	-	57,57,57,57	0
56	MG	2A	3316	1/1	0.91	0.17	-	54,54,54,54	0
56	MG	1A	3266	1/1	0.93	0.22	-	52,52,52,52	0
56	MG	1B	3025	1/1	0.84	0.16	-	77,77,77,77	0
56	MG	1a	1736	1/1	0.96	0.12	-	57,57,57,57	0
56	MG	1A	3787	1/1	0.76	0.14	-	55,55,55,55	0
56	MG	1A	3583	1/1	0.95	0.37	-	42,42,42,42	0
56	MG	1A	4019	1/1	0.92	0.20	-	42,42,42,42	0
56	MG	1A	3639	1/1	0.89	0.23	-	41,41,41,41	0
56	MG	2A	3015	1/1	0.94	0.20	-	43,43,43,43	0
56	MG	2A	3482	1/1	0.86	0.16	-	63,63,63,63	0
56	MG	1A	3846	1/1	0.91	0.12	-	53,53,53,53	0
56	MG	2A	3202	1/1	0.85	0.26	-	56,56,56,56	0
56	MG	2A	3474	1/1	0.81	0.19	-	55,55,55,55	0
56	MG	20	3001	1/1	0.93	0.17	-	59,59,59,59	0
56	MG	1A	3163	1/1	0.94	0.29	-	52,52,52,52	0
56	MG	2A	3604	1/1	0.94	0.20	-	64,64,64,64	0
56	MG	1A	3964	1/1	0.97	0.15	-	45,45,45,45	0
56	MG	2A	3392	1/1	0.97	0.11	-	55,55,55,55	0
56	MG	1v	3001	1/1	0.82	0.13	-	77,77,77,77	0
56	MG	2A	3689	1/1	0.97	0.08	-	71,71,71,71	0
56	MG	18	103	1/1	0.23	0.17	-	72,72,72,72	0
56	MG	1s	101	1/1	0.90	0.17	-	65,65,65,65	0
56	MG	1A	3094	1/1	0.95	0.10	-	52,52,52,52	0
56	MG	1A	4088	1/1	0.47	0.07	-	57,57,57,57	0
56	MG	1A	3685	1/1	0.96	0.23	-	60,60,60,60	0
56	MG	1A	3911	1/1	0.89	0.10	-	65,65,65,65	0
56	MG	1A	3096	1/1	0.76	0.27	-	49,49,49,49	0
56	MG	2A	3369	1/1	0.94	0.07	-	47,47,47,47	0
56	MG	2A	3686	1/1	0.83	0.14	-	57,57,57,57	0
56	MG	2A	3469	1/1	0.94	0.11	-	55,55,55,55	0
56	MG	1A	3137	1/1	0.97	0.20	-	33,33,33,33	0
56	MG	1A	3146	1/1	0.97	0.16	-	36,36,36,36	0
56	MG	2A	3728	1/1	0.94	0.09	-	58,58,58,58	0
56	MG	2A	3617	1/1	0.88	0.12	-	38,38,38,38	0
56	MG	2A	3350	1/1	0.93	0.21	-	61,61,61,61	0
56	MG	2A	3749	1/1	0.92	0.11	-	48,48,48,48	0
56	MG	2A	3232	1/1	0.81	0.12	-	64,64,64,64	0
56	MG	2a	3164	1/1	0.94	0.21	-	73,73,73,73	0
56	MG	1A	3182	1/1	0.80	0.12	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3640	1/1	0.95	0.26	-	45,45,45,45	0
56	MG	1A	3253	1/1	0.76	0.21	-	61,61,61,61	0
56	MG	2A	3302	1/1	0.96	0.19	-	66,66,66,66	0
56	MG	2A	3118	1/1	0.89	0.13	-	50,50,50,50	0
56	MG	1A	3088	1/1	0.95	0.11	-	47,47,47,47	0
56	MG	1A	3124	1/1	0.90	0.22	-	44,44,44,44	0
56	MG	1A	3676	1/1	0.97	0.21	-	24,24,24,24	0
