



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:40 PM GMT

PDB ID : 1VY5
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the post-catalysis state of peptide bond formation containing dipeptidyl-tRNA in the A site and deacylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.55 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

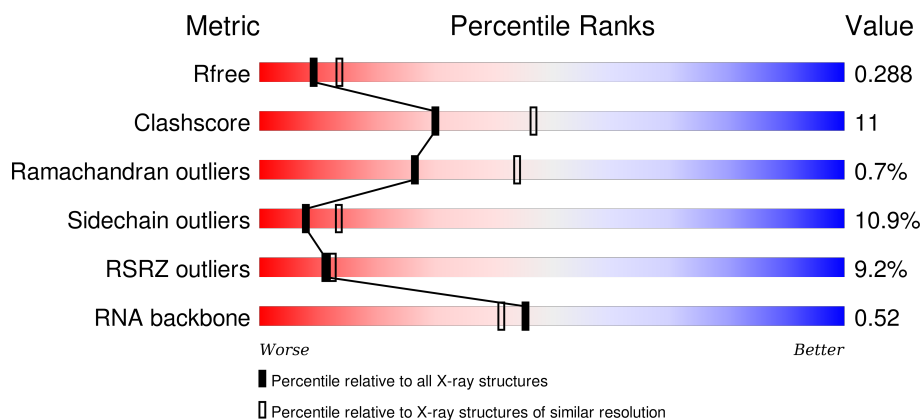
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)
RNA backbone	2183	1093 (3.00-2.08)

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	AA	1521	<div> <div>2%</div> <div>52%</div> <div>37%</div> <div>9%</div> <div>..</div> </div>
1	CA	1521	<div> <div>5%</div> <div>45%</div> <div>42%</div> <div>10%</div> <div>..</div> </div>
2	AB	256	<div> <div>13%</div> <div>42%</div> <div>41%</div> <div>6%</div> <div>10%</div> </div>
2	CB	256	<div> <div>23%</div> <div>36%</div> <div>43%</div> <div>11%</div> <div>10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	76	
23	CW	76	
24	AX	77	
24	CX	77	
25	AY	76	
25	CY	76	
26	BA	2915	
26	DA	2915	
27	BB	121	
27	DB	121	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	
52	B5	60	
52	D5	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

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
57	MG	AA	3018	-	-	-	X
57	MG	AA	3080	-	-	-	X
57	MG	AA	3084	-	-	-	X
57	MG	AA	3095	-	-	-	X
57	MG	AA	3138	-	-	-	X
57	MG	AA	3156	-	-	-	X
57	MG	AA	3205	-	-	-	X
57	MG	AF	3001	-	-	-	X
57	MG	AY	3003	-	-	-	X
57	MG	B1	101	-	-	-	X
57	MG	BA	3029	-	-	-	X
57	MG	BA	3040	-	-	-	X
57	MG	BA	3046	-	-	-	X
57	MG	BA	3054	-	-	-	X
57	MG	BA	3069	-	-	-	X
57	MG	BA	3082	-	-	-	X
57	MG	BA	3085	-	-	-	X
57	MG	BA	3115	-	-	-	X
57	MG	BA	3139	-	-	-	X
57	MG	BA	3141	-	-	-	X
57	MG	BA	3143	-	-	-	X
57	MG	BA	3151	-	-	-	X
57	MG	BA	3153	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3156	-	-	-	X
57	MG	BA	3196	-	-	-	X
57	MG	BA	3203	-	-	-	X
57	MG	BA	3213	-	-	-	X
57	MG	BA	3215	-	-	-	X
57	MG	BA	3232	-	-	-	X
57	MG	BA	3239	-	-	-	X
57	MG	BA	3240	-	-	-	X
57	MG	BA	3246	-	-	-	X
57	MG	BA	3248	-	-	-	X
57	MG	BA	3250	-	-	-	X
57	MG	BA	3284	-	-	-	X
57	MG	BA	3289	-	-	-	X
57	MG	BA	3290	-	-	-	X
57	MG	BA	3328	-	-	-	X
57	MG	BA	3330	-	-	-	X
57	MG	BA	3335	-	-	-	X
57	MG	BA	3367	-	-	-	X
57	MG	BA	3549	-	-	-	X
57	MG	BA	3613	-	-	-	X
57	MG	BA	3626	-	-	-	X
57	MG	BA	3639	-	-	-	X
57	MG	BA	3670	-	-	-	X
57	MG	BA	3698	-	-	-	X
57	MG	BA	3699	-	-	-	X
57	MG	BA	3728	-	-	-	X
57	MG	BA	3732	-	-	-	X
57	MG	BA	3771	-	-	-	X
57	MG	BA	3801	-	-	-	X
57	MG	BA	3802	-	-	-	X
57	MG	BA	3804	-	-	-	X
57	MG	BA	3812	-	-	-	X
57	MG	BB	202	-	-	-	X
57	MG	BB	218	-	-	-	X
57	MG	BD	302	-	-	-	X
57	MG	BD	306	-	-	-	X
57	MG	BF	303	-	-	-	X
57	MG	BF	306	-	-	-	X
57	MG	BN	3001	-	-	-	X
57	MG	BP	201	-	-	-	X
57	MG	BU	206	-	-	-	X
57	MG	BV	201	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BX	3001	-	-	-	X
57	MG	CA	3045	-	-	-	X
57	MG	CA	3057	-	-	-	X
57	MG	CA	3061	-	-	-	X
57	MG	CA	3079	-	-	-	X
57	MG	CA	3087	-	-	-	X
57	MG	CA	3133	-	-	-	X
57	MG	CA	3152	-	-	-	X
57	MG	CA	3169	-	-	-	X
57	MG	DA	3016	-	-	-	X
57	MG	DA	3019	-	-	-	X
57	MG	DA	3027	-	-	-	X
57	MG	DA	3028	-	-	-	X
57	MG	DA	3029	-	-	-	X
57	MG	DA	3031	-	-	-	X
57	MG	DA	3045	-	-	-	X
57	MG	DA	3059	-	-	-	X
57	MG	DA	3067	-	-	-	X
57	MG	DA	3081	-	-	-	X
57	MG	DA	3096	-	-	-	X
57	MG	DA	3115	-	-	-	X
57	MG	DA	3116	-	-	-	X
57	MG	DA	3119	-	-	-	X
57	MG	DA	3132	-	-	-	X
57	MG	DA	3168	-	-	-	X
57	MG	DA	3182	-	-	-	X
57	MG	DA	3208	-	-	-	X
57	MG	DA	3213	-	-	-	X
57	MG	DA	3226	-	-	-	X
57	MG	DA	3236	-	-	-	X
57	MG	DA	3426	-	-	-	X
57	MG	DA	3439	-	-	-	X
57	MG	DA	3471	-	-	-	X
57	MG	DA	3481	-	-	-	X
57	MG	DA	3510	-	-	-	X
57	MG	DA	3518	-	-	-	X
57	MG	DA	3588	-	-	-	X
57	MG	DA	3594	-	-	-	X
57	MG	DA	3610	-	-	-	X
57	MG	DA	3629	-	-	-	X
57	MG	DA	3637	-	-	-	X
57	MG	DA	3642	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3668	-	-	-	X
57	MG	DA	3669	-	-	-	X
57	MG	DA	3676	-	-	-	X
57	MG	DB	3008	-	-	-	X
57	MG	DB	3009	-	-	-	X
57	MG	DD	304	-	-	-	X
57	MG	DD	307	-	-	-	X
57	MG	DD	308	-	-	-	X
57	MG	DE	301	-	-	-	X
57	MG	DF	3003	-	-	-	X
57	MG	DU	3002	-	-	-	X
59	ZN	B5	102	-	-	-	X
59	ZN	B6	103	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 297141 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 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1498	Total	C	N	O	P	0	0	0
			32205	14333	5970	10404	1498			
1	CA	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1552	976	302	273	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1659	1040	326	286	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			806	511	143	149	3			
6	CF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
8	CH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			983	623	193	167			
9	CI	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	97	Total	C	N	O	0	0	0
			709	440	138	131			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O			
			714	445	138	131	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	AK	114	Total	C	N	O	S		
			829	516	155	155	3	0	0
11	CK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0
12	CL	122	Total	C	N	O	S		
			930	585	185	159	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0
14	CN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0
15	CO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	CP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	CR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
19	CS	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
20	CT	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

- Molecule 23 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	S	0	0	0
			1607	727	288	516	73	3			
23	CW	72	Total	C	N	O	P	S	0	0	0
			1560	702	281	503	72	2			

- Molecule 24 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 25 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
25	AY	74	Total	C	N	O	P	S	0	0	0
			1581	707	285	515	73	1			
25	CY	73	Total	C	N	O	P	S	0	0	0
			1561	698	283	507	72	1			

- Molecule 26 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BA	2819	Total	C	N	O	P	0	0	0
			60729	27026	11370	19515	2818			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	DA	2800	Total	C	N	O	P	0	0	0
			60311	26840	11284	19388	2799			

- Molecule 27 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
27	DB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
28	DD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
29	DE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	181	Total	C	N	O	S	0	0	0
			1425	914	256	251	4			
31	DG	181	Total	C	N	O	S	0	0	0
			1424	911	258	251	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
32	DH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	146	Total	C	N	O	S	0	0	0
			1085	693	189	202	1			
33	DI	146	Total	C	N	O	S	0	0	0
			1061	680	186	194	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
34	DN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
35	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
36	DP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
37	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
38	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BS	110	Total	C	N	O	0	0	0
			877	553	175	149			
39	DS	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
40	DT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
41	DU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
43	DW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
44	DX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
45	DY	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	171	Total	C	N	O	S	0	0	0
			1349	862	243	242	2			
46	DZ	174	Total	C	N	O	S	0	0	0
			1360	870	243	245	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
47	D0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
48	D1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
49	D2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	B3	59	Total	C	N	O	0	0	0
			469	298	90	81			
50	D3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	69	Total	C	N	O	S	0	0	0
			558	352	102	99	5			
51	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
52	D5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
53	D6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
54	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	64	Total	C	N	O	S	0	0	0
			511	328	99	82	2			
55	D8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
56	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B4	1	Total	Mg	0	0
			1	1		
57	BA	812	Total	Mg	0	0
			812	812		
57	AK	1	Total	Mg	0	0
			1	1		
57	DQ	4	Total	Mg	0	0
			4	4		
57	D3	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DF	4	Total 4	Mg 4	0	0
57	CV	1	Total 1	Mg 1	0	0
57	B8	1	Total 1	Mg 1	0	0
57	BE	8	Total 8	Mg 8	0	0
57	AW	4	Total 4	Mg 4	0	0
57	DU	2	Total 2	Mg 2	0	0
57	B1	1	Total 1	Mg 1	0	0
57	AN	2	Total 2	Mg 2	0	0
57	BP	5	Total 5	Mg 5	0	0
57	AX	15	Total 15	Mg 15	0	0
57	DN	1	Total 1	Mg 1	0	0
57	CA	170	Total 170	Mg 170	0	0
57	B5	1	Total 1	Mg 1	0	0
57	BB	20	Total 20	Mg 20	0	0
57	D8	1	Total 1	Mg 1	0	0
57	AE	3	Total 3	Mg 3	0	0
57	DG	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	BF	9	Total 9	Mg 9	0	0
57	BX	3	Total 3	Mg 3	0	0
57	B2	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	214	Total 214	Mg 214	0	0
57	BQ	5	Total 5	Mg 5	0	0
57	CX	3	Total 3	Mg 3	0	0
57	DV	3	Total 3	Mg 3	0	0
57	B6	2	Total 2	Mg 2	0	0
57	AM	1	Total 1	Mg 1	0	0
57	BU	8	Total 8	Mg 8	0	0
57	DR	1	Total 1	Mg 1	0	0
57	BN	6	Total 6	Mg 6	0	0
57	CT	1	Total 1	Mg 1	0	0
57	D0	1	Total 1	Mg 1	0	0
57	BG	3	Total 3	Mg 3	0	0
57	BY	1	Total 1	Mg 1	0	0
57	DE	4	Total 4	Mg 4	0	0
57	B3	2	Total 2	Mg 2	0	0
57	CJ	1	Total 1	Mg 1	0	0
57	BR	2	Total 2	Mg 2	0	0
57	DA	677	Total 677	Mg 677	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DW	4	Total 4	Mg 4	0	0
57	B7	5	Total 5	Mg 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CF	1	Total 1	Mg 1	0	0
57	BV	5	Total 5	Mg 5	0	0
57	DO	1	Total 1	Mg 1	0	0
57	BO	2	Total 2	Mg 2	0	0
57	DX	1	Total 1	Mg 1	0	0
57	BZ	1	Total 1	Mg 1	0	0
57	DY	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0
57	CD	1	Total 1	Mg 1	0	0
57	BD	9	Total 9	Mg 9	0	0
57	B0	3	Total 3	Mg 3	0	0
57	CE	1	Total 1	Mg 1	0	0
57	BW	4	Total 4	Mg 4	0	0
57	AY	3	Total 3	Mg 3	0	0
57	DD	9	Total 9	Mg 9	0	0
57	CK	1	Total 1	Mg 1	0	0
57	AF	1	Total 1	Mg 1	0	0
57	DB	13	Total 13	Mg 13	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AD	1	Total	Fe	S	0	0
			8	4	4		
58	CD	1	Total	Fe	S	0	0
			8	4	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B5	1	Total	Zn	0	0
			1	1		
59	B4	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		
59	BY	1	Total	Zn	0	0
			1	1		
59	B9	1	Total	Zn	0	0
			1	1		
59	DY	1	Total	Zn	0	0
			1	1		
59	D5	1	Total	Zn	0	0
			1	1		
59	D4	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	D6	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D9	1	Total 1	Zn 1	0	0
59	B6	1	Total 1	Zn 1	0	0

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AX	1	Total 1	K 1	0	0
60	CX	1	Total 1	K 1	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	227	Total 227	O 227	0	0
61	AE	2	Total 2	O 2	0	0
61	AJ	1	Total 1	O 1	0	0
61	AL	1	Total 1	O 1	0	0
61	AM	1	Total 1	O 1	0	0
61	AU	1	Total 1	O 1	0	0
61	AV	3	Total 3	O 3	0	0
61	AW	3	Total 3	O 3	0	0
61	AX	6	Total 6	O 6	0	0
61	AY	1	Total 1	O 1	0	0
61	BA	1383	Total 1383	O 1383	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	12	Total 12	O 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BE	14	Total 14	O 14	0	0
61	BF	8	Total 8	O 8	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0
61	BO	4	Total 4	O 4	0	0
61	BP	16	Total 16	O 16	0	0
61	BQ	4	Total 4	O 4	0	0
61	BR	2	Total 2	O 2	0	0
61	BT	2	Total 2	O 2	0	0
61	BU	3	Total 3	O 3	0	0
61	BV	2	Total 2	O 2	0	0
61	BW	1	Total 1	O 1	0	0
61	BX	4	Total 4	O 4	0	0
61	BZ	1	Total 1	O 1	0	0
61	B0	3	Total 3	O 3	0	0
61	B1	1	Total 1	O 1	0	0
61	B3	2	Total 2	O 2	0	0
61	B5	2	Total 2	O 2	0	0
61	B6	1	Total 1	O 1	0	0
61	B7	2	Total 2	O 2	0	0
61	B8	8	Total 8	O 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CA	185	Total 185	O 185	0	0
61	CJ	2	Total 2	O 2	0	0
61	CL	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CV	1	Total 1	O 1	0	0
61	CW	2	Total 2	O 2	0	0
61	DA	1025	Total 1025	O 1025	0	0
61	DB	9	Total 9	O 9	0	0
61	DD	19	Total 19	O 19	0	0
61	DE	11	Total 11	O 11	0	0
61	DF	3	Total 3	O 3	0	0
61	DN	2	Total 2	O 2	0	0
61	DO	1	Total 1	O 1	0	0
61	DP	16	Total 16	O 16	0	0
61	DR	1	Total 1	O 1	0	0
61	DT	3	Total 3	O 3	0	0
61	DU	2	Total 2	O 2	0	0
61	DX	3	Total 3	O 3	0	0
61	DY	2	Total 2	O 2	0	0
61	D0	3	Total 3	O 3	0	0
61	D1	1	Total 1	O 1	0	0

Continued on next page...

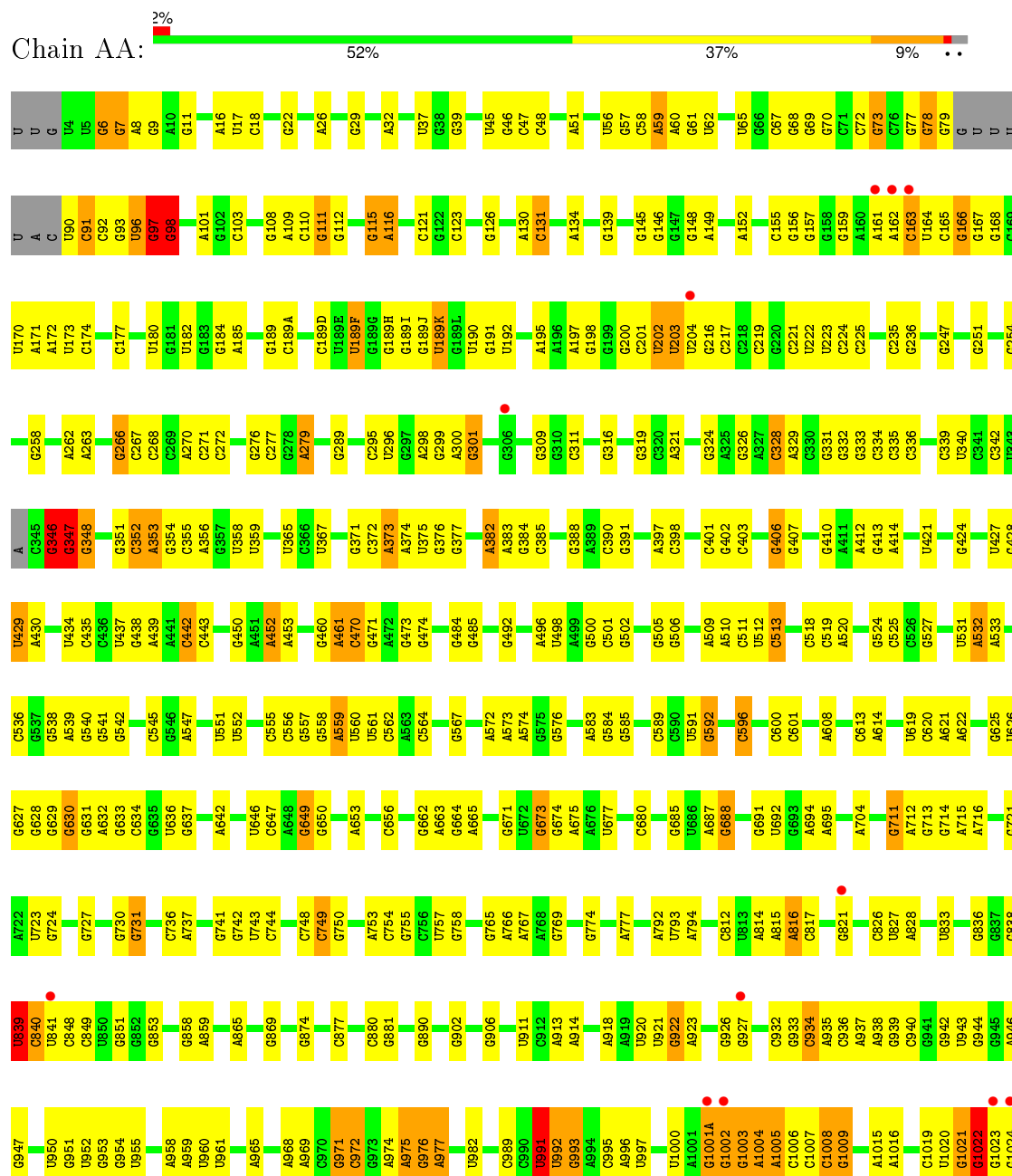
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	D3	1	Total	O	0	0
			1	1		
61	D7	3	Total	O	0	0
			3	3		
61	D8	4	Total	O	0	0
			4	4		