56	MG	2A	3229	1/1	0.89	0.10	-	41,41,41,41	0
56	MG	2A	3395	1/1	0.93	0.21	-	50,50,50,50	0
56	MG	1A	3201	1/1	0.92	0.24	-	45,45,45,45	0
56	MG	2a	3003	1/1	0.84	0.16	-	64,64,64,64	0
56	MG	2A	3462	1/1	0.90	0.27	-	59,59,59,59	0
56	MG	2A	3463	1/1	0.72	0.14	-	57,57,57,57	0
56	MG	1A	3819	1/1	0.94	0.11	-	48,48,48,48	0
56	MG	1A	3617	1/1	0.93	0.16	-	33,33,33,33	0
56	MG	2B	3019	1/1	0.79	0.12	-	76,76,76,76	0
56	MG	1A	3876	1/1	0.94	0.18	-	49,49,49,49	0
56	MG	1A	3224	1/1	0.97	0.19	-	50,50,50,50	0
56	MG	1A	3127	1/1	0.85	0.44	-	51,51,51,51	0
56	MG	2A	3632	1/1	0.92	0.13	-	41,41,41,41	0
56	MG	2B	3003	1/1	0.82	0.20	-	74,74,74,74	0
56	MG	2A	3435	1/1	0.98	0.07	-	49,49,49,49	0
56	MG	1A	3571	1/1	0.91	0.21	-	57,57,57,57	0
56	MG	2a	3029	1/1	0.84	0.15	-	67,67,67,67	0
56	MG	2A	3442	1/1	0.94	0.14	-	50,50,50,50	0
56	MG	2A	3801	1/1	0.92	0.27	-	64,64,64,64	0
56	MG	2A	3343	1/1	0.89	0.11	-	57,57,57,57	0
56	MG	2A	3595	1/1	0.97	0.11	-	49,49,49,49	0
56	MG	2A	3215	1/1	0.95	0.17	-	37,37,37,37	0
56	MG	2a	3037	1/1	0.91	0.38	-	77,77,77,77	0
56	MG	2A	3703	1/1	0.89	0.13	-	47,47,47,47	0
56	MG	2A	3331	1/1	0.95	0.18	-	56,56,56,56	0
56	MG	1A	4067	1/1	0.92	0.14	-	56,56,56,56	0
56	MG	2A	3528	1/1	0.96	0.34	-	57,57,57,57	0
56	MG	1A	3721	1/1	0.90	0.19	-	57,57,57,57	0
56	MG	2A	3300	1/1	0.93	0.14	-	55,55,55,55	0
56	MG	2A	3523	1/1	0.92	0.13	-	27,27,27,27	0
56	MG	2A	3477	1/1	0.92	0.34	-	56,56,56,56	0
56	MG	2A	3739	1/1	0.96	0.10	-	59,59,59,59	0
56	MG	2y	3001	1/1	0.90	0.18	-	59,59,59,59	0
56	MG	2A	3790	1/1	0.74	0.21	-	65,65,65,65	0
56	MG	1A	3690	1/1	0.97	0.14	-	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1a	1641	1/1	0.91	0.18	-	58,58,58,58	0
56	MG	2a	3228	1/1	0.69	0.11	-	86,86,86,86	0
56	MG	2A	3439	1/1	0.90	0.21	-	60,60,60,60	0
56	MG	2a	3087	1/1	0.91	0.08	-	63,63,63,63	0
56	MG	1A	3290	1/1	0.98	0.24	-	46,46,46,46	0
56	MG	1A	3792	1/1	0.88	0.14	-	35,35,35,35	0
56	MG	1A	3179	1/1	0.95	0.21	-	36,36,36,36	0
56	MG	2A	3309	1/1	0.83	0.13	-	53,53,53,53	0
56	MG	1A	3588	1/1	0.80	0.19	-	46,46,46,46	0
56	MG	1B	3016	1/1	0.86	0.16	-	54,54,54,54	0
56	MG	1A	3336	1/1	0.97	0.27	-	41,41,41,41	0
56	MG	2a	3179	1/1	0.47	0.50	-	100,100,100,100	0
56	MG	2A	3141	1/1	0.96	0.09	-	51,51,51,51	0
56	MG	2A	3767	1/1	0.95	0.09	-	56,56,56,56	0
56	MG	1A	3345	1/1	0.97	0.28	-	47,47,47,47	0
56	MG	1A	3428	1/1	0.88	0.16	-	51,51,51,51	0
56	MG	1A	3028	1/1	0.98	0.24	-	34,34,34,34	0
56	MG	2A	3782	1/1	0.94	0.08	-	51,51,51,51	0
56	MG	2A	3764	1/1	0.95	0.11	-	66,66,66,66	0
56	MG	2a	3022	1/1	0.85	0.09	-	72,72,72,72	0
56	MG	1Z	303	1/1	0.97	0.17	-	56,56,56,56	0
56	MG	1b	3002	1/1	0.85	0.17	-	61,61,61,61	0
56	MG	1A	3446	1/1	0.60	0.18	-	61,61,61,61	0
56	MG	1A	3134	1/1	0.90	0.32	-	54,54,54,54	0
56	MG	1A	3918	1/1	0.88	0.13	-	56,56,56,56	0
56	MG	1a	1762	1/1	0.89	0.13	-	78,78,78,78	0
56	MG	1B	3032	1/1	0.69	0.23	-	80,80,80,80	0
56	MG	2A	3791	1/1	0.91	0.21	-	46,46,46,46	0
56	MG	2Z	8001	1/1	0.89	0.07	-	78,78,78,78	0
56	MG	2a	3141	1/1	0.89	0.18	-	94,94,94,94	0
56	MG	2A	3368	1/1	0.94	0.06	-	47,47,47,47	0
56	MG	1A	3131	1/1	0.89	0.17	-	72,72,72,72	0
56	MG	1A	3416	1/1	0.93	0.17	-	47,47,47,47	0
56	MG	2a	3012	1/1	0.76	0.14	-	71,71,71,71	0
56	MG	1A	3739	1/1	0.93	0.18	-	39,39,39,39	0
56	MG	2A	3113	1/1	0.80	0.13	-	52,52,52,52	0
56	MG	2a	3116	1/1	0.87	0.08	-	67,67,67,67	0
56	MG	2a	3052	1/1	0.93	0.15	-	62,62,62,62	0
56	MG	1A	3529	1/1	0.96	0.19	-	43,43,43,43	0
56	MG	1A	3370	1/1	0.74	0.27	-	57,57,57,57	0
56	MG	1A	3959	1/1	0.94	0.14	-	56,56,56,56	0
56	MG	2A	3374	1/1	0.64	0.26	-	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2A	3084	1/1	0.93	0.10	-	45,45,45,45	0
56	MG	2A	3517	1/1	0.97	0.12	-	42,42,42,42	0
56	MG	2A	3525	1/1	0.98	0.13	-	34,34,34,34	0
56	MG	1A	3143	1/1	0.91	0.18	-	55,55,55,55	0
56	MG	1A	3406	1/1	0.93	0.29	-	47,47,47,47	0
56	MG	2A	3758	1/1	0.95	0.23	-	58,58,58,58	0
56	MG	1a	1627	1/1	0.89	0.14	-	55,55,55,55	0
56	MG	2A	3519	1/1	0.92	0.17	-	33,33,33,33	0
56	MG	1A	3743	1/1	0.90	0.22	-	60,60,60,60	0
56	MG	1A	3558	1/1	0.91	0.12	-	52,52,52,52	0
56	MG	1A	3233	1/1	0.95	0.13	-	49,49,49,49	0
56	MG	2A	3327	1/1	0.95	0.12	-	50,50,50,50	0
56	MG	1A	3895	1/1	0.96	0.14	-	61,61,61,61	0
56	MG	2A	3201	1/1	0.95	0.10	-	51,51,51,51	0
56	MG	1A	3566	1/1	0.86	0.31	-	72,72,72,72	0