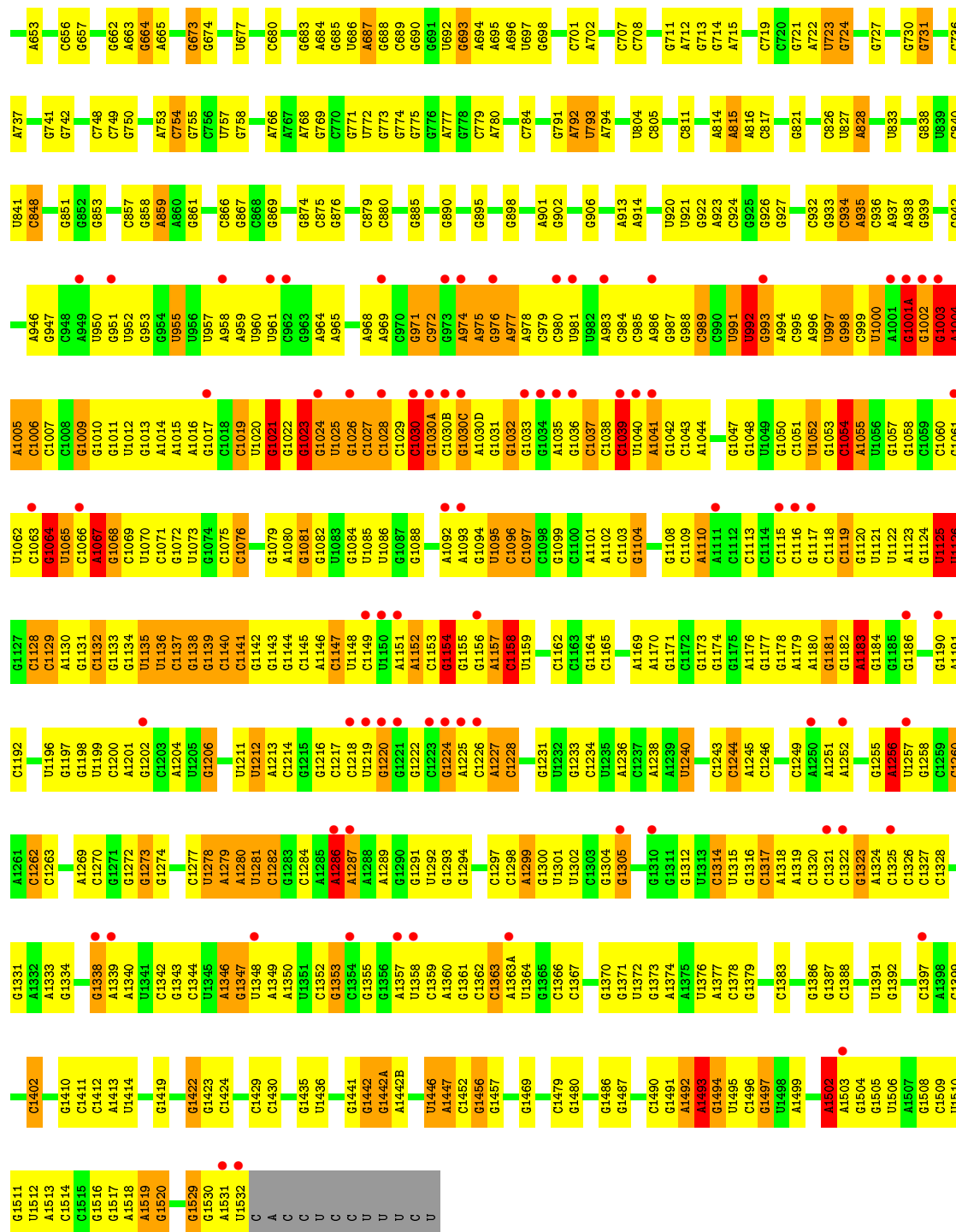
3 Residue-property plots

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

- Molecule 1: 16S Ribosomal RNA



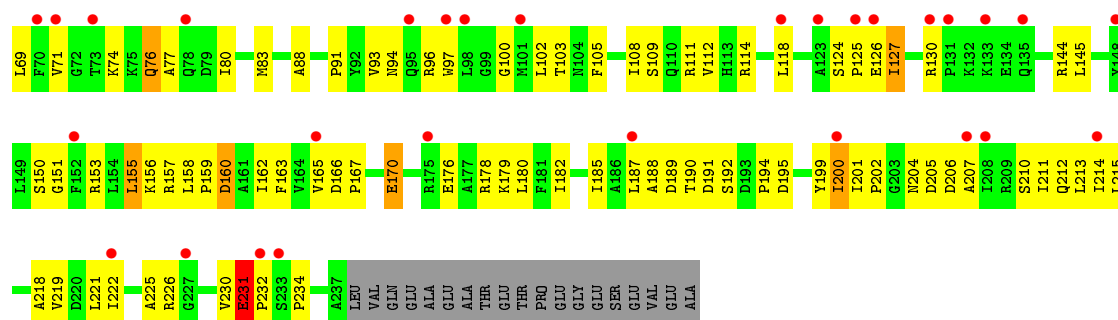




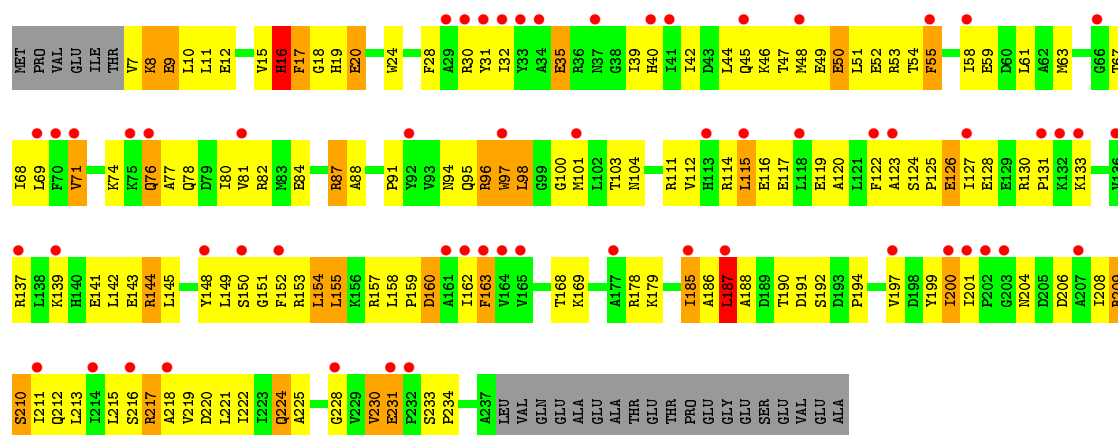
• Molecule 2: 30S ribosomal protein S2

Chain AB: 13% 42% 41% 6% 10%

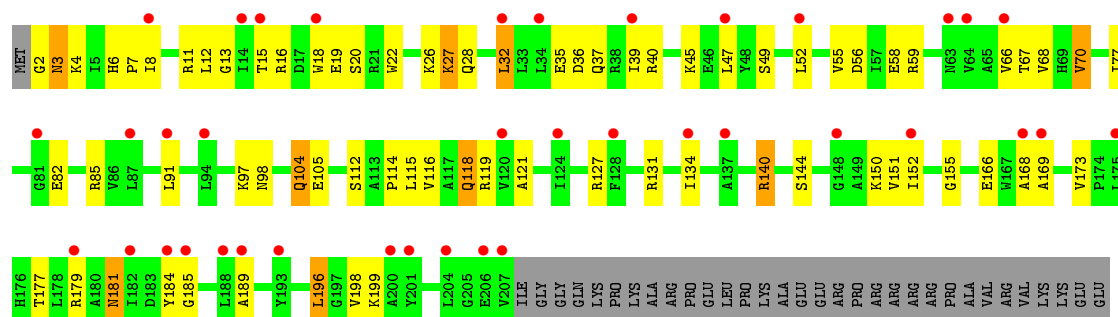




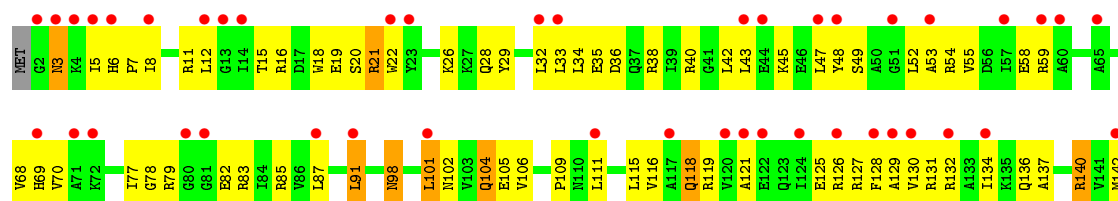
• Molecule 2: 30S ribosomal protein S2

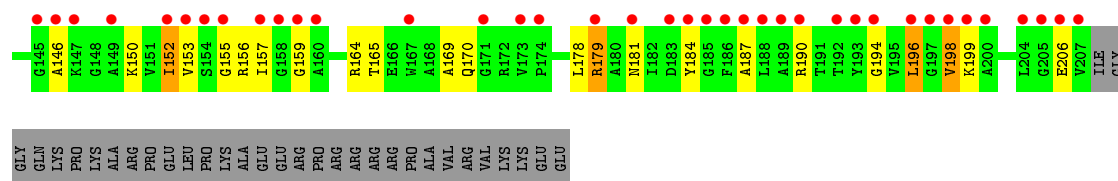


• Molecule 3: 30S ribosomal protein S3

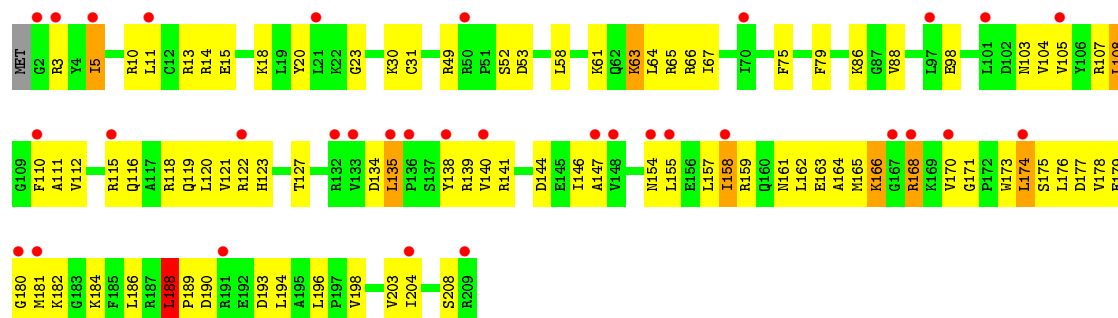


• Molecule 3: 30S ribosomal protein S3

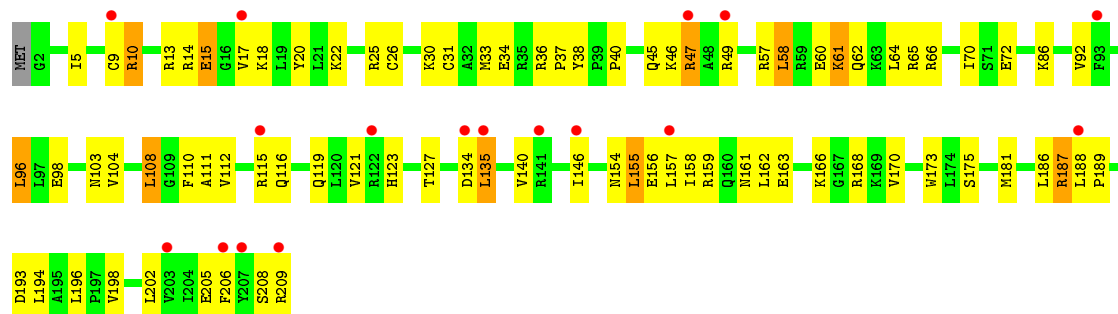




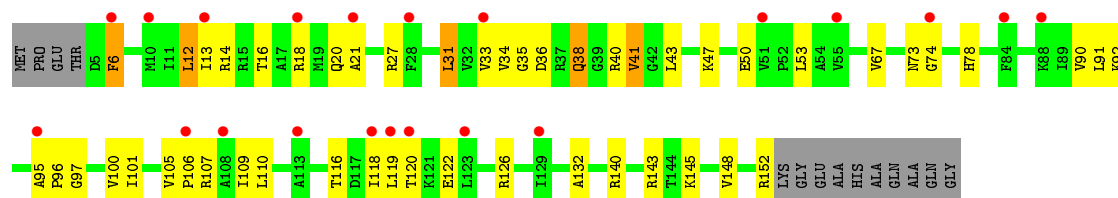
• Molecule 4: 30S ribosomal protein S4



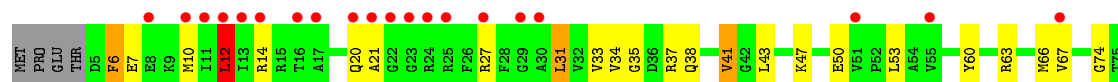
• Molecule 4: 30S ribosomal protein S4

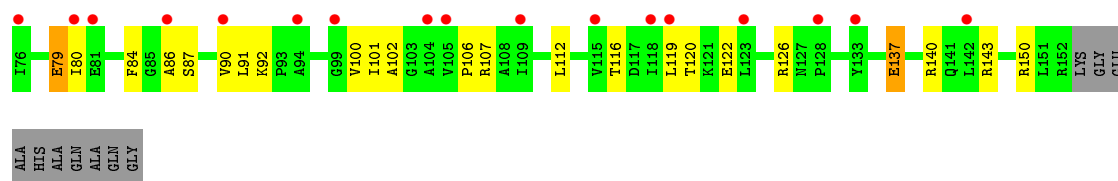


• Molecule 5: 30S ribosomal protein S5

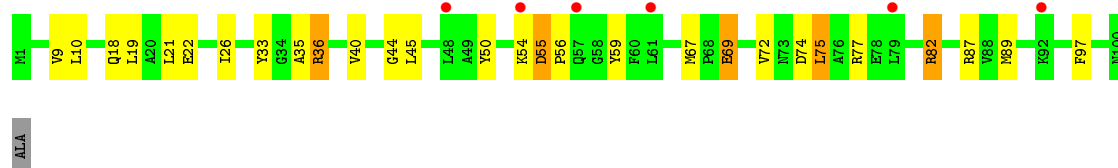
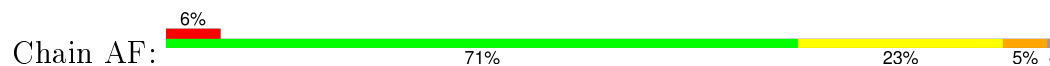


• Molecule 5: 30S ribosomal protein S5

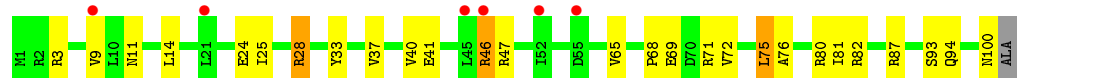
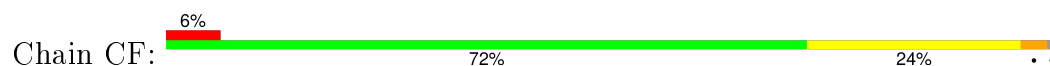




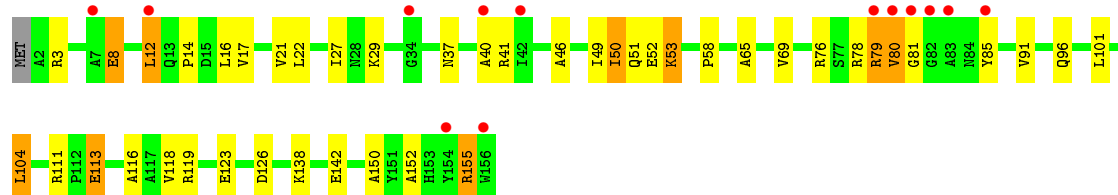
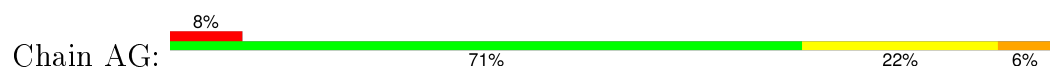
- Molecule 6: 30S ribosomal protein S6



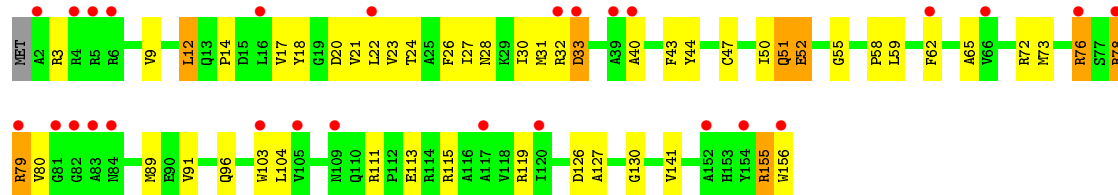
- Molecule 6: 30S ribosomal protein S6



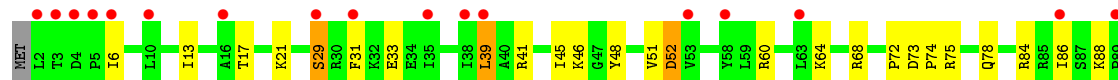
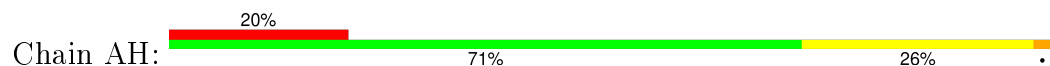
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7

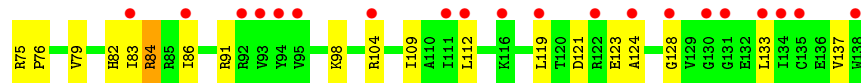
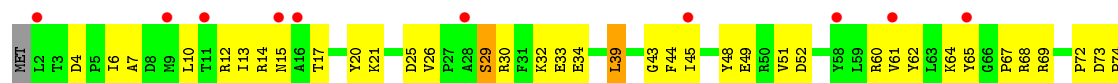


- Molecule 8: 30S ribosomal protein S8

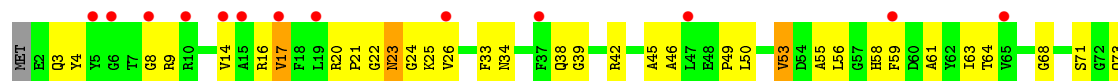




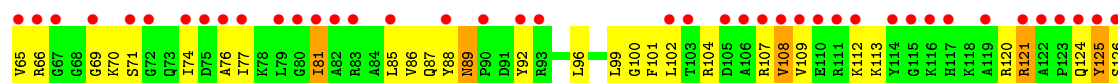
- Molecule 8: 30S ribosomal protein S8



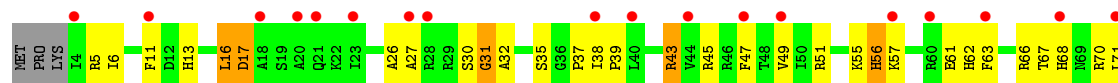
- Molecule 9: 30S ribosomal protein S9



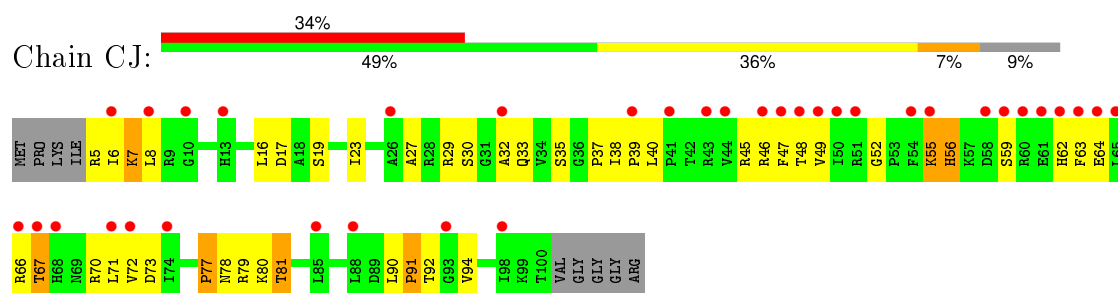
- Molecule 9: 30S ribosomal protein S9



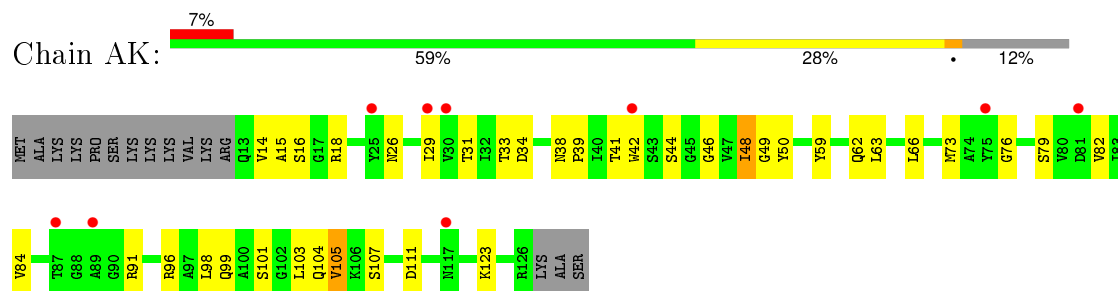
- Molecule 10: 30S ribosomal protein S10



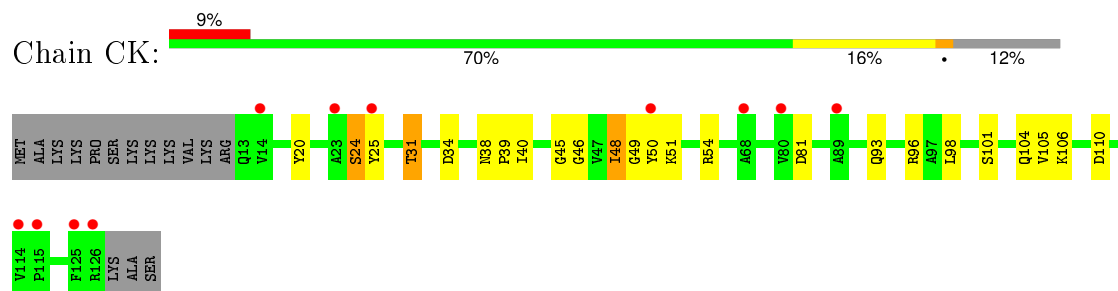
- Molecule 10: 30S ribosomal protein S10



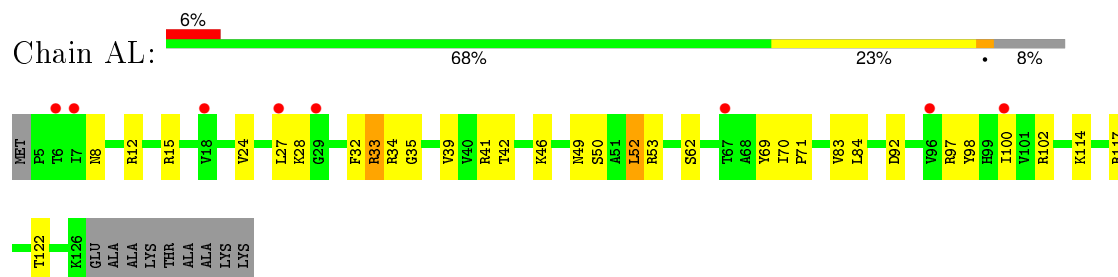
- Molecule 11: 30S ribosomal protein S11



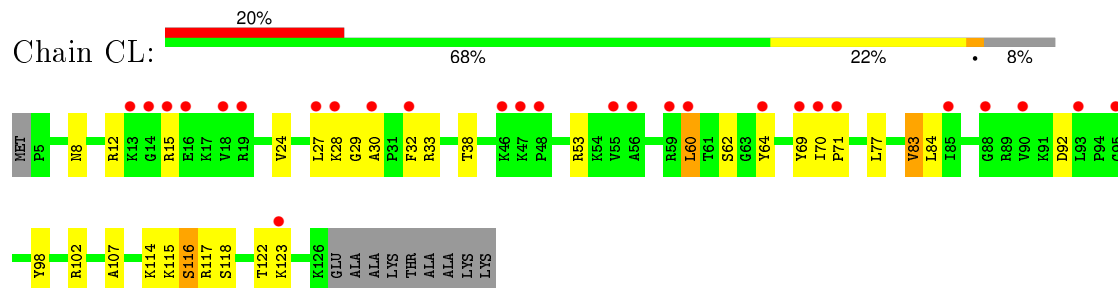
- Molecule 11: 30S ribosomal protein S11



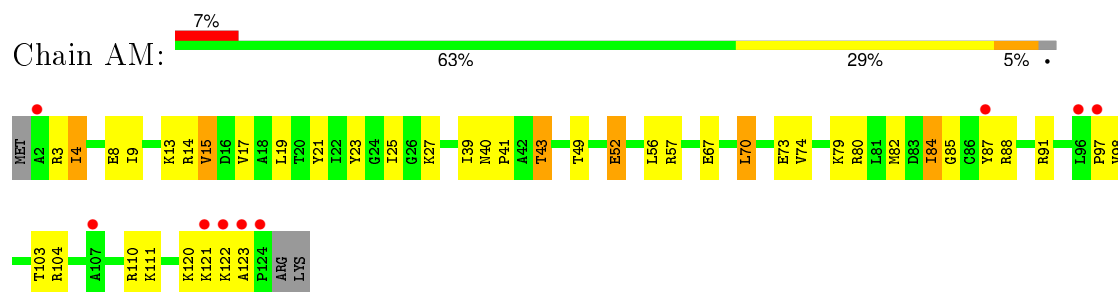
- Molecule 12: 30S ribosomal protein S12



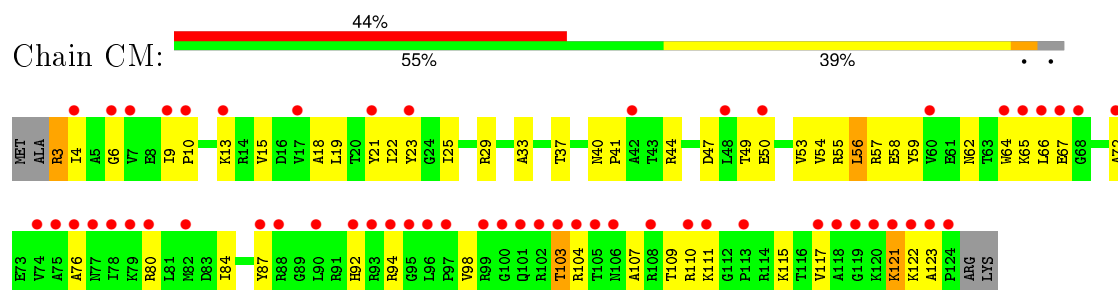
- Molecule 12: 30S ribosomal protein S12



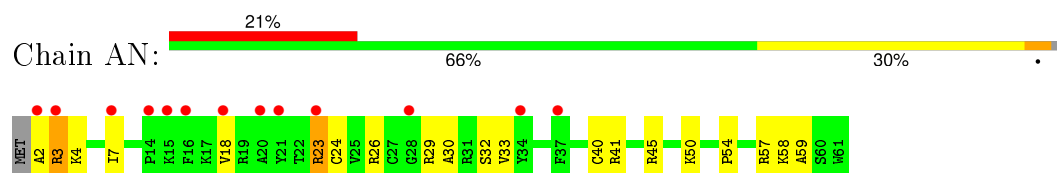
- Molecule 13: 30S ribosomal protein S13



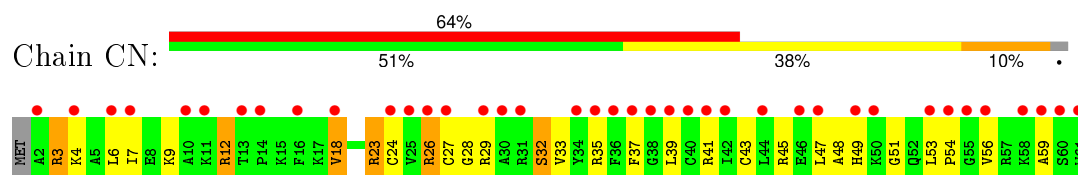
- Molecule 13: 30S ribosomal protein S13



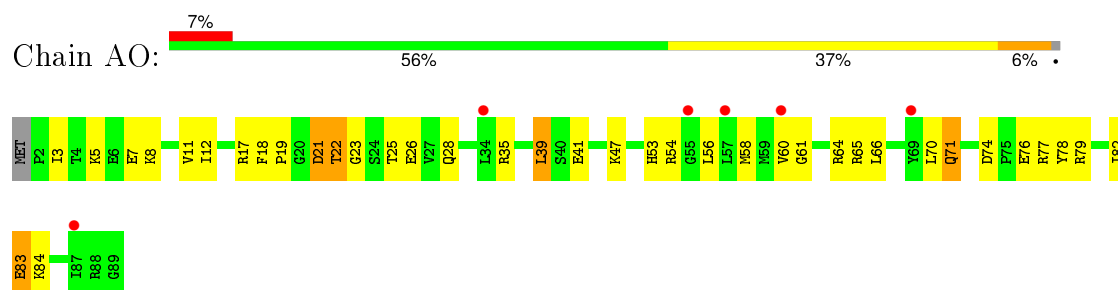
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z

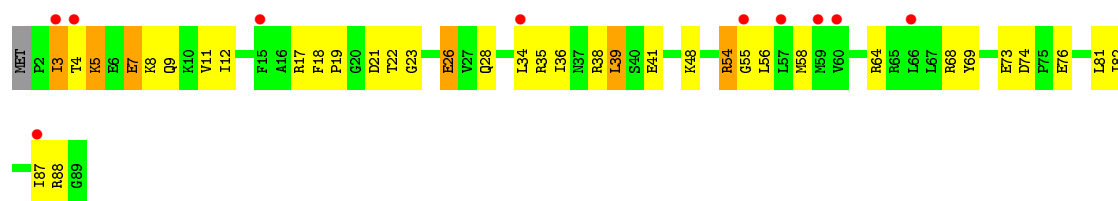


- Molecule 15: 30S ribosomal protein S15

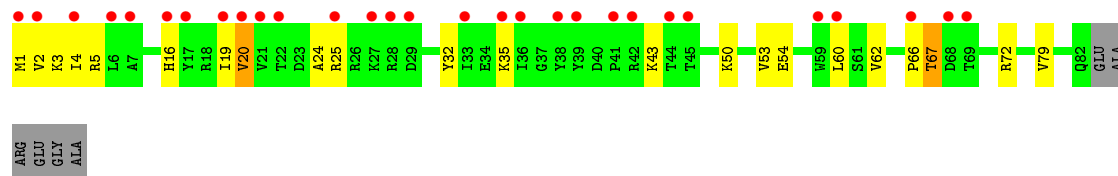


- Molecule 15: 30S ribosomal protein S15

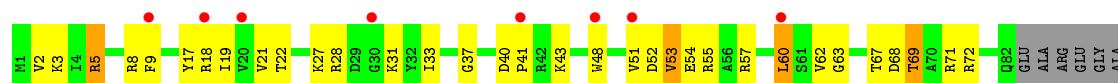




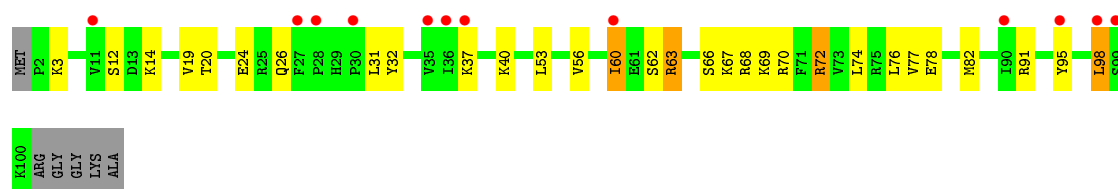
- Molecule 16: 30S ribosomal protein S16



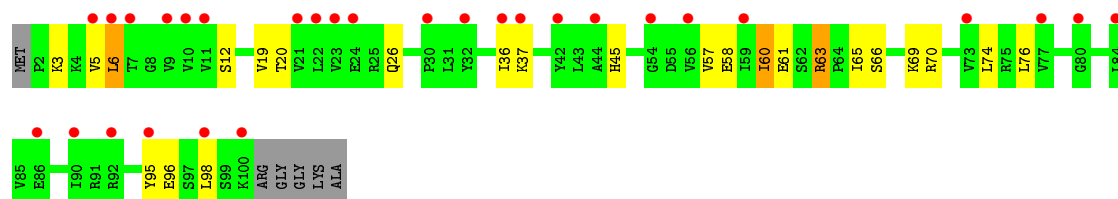
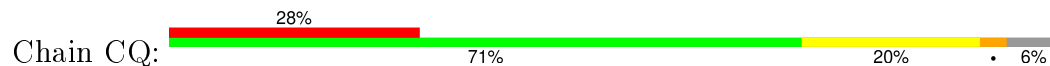
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

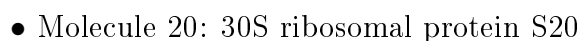
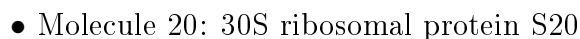
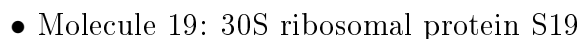
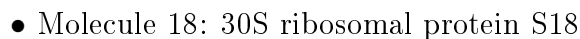


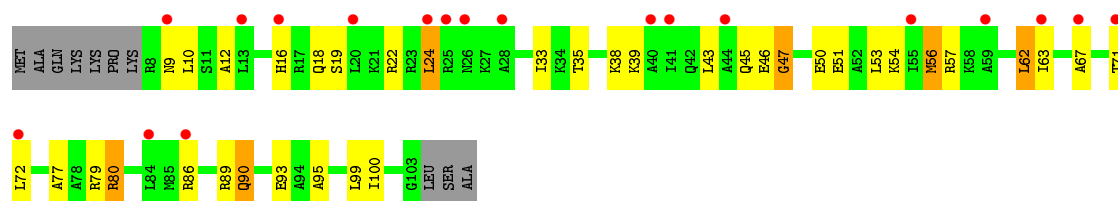
- Molecule 17: 30S ribosomal protein S17



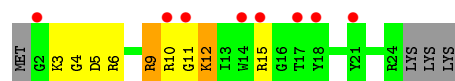
- Molecule 18: 30S ribosomal protein S18







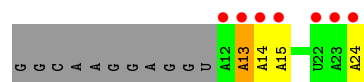
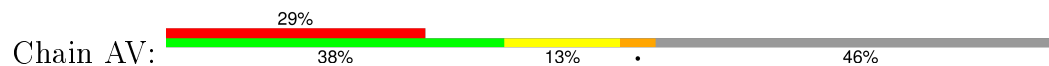
- Molecule 21: 30S ribosomal protein Thx



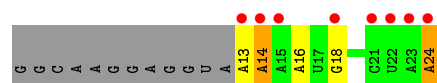
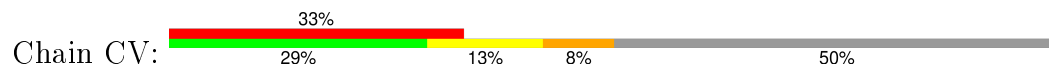
- Molecule 21: 30S ribosomal protein Thx



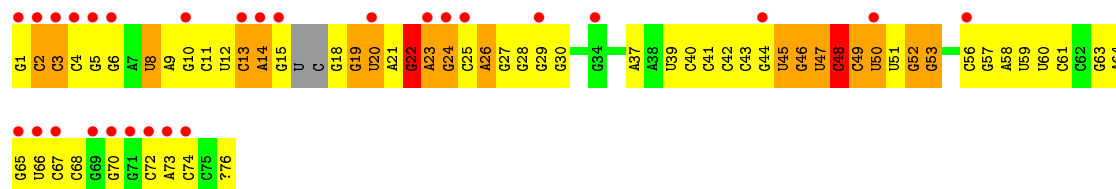
- Molecule 22: mRNA



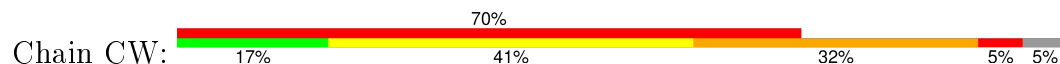
- Molecule 22: mRNA

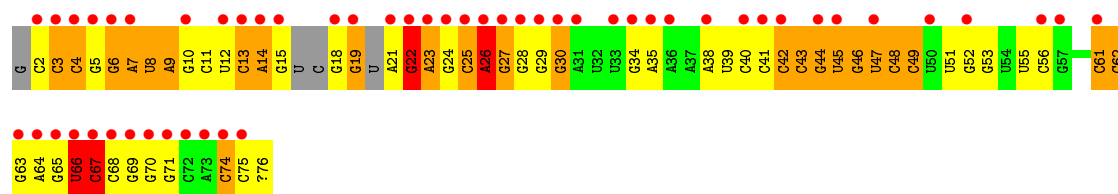


- Molecule 23: A-site tRNA



- Molecule 23: A-site tRNA

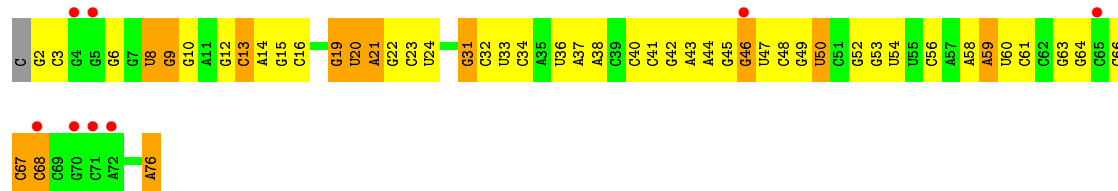




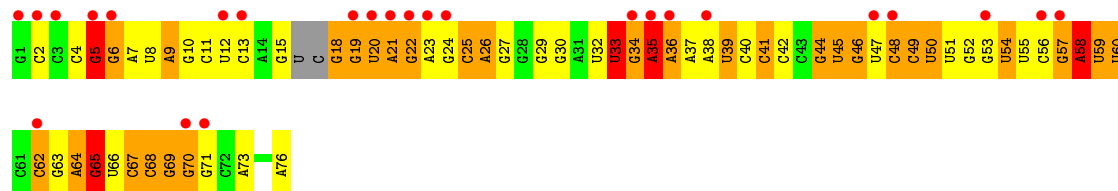
- Molecule 24: P-site tRNA



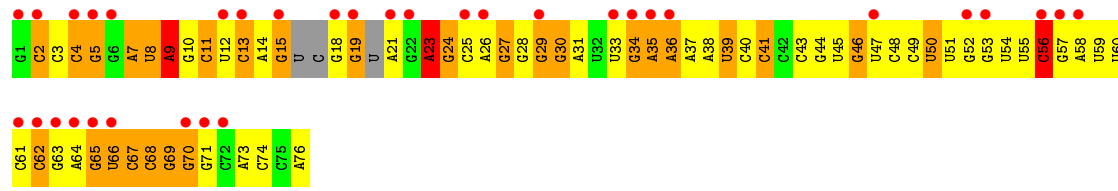
- Molecule 24: P-site tRNA



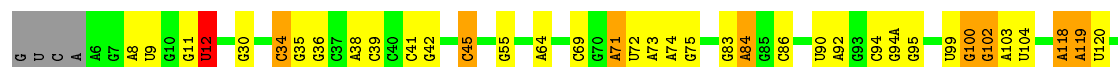
- Molecule 25: E-site tRNA



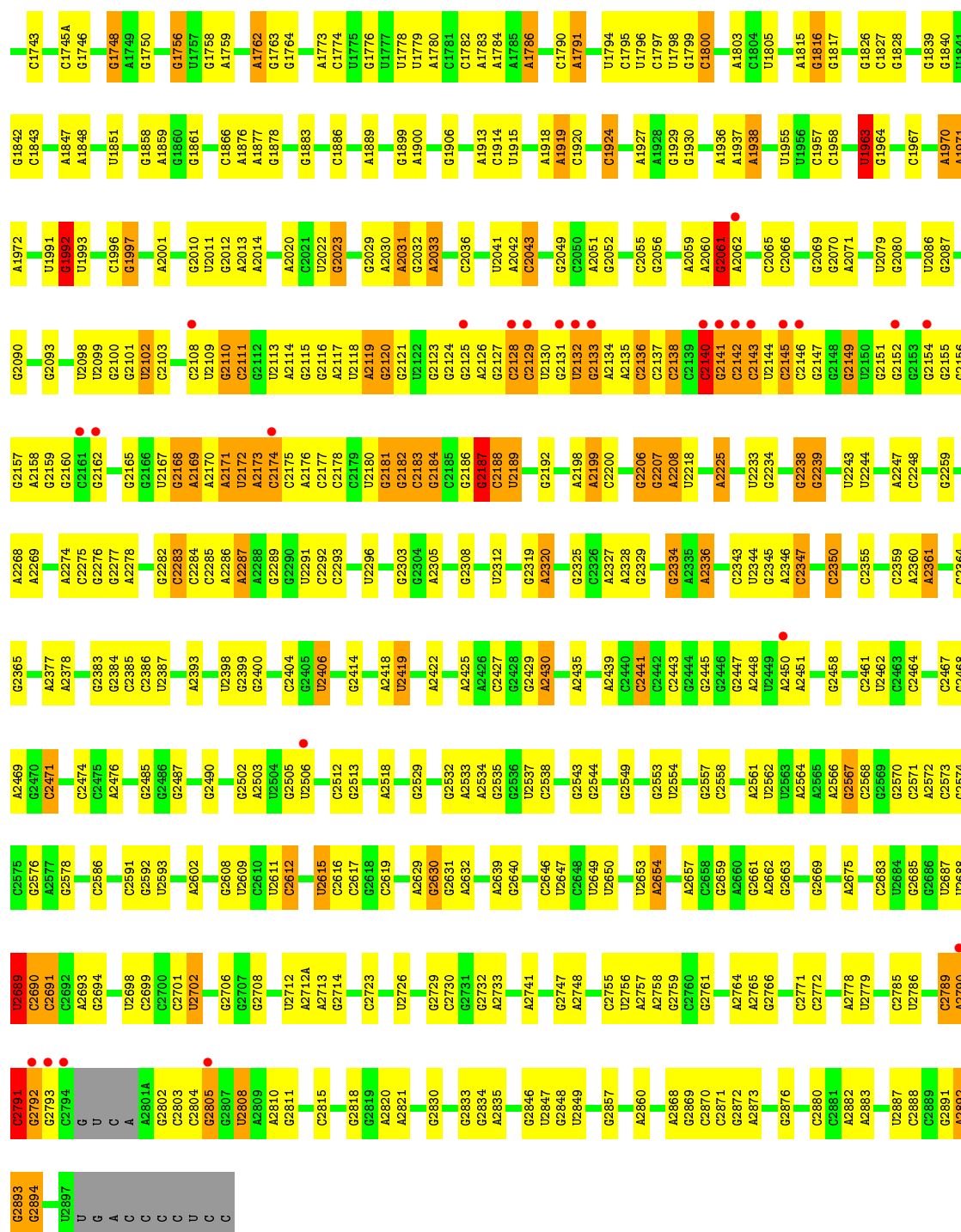
- Molecule 25: E-site tRNA



- Molecule 26: 23S Ribosomal RNA

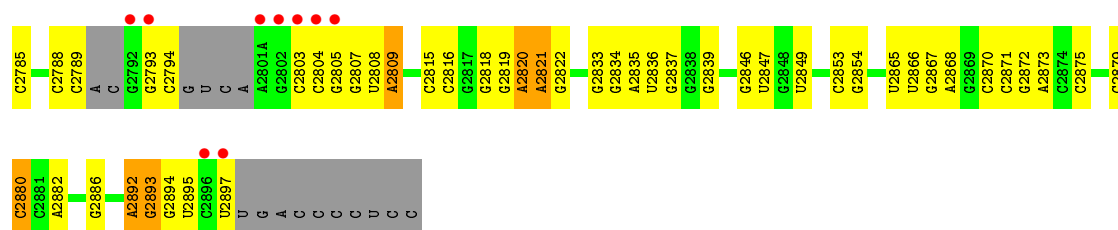






U1263	G1179	C	4887	G966	G809	G721	A637	A	C456	G272B	A204	A82
G1264	C1180	A	C888	C967	G810	C721	G638	G549	A457	G272E	G205	G93
A1265	G1266	C	C889	C971	U810	U724	U639	G556	G465	C272J	C208	C94
G1266	G1184	A	A890	C971	U811	G725	G640	U557	G370	G274	C209	G94A
U1267	G1184	G	G892	G974	C812	G726	G641	G563	A371	G275	G212	G95
A1268	G1185	G	C893	C975	U813	G729	A643	G564	G372	A276	G213	G100
G1269	G1186	A	U895	C975	C816	C730	G644	C565	G373	C277	G214	A103
A1269	G1187	C	A896	A983	C817	C645	A646	C566	A374	A278	G215	G109
C1270	U1188	G	C897	A983	G818	C731	G647	U566	C375	C278	A216	G117
G1271	A1189	A	C898	C987	A819	G734	G648	A567	A479	G279	A217	A118
U1272	U1273	C	A899	C987	A820	A734	G649	A480	A478	C285	G218	A119
A1278	G1196	C	A900	A988	A821	U740	G649	G481	A479	C286	A221	U120
G1283	G1197	A	A901	A990	A821	G741	A652B	A482	A480	C287	A222	G121
A1284	U1199	G	G902	A990	U827	G741	G652C	A483	G481	C288	A223	G125
G1285	G1117	A	C903	C992	U828	G744	G652D	A484	G482	A289	G226	G131
C1201	G1117	G	C904	C993	A829	G744	G652E	C485	A483	G292	G227	G140
G1286	C1118	G	G904	C994	G830	G745	G	C485	A484	C293	G228	A141
A1287	G1122	U	U910	C995	G831	A746	G	A492	G485	A294	G229	G143
U1288	U1205	U	A911	A996	G832	G747	G	G493	A478	A299	A228	C143A
G1293	G1209	G	C912	C998	G833	G748	C	G494	A479	A300	A229	G145
C1293	A1126	G	U913	C998	G833	G748	C	G498	A480	G301	U230	A149
U1211	A1127	C	C914	C999	U839	A752	G	G498	G481	U305	A233	G154A
G1219	A1128	U	A917	A1001	C940	C753	C	U499	G482	U306	C234	U157
A1301	U1130	A	A918	G1002	G848	C754	A	G500	A483	G307	U235	G
A1302	G1131	G	G921	C1005	U851	C755	C	A503	A484	G308	A241	G143
G1303	C1135	A	U922	C1006	G852	G760	G	A504	A485	G309	G245	G144
C1304	G1136	G	C923	C1007	G853	A761	G	A505	A486	A310	G246	G145
G1305	C1136	C	G924	C1008	G854	G762	G	A509	A487	A311	C247	A149
G1309	G1139	A	G927	G1011	G855	A764	C	G510	A488	G315	G248	G171
G1340	C1140	G	U928	U1012	C856	G765	C	U511	A489	C316	G249	G172
U1313	U1141	C	G932	C1013	C857	G770	G652T	A512	A490	G320	G250	G173
G1314	U1142	C	A933	U1014	U858	A774	G655	A513	A491	A321	A251	G
C1315	A1143	A	G934	G1015	U859	G775	G656	C516	A492	A322	G252	G
G1324	G1144	U	U937	G1016	A861	G776	U657	C517	A493	G323	C263	G
C1327	G1151	U	G938	C1017	G862	A782	G659	G521	A494	A324	A265	G178
G1332	C1152	U	A941	U1019	G864	A783	G662	A526	A495	G325	G266	G
A1336	G1153	A	U942	U1020	C865	A784	G663	G527	A496	G326	A270	A181
G1337	A1155	A	U943	G1022	A866	G785	G668	A528	A497	U328	A182	A182
U1338	G1160	G	G944	U1023	C867	G785	G669	A529	A498	A330	C183	C183
G1341	C1161	A	A945	G1024	U868	A788	G674	G530	A499	A331	U184	U185
A1342	G1162	U	G946	G1025	G869	C790	G674	A532	A500	A332	U271K	U185
G1353	U1167	C	G950	A1027	G874	C791	G686	G533	A501	G333	U271L	A191
A1354	G1168	G	G952	A1028	G875	G792	G686	U534	A502	C334	G271M	A191
A1359	C1169	A	A953	U1032	A878	A793	G692	C535	A503	A442	U271N	C192
G1363	G1170	U	G954	U1033	G879	C795	G698	C537	A504	A443	G271R	U193
A1364	G1171	A	U957	G1034	G880	C796	A699	C538	A505	A444	G194	A195
G1365	G	A	G958	U1035	G881	C797	G700	C540	A506	A445	G271V	A196
C1261	U	U	U959	G1037	G882	G798	G700	C541	A507	A446	G271W	A197
A1262	G	C	G961	G1039	G883	U803	G710	C	A508	U448	G271H	C198
G1369	C1178	U	C961	G1039	C884	A804	G715	A	A509	A449	U272A	A199
					C885	G805			A510	G363	G272B	C203
					C886						G272C	





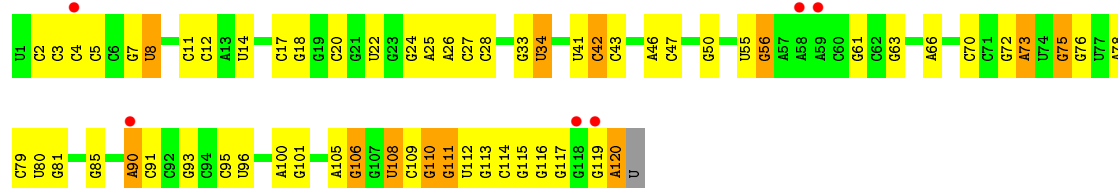
• Molecule 27: 5S Ribosomal RNA

Chain BB: 75% 18% 6% .



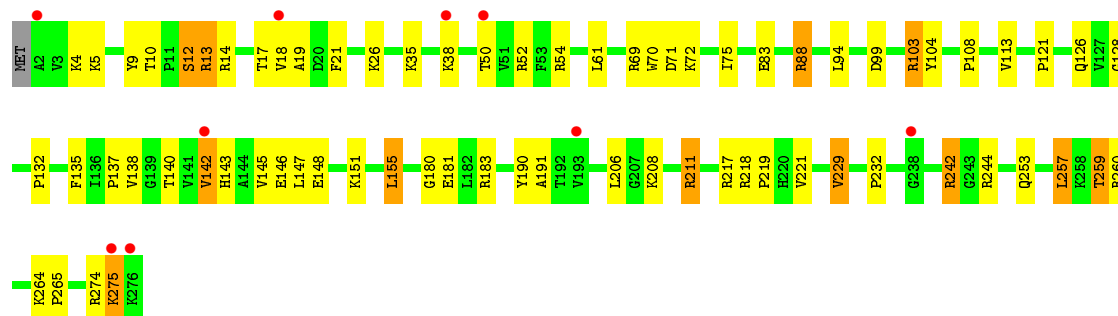
• Molecule 27: 5S Ribosomal RNA

Chain DB: 5% 48% 41% 10% .