56	MG	1A	3487	1/1	0.82	0.23	-	70,70,70,70	0
56	MG	2W	203	1/1	0.84	0.25	-	59,59,59,59	0
56	MG	2A	3558	1/1	0.93	0.17	-	31,31,31,31	0
56	MG	1a	1648	1/1	0.89	0.16	-	59,59,59,59	0
56	MG	2B	3002	1/1	0.88	0.11	-	49,49,49,49	0
56	MG	2a	3194	1/1	0.94	0.11	-	68,68,68,68	0
56	MG	2a	3067	1/1	0.93	0.15	-	65,65,65,65	0
56	MG	1A	3186	1/1	0.96	0.32	-	39,39,39,39	0
56	MG	1A	4044	1/1	0.64	0.25	-	79,79,79,79	0
56	MG	2A	3049	1/1	0.99	0.16	-	23,23,23,23	0
56	MG	1A	3093	1/1	0.91	0.22	-	33,33,33,33	0
56	MG	2A	3171	1/1	0.90	0.12	-	38,38,38,38	0
56	MG	1A	3469	1/1	0.92	0.23	-	53,53,53,53	0
56	MG	2a	3004	1/1	0.82	0.16	-	57,57,57,57	0
56	MG	2A	3787	1/1	0.90	0.04	-	64,64,64,64	0
56	MG	1A	3551	1/1	0.96	0.16	-	37,37,37,37	0
56	MG	2a	3133	1/1	0.96	0.13	-	54,54,54,54	0
56	MG	1A	3884	1/1	0.92	0.09	-	48,48,48,48	0
56	MG	2A	3351	1/1	0.92	0.11	-	54,54,54,54	0
56	MG	1A	3724	1/1	0.90	0.21	-	58,58,58,58	0
56	MG	1A	3989	1/1	0.57	0.08	-	60,60,60,60	0
56	MG	2a	3181	1/1	0.56	0.10	-	69,69,69,69	0
56	MG	1A	4023	1/1	0.98	0.14	-	47,47,47,47	0
56	MG	2a	3209	1/1	0.97	0.14	-	77,77,77,77	0
56	MG	1A	3601	1/1	0.99	0.18	-	11,11,11,11	0
56	MG	2A	3809	1/1	0.91	0.08	-	59,59,59,59	0
56	MG	1a	1631	1/1	0.89	0.24	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	2a	3132	1/1	0.95	0.21	-	63,63,63,63	0
56	MG	2a	3231	1/1	0.83	0.11	-	68,68,68,68	0
56	MG	1A	3006	1/1	0.80	0.33	-	57,57,57,57	0
56	MG	2A	3664	1/1	0.96	0.15	-	54,54,54,54	0
56	MG	2A	3691	1/1	0.73	0.31	-	68,68,68,68	0
56	MG	1B	3007	1/1	0.51	0.25	-	85,85,85,85	0
56	MG	2A	3009	1/1	0.98	0.13	-	31,31,31,31	0
56	MG	2a	3073	1/1	0.92	0.12	-	66,66,66,66	0
56	MG	2A	3654	1/1	0.96	0.09	-	62,62,62,62	0
56	MG	2A	3012	1/1	0.96	0.13	-	39,39,39,39	0
56	MG	1A	4031	1/1	0.82	0.15	-	54,54,54,54	0
56	MG	1E	301	1/1	0.94	0.19	-	37,37,37,37	0
56	MG	13	103	1/1	0.92	0.21	-	47,47,47,47	0
56	MG	2A	3662	1/1	0.91	0.12	-	48,48,48,48	0
56	MG	2A	3842	1/1	0.95	0.14	-	59,59,59,59	0
56	MG	1A	3061	1/1	0.94	0.35	-	62,62,62,62	0
56	MG	2A	3219	1/1	0.93	0.20	-	51,51,51,51	0
56	MG	1a	1722	1/1	0.84	0.08	-	65,65,65,65	0
56	MG	1a	1609	1/1	0.97	0.11	-	54,54,54,54	0
56	MG	1a	1710	1/1	0.84	0.13	-	77,77,77,77	0
56	MG	1A	3682	1/1	0.92	0.21	-	35,35,35,35	0
56	MG	2a	3172	1/1	0.94	0.09	-	66,66,66,66	0
56	MG	2A	3341	1/1	0.79	0.11	-	52,52,52,52	0
56	MG	2A	3838	1/1	0.96	0.16	-	47,47,47,47	0
56	MG	2A	3373	1/1	0.92	0.06	-	52,52,52,52	0
56	MG	2a	3124	1/1	0.98	0.13	-	61,61,61,61	0
56	MG	1A	3286	1/1	0.99	0.41	-	49,49,49,49	0
56	MG	2A	3087	1/1	0.81	0.20	-	53,53,53,53	0
56	MG	1A	3943	1/1	0.94	0.19	-	81,81,81,81	0
56	MG	1A	3005	1/1	0.95	0.16	-	41,41,41,41	0
56	MG	2A	3646	1/1	0.88	0.15	-	55,55,55,55	0
56	MG	2a	3236	1/1	0.82	0.13	-	75,75,75,75	0
56	MG	2A	3263	1/1	0.95	0.13	-	55,55,55,55	0
56	MG	1A	3383	1/1	0.91	0.16	-	55,55,55,55	0
56	MG	1A	3485	1/1	0.93	0.18	-	48,48,48,48	0
56	MG	1a	1690	1/1	0.94	0.14	-	70,70,70,70	0
56	MG	1X	105	1/1	0.89	0.13	-	47,47,47,47	0
56	MG	2a	3013	1/1	0.75	0.11	-	78,78,78,78	0
56	MG	1A	3129	1/1	0.86	0.23	-	51,51,51,51	0
56	MG	2a	3185	1/1	0.96	0.15	-	47,47,47,47	0
56	MG	2A	3222	1/1	0.95	0.16	-	38,38,38,38	0
56	MG	1A	3118	1/1	0.93	0.22	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3385	1/1	0.93	0.15	-	58,58,58,58	0
56	MG	2A	3592	1/1	0.97	0.20	-	57,57,57,57	0
56	MG	2A	3696	1/1	0.78	0.13	-	58,58,58,58	0
56	MG	1X	106	1/1	0.96	0.19	-	29,29,29,29	0
56	MG	2A	3125	1/1	0.96	0.16	-	44,44,44,44	0
56	MG	1A	3149	1/1	0.91	0.15	-	33,33,33,33	0
56	MG	1A	3069	1/1	0.98	0.25	-	20,20,20,20	0
56	MG	1A	3544	1/1	0.91	0.17	-	47,47,47,47	0
56	MG	2A	3224	1/1	0.88	0.22	-	52,52,52,52	0
56	MG	2A	3785	1/1	0.97	0.26	-	45,45,45,45	0
56	MG	1A	3207	1/1	0.81	0.28	-	54,54,54,54	0
56	MG	2A	3380	1/1	0.83	0.12	-	55,55,55,55	0
56	MG	2A	3355	1/1	0.93	0.10	-	51,51,51,51	0
56	MG	1a	1703	1/1	0.92	0.27	-	55,55,55,55	0
56	MG	2A	3795	1/1	0.76	0.11	-	37,37,37,37	0
56	MG	1A	3361	1/1	0.84	0.11	-	49,49,49,49	0
56	MG	2A	3498	1/1	0.90	0.11	-	55,55,55,55	0
56	MG	1A	3970	1/1	0.42	0.13	-	70,70,70,70	0
56	MG	2x	102	1/1	0.52	0.17	-	77,77,77,77	0
56	MG	2A	3002	1/1	0.97	0.30	-	57,57,57,57	0
56	MG	2j	8001	1/1	0.86	0.09	-	75,75,75,75	0
56	MG	1B	3002	1/1	0.80	0.33	-	58,58,58,58	0
56	MG	1A	3978	1/1	0.83	0.08	-	65,65,65,65	0