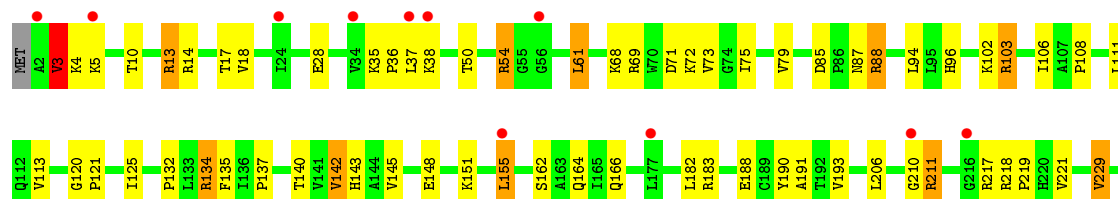
• Molecule 28: 50S ribosomal protein L2

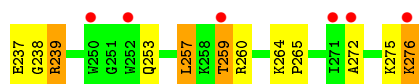
Chain BD: 3% 74% 21% .



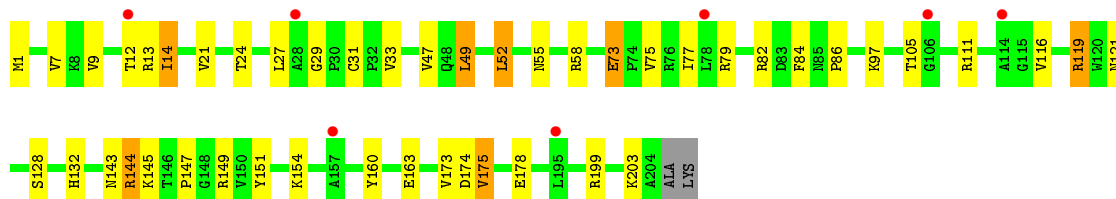
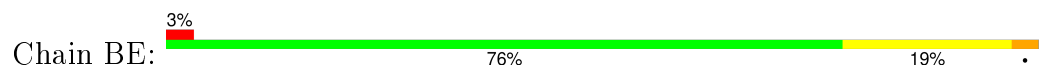
• Molecule 28: 50S ribosomal protein L2

Chain DD: 6% 72% 22% 5% .

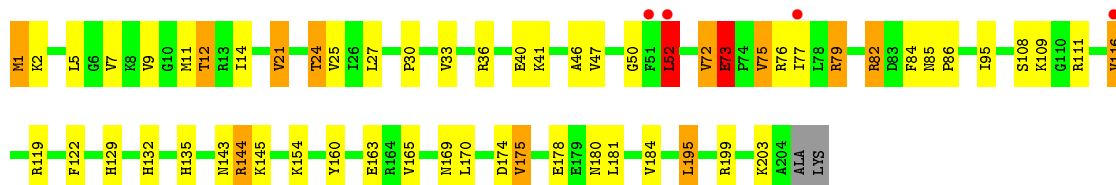




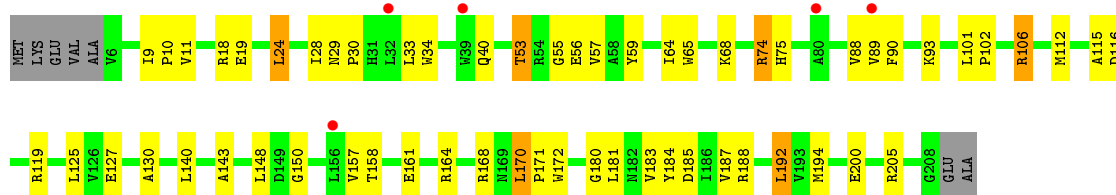
- Molecule 29: 50S ribosomal protein L3



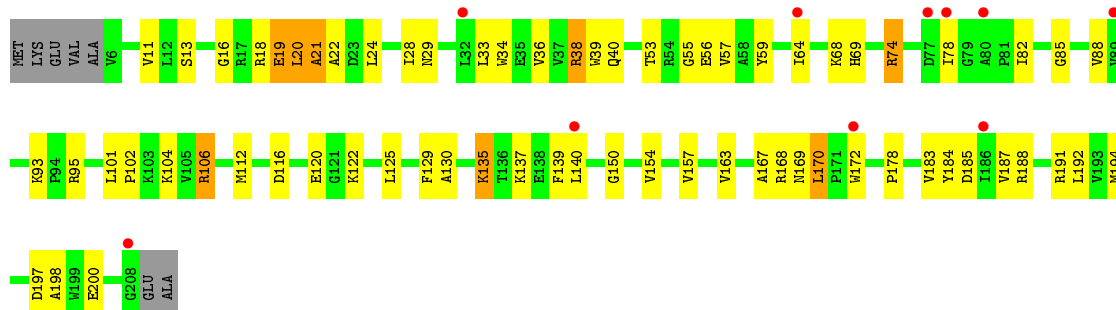
- Molecule 29: 50S ribosomal protein L3



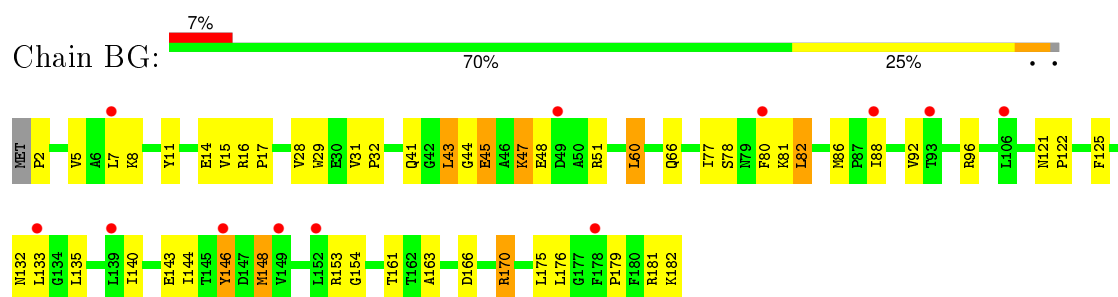
- Molecule 30: 50S ribosomal protein L4



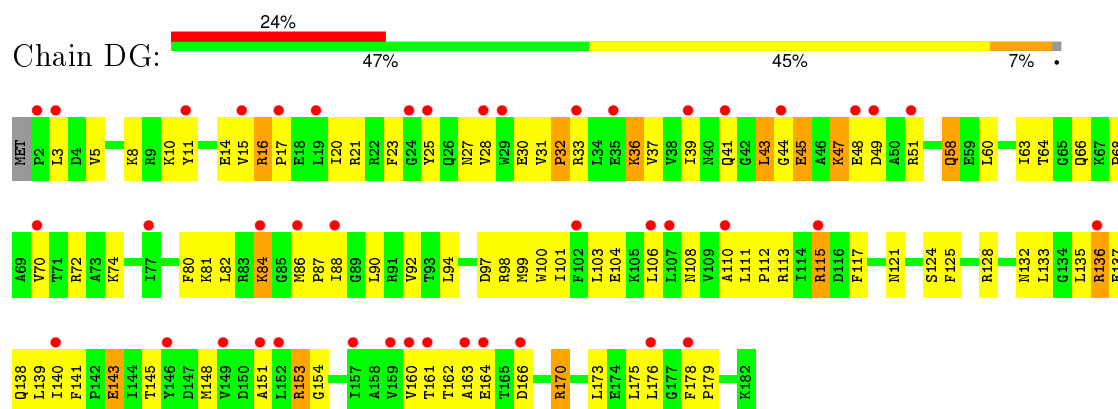
- Molecule 30: 50S ribosomal protein L4



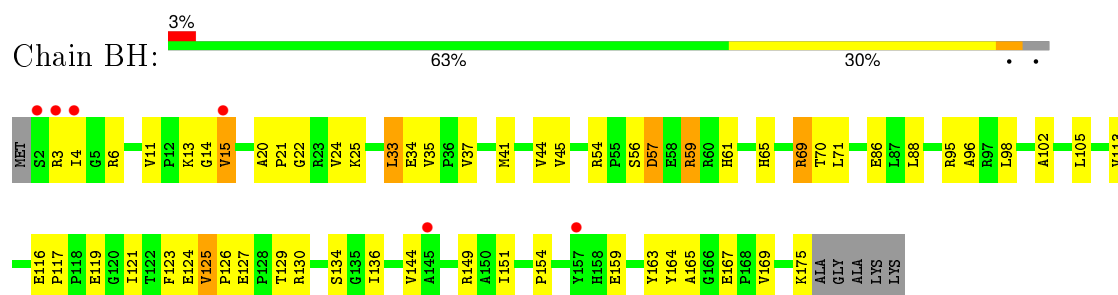
- Molecule 31: 50S ribosomal protein L5



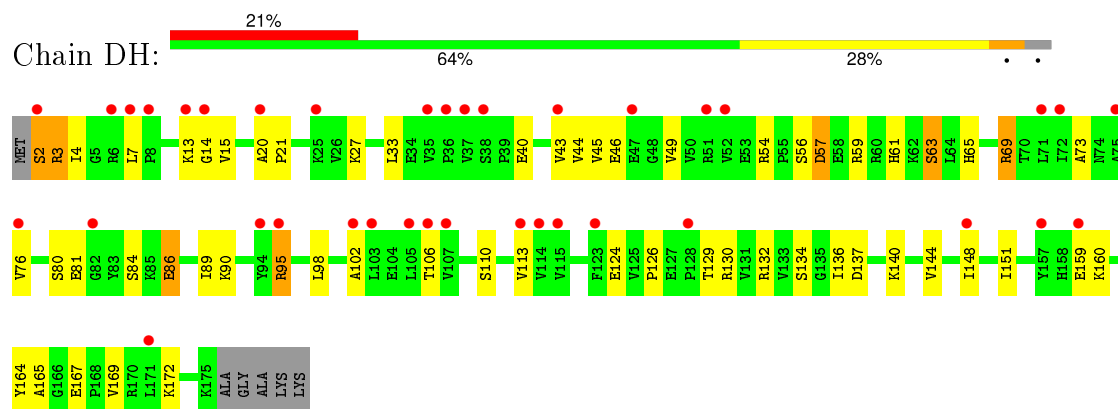
• Molecule 31: 50S ribosomal protein L5



• Molecule 32: 50S ribosomal protein L6

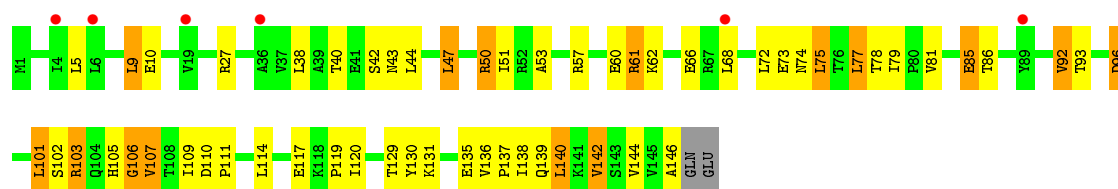


• Molecule 32: 50S ribosomal protein L6

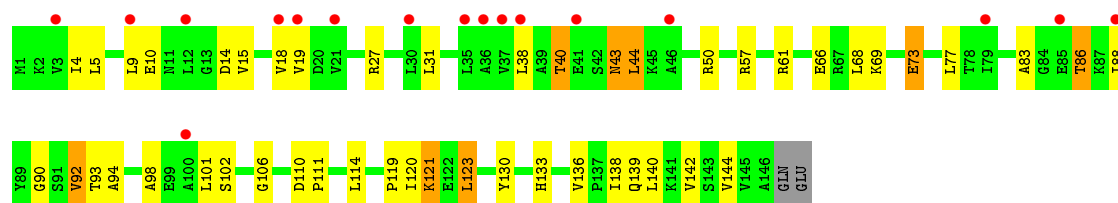


• Molecule 33: 50S ribosomal protein L9

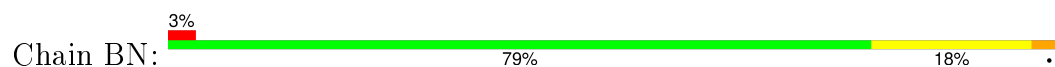




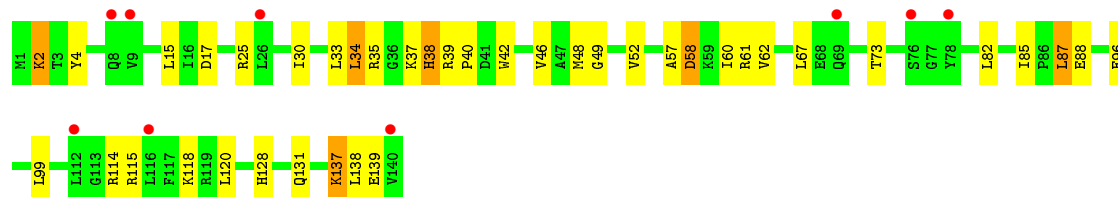
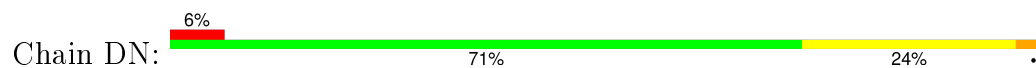
• Molecule 33: 50S ribosomal protein L9



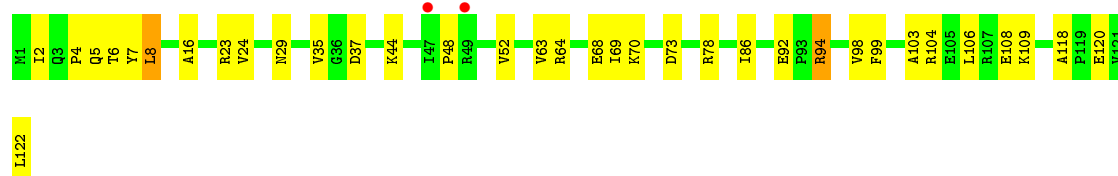
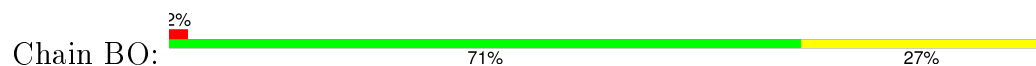
• Molecule 34: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L13

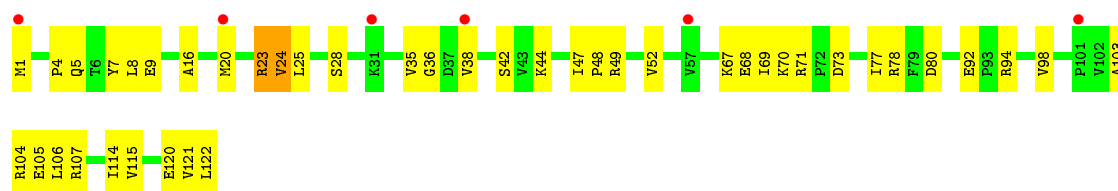


• Molecule 35: 50S ribosomal protein L14

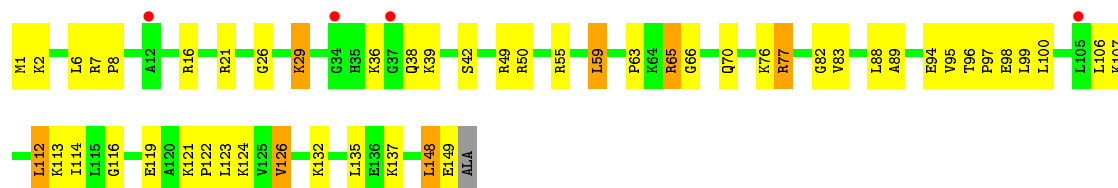


• Molecule 35: 50S ribosomal protein L14

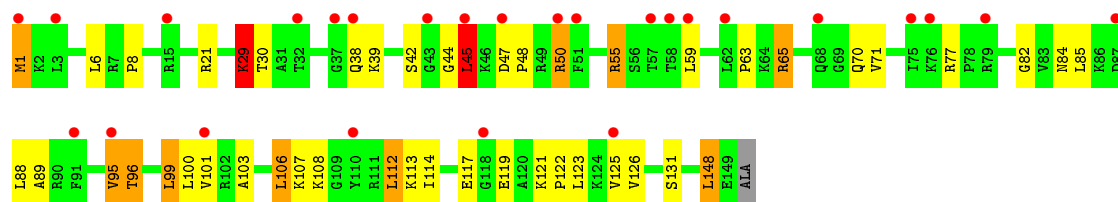




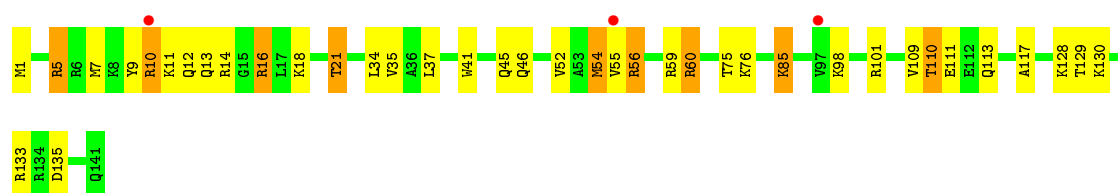
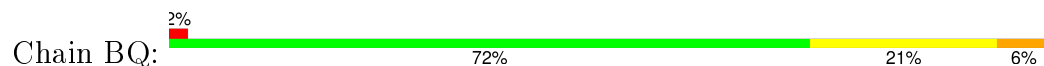
- Molecule 36: 50S ribosomal protein L15



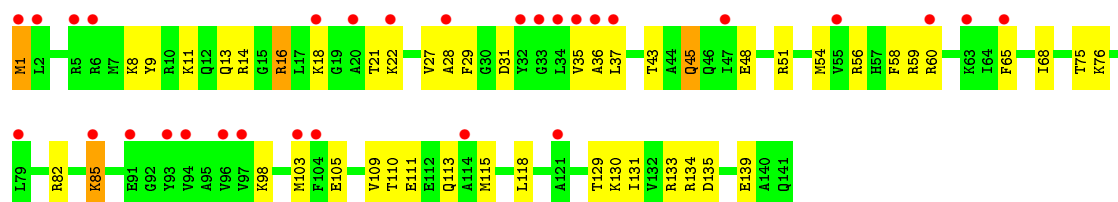
- Molecule 36: 50S ribosomal protein L15



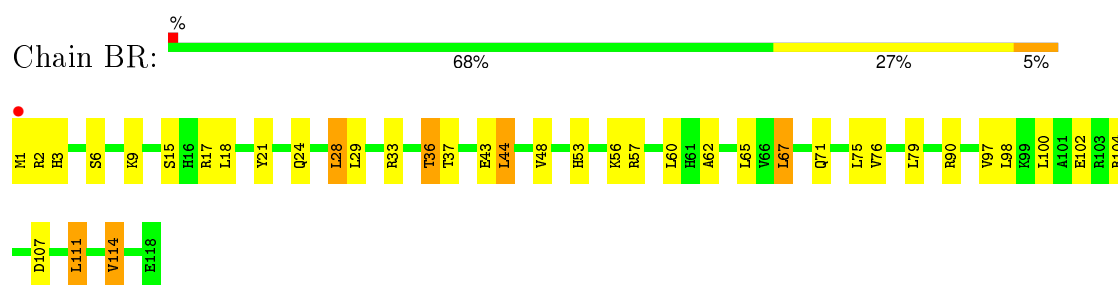
- Molecule 37: 50S ribosomal protein L16



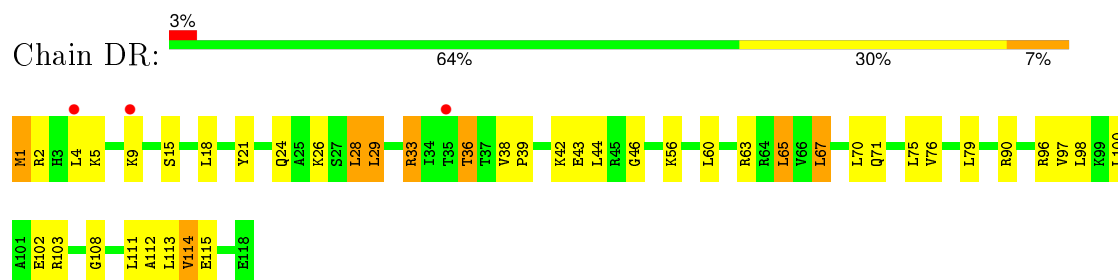
- Molecule 37: 50S ribosomal protein L16



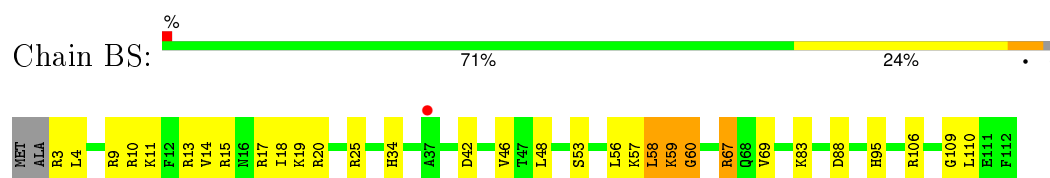
- Molecule 38: 50S ribosomal protein L17



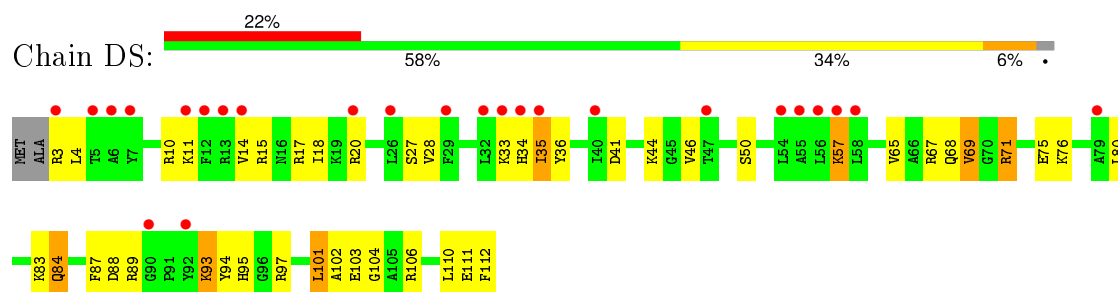
- Molecule 38: 50S ribosomal protein L17



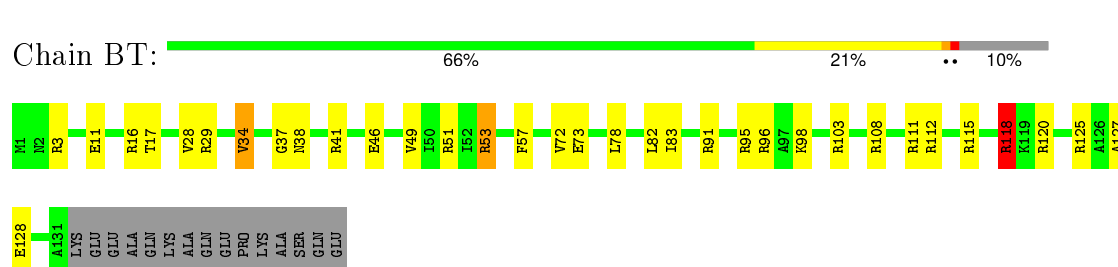
- Molecule 39: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L18