56	MG	1a	1820	1/1	0.93	0.08	-	57,57,57,57	0
56	MG	2A	3022	1/1	0.94	0.27	-	47,47,47,47	0
56	MG	2A	3802	1/1	0.84	0.13	-	56,56,56,56	0
56	MG	2A	3273	1/1	0.95	0.14	-	51,51,51,51	0
56	MG	10	104	1/1	0.83	0.30	-	64,64,64,64	0
56	MG	1a	1604	1/1	0.91	0.11	-	58,58,58,58	0
56	MG	1A	3045	1/1	0.96	0.20	-	36,36,36,36	0
56	MG	2A	3064	1/1	0.92	0.13	-	51,51,51,51	0
56	MG	1A	4048	1/1	0.85	0.08	-	48,48,48,48	0
56	MG	2A	3653	1/1	0.96	0.18	-	58,58,58,58	0
56	MG	2A	3766	1/1	0.80	0.11	-	52,52,52,52	0
56	MG	1A	3711	1/1	0.78	0.15	-	61,61,61,61	0
56	MG	1A	3589	1/1	0.95	0.23	-	52,52,52,52	0
56	MG	1a	1733	1/1	0.93	0.14	-	58,58,58,58	0
56	MG	2A	3546	1/1	0.78	0.12	-	44,44,44,44	0
56	MG	1A	3111	1/1	0.98	0.15	-	40,40,40,40	0
56	MG	1A	4087	1/1	0.90	0.21	-	54,54,54,54	0
56	MG	2a	3120	1/1	0.70	0.19	-	72,72,72,72	0
56	MG	1A	3333	1/1	0.85	0.11	-	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3563	1/1	0.96	0.26	-	43,43,43,43	0
56	MG	1A	3397	1/1	0.90	0.23	-	47,47,47,47	0
56	MG	1A	3848	1/1	0.92	0.14	-	56,56,56,56	0
56	MG	1U	201	1/1	0.88	0.18	-	52,52,52,52	0
56	MG	1A	4065	1/1	0.91	0.18	-	51,51,51,51	0
56	MG	1A	3553	1/1	0.91	0.26	-	49,49,49,49	0
56	MG	2A	3178	1/1	0.93	0.24	-	57,57,57,57	0
56	MG	1A	3762	1/1	0.91	0.12	-	60,60,60,60	0
56	MG	2A	3483	1/1	0.95	0.16	-	55,55,55,55	0
56	MG	1A	3592	1/1	0.96	0.20	-	21,21,21,21	0
56	MG	2A	3695	1/1	0.98	0.09	-	38,38,38,38	0
56	MG	2A	3047	1/1	0.91	0.16	-	46,46,46,46	0
56	MG	1B	3035	1/1	0.95	0.11	-	59,59,59,59	0
56	MG	2A	3319	1/1	0.99	0.07	-	49,49,49,49	0
56	MG	2A	3596	1/1	0.87	0.11	-	47,47,47,47	0
56	MG	1a	1796	1/1	0.96	0.06	-	59,59,59,59	0
56	MG	1A	3393	1/1	0.98	0.18	-	50,50,50,50	0
56	MG	2A	3447	1/1	0.92	0.28	-	46,46,46,46	0
56	MG	1A	3215	1/1	0.95	0.06	-	65,65,65,65	0
56	MG	2A	3147	1/1	0.85	0.29	-	58,58,58,58	0
56	MG	2A	3259	1/1	0.78	0.15	-	61,61,61,61	0
56	MG	2A	3628	1/1	0.87	0.07	-	52,52,52,52	0
56	MG	2E	301	1/1	0.94	0.17	-	50,50,50,50	0
56	MG	1A	3044	1/1	0.93	0.20	-	37,37,37,37	0
56	MG	2A	3349	1/1	0.95	0.87	-	58,58,58,58	0
56	MG	2a	3102	1/1	0.98	0.14	-	58,58,58,58	0
56	MG	2A	3822	1/1	0.83	0.11	-	66,66,66,66	0