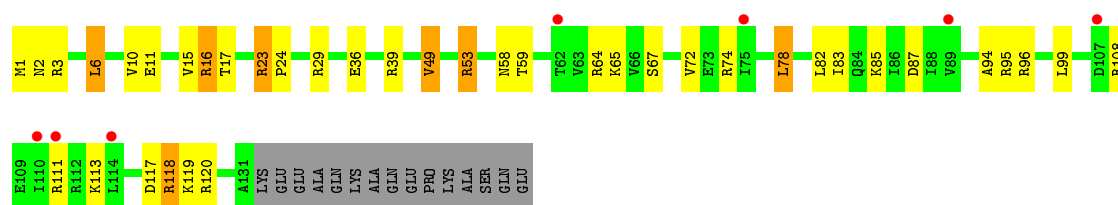


- Molecule 40: 50S ribosomal protein L19

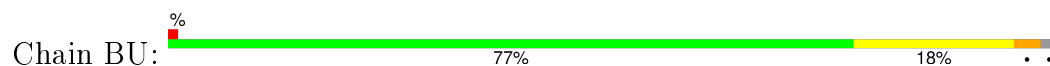


- Molecule 40: 50S ribosomal protein L19

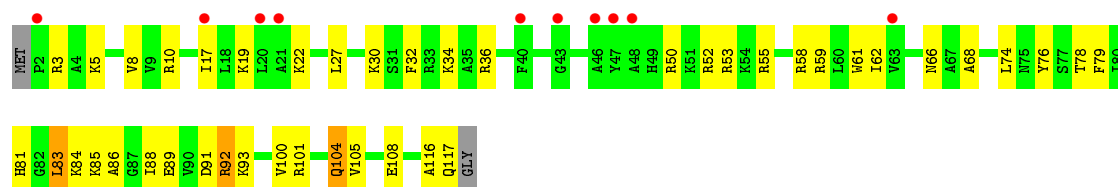




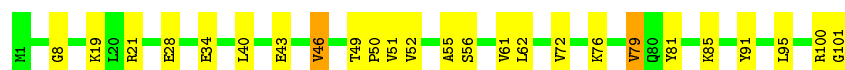
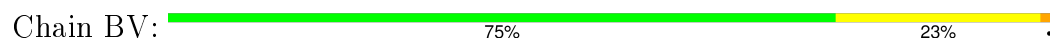
- Molecule 41: 50S ribosomal protein L20



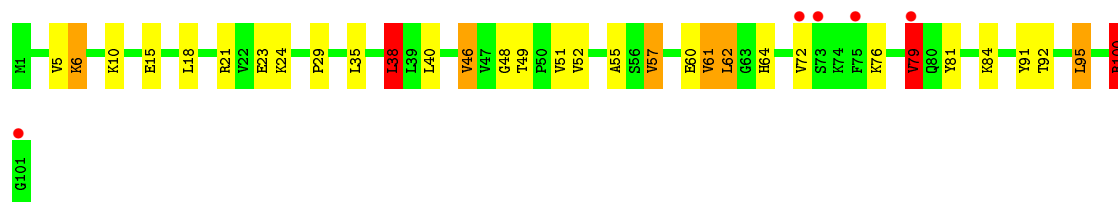
- Molecule 41: 50S ribosomal protein L20



- Molecule 42: 50S ribosomal protein L21



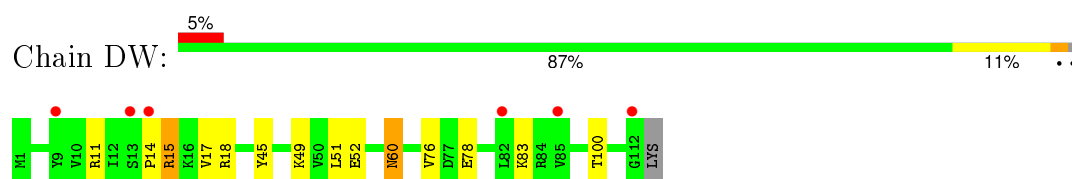
- Molecule 42: 50S ribosomal protein L21



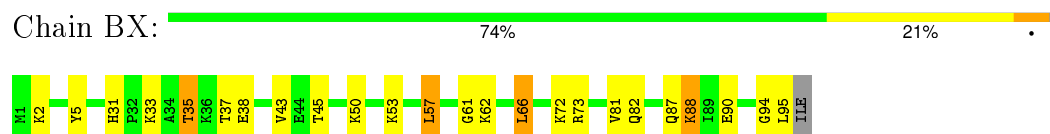
- Molecule 43: 50S ribosomal protein L22



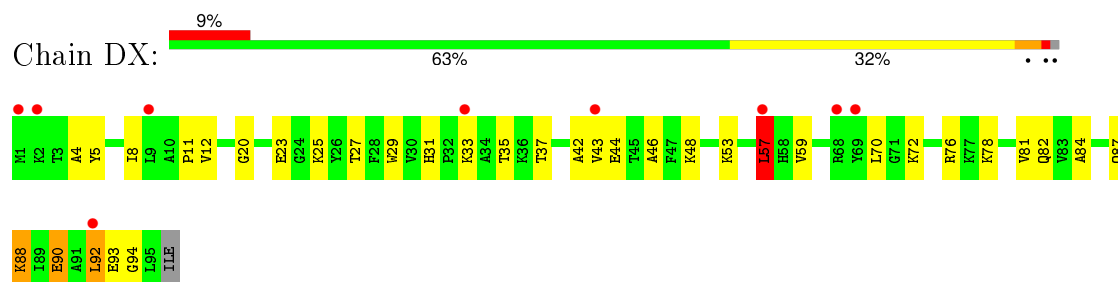
- Molecule 43: 50S ribosomal protein L22



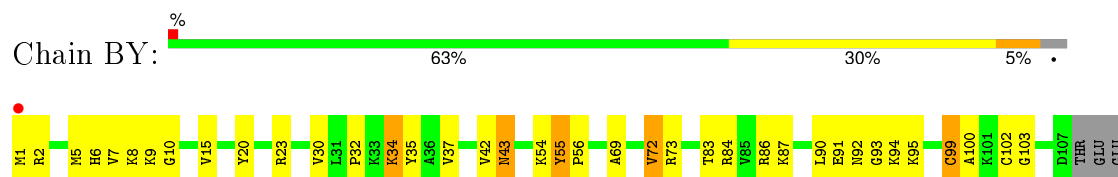
- Molecule 44: 50S ribosomal protein L23



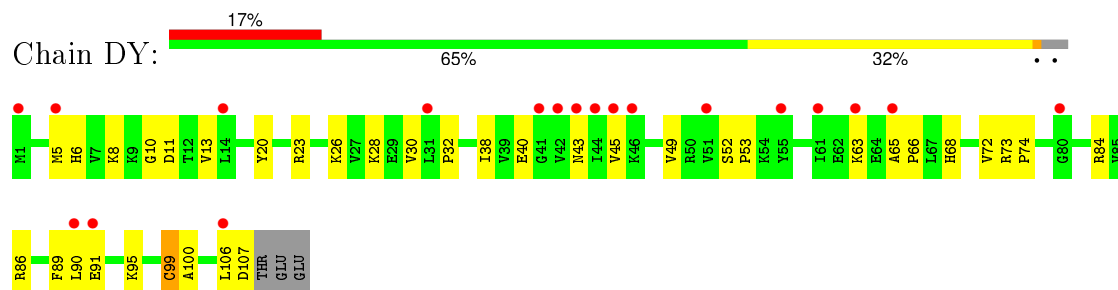
- Molecule 44: 50S ribosomal protein L23



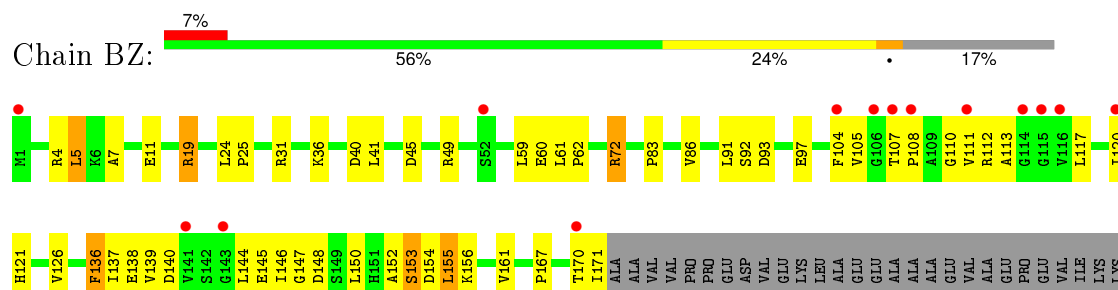
- Molecule 45: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L24

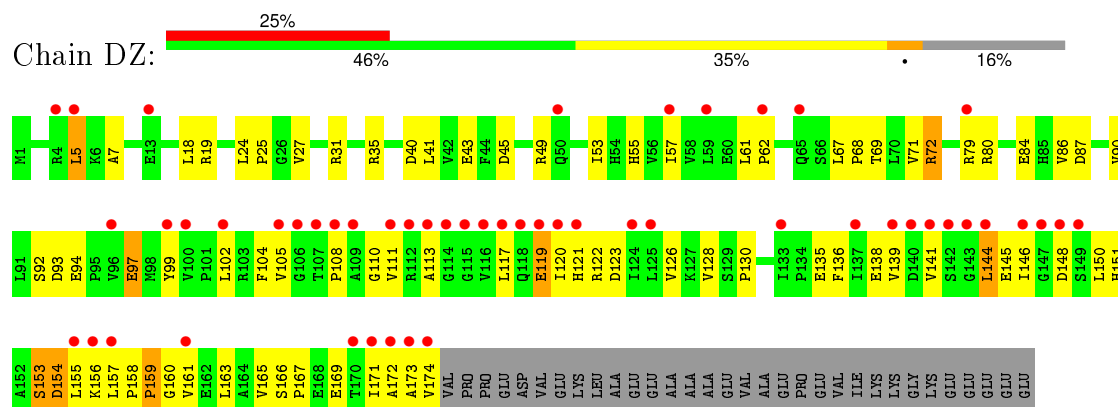


- Molecule 46: 50S ribosomal protein L25

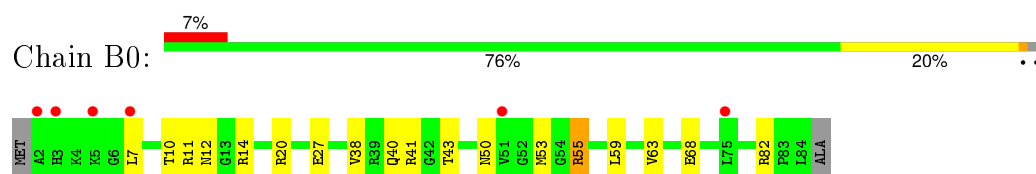


GLY
LYS
GLU
GLU
GLU
GLU

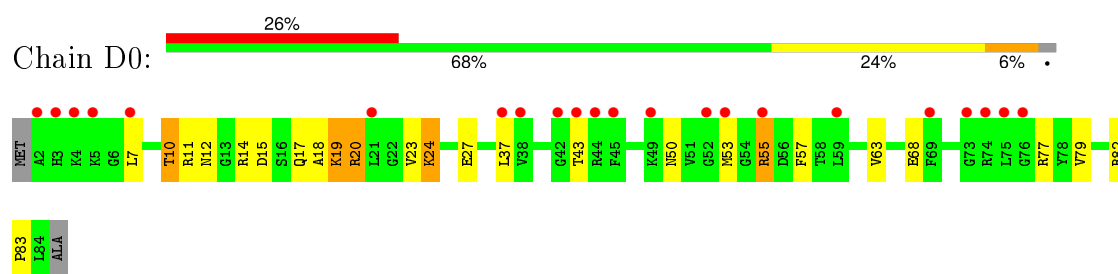
- Molecule 46: 50S ribosomal protein L25



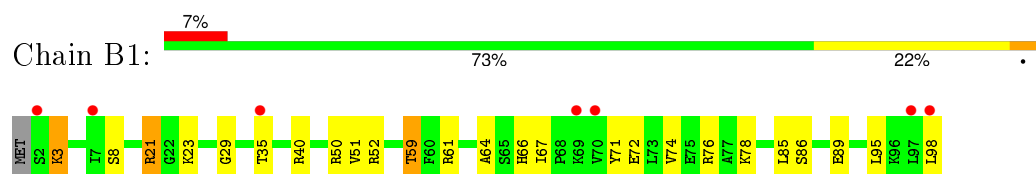
- Molecule 47: 50S ribosomal protein L27



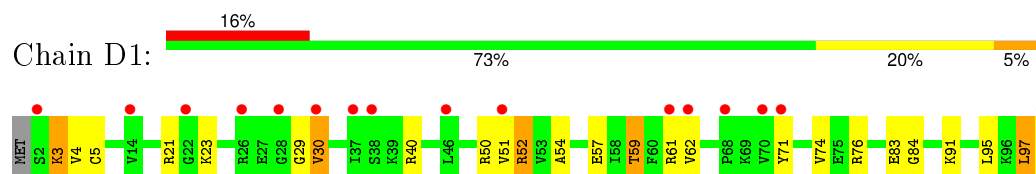
- Molecule 47: 50S ribosomal protein L27



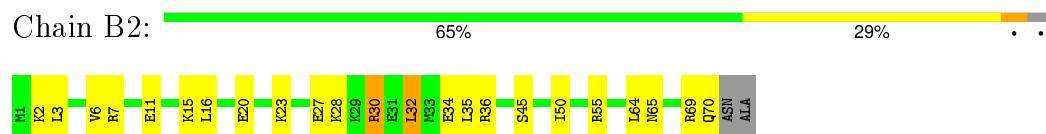
- Molecule 48: 50S ribosomal protein L28



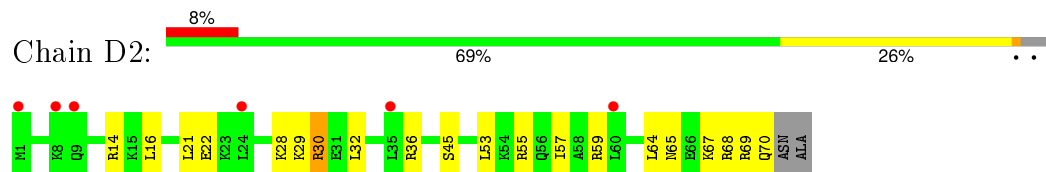
- Molecule 48: 50S ribosomal protein L28



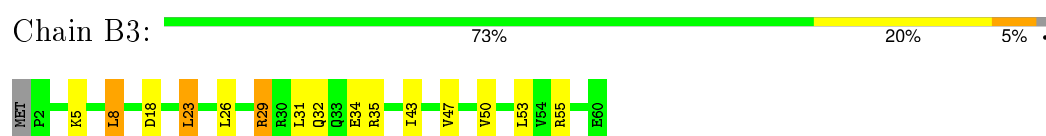
- Molecule 49: 50S ribosomal protein L29



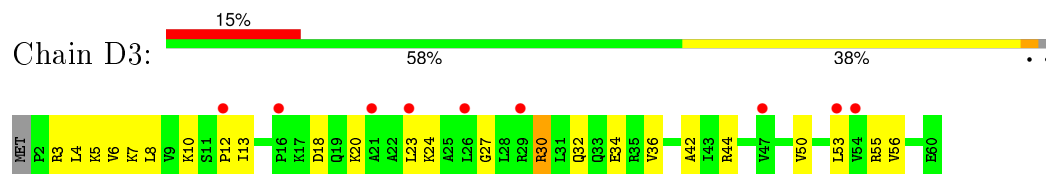
- Molecule 49: 50S ribosomal protein L29



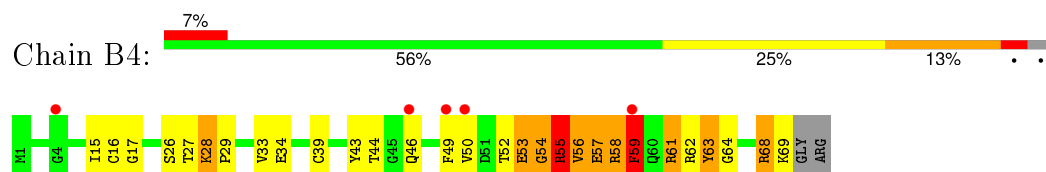
- Molecule 50: 50S ribosomal protein L30



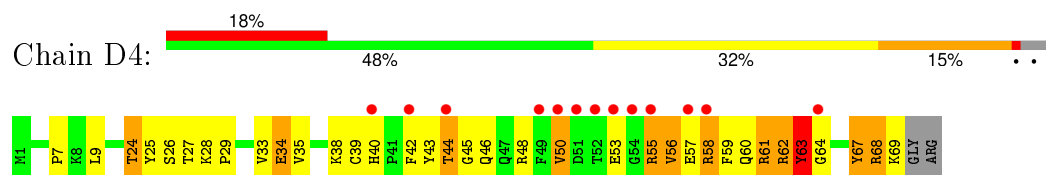
- Molecule 50: 50S ribosomal protein L30



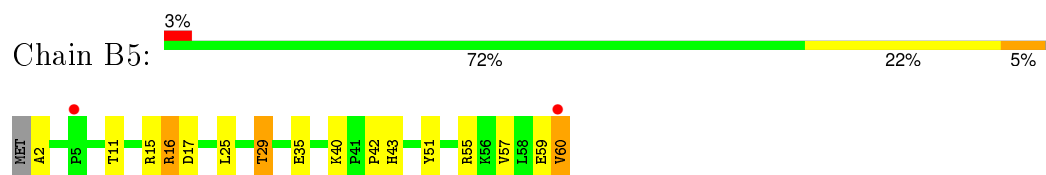
- Molecule 51: 50S ribosomal protein L31



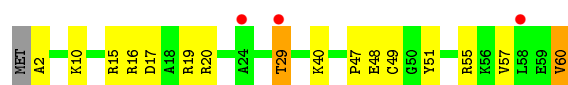
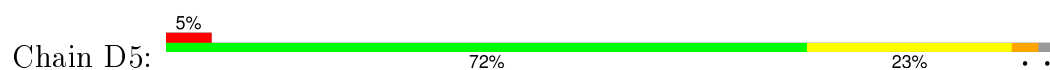
- Molecule 51: 50S ribosomal protein L31



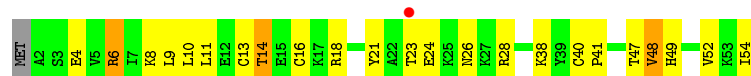
- Molecule 52: 50S ribosomal protein L32



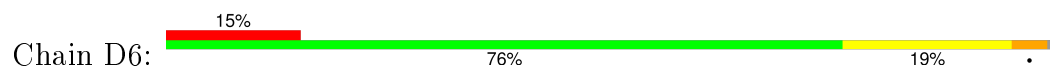
- Molecule 52: 50S ribosomal protein L32



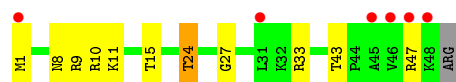
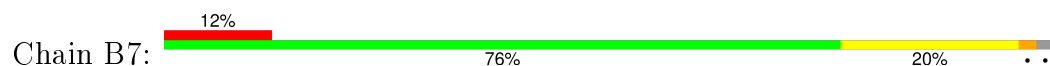
- Molecule 53: 50S ribosomal protein L33



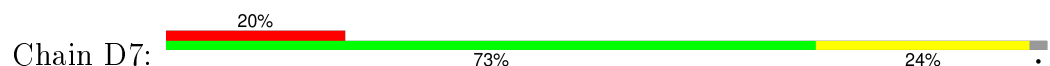
- Molecule 53: 50S ribosomal protein L33



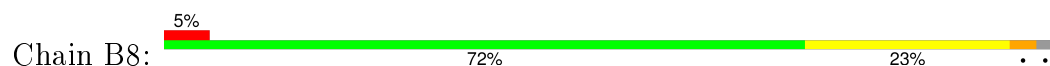
- Molecule 54: 50S ribosomal protein L34



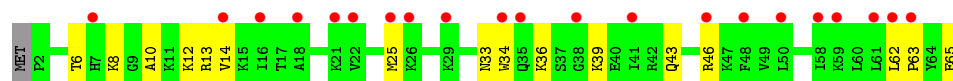
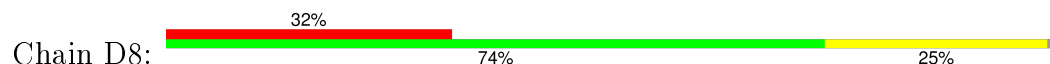
- Molecule 54: 50S ribosomal protein L34



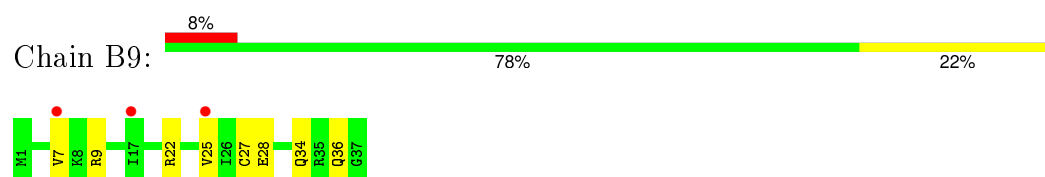
- Molecule 55: 50S ribosomal protein L35