56	MG	1A	3547	1/1	0.98	0.14	-	53,53,53,53	0
56	MG	1B	3033	1/1	0.93	0.17	-	56,56,56,56	0
56	MG	2A	3174	1/1	0.94	0.15	-	53,53,53,53	0
56	MG	1A	3924	1/1	0.95	0.09	-	50,50,50,50	0
56	MG	2A	3710	1/1	0.85	0.14	-	63,63,63,63	0
56	MG	2a	3061	1/1	0.94	0.20	-	54,54,54,54	0
56	MG	2A	3430	1/1	0.89	0.10	-	51,51,51,51	0
56	MG	2A	3563	1/1	0.93	0.14	-	49,49,49,49	0
56	MG	1A	3517	1/1	0.98	0.14	-	37,37,37,37	0
56	MG	1A	3992	1/1	0.79	0.24	-	75,75,75,75	0
56	MG	1A	3444	1/1	0.96	0.22	-	63,63,63,63	0
56	MG	2A	3887	1/1	0.94	0.08	-	48,48,48,48	0
56	MG	1a	1797	1/1	0.93	0.13	-	64,64,64,64	0
56	MG	2A	3502	1/1	0.91	0.09	-	43,43,43,43	0
56	MG	12	101	1/1	0.88	0.21	-	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	MG	1A	3246	1/1	0.90	0.31	-	58,58,58,58	0
56	MG	1A	3390	1/1	0.87	0.18	-	35,35,35,35	0
56	MG	1A	3986	1/1	0.93	0.24	-	22,22,22,22	0
56	MG	1A	3969	1/1	0.69	0.14	-	66,66,66,66	0
56	MG	2A	3396	1/1	0.93	0.09	-	56,56,56,56	0
56	MG	2A	3642	1/1	0.80	0.18	-	47,47,47,47	0
56	MG	1a	1605	1/1	0.75	0.17	-	65,65,65,65	0
56	MG	1A	3760	1/1	0.95	0.22	-	35,35,35,35	0
56	MG	2A	3029	1/1	0.81	0.22	-	44,44,44,44	0
56	MG	1A	3470	1/1	0.92	0.17	-	47,47,47,47	0
56	MG	1E	306	1/1	0.88	0.15	-	31,31,31,31	0
56	MG	1A	3684	1/1	0.97	0.27	-	32,32,32,32	0
56	MG	1A	3534	1/1	0.97	0.18	-	33,33,33,33	0
56	MG	2A	3129	1/1	0.91	0.14	-	50,50,50,50	0
56	MG	2a	3125	1/1	0.95	0.10	-	65,65,65,65	0
56	MG	1A	3251	1/1	0.79	0.10	-	58,58,58,58	0
56	MG	2a	3023	1/1	0.95	0.08	-	47,47,47,47	0
56	MG	2A	3427	1/1	0.98	0.13	-	45,45,45,45	0
56	MG	1A	3493	1/1	0.95	0.20	-	36,36,36,36	0
56	MG	1a	1644	1/1	0.92	0.15	-	66,66,66,66	0
56	MG	1A	3279	1/1	0.91	0.17	-	38,38,38,38	0
56	MG	1A	3423	1/1	0.79	0.30	-	67,67,67,67	0
56	MG	2A	3826	1/1	0.86	0.11	-	54,54,54,54	0
56	MG	1A	3113	1/1	0.96	0.14	-	35,35,35,35	0
56	MG	2A	3176	1/1	0.95	0.13	-	46,46,46,46	0
56	MG	2A	3333	1/1	0.92	0.13	-	55,55,55,55	0
56	MG	2A	3216	1/1	0.89	0.13	-	56,56,56,56	0
56	MG	2a	3072	1/1	0.94	0.14	-	53,53,53,53	0
56	MG	1a	1786	1/1	0.86	0.09	-	64,64,64,64	0
56	MG	1A	3480	1/1	0.92	0.10	-	52,52,52,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.