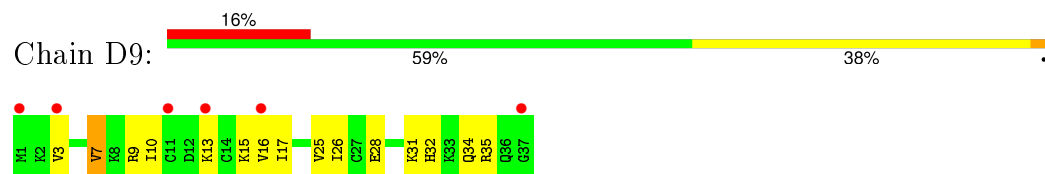
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.32Å 450.06Å 622.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.51 – 2.55 255.92 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.8 (152.51-2.55) 95.8 (255.92-2.55)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.233 , 0.280 0.244 , 0.288	Depositor DCC
R_{free} test set	90444 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 1802139 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	297141	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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, 31M, MIA, SF4, MG, 5MC, 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	AA	0.37	0/36049	0.91	42/56261 (0.1%)
1	CA	0.40	6/36170 (0.0%)	1.00	88/56452 (0.2%)
2	AB	0.31	0/1881	0.60	0/2542
2	CB	0.33	0/1860	0.65	1/2518 (0.0%)
3	AC	0.28	0/1576	0.52	0/2130
3	CC	0.32	0/1566	0.61	0/2119
4	AD	0.29	0/1689	0.58	2/2267 (0.1%)
4	CD	0.30	0/1704	0.54	0/2284
5	AE	0.30	0/1145	0.55	0/1543
5	CE	0.31	0/1149	0.62	1/1548 (0.1%)
6	AF	0.28	0/819	0.49	0/1111
6	CF	0.31	0/829	0.52	0/1123
7	AG	0.27	0/1250	0.51	0/1679
7	CG	0.28	0/1254	0.53	0/1683
8	AH	0.27	0/1108	0.50	0/1494
8	CH	0.27	0/1108	0.52	0/1494
9	AI	0.30	0/1002	0.59	0/1346
9	CI	0.30	0/997	0.57	0/1343
10	AJ	0.28	0/722	0.59	0/982
10	CJ	0.31	0/727	0.59	0/988
11	AK	0.28	0/844	0.60	1/1145 (0.1%)
11	CK	0.28	0/848	0.53	0/1149
12	AL	0.30	0/946	0.52	0/1274
12	CL	0.30	0/946	0.55	0/1274
13	AM	0.28	0/969	0.61	0/1302
13	CM	0.29	0/961	0.57	0/1291
14	AN	0.30	0/501	0.50	0/664
14	CN	0.33	0/501	0.57	0/664
15	AO	0.28	0/739	0.55	0/985
15	CO	0.30	0/739	0.54	0/985
16	AP	0.28	0/697	0.52	0/939
16	CP	0.31	0/693	0.51	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.28	0/836	0.53	0/1117
17	CQ	0.29	0/836	0.50	0/1117
18	AR	0.27	0/560	0.56	0/746
18	CR	0.28	0/560	0.56	0/746
19	AS	0.29	0/667	0.58	0/900
19	CS	0.32	0/661	0.67	0/893
20	AT	0.28	0/730	0.58	0/965
20	CT	0.28	0/729	0.52	0/965
21	AU	0.26	0/203	0.52	0/266
21	CU	0.35	0/203	0.52	0/266
22	AV	0.41	0/310	0.94	0/480
22	CV	0.45	0/282	1.06	1/437 (0.2%)
23	AW	0.47	0/1577	1.18	6/2454 (0.2%)
23	CW	0.59	0/1531	1.46	25/2379 (1.1%)
24	AX	0.51	0/1725	1.17	14/2689 (0.5%)
24	CX	0.44	0/1725	1.12	10/2689 (0.4%)
25	AY	0.62	0/1602	1.43	22/2493 (0.9%)
25	CY	0.64	0/1579	1.46	32/2455 (1.3%)
26	BA	0.48	2/68013 (0.0%)	0.95	84/106165 (0.1%)
26	DA	0.42	1/67542 (0.0%)	0.94	72/105428 (0.1%)
27	BB	0.41	0/2878	0.88	0/4490
27	DB	0.44	0/2878	0.94	0/4490
28	BD	0.37	0/2186	0.59	0/2944
28	DD	0.33	0/2186	0.55	0/2944
29	BE	0.36	0/1592	0.57	0/2149
29	DE	0.34	0/1592	0.60	1/2149 (0.0%)
30	BF	0.35	0/1619	0.55	0/2193
30	DF	0.32	0/1615	0.58	0/2188
31	BG	0.31	0/1450	0.54	0/1959
31	DG	0.33	0/1449	0.57	0/1958
32	BH	0.33	0/1356	0.54	0/1834
32	DH	0.30	0/1356	0.52	0/1834
33	BI	0.29	0/1100	0.60	0/1501
33	DI	0.28	0/1076	0.57	0/1471
34	BN	0.32	0/1144	0.53	0/1543
34	DN	0.31	0/1144	0.54	0/1543
35	BO	0.34	0/943	0.58	1/1269 (0.1%)
35	DO	0.31	0/943	0.51	0/1269
36	BP	0.34	0/1152	0.58	0/1533
36	DP	0.31	0/1152	0.59	0/1533
37	BQ	0.34	0/1143	0.53	0/1527
37	DQ	0.31	0/1143	0.52	0/1527
38	BR	0.35	0/982	0.58	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.29	0/982	0.52	0/1312
39	BS	0.31	0/887	0.63	2/1180 (0.2%)
39	DS	0.29	0/880	0.61	0/1172
40	BT	0.33	0/1105	0.59	1/1477 (0.1%)
40	DT	0.29	0/1097	0.56	0/1468
41	BU	0.37	0/977	0.56	0/1301
41	DU	0.31	0/977	0.50	0/1301
42	BV	0.39	0/782	0.58	0/1049
42	DV	0.32	0/782	0.64	2/1049 (0.2%)
43	BW	0.38	0/897	0.57	0/1205
43	DW	0.31	0/897	0.52	0/1205
44	BX	0.39	0/764	0.59	1/1025 (0.1%)
44	DX	0.32	0/764	0.56	1/1025 (0.1%)
45	BY	0.34	0/819	0.57	0/1095
45	DY	0.31	0/819	0.55	0/1095
46	BZ	0.31	0/1379	0.61	0/1873
46	DZ	0.29	0/1390	0.57	0/1890
47	B0	0.35	0/662	0.57	0/881
47	D0	0.29	0/662	0.49	0/881
48	B1	0.34	0/762	0.56	0/1014
48	D1	0.32	0/762	0.54	0/1014
49	B2	0.32	0/590	0.56	0/781
49	D2	0.27	0/590	0.46	0/781
50	B3	0.36	0/474	0.58	0/635
50	D3	0.27	0/469	0.50	0/630
51	B4	0.35	0/571	0.71	0/768
51	D4	0.34	0/545	0.70	0/737
52	B5	0.38	0/469	0.60	0/635
52	D5	0.33	0/469	0.52	0/635
53	B6	0.36	0/460	0.51	0/613
53	D6	0.30	0/456	0.48	0/608
54	B7	0.39	0/426	0.55	0/561
54	D7	0.33	0/426	0.59	0/561
55	B8	0.36	0/519	0.58	0/684
55	D8	0.32	0/525	0.52	0/691
56	B9	0.35	0/310	0.51	0/407
56	D9	0.31	0/310	0.56	0/407
All	All	0.40	9/316594 (0.0%)	0.88	410/473970 (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
2	AB	0	4
7	AG	0	2
7	CG	0	1
20	CT	0	1
28	BD	0	1
39	BS	0	1
51	B4	0	2
51	D4	0	1
All	All	0	13

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	N1-C2	-11.01	1.28	1.37
1	CA	1154	G	C6-N1	-10.68	1.32	1.39
1	CA	1119	C	N3-C4	-9.86	1.27	1.33
1	CA	1154	G	N7-C5	-7.17	1.34	1.39
26	BA	330	A	N9-C4	-6.79	1.33	1.37

The worst 5 of 410 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1119	C	N1-C2-O2	32.18	138.21	118.90
1	CA	1154	G	N3-C2-N2	24.48	137.03	119.90
1	CA	1154	G	C5-C6-O6	24.01	143.00	128.60
1	CA	1154	G	N1-C2-N2	-21.95	96.45	116.20
1	CA	1119	C	N3-C2-O2	-20.26	107.72	121.90

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	18	GLY	Peptide
2	AB	231	GLU	Peptide
2	AB	8	LYS	Peptide
2	AB	9	GLU	Peptide
7	AG	78	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16254	495	0
1	CA	32312	0	16307	663	0
2	AB	1846	0	1867	92	0
2	CB	1825	0	1828	102	0
3	AC	1552	0	1546	53	0
3	CC	1542	0	1517	81	0
4	AD	1659	0	1676	73	0
4	CD	1674	0	1714	61	0
5	AE	1129	0	1185	34	0
5	CE	1133	0	1191	33	0
6	AF	806	0	793	24	0
6	CF	816	0	808	18	0
7	AG	1231	0	1238	28	0
7	CG	1235	0	1249	37	0
8	AH	1088	0	1126	26	0
8	CH	1088	0	1126	42	0
9	AI	983	0	986	47	0
9	CI	978	0	966	47	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	36	0
11	AK	829	0	825	20	0
11	CK	833	0	836	14	0
12	AL	930	0	980	24	0
12	CL	930	0	980	27	0
13	AM	958	0	1002	31	0
13	CM	950	0	988	39	0
14	AN	492	0	529	16	0
14	CN	492	0	529	33	0
15	AO	728	0	760	20	0
15	CO	728	0	760	31	0
16	AP	681	0	697	12	0
16	CP	677	0	686	23	0
17	AQ	823	0	891	22	0
17	CQ	823	0	891	15	0
18	AR	555	0	618	17	0
18	CR	555	0	618	16	0
19	AS	652	0	662	31	0
19	CS	646	0	644	42	0
20	AT	728	0	798	32	0
20	CT	727	0	796	25	0
21	AU	199	0	208	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	CU	199	0	208	10	0
22	AV	277	0	140	2	0
22	CV	252	0	130	7	0
23	AW	1607	0	839	55	0
23	CW	1560	0	803	55	0
24	AX	1625	0	828	34	0
24	CX	1625	0	828	33	0
25	AY	1581	0	805	96	0
25	CY	1561	0	796	79	0
26	BA	60729	0	30621	669	0
26	DA	60311	0	30409	876	0
27	BB	2573	0	1306	19	0
27	DB	2573	0	1306	50	0
28	BD	2136	0	2218	51	0
28	DD	2136	0	2218	61	0
29	BE	1559	0	1618	30	0
29	DE	1559	0	1618	45	0
30	BF	1584	0	1625	47	0
30	DF	1580	0	1619	50	0
31	BG	1425	0	1443	38	0
31	DG	1424	0	1434	66	0
32	BH	1330	0	1407	28	0
32	DH	1330	0	1407	30	0
33	BI	1085	0	1114	41	0
33	DI	1061	0	1080	25	0
34	BN	1117	0	1183	17	0
34	DN	1117	0	1184	27	0
35	BO	933	0	996	20	0
35	DO	933	0	996	29	0
36	BP	1135	0	1212	38	0
36	DP	1135	0	1212	43	0
37	BQ	1122	0	1179	31	0
37	DQ	1122	0	1179	35	0
38	BR	968	0	1033	18	0
38	DR	968	0	1033	28	0
39	BS	877	0	938	23	0
39	DS	870	0	923	34	0
40	BT	1091	0	1151	27	0
40	DT	1083	0	1136	31	0
41	BU	959	0	1019	17	0
41	DU	959	0	1019	38	0
42	BV	771	0	830	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	DV	771	0	830	25	0
43	BW	886	0	939	12	0
43	DW	886	0	940	9	0
44	BX	750	0	814	16	0
44	DX	750	0	814	23	0
45	BY	806	0	881	23	0
45	DY	806	0	881	26	0
46	BZ	1349	0	1355	44	0
46	DZ	1360	0	1363	61	0
47	B0	653	0	674	14	0
47	D0	653	0	674	20	0
48	B1	755	0	826	18	0
48	D1	755	0	826	18	0
49	B2	588	0	643	11	0
49	D2	588	0	643	12	0
50	B3	469	0	518	9	0
50	D3	464	0	514	12	0
51	B4	558	0	544	22	0
51	D4	532	0	503	31	0
52	B5	455	0	465	11	0
52	D5	455	0	465	12	0
53	B6	453	0	473	13	0
53	D6	449	0	469	9	0
54	B7	418	0	467	9	0
54	D7	418	0	467	10	0
55	B8	511	0	571	21	0
55	D8	517	0	582	10	0
56	B9	307	0	335	7	0
56	D9	307	0	335	13	0
57	AA	214	0	0	0	0
57	AE	3	0	0	0	0
57	AF	1	0	0	0	0
57	AK	1	0	0	0	0
57	AM	1	0	0	0	0
57	AN	2	0	0	0	0
57	AW	4	0	0	0	0
57	AX	15	0	0	0	0
57	AY	3	0	0	0	0
57	B0	3	0	0	0	0
57	B1	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B4	1	0	0	0	0
57	B5	1	0	0	0	0
57	B6	2	0	0	0	0
57	B7	5	0	0	0	0
57	B8	1	0	0	0	0
57	B9	1	0	0	0	0
57	BA	812	0	0	0	0
57	BB	20	0	0	0	0
57	BD	9	0	0	0	0
57	BE	8	0	0	0	0
57	BF	9	0	0	0	0
57	BG	3	0	0	0	0
57	BN	6	0	0	0	0
57	BO	2	0	0	0	0
57	BP	5	0	0	0	0
57	BQ	5	0	0	0	0
57	BR	2	0	0	0	0
57	BU	8	0	0	0	0
57	BV	5	0	0	0	0
57	BW	4	0	0	0	0
57	BX	3	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	1	0	0	0	0
57	CA	170	0	0	0	0
57	CD	1	0	0	0	0
57	CE	1	0	0	0	0
57	CF	1	0	0	0	0
57	CJ	1	0	0	0	0
57	CK	1	0	0	0	0
57	CT	1	0	0	0	0
57	CV	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	3	0	0	1	0
57	D0	1	0	0	0	0
57	D3	1	0	0	0	0
57	D8	1	0	0	0	0
57	DA	677	0	0	0	0
57	DB	13	0	0	0	0
57	DD	9	0	0	0	0
57	DE	4	0	0	0	0
57	DF	4	0	0	0	0
57	DG	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	4	0	0	0	0
57	DR	1	0	0	0	0
57	DU	2	0	0	0	0
57	DV	3	0	0	0	0
57	DW	4	0	0	0	0
57	DX	1	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	0	0
58	CD	8	0	0	0	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	227	0	0	17	0
61	AE	2	0	0	0	0
61	AJ	1	0	0	0	0
61	AL	1	0	0	1	0
61	AM	1	0	0	0	0
61	AU	1	0	0	1	0
61	AV	3	0	0	0	0
61	AW	3	0	0	0	0
61	AX	6	0	0	2	0
61	AY	1	0	0	0	0
61	B0	3	0	0	0	0
61	B1	1	0	0	0	0
61	B3	2	0	0	0	0
61	B5	2	0	0	0	0
61	B6	1	0	0	0	0
61	B7	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B8	8	0	0	1	0
61	BA	1383	0	0	61	0
61	BB	36	0	0	1	0
61	BD	12	0	0	1	0
61	BE	14	0	0	4	0
61	BF	8	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BO	4	0	0	0	0
61	BP	16	0	0	3	0
61	BQ	4	0	0	0	0
61	BR	2	0	0	0	0
61	BT	2	0	0	0	0
61	BU	3	0	0	0	0
61	BV	2	0	0	0	0
61	BW	1	0	0	0	0
61	BX	4	0	0	0	0
61	BZ	1	0	0	0	0
61	CA	185	0	0	17	0
61	CJ	2	0	0	1	0
61	CL	1	0	0	0	0
61	CT	1	0	0	0	0
61	CV	1	0	0	0	0
61	CW	2	0	0	0	0
61	D0	3	0	0	0	0
61	D1	1	0	0	0	0
61	D3	1	0	0	1	0
61	D7	3	0	0	0	0
61	D8	4	0	0	0	0
61	DA	1025	0	0	79	0
61	DB	9	0	0	0	0
61	DD	19	0	0	4	0
61	DE	11	0	0	0	0
61	DF	3	0	0	0	0
61	DN	2	0	0	1	0
61	DO	1	0	0	0	0
61	DP	16	0	0	2	0
61	DR	1	0	0	0	0
61	DT	3	0	0	0	0
61	DU	2	0	0	0	0
61	DX	3	0	0	0	0
61	DY	2	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	297141	0	196251	5228	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 11.

The worst 5 of 5228 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)
25:CY:7:A:N6	25:CY:66:U:H3	1.37	1.21
25:AY:49:C:N4	25:AY:65:G:H1	1.44	1.16
26:DA:2139:C:N4	26:DA:2152:G:H1	1.42	1.16
1:CA:1000:U:H3	1:CA:1041:A:N6	1.44	1.15
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.12

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	
2	AB	229/256 (90%)	208 (91%)	14 (6%)	7 (3%)	5	6
2	CB	229/256 (90%)	206 (90%)	16 (7%)	7 (3%)	5	6
3	AC	204/239 (85%)	195 (96%)	8 (4%)	1 (0%)	34	54
3	CC	204/239 (85%)	189 (93%)	15 (7%)	0	100	100
4	AD	206/209 (99%)	197 (96%)	7 (3%)	2 (1%)	19	33
4	CD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	34	54
5	AE	146/162 (90%)	142 (97%)	4 (3%)	0	100	100
5	CE	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
6	AF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	CF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	AG	153/156 (98%)	144 (94%)	5 (3%)	4 (3%)	7	9
7	CG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	26	44
8	AH	135/138 (98%)	134 (99%)	1 (1%)	0	100	100
8	CH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
9	AI	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
9	CI	125/128 (98%)	119 (95%)	5 (4%)	1 (1%)	24	40
10	AJ	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	3	3
10	CJ	94/105 (90%)	85 (90%)	4 (4%)	5 (5%)	2	2
11	AK	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	11	17
11	CK	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	11	17
12	AL	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
12	CL	120/132 (91%)	118 (98%)	2 (2%)	0	100	100
13	AM	121/126 (96%)	116 (96%)	5 (4%)	0	100	100
13	CM	120/126 (95%)	113 (94%)	7 (6%)	0	100	100
14	AN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
15	CO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/88 (91%)	79 (99%)	1 (1%)	0	100	100
16	CP	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	15	25
17	AQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
17	CQ	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	AR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
18	CR	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	AS	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	16	27
19	CS	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
20	AT	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	3	3
20	CT	94/106 (89%)	88 (94%)	3 (3%)	3 (3%)	5	6
21	AU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
21	CU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	BD	273/276 (99%)	264 (97%)	8 (3%)	1 (0%)	39	60
28	DD	273/276 (99%)	263 (96%)	8 (3%)	2 (1%)	26	44
29	BE	202/206 (98%)	196 (97%)	5 (2%)	1 (0%)	34	54
29	DE	202/206 (98%)	196 (97%)	4 (2%)	2 (1%)	19	33
30	BF	201/210 (96%)	200 (100%)	0	1 (0%)	34	54
30	DF	201/210 (96%)	199 (99%)	0	2 (1%)	19	33
31	BG	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	30	48
31	DG	179/182 (98%)	171 (96%)	5 (3%)	3 (2%)	11	18
32	BH	172/180 (96%)	168 (98%)	3 (2%)	1 (1%)	30	48
32	DH	172/180 (96%)	166 (96%)	5 (3%)	1 (1%)	30	48
33	BI	144/148 (97%)	130 (90%)	11 (8%)	3 (2%)	9	13
33	DI	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	26	44
34	BN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
34	DN	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	26	44
35	BO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
35	DO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
36	BP	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	26	44
36	DP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	14	23
37	BQ	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	26	44
38	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
39	BS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	21	36
39	DS	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	21	36
40	BT	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
40	DT	129/146 (88%)	127 (98%)	2 (2%)	0	100	100
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	114 (100%)	0	0	100	100
42	BV	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
42	DV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	19	33
43	BW	110/113 (97%)	110 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	DW	110/113 (97%)	110 (100%)	0	0	100	100
44	BX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
44	DX	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
45	BY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
45	DY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
46	BZ	169/206 (82%)	153 (90%)	15 (9%)	1 (1%)	30	48
46	DZ	172/206 (84%)	161 (94%)	11 (6%)	0	100	100
47	B0	81/85 (95%)	81 (100%)	0	0	100	100
47	D0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
48	B1	95/98 (97%)	94 (99%)	0	1 (1%)	17	30
48	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	30
49	B2	68/72 (94%)	68 (100%)	0	0	100	100
49	D2	68/72 (94%)	68 (100%)	0	0	100	100
50	B3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	3	3
51	D4	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	1
52	B5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
52	D5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
53	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
53	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
54	B7	46/49 (94%)	46 (100%)	0	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	8	12
55	B8	62/65 (95%)	62 (100%)	0	0	100	100
55	D8	62/65 (95%)	62 (100%)	0	0	100	100
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10908 (96%)	416 (4%)	85 (1%)	26	44

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	AG	80	VAL
20	AT	10	LEU
20	AT	96	GLY
28	BD	275	LYS

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	
2	AB	192/220 (87%)	163 (85%)	29 (15%)	3	6
2	CB	187/220 (85%)	149 (80%)	38 (20%)	1	2
3	AC	143/188 (76%)	121 (85%)	22 (15%)	3	5
3	CC	140/188 (74%)	124 (89%)	16 (11%)	7	12
4	AD	170/181 (94%)	152 (89%)	18 (11%)	8	15
4	CD	173/181 (96%)	152 (88%)	21 (12%)	6	10
5	AE	113/123 (92%)	105 (93%)	8 (7%)	18	32
5	CE	114/123 (93%)	101 (89%)	13 (11%)	7	12
6	AF	83/90 (92%)	76 (92%)	7 (8%)	14	24
6	CF	85/90 (94%)	80 (94%)	5 (6%)	24	42
7	AG	119/127 (94%)	108 (91%)	11 (9%)	11	20
7	CG	120/127 (94%)	109 (91%)	11 (9%)	11	20
8	AH	114/119 (96%)	105 (92%)	9 (8%)	15	27
8	CH	114/119 (96%)	107 (94%)	7 (6%)	23	40
9	AI	90/99 (91%)	76 (84%)	14 (16%)	3	5
9	CI	89/99 (90%)	76 (85%)	13 (15%)	4	6
10	AJ	66/92 (72%)	58 (88%)	8 (12%)	6	10
10	CJ	69/92 (75%)	63 (91%)	6 (9%)	13	22
11	AK	82/99 (83%)	77 (94%)	5 (6%)	23	40
11	CK	83/99 (84%)	76 (92%)	7 (8%)	14	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	97/109 (89%)	93 (96%)	4 (4%)	37	61
12	CL	97/109 (89%)	93 (96%)	4 (4%)	37	61
13	AM	93/101 (92%)	82 (88%)	11 (12%)	6	11
13	CM	92/101 (91%)	80 (87%)	12 (13%)	5	9
14	AN	49/50 (98%)	42 (86%)	7 (14%)	4	7
14	CN	49/50 (98%)	41 (84%)	8 (16%)	3	4
15	AO	78/80 (98%)	64 (82%)	14 (18%)	2	3
15	CO	78/80 (98%)	69 (88%)	9 (12%)	7	12
16	AP	69/74 (93%)	60 (87%)	9 (13%)	5	9
16	CP	68/74 (92%)	61 (90%)	7 (10%)	9	15
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	10	18
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	17	30
18	AR	59/77 (77%)	54 (92%)	5 (8%)	13	23
18	CR	59/77 (77%)	52 (88%)	7 (12%)	6	11
19	AS	69/80 (86%)	64 (93%)	5 (7%)	18	31
19	CS	67/80 (84%)	63 (94%)	4 (6%)	24	41
20	AT	70/82 (85%)	62 (89%)	8 (11%)	7	12
20	CT	70/82 (85%)	62 (89%)	8 (11%)	7	12
21	AU	18/22 (82%)	15 (83%)	3 (17%)	3	4
21	CU	18/22 (82%)	17 (94%)	1 (6%)	26	45
28	BD	215/218 (99%)	195 (91%)	20 (9%)	11	19
28	DD	215/218 (99%)	193 (90%)	22 (10%)	9	16
29	BE	164/166 (99%)	146 (89%)	18 (11%)	8	13
29	DE	164/166 (99%)	145 (88%)	19 (12%)	7	12
30	BF	160/166 (96%)	149 (93%)	11 (7%)	19	34
30	DF	159/166 (96%)	144 (91%)	15 (9%)	11	19
31	BG	143/156 (92%)	128 (90%)	15 (10%)	8	15
31	DG	142/156 (91%)	122 (86%)	20 (14%)	4	7
32	BH	144/148 (97%)	126 (88%)	18 (12%)	6	10
32	DH	144/148 (97%)	126 (88%)	18 (12%)	6	10
33	BI	110/124 (89%)	86 (78%)	24 (22%)	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DI	104/124 (84%)	88 (85%)	16 (15%)	3	5
34	BN	118/119 (99%)	103 (87%)	15 (13%)	5	9
34	DN	118/119 (99%)	106 (90%)	12 (10%)	9	16
35	BO	100/100 (100%)	93 (93%)	7 (7%)	19	33
35	DO	100/100 (100%)	93 (93%)	7 (7%)	19	33
36	BP	115/116 (99%)	98 (85%)	17 (15%)	4	6
36	DP	115/116 (99%)	100 (87%)	15 (13%)	5	9
37	BQ	111/111 (100%)	95 (86%)	16 (14%)	4	6
37	DQ	111/111 (100%)	99 (89%)	12 (11%)	8	14
38	BR	101/101 (100%)	82 (81%)	19 (19%)	2	3
38	DR	101/101 (100%)	83 (82%)	18 (18%)	2	3
39	BS	87/88 (99%)	81 (93%)	6 (7%)	19	34
39	DS	85/88 (97%)	75 (88%)	10 (12%)	6	11
40	BT	115/127 (91%)	106 (92%)	9 (8%)	16	28
40	DT	113/127 (89%)	103 (91%)	10 (9%)	12	22
41	BU	93/94 (99%)	84 (90%)	9 (10%)	10	18
41	DU	93/94 (99%)	85 (91%)	8 (9%)	13	23
42	BV	80/82 (98%)	68 (85%)	12 (15%)	3	6
42	DV	80/82 (98%)	67 (84%)	13 (16%)	3	4
43	BW	90/92 (98%)	83 (92%)	7 (8%)	16	28
43	DW	90/92 (98%)	83 (92%)	7 (8%)	16	28
44	BX	77/78 (99%)	71 (92%)	6 (8%)	16	28
44	DX	77/78 (99%)	71 (92%)	6 (8%)	16	28
45	BY	85/91 (93%)	75 (88%)	10 (12%)	6	11
45	DY	85/91 (93%)	79 (93%)	6 (7%)	18	32
46	BZ	145/179 (81%)	133 (92%)	12 (8%)	14	25
46	DZ	145/179 (81%)	129 (89%)	16 (11%)	8	13
47	B0	65/67 (97%)	62 (95%)	3 (5%)	33	55
47	D0	65/67 (97%)	60 (92%)	5 (8%)	16	28
48	B1	80/83 (96%)	73 (91%)	7 (9%)	12	22
48	D1	80/83 (96%)	71 (89%)	9 (11%)	7	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B2	65/67 (97%)	57 (88%)	8 (12%)	6	10
49	D2	65/67 (97%)	59 (91%)	6 (9%)	11	20
50	B3	51/52 (98%)	46 (90%)	5 (10%)	10	17
50	D3	50/52 (96%)	44 (88%)	6 (12%)	6	11
51	B4	60/63 (95%)	47 (78%)	13 (22%)	1	2
51	D4	53/63 (84%)	43 (81%)	10 (19%)	2	3
52	B5	50/52 (96%)	45 (90%)	5 (10%)	9	17
52	D5	50/52 (96%)	46 (92%)	4 (8%)	15	26
53	B6	51/52 (98%)	44 (86%)	7 (14%)	4	7
53	D6	50/52 (96%)	48 (96%)	2 (4%)	38	62
54	B7	41/42 (98%)	38 (93%)	3 (7%)	17	31
54	D7	41/42 (98%)	38 (93%)	3 (7%)	17	31
55	B8	53/55 (96%)	49 (92%)	4 (8%)	17	30
55	D8	54/55 (98%)	51 (94%)	3 (6%)	26	45
56	B9	34/34 (100%)	34 (100%)	0	100	100
56	D9	34/34 (100%)	32 (94%)	2 (6%)	24	42
All	All	9320/10066 (93%)	8304 (89%)	1016 (11%)	8	13

5 of 1016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	B0	82	ARG
4	CD	31	CYS
44	DX	57	LEU
49	B2	64	LEU
2	CB	24	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
40	BT	123	GLN
3	CC	28	GLN
40	DT	123	GLN
44	BX	31	HIS
51	B4	46	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	304 (20%)	25 (1%)
1	CA	1501/1521 (98%)	316 (21%)	28 (1%)
22	AV	12/24 (50%)	3 (25%)	0
22	CV	11/24 (45%)	2 (18%)	0
23	AW	70/76 (92%)	30 (42%)	2 (2%)
23	CW	67/76 (88%)	32 (47%)	2 (2%)
24	AX	75/77 (97%)	16 (21%)	0
24	CX	75/77 (97%)	21 (28%)	0
25	AY	71/76 (93%)	35 (49%)	4 (5%)
25	CY	69/76 (90%)	32 (46%)	1 (1%)
26	BA	2811/2915 (96%)	450 (16%)	34 (1%)
26	DA	2791/2915 (95%)	552 (19%)	30 (1%)
27	BB	119/121 (98%)	14 (11%)	0
27	DB	119/121 (98%)	17 (14%)	0
All	All	9286/9620 (96%)	1824 (19%)	126 (1%)

5 of 1824 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	22	G
1	AA	29	G

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2126	A
1	CA	509	A
26	DA	1992	G
26	BA	2183	C
26	BA	2756	U

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

38 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
23	PSU	AW	32	23	13,21,22	1.17	1 (7%)	18,30,33	3.46	6 (33%)
23	MIA	AW	37	23	21,31,32	1.70	2 (9%)	26,44,47	1.54	6 (23%)
23	PSU	AW	39	23	13,21,22	1.43	1 (7%)	18,30,33	3.54	6 (33%)
23	7MG	AW	46	23	19,26,27	1.11	1 (5%)	24,39,42	3.10	7 (29%)
23	5MU	AW	54	23	12,22,23	0.32	0	14,32,35	2.50	2 (14%)
23	PSU	AW	55	23	13,21,22	1.28	1 (7%)	18,30,33	3.56	6 (33%)
23	31M	AW	76	23	35,44,45	1.39	4 (11%)	40,61,64	2.17	6 (15%)
23	4SU	AW	8	23	11,21,22	1.20	1 (9%)	13,30,33	1.13	1 (7%)
24	5MC	AX	32	24	13,22,23	1.42	1 (7%)	15,32,35	1.02	1 (6%)
24	5MU	AX	54	24,57	12,22,23	0.31	0	14,32,35	2.40	2 (14%)
24	PSU	AX	55	24,57	13,21,22	1.49	1 (7%)	18,30,33	3.39	6 (33%)
24	4SU	AX	8	24	11,21,22	1.17	1 (9%)	13,30,33	1.64	1 (7%)
25	PSU	AY	32	25	13,21,22	1.02	1 (7%)	18,30,33	3.34	6 (33%)
25	MIA	AY	37	25	15,24,32	1.21	2 (13%)	16,35,47	2.01	2 (12%)
25	PSU	AY	39	25	13,21,22	1.30	2 (15%)	18,30,33	3.68	4 (22%)
25	7MG	AY	46	25	19,26,27	1.11	1 (5%)	24,39,42	3.34	8 (33%)
25	5MU	AY	54	25	12,22,23	0.43	0	14,32,35	2.26	2 (14%)
25	PSU	AY	55	25	13,21,22	1.74	2 (15%)	18,30,33	3.07	6 (33%)
25	4SU	AY	8	25	11,21,22	1.22	1 (9%)	13,30,33	1.22	1 (7%)
23	PSU	CW	32	23	13,21,22	1.33	1 (7%)	18,30,33	3.29	5 (27%)
23	MIA	CW	37	23	15,24,32	1.21	2 (13%)	16,35,47	1.95	2 (12%)
23	PSU	CW	39	23	13,21,22	1.48	1 (7%)	18,30,33	3.63	6 (33%)
23	7MG	CW	46	23	19,26,27	1.06	1 (5%)	24,39,42	2.89	6 (25%)
23	5MU	CW	54	23	12,22,23	0.42	0	14,32,35	2.46	2 (14%)
23	PSU	CW	55	23	13,21,22	1.09	1 (7%)	18,30,33	3.37	6 (33%)
23	31M	CW	76	23	35,44,45	1.40	4 (11%)	40,61,64	1.97	3 (7%)
23	4SU	CW	8	23	11,21,22	1.25	1 (9%)	13,30,33	1.21	1 (7%)
24	5MC	CX	32	24	13,22,23	1.34	1 (7%)	15,32,35	0.95	1 (6%)
24	5MU	CX	54	24	12,22,23	0.36	0	14,32,35	2.17	2 (14%)
24	PSU	CX	55	24	13,21,22	1.21	1 (7%)	18,30,33	3.31	6 (33%)
24	4SU	CX	8	24	11,21,22	1.15	1 (9%)	13,30,33	1.67	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PSU	CY	32	25	13,21,22	1.13	1 (7%)	18,30,33	3.38	5 (27%)
25	MIA	CY	37	25	15,24,32	1.26	2 (13%)	16,35,47	1.96	2 (12%)
25	PSU	CY	39	25	13,21,22	1.32	1 (7%)	18,30,33	2.98	6 (33%)
25	7MG	CY	46	25	19,26,27	1.02	1 (5%)	24,39,42	2.92	7 (29%)
25	5MU	CY	54	25	12,22,23	0.37	0	14,32,35	2.16	2 (14%)
25	PSU	CY	55	25	13,21,22	0.82	1 (7%)	18,30,33	3.36	6 (33%)
25	4SU	CY	8	25	11,21,22	1.32	1 (9%)	13,30,33	1.02	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
23	PSU	AW	32	23	-	0/7/25/26	0/2/2/2
23	MIA	AW	37	23	-	0/11/33/34	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	0/7/37/38	0/3/3/3
23	5MU	AW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	31M	AW	76	23	-	0/27/49/50	0/4/4/4
23	4SU	AW	8	23	-	0/3/25/26	0/2/2/2
24	5MC	AX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	AX	54	24,57	-	0/3/25/26	0/2/2/2
24	PSU	AX	55	24,57	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/3/25/26	0/2/2/2
25	PSU	AY	32	25	-	0/7/25/26	0/2/2/2
25	MIA	AY	37	25	-	0/3/25/34	0/3/3/3
25	PSU	AY	39	25	-	0/7/25/26	0/2/2/2
25	7MG	AY	46	25	-	0/7/37/38	0/3/3/3
25	5MU	AY	54	25	-	0/3/25/26	0/2/2/2
25	PSU	AY	55	25	-	0/7/25/26	0/2/2/2
25	4SU	AY	8	25	-	0/3/25/26	0/2/2/2
23	PSU	CW	32	23	-	0/7/25/26	0/2/2/2
23	MIA	CW	37	23	-	0/3/25/34	0/3/3/3
23	PSU	CW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	CW	46	23	-	0/7/37/38	0/3/3/3
23	5MU	CW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	CW	55	23	-	0/7/25/26	0/2/2/2
23	31M	CW	76	23	-	0/27/49/50	0/4/4/4
23	4SU	CW	8	23	-	0/3/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	5MC	CX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
24	4SU	CX	8	24	-	0/3/25/26	0/2/2/2
25	PSU	CY	32	25	-	0/7/25/26	0/2/2/2
25	MIA	CY	37	25	-	0/3/25/34	0/3/3/3
25	PSU	CY	39	25	-	0/7/25/26	0/2/2/2
25	7MG	CY	46	25	-	0/7/37/38	0/3/3/3
25	5MU	CY	54	25	-	0/3/25/26	0/2/2/2
25	PSU	CY	55	25	-	0/7/25/26	0/2/2/2
25	4SU	CY	8	25	-	0/3/25/26	0/2/2/2

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	37	MIA	C2-S10	-6.35	1.70	1.75
25	AY	55	PSU	C5-C1'	-5.72	1.47	1.52
23	AW	76	31M	CB-CG	-4.92	1.39	1.51
23	CW	39	PSU	C5-C1'	-4.87	1.48	1.52
24	AX	55	PSU	C5-C1'	-4.77	1.48	1.52

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AW	76	31M	N3-C2-N1	-11.49	120.09	128.89
25	AY	39	PSU	N1-C2-N3	-11.29	121.13	128.33
23	CW	39	PSU	N1-C2-N3	-11.15	121.22	128.33
23	CW	76	31M	N3-C2-N1	-11.12	120.38	128.89
23	AW	39	PSU	N1-C2-N3	-10.87	121.40	128.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	37	MIA	1	0
23	AW	39	PSU	1	0
23	AW	46	7MG	1	0
23	AW	76	31M	4	0
23	AW	8	4SU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AX	32	5MC	3	0
24	AX	55	PSU	1	0
24	AX	8	4SU	2	0
25	AY	32	PSU	2	0
25	AY	37	MIA	3	0
25	AY	39	PSU	4	0
25	AY	46	7MG	3	0
25	AY	54	5MU	2	0
25	AY	55	PSU	4	0
25	AY	8	4SU	1	0
23	CW	39	PSU	3	0
23	CW	46	7MG	1	0
23	CW	55	PSU	1	0
23	CW	76	31M	7	0
23	CW	8	4SU	2	0
24	CX	32	5MC	2	0
24	CX	54	5MU	2	0
24	CX	8	4SU	2	0
25	CY	37	MIA	2	0
25	CY	39	PSU	4	0
25	CY	46	7MG	1	0
25	CY	55	PSU	4	0
25	CY	8	4SU	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2093 ligands modelled in this entry, 2091 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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	SF4	AD	501	4	0,12,12	0.00	-	0,24,24	0.00	-
58	SF4	CD	302	4	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
58	SF4	AD	501	4	-	0/0/48/48	0/6/5/5
58	SF4	CD	302	4	-	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1498/1521 (98%)	0.52	34 (2%) 64 69	42, 72, 93, 108	0
1	CA	1503/1521 (98%)	0.55	81 (5%) 29 34	44, 74, 94, 109	0
2	AB	231/256 (90%)	0.85	33 (14%) 4 4	72, 82, 90, 94	0
2	CB	231/256 (90%)	1.53	59 (25%) 1 1	73, 84, 90, 95	0
3	AC	206/239 (86%)	1.04	38 (18%) 2 2	68, 79, 87, 94	0
3	CC	206/239 (86%)	1.95	82 (39%) 0 0	71, 81, 89, 94	0
4	AD	208/209 (99%)	1.05	33 (15%) 3 3	57, 72, 81, 90	0
4	CD	208/209 (99%)	0.88	17 (8%) 14 16	58, 71, 80, 91	0
5	AE	148/162 (91%)	1.09	21 (14%) 4 4	58, 71, 80, 85	0
5	CE	148/162 (91%)	1.30	37 (25%) 1 1	60, 73, 81, 86	0
6	AF	100/101 (99%)	0.62	6 (6%) 25 29	56, 69, 78, 82	0
6	CF	100/101 (99%)	0.50	6 (6%) 25 29	57, 70, 78, 82	0
7	AG	155/156 (99%)	0.92	13 (8%) 14 15	65, 75, 83, 91	0
7	CG	155/156 (99%)	1.22	27 (17%) 2 2	66, 76, 84, 92	0
8	AH	137/138 (99%)	1.05	27 (19%) 1 1	62, 72, 79, 87	0
8	CH	137/138 (99%)	1.17	30 (21%) 1 1	64, 74, 80, 87	0
9	AI	127/128 (99%)	1.20	28 (22%) 1 1	65, 80, 86, 89	0
9	CI	127/128 (99%)	2.63	76 (59%) 0 0	68, 82, 88, 91	0
10	AJ	97/105 (92%)	1.27	23 (23%) 1 1	64, 82, 90, 93	0
10	CJ	96/105 (91%)	1.83	36 (37%) 0 0	67, 84, 91, 93	0
11	AK	114/129 (88%)	0.90	9 (7%) 15 17	48, 70, 79, 84	0
11	CK	114/129 (88%)	0.83	11 (9%) 10 11	51, 71, 79, 84	0
12	AL	122/132 (92%)	0.84	8 (6%) 22 25	50, 65, 73, 78	0
12	CL	122/132 (92%)	1.26	27 (22%) 1 1	53, 67, 75, 80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	0.78	9 (7%) 18 20	55, 70, 81, 89	0
13	CM	122/126 (96%)	2.18	56 (45%) 0 0	70, 84, 91, 99	0
14	AN	60/61 (98%)	1.29	13 (21%) 1 1	67, 74, 83, 84	0
14	CN	60/61 (98%)	3.14	39 (65%) 0 0	69, 77, 84, 88	0
15	AO	88/89 (98%)	0.74	6 (6%) 20 23	56, 67, 80, 81	0
15	CO	88/89 (98%)	1.01	10 (11%) 7 7	59, 69, 80, 83	0
16	AP	82/88 (93%)	1.68	29 (35%) 0 0	57, 71, 80, 84	0
16	CP	82/88 (93%)	1.05	8 (9%) 10 11	58, 70, 80, 84	0
17	AQ	99/105 (94%)	0.89	12 (12%) 6 6	59, 71, 80, 84	0
17	CQ	99/105 (94%)	1.39	29 (29%) 1 0	61, 71, 81, 85	0
18	AR	68/88 (77%)	0.82	5 (7%) 17 20	59, 68, 81, 83	0
18	CR	68/88 (77%)	0.67	3 (4%) 38 44	61, 70, 80, 84	0
19	AS	83/93 (89%)	0.68	4 (4%) 34 40	71, 80, 86, 95	0
19	CS	83/93 (89%)	2.05	34 (40%) 0 0	74, 82, 89, 96	0
20	AT	96/106 (90%)	1.03	16 (16%) 2 2	57, 71, 81, 85	0
20	CT	96/106 (90%)	1.24	19 (19%) 1 1	58, 70, 82, 85	0
21	AU	23/27 (85%)	1.76	8 (34%) 0 0	67, 74, 77, 81	0
21	CU	23/27 (85%)	2.92	15 (65%) 0 0	71, 75, 80, 84	0
22	AV	13/24 (54%)	3.01	7 (53%) 0 0	58, 81, 96, 99	0
22	CV	12/24 (50%)	3.80	8 (66%) 0 0	63, 84, 93, 94	0
23	AW	66/76 (86%)	2.11	28 (42%) 0 0	68, 96, 103, 105	0
23	CW	64/76 (84%)	3.73	53 (82%) 0 0	73, 97, 103, 106	0
24	AX	72/77 (93%)	0.61	1 (1%) 78 81	39, 68, 87, 91	0
24	CX	72/77 (93%)	0.89	8 (11%) 7 8	53, 82, 93, 97	0
25	AY	67/76 (88%)	1.57	25 (37%) 0 0	44, 97, 102, 105	0
25	CY	66/76 (86%)	2.48	34 (51%) 0 0	47, 97, 102, 105	0
26	BA	2819/2915 (96%)	0.84	37 (1%) 79 83	26, 45, 89, 104	0
26	DA	2800/2915 (96%)	0.35	73 (2%) 59 64	30, 49, 90, 108	0
27	BB	120/121 (99%)	0.72	0 100 100	40, 64, 73, 86	0
27	DB	120/121 (99%)	0.38	6 (5%) 32 38	46, 69, 76, 90	0
28	BD	275/276 (99%)	0.89	9 (3%) 50 56	27, 43, 58, 82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	275/276 (99%)	0.77	17 (6%) 24 27	29, 45, 61, 81	0
29	BE	204/206 (99%)	0.87	7 (3%) 49 55	25, 48, 66, 80	0
29	DE	204/206 (99%)	0.64	4 (1%) 68 73	29, 52, 67, 81	0
30	BF	203/210 (96%)	0.82	5 (2%) 61 66	26, 53, 76, 87	0
30	DF	203/210 (96%)	0.64	10 (4%) 33 39	30, 58, 77, 87	0
31	BG	181/182 (99%)	0.89	12 (6%) 22 25	51, 69, 81, 88	0
31	DG	181/182 (99%)	1.36	43 (23%) 1 1	56, 73, 82, 90	0
32	BH	174/180 (96%)	0.82	6 (3%) 49 55	51, 65, 75, 88	0
32	DH	174/180 (96%)	1.17	37 (21%) 1 1	55, 70, 78, 88	0
33	BI	146/148 (98%)	0.63	6 (4%) 41 47	50, 74, 82, 87	0
33	DI	146/148 (98%)	0.67	17 (11%) 6 7	52, 75, 82, 86	0
34	BN	140/140 (100%)	0.98	4 (2%) 55 61	32, 50, 67, 76	0
34	DN	140/140 (100%)	0.75	9 (6%) 23 26	36, 55, 70, 77	0
35	BO	122/122 (100%)	0.65	2 (1%) 74 79	30, 43, 59, 70	0
35	DO	122/122 (100%)	0.83	6 (4%) 33 39	45, 59, 73, 78	0
36	BP	149/150 (99%)	0.90	4 (2%) 58 63	26, 55, 75, 83	0
36	DP	149/150 (99%)	1.03	26 (17%) 2 2	30, 59, 77, 85	0
37	BQ	141/141 (100%)	0.91	3 (2%) 67 72	36, 52, 67, 80	0
37	DQ	141/141 (100%)	1.34	30 (21%) 1 1	41, 57, 70, 82	0
38	BR	118/118 (100%)	0.76	1 (0%) 87 89	25, 36, 54, 59	0
38	DR	118/118 (100%)	0.72	3 (2%) 61 66	41, 54, 65, 72	0
39	BS	110/112 (98%)	0.57	1 (0%) 85 88	38, 51, 65, 72	0
39	DS	110/112 (98%)	1.31	25 (22%) 1 1	63, 77, 84, 92	0
40	BT	131/146 (89%)	0.58	0 100 100	32, 47, 69, 82	0
40	DT	131/146 (89%)	0.74	7 (5%) 30 35	48, 63, 79, 85	0
41	BU	116/118 (98%)	0.88	1 (0%) 85 88	18, 33, 49, 59	0
41	DU	116/118 (98%)	0.90	10 (8%) 13 14	42, 61, 78, 84	0
42	BV	101/101 (100%)	0.62	0 100 100	21, 41, 58, 67	0
42	DV	101/101 (100%)	0.70	5 (4%) 32 38	41, 71, 83, 91	0
43	BW	112/113 (99%)	0.81	0 100 100	23, 34, 54, 79	0
43	DW	112/113 (99%)	0.77	6 (5%) 29 34	39, 50, 67, 83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
44	BX	95/96 (98%)	0.63	0	100 100	23, 38, 61, 84	0
44	DX	95/96 (98%)	1.06	9 (9%)	10 11	43, 60, 76, 79	0
45	BY	107/110 (97%)	0.58	1 (0%)	85 88	32, 50, 69, 83	0
45	DY	107/110 (97%)	1.29	19 (17%)	2 2	57, 71, 81, 88	0
46	BZ	171/206 (83%)	0.77	14 (8%)	14 16	39, 64, 91, 95	0
46	DZ	174/206 (84%)	1.64	52 (29%)	1 0	66, 84, 94, 101	0
47	B0	83/85 (97%)	0.96	6 (7%)	18 21	27, 39, 61, 73	0
47	D0	83/85 (97%)	1.60	22 (26%)	1 1	47, 66, 75, 82	0
48	B1	97/98 (98%)	0.88	7 (7%)	18 21	30, 48, 70, 76	0
48	D1	97/98 (98%)	1.04	16 (16%)	2 2	38, 58, 74, 83	0
49	B2	70/72 (97%)	0.64	0	100 100	34, 50, 64, 79	0
49	D2	70/72 (97%)	0.73	6 (8%)	13 14	56, 70, 80, 86	0
50	B3	59/60 (98%)	0.70	0	100 100	24, 37, 63, 71	0
50	D3	59/60 (98%)	1.05	9 (15%)	3 3	49, 64, 79, 85	0
51	B4	69/71 (97%)	0.55	5 (7%)	18 21	54, 73, 87, 92	0
51	D4	69/71 (97%)	1.21	13 (18%)	2 2	74, 88, 94, 99	0
52	B5	59/60 (98%)	0.71	2 (3%)	49 55	20, 33, 54, 67	0
52	D5	59/60 (98%)	0.63	3 (5%)	32 37	36, 51, 67, 73	0
53	B6	53/54 (98%)	0.67	1 (1%)	70 74	31, 44, 61, 68	0
53	D6	53/54 (98%)	1.20	8 (15%)	3 3	52, 63, 76, 79	0
54	B7	48/49 (97%)	1.12	6 (12%)	5 6	21, 30, 62, 76	0
54	D7	48/49 (97%)	1.41	10 (20%)	1 1	33, 42, 61, 70	0
55	B8	64/65 (98%)	0.82	3 (4%)	35 41	25, 36, 45, 60	0
55	D8	64/65 (98%)	1.61	21 (32%)	0 0	46, 58, 66, 72	0
56	B9	37/37 (100%)	1.16	3 (8%)	15 16	31, 49, 73, 74	0
56	D9	37/37 (100%)	1.37	6 (16%)	3 2	46, 57, 73, 76	0
All	All	20897/21748 (96%)	0.86	1915 (9%)	11 12	18, 64, 89, 109	0

The worst 5 of 1915 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	CM	124	PRO	13.3
2	CB	165	VAL	13.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	AM	124	PRO	11.8
7	CG	83	ALA	11.1
23	CW	71	G	10.9

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
23	5MU	CW	54	21/22	0.84	0.23	-	74,88,99,101	0
24	5MC	AX	32	21/22	0.95	0.21	-	43,53,62,78	0
23	MIA	AW	37	29/30	0.94	0.26	-	59,71,81,86	0
25	PSU	CY	55	20/21	0.67	0.49	-	94,102,110,124	0
23	4SU	AW	8	20/21	0.81	0.19	-	86,95,112,128	0
23	PSU	CW	39	20/21	0.87	0.42	-	78,84,97,98	0
25	MIA	CY	37	22/30	0.61	0.38	-	72,95,113,138	0
24	5MC	CX	32	21/22	0.96	0.21	-	63,76,86,88	0
23	PSU	AW	32	20/21	0.88	0.25	-	77,83,92,98	0
23	PSU	CW	32	20/21	0.88	0.45	-	81,87,94,103	0
25	7MG	CY	46	24/25	0.48	0.37	-	86,105,111,137	0
23	31M	CW	76	41/42	0.89	0.41	-	50,63,73,88	20
25	4SU	AY	8	20/21	0.78	0.16	-	82,96,103,118	0
23	PSU	AW	55	20/21	0.84	0.26	-	77,90,98,104	0
24	PSU	AX	55	20/21	0.95	0.21	-	50,63,73,83	0
25	PSU	AY	55	20/21	0.70	0.29	-	93,101,108,122	0
25	PSU	CY	32	20/21	0.79	0.21	-	80,92,101,107	0
23	PSU	CW	55	20/21	0.79	0.30	-	79,89,99,104	0
24	5MU	CX	54	21/22	0.92	0.22	-	70,81,89,99	0
24	4SU	CX	8	20/21	0.91	0.17	-	77,87,95,97	0
25	PSU	AY	32	20/21	0.83	0.24	-	78,93,100,106	0
24	4SU	AX	8	20/21	0.94	0.18	-	54,66,82,89	0
23	MIA	CW	37	22/30	0.84	0.32	-	75,85,92,100	0
23	5MU	AW	54	21/22	0.91	0.20	-	65,82,91,93	0
23	7MG	AW	46	24/25	0.72	0.23	-	84,99,117,133	0
24	PSU	CX	55	20/21	0.89	0.15	-	70,80,91,96	0
23	7MG	CW	46	24/25	0.67	0.27	-	79,96,109,133	0
25	PSU	CY	39	20/21	0.77	0.30	-	79,90,116,130	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	PSU	AW	39	20/21	0.93	0.23	-	73,82,95,97	0
25	MIA	AY	37	22/30	0.80	0.22	-	77,90,111,119	0
23	31M	AW	76	41/42	0.94	0.33	-	37,54,66,83	9
25	5MU	AY	54	21/22	0.73	0.26	-	80,96,105,131	0
25	4SU	CY	8	20/21	0.68	0.22	-	93,103,113,128	0
25	5MU	CY	54	21/22	0.63	0.53	-	78,94,109,140	0
25	PSU	AY	39	20/21	0.76	0.30	-	78,90,117,123	0
25	7MG	AY	46	24/25	0.76	0.28	-	75,101,111,123	0
24	5MU	AX	54	21/22	0.95	0.20	-	49,68,79,84	0
23	4SU	CW	8	20/21	0.69	0.30	-	81,98,120,127	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
57	MG	BA	3639	1/1	0.93	0.46	38.70	48,48,48,48	0
57	MG	BF	303	1/1	0.96	0.54	32.51	49,49,49,49	0
57	MG	BX	3001	1/1	0.92	0.83	32.24	48,48,48,48	0
57	MG	DA	3116	1/1	0.91	0.48	27.40	52,52,52,52	0
57	MG	DA	3226	1/1	0.95	0.38	22.29	45,45,45,45	0
57	MG	BA	3250	1/1	0.93	0.67	21.11	42,42,42,42	0
57	MG	BA	3367	1/1	0.98	0.25	16.63	29,29,29,29	0
57	MG	DA	3031	1/1	0.99	0.43	16.26	43,43,43,43	0
57	MG	BA	3054	1/1	0.94	0.28	15.40	36,36,36,36	0
57	MG	DA	3213	1/1	0.64	0.32	12.85	63,63,63,63	0
57	MG	DA	3208	1/1	0.89	0.37	12.01	58,58,58,58	0
57	MG	B1	101	1/1	0.91	0.50	11.81	51,51,51,51	0
57	MG	DA	3168	1/1	0.97	0.29	11.65	45,45,45,45	0
57	MG	BA	3239	1/1	0.92	0.34	11.60	48,48,48,48	0
57	MG	BA	3029	1/1	0.97	0.49	11.56	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
57	MG	DA	3016	1/1	0.97	0.34	10.49	50,50,50,50	0
57	MG	BA	3804	1/1	0.96	0.42	10.05	53,53,53,53	0
57	MG	BA	3248	1/1	0.96	0.30	9.77	42,42,42,42	0
57	MG	BA	3802	1/1	0.83	0.47	9.63	54,54,54,54	0
57	MG	BA	3246	1/1	0.95	0.35	9.56	39,39,39,39	0
57	MG	BA	3240	1/1	0.91	0.40	9.54	47,47,47,47	0
57	MG	AA	3156	1/1	0.95	0.25	9.33	63,63,63,63	0
57	MG	BA	3115	1/1	0.97	0.23	9.29	59,59,59,59	0
57	MG	DA	3588	1/1	0.91	0.30	9.19	65,65,65,65	0
57	MG	BA	3328	1/1	0.93	0.27	9.14	40,40,40,40	0
57	MG	DA	3019	1/1	0.97	0.29	9.06	37,37,37,37	0
57	MG	DA	3067	1/1	0.94	0.26	8.76	57,57,57,57	0
57	MG	DA	3045	1/1	0.93	0.29	8.34	51,51,51,51	0
57	MG	DU	3002	1/1	0.85	0.40	8.22	55,55,55,55	0
57	MG	DA	3594	1/1	0.94	0.31	8.03	54,54,54,54	0
57	MG	DA	3081	1/1	0.96	0.28	7.99	55,55,55,55	0
57	MG	BA	3670	1/1	0.43	0.25	7.81	61,61,61,61	0
57	MG	DA	3028	1/1	0.97	0.36	7.66	52,52,52,52	0
57	MG	BA	3728	1/1	0.80	0.33	7.42	48,48,48,48	0
57	MG	DA	3481	1/1	0.89	0.41	7.36	55,55,55,55	0
57	MG	BA	3613	1/1	0.96	0.42	7.18	42,42,42,42	0
57	MG	DA	3027	1/1	0.99	0.57	7.18	51,51,51,51	0
57	MG	BA	3771	1/1	0.78	0.29	7.12	50,50,50,50	0
57	MG	DD	308	1/1	0.98	0.29	7.00	48,48,48,48	0
57	MG	DA	3132	1/1	0.90	0.23	6.91	52,52,52,52	0
57	MG	DA	3236	1/1	0.91	0.26	6.82	47,47,47,47	0
57	MG	DA	3642	1/1	0.76	0.28	6.77	54,54,54,54	0
57	MG	BA	3069	1/1	0.99	0.27	6.68	22,22,22,22	0
57	MG	CA	3152	1/1	0.80	0.20	6.41	76,76,76,76	0
57	MG	BA	3732	1/1	0.87	0.26	6.38	51,51,51,51	0
57	MG	BU	206	1/1	0.99	0.40	6.17	35,35,35,35	0
57	MG	BA	3156	1/1	0.95	0.29	6.05	41,41,41,41	0
57	MG	DA	3676	1/1	0.87	0.33	5.70	67,67,67,67	0
57	MG	DA	3637	1/1	0.92	0.59	5.65	58,58,58,58	0
57	MG	DA	3029	1/1	0.93	0.35	5.65	49,49,49,49	0
57	MG	BA	3139	1/1	0.97	0.33	5.63	40,40,40,40	0
57	MG	BA	3040	1/1	0.98	0.36	5.54	35,35,35,35	0
57	MG	AY	3003	1/1	0.92	0.30	5.53	53,53,53,53	0
57	MG	BA	3046	1/1	0.97	0.28	5.28	41,41,41,41	0
57	MG	DE	301	1/1	0.98	0.40	5.26	46,46,46,46	0
57	MG	BA	3232	1/1	0.97	0.21	5.08	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
57	MG	BA	3812	1/1	0.92	0.28	5.08	47,47,47,47	0
57	MG	BB	202	1/1	0.86	0.28	5.05	59,59,59,59	0
57	MG	AA	3095	1/1	0.93	0.29	5.02	60,60,60,60	0
57	MG	BA	3549	1/1	0.97	0.29	4.92	39,39,39,39	0
57	MG	BA	3085	1/1	0.98	0.27	4.87	35,35,35,35	0
57	MG	DD	307	1/1	0.97	0.32	4.81	43,43,43,43	0
57	MG	BA	3213	1/1	0.86	0.26	4.80	40,40,40,40	0
57	MG	BA	3153	1/1	0.96	0.31	4.76	47,47,47,47	0
57	MG	BP	201	1/1	0.95	0.28	4.46	41,41,41,41	0
57	MG	BA	3335	1/1	0.82	0.23	4.46	52,52,52,52	0
57	MG	BA	3801	1/1	0.94	0.31	4.32	50,50,50,50	0
57	MG	BA	3143	1/1	0.91	0.26	4.26	45,45,45,45	0
57	MG	DB	3008	1/1	0.76	0.20	4.14	67,67,67,67	0
57	MG	DA	3059	1/1	0.96	0.26	4.12	43,43,43,43	0
57	MG	CA	3169	1/1	0.95	0.24	4.04	51,51,51,51	0
57	MG	DA	3182	1/1	0.97	0.24	3.94	51,51,51,51	0
57	MG	DA	3668	1/1	0.92	0.39	3.81	60,60,60,60	0
57	MG	DA	3629	1/1	0.95	0.27	3.69	62,62,62,62	0
57	MG	DF	3003	1/1	0.97	0.40	3.67	43,43,43,43	0
57	MG	AA	3084	1/1	0.78	0.24	3.62	51,51,51,51	0
57	MG	DA	3426	1/1	0.93	0.22	3.60	49,49,49,49	0
57	MG	BA	3082	1/1	0.97	0.22	3.54	39,39,39,39	0
57	MG	BA	3196	1/1	0.94	0.25	3.53	38,38,38,38	0
57	MG	DA	3669	1/1	0.81	0.25	3.52	55,55,55,55	0
57	MG	DA	3439	1/1	0.95	0.23	3.51	42,42,42,42	0
57	MG	BA	3290	1/1	0.92	0.28	3.47	40,40,40,40	0
57	MG	BA	3141	1/1	0.98	0.28	3.42	42,42,42,42	0
57	MG	CA	3057	1/1	0.90	0.18	3.42	76,76,76,76	0
57	MG	BA	3284	1/1	0.86	0.26	3.35	43,43,43,43	0
57	MG	BA	3626	1/1	0.95	0.25	3.32	44,44,44,44	0
57	MG	DD	304	1/1	0.92	0.38	3.28	52,52,52,52	0
57	MG	BA	3699	1/1	0.96	0.23	3.17	35,35,35,35	0
57	MG	CA	3061	1/1	0.89	0.28	3.13	66,66,66,66	0
57	MG	BV	201	1/1	0.98	0.31	3.13	33,33,33,33	0
57	MG	BF	306	1/1	0.97	0.28	3.10	31,31,31,31	0
57	MG	AA	3018	1/1	0.97	0.24	2.91	56,56,56,56	0
57	MG	AA	3138	1/1	0.81	0.18	2.83	71,71,71,71	0
57	MG	DA	3115	1/1	0.98	0.24	2.79	40,40,40,40	0
57	MG	BA	3151	1/1	0.92	0.26	2.76	52,52,52,52	0
57	MG	DA	3119	1/1	0.90	0.21	2.69	39,39,39,39	0
57	MG	DA	3471	1/1	0.98	0.22	2.54	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
57	MG	CA	3133	1/1	0.98	0.21	2.53	59,59,59,59	0
59	ZN	B6	103	1/1	0.98	0.24	2.50	49,49,49,49	0
57	MG	BA	3203	1/1	0.92	0.25	2.49	40,40,40,40	0
57	MG	BD	306	1/1	0.97	0.25	2.48	38,38,38,38	0
57	MG	BA	3289	1/1	0.94	0.21	2.47	56,56,56,56	0
57	MG	BA	3215	1/1	0.95	0.27	2.46	36,36,36,36	0
57	MG	DB	3009	1/1	0.94	0.18	2.46	59,59,59,59	0
57	MG	BA	3330	1/1	0.97	0.23	2.44	37,37,37,37	0
57	MG	BN	3001	1/1	0.96	0.31	2.43	53,53,53,53	0
57	MG	DA	3610	1/1	0.78	0.22	2.41	64,64,64,64	0
57	MG	CA	3087	1/1	0.83	0.19	2.38	67,67,67,67	0
57	MG	BD	302	1/1	0.91	0.28	2.37	50,50,50,50	0
57	MG	CA	3045	1/1	0.96	0.24	2.36	54,54,54,54	0
57	MG	AA	3205	1/1	0.95	0.22	2.24	51,51,51,51	0
57	MG	AF	3001	1/1	0.95	0.26	2.20	44,44,44,44	0
57	MG	CA	3079	1/1	0.94	0.21	2.19	66,66,66,66	0
57	MG	DA	3096	1/1	0.97	0.23	2.17	42,42,42,42	0
57	MG	AA	3080	1/1	0.92	0.21	2.16	58,58,58,58	0
57	MG	BA	3698	1/1	0.97	0.22	2.14	31,31,31,31	0
59	ZN	B5	102	1/1	0.99	0.22	2.10	48,48,48,48	0
57	MG	DA	3510	1/1	0.95	0.25	2.10	49,49,49,49	0
57	MG	DA	3518	1/1	0.66	0.24	2.04	54,54,54,54	0
57	MG	BB	218	1/1	0.82	0.22	2.00	77,77,77,77	0
57	MG	B7	104	1/1	0.91	0.27	1.99	48,48,48,48	0
57	MG	BA	3014	1/1	0.93	0.29	1.96	42,42,42,42	0
57	MG	BU	205	1/1	0.94	0.24	1.95	47,47,47,47	0
57	MG	DA	3113	1/1	0.95	0.19	1.89	60,60,60,60	0
57	MG	BA	3228	1/1	0.93	0.25	1.85	59,59,59,59	0
57	MG	BA	3742	1/1	0.87	0.24	1.81	65,65,65,65	0
57	MG	BA	3279	1/1	0.94	0.24	1.78	43,43,43,43	0
57	MG	DA	3014	1/1	0.96	0.21	1.73	46,46,46,46	0
57	MG	DD	306	1/1	0.94	0.28	1.73	39,39,39,39	0
57	MG	CA	3067	1/1	0.96	0.31	1.71	61,61,61,61	0
57	MG	BA	3796	1/1	0.95	0.25	1.69	45,45,45,45	0
57	MG	DV	3002	1/1	0.97	0.31	1.67	49,49,49,49	0
57	MG	BA	3212	1/1	0.88	0.24	1.65	54,54,54,54	0
57	MG	BA	3159	1/1	0.97	0.25	1.65	50,50,50,50	0
57	MG	DA	3117	1/1	0.95	0.20	1.64	52,52,52,52	0
57	MG	AA	3025	1/1	0.84	0.25	1.62	62,62,62,62	0
57	MG	BA	3087	1/1	0.95	0.24	1.56	42,42,42,42	0
57	MG	DA	3347	1/1	0.99	0.20	1.56	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	ZN	D5	501	1/1	0.99	0.20	1.45	58,58,58,58	0
57	MG	BA	3321	1/1	0.91	0.24	1.39	55,55,55,55	0
57	MG	BA	3628	1/1	0.92	0.25	1.38	49,49,49,49	0
57	MG	BA	3078	1/1	0.93	0.24	1.36	51,51,51,51	0
57	MG	DV	3001	1/1	0.93	0.23	1.24	70,70,70,70	0
57	MG	BA	3607	1/1	0.98	0.24	1.24	38,38,38,38	0
57	MG	BA	3787	1/1	0.97	0.23	1.23	45,45,45,45	0
57	MG	DW	3004	1/1	0.97	0.22	1.22	52,52,52,52	0
57	MG	DA	3462	1/1	0.86	0.20	1.21	42,42,42,42	0
57	MG	BA	3096	1/1	0.94	0.23	1.14	54,54,54,54	0
57	MG	BA	3443	1/1	0.85	0.23	1.14	37,37,37,37	0
57	MG	BA	3794	1/1	0.84	0.26	1.09	51,51,51,51	0
57	MG	DA	3104	1/1	0.94	0.29	1.08	53,53,53,53	0
57	MG	DA	3431	1/1	0.84	0.23	1.04	50,50,50,50	0
57	MG	BA	3543	1/1	0.94	0.23	1.03	37,37,37,37	0
57	MG	BA	3206	1/1	0.87	0.23	1.03	49,49,49,49	0
57	MG	DA	3169	1/1	0.96	0.24	1.03	47,47,47,47	0
57	MG	CA	3138	1/1	0.87	0.19	0.97	80,80,80,80	0
57	MG	CA	3150	1/1	0.91	0.21	0.92	56,56,56,56	0
57	MG	BE	302	1/1	0.97	0.23	0.89	39,39,39,39	0
57	MG	BA	3264	1/1	0.96	0.21	0.89	58,58,58,58	0
57	MG	DA	3413	1/1	0.66	0.23	0.88	48,48,48,48	0
57	MG	AA	3155	1/1	0.93	0.24	0.87	48,48,48,48	0
57	MG	AA	3125	1/1	0.97	0.24	0.85	37,37,37,37	0
57	MG	DA	3470	1/1	0.89	0.19	0.79	45,45,45,45	0
57	MG	BA	3254	1/1	0.97	0.22	0.78	25,25,25,25	0
57	MG	BA	3216	1/1	0.99	0.23	0.74	37,37,37,37	0
57	MG	BA	3098	1/1	0.92	0.22	0.73	40,40,40,40	0
57	MG	AA	3071	1/1	0.93	0.22	0.72	53,53,53,53	0
57	MG	BF	307	1/1	0.97	0.24	0.71	37,37,37,37	0
57	MG	BA	3273	1/1	0.82	0.22	0.67	54,54,54,54	0
57	MG	DQ	3004	1/1	0.87	0.28	0.65	54,54,54,54	0
57	MG	BA	3041	1/1	0.96	0.23	0.63	40,40,40,40	0
57	MG	CA	3116	1/1	0.84	0.22	0.62	68,68,68,68	0
57	MG	BA	3044	1/1	0.98	0.22	0.61	20,20,20,20	0
57	MG	BA	3412	1/1	0.92	0.23	0.49	40,40,40,40	0
57	MG	BQ	3002	1/1	0.96	0.23	0.49	43,43,43,43	0
57	MG	DA	3180	1/1	0.85	0.20	0.46	42,42,42,42	0
57	MG	DA	3336	1/1	0.94	0.19	0.45	40,40,40,40	0
57	MG	BD	301	1/1	0.95	0.23	0.44	40,40,40,40	0
57	MG	BA	3209	1/1	0.95	0.24	0.44	54,54,54,54	0
57	MG	BG	202	1/1	0.92	0.21	0.43	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
57	MG	DA	3459	1/1	0.98	0.19	0.43	47,47,47,47	0
57	MG	DA	3256	1/1	0.67	0.19	0.41	62,62,62,62	0
57	MG	BA	3747	1/1	0.94	0.20	0.40	52,52,52,52	0
57	MG	BA	3259	1/1	0.98	0.21	0.39	25,25,25,25	0
57	MG	DA	3558	1/1	0.87	0.17	0.38	61,61,61,61	0
57	MG	BA	3079	1/1	0.93	0.19	0.36	39,39,39,39	0
57	MG	DA	3210	1/1	0.94	0.17	0.32	53,53,53,53	0
57	MG	DU	3001	1/1	0.98	0.32	0.29	55,55,55,55	0
57	MG	BA	3268	1/1	0.94	0.22	0.26	55,55,55,55	0
57	MG	BA	3518	1/1	0.97	0.20	0.25	44,44,44,44	0
57	MG	DA	3268	1/1	0.83	0.17	0.18	51,51,51,51	0
57	MG	CA	3167	1/1	0.97	0.17	0.13	60,60,60,60	0
57	MG	BA	3399	1/1	0.89	0.20	0.10	45,45,45,45	0
57	MG	BA	3056	1/1	0.95	0.21	0.09	40,40,40,40	0
57	MG	CA	3051	1/1	0.66	0.19	0.03	81,81,81,81	0
59	ZN	B4	501	1/1	0.95	0.15	0.03	89,89,89,89	0
57	MG	AA	3120	1/1	0.97	0.19	-0.00	45,45,45,45	0
57	MG	DA	3630	1/1	0.82	0.19	0.00	61,61,61,61	0
57	MG	DA	3578	1/1	0.93	0.18	-0.02	59,59,59,59	0
57	MG	CA	3134	1/1	0.97	0.16	-0.04	69,69,69,69	0
57	MG	DA	3641	1/1	0.86	0.20	-0.06	69,69,69,69	0
57	MG	AX	3002	1/1	0.88	0.17	-0.08	58,58,58,58	0
57	MG	AA	3148	1/1	0.97	0.22	-0.08	57,57,57,57	0
57	MG	DA	3015	1/1	0.95	0.20	-0.08	52,52,52,52	0
57	MG	BA	3583	1/1	0.87	0.21	-0.11	45,45,45,45	0
57	MG	BA	3416	1/1	0.98	0.21	-0.14	21,21,21,21	0
59	ZN	AN	501	1/1	0.98	0.19	-0.15	69,69,69,69	0
57	MG	AA	3213	1/1	0.95	0.23	-0.19	54,54,54,54	0
57	MG	BD	304	1/1	0.95	0.22	-0.25	32,32,32,32	0
57	MG	BX	3002	1/1	0.87	0.19	-0.27	46,46,46,46	0
57	MG	BA	3357	1/1	0.92	0.23	-0.28	25,25,25,25	0
57	MG	DA	3020	1/1	0.97	0.16	-0.29	55,55,55,55	0
57	MG	DA	3640	1/1	0.95	0.19	-0.33	43,43,43,43	0
57	MG	BA	3588	1/1	0.98	0.23	-0.34	31,31,31,31	0
57	MG	DA	3295	1/1	0.95	0.21	-0.34	44,44,44,44	0
57	MG	BA	3245	1/1	0.97	0.23	-0.34	34,34,34,34	0
57	MG	BW	203	1/1	0.96	0.20	-0.34	44,44,44,44	0
57	MG	BA	3283	1/1	0.95	0.20	-0.35	35,35,35,35	0
57	MG	BA	3094	1/1	0.96	0.21	-0.36	36,36,36,36	0
57	MG	D3	3001	1/1	0.92	0.20	-0.38	57,57,57,57	0
57	MG	BA	3028	1/1	0.97	0.22	-0.39	51,51,51,51	0
57	MG	AA	3099	1/1	0.97	0.20	-0.39	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
57	MG	DA	3267	1/1	0.92	0.16	-0.40	49,49,49,49	0
57	MG	BA	3530	1/1	0.86	0.22	-0.40	49,49,49,49	0
57	MG	DF	3002	1/1	0.98	0.17	-0.43	48,48,48,48	0
57	MG	BA	3045	1/1	0.99	0.21	-0.45	36,36,36,36	0
59	ZN	D6	501	1/1	0.99	0.17	-0.45	71,71,71,71	0
57	MG	D8	5001	1/1	0.65	0.23	-0.45	66,66,66,66	0
57	MG	DA	3322	1/1	0.97	0.19	-0.47	51,51,51,51	0
57	MG	AK	3001	1/1	0.97	0.18	-0.48	44,44,44,44	0
57	MG	BA	3135	1/1	0.98	0.20	-0.57	43,43,43,43	0
57	MG	BA	3050	1/1	0.98	0.20	-0.58	38,38,38,38	0
57	MG	BA	3124	1/1	0.98	0.21	-0.58	19,19,19,19	0
57	MG	CK	3001	1/1	0.95	0.17	-0.61	45,45,45,45	0
57	MG	DA	3143	1/1	0.97	0.18	-0.61	38,38,38,38	0
57	MG	BA	3042	1/1	0.97	0.20	-0.63	43,43,43,43	0
57	MG	AA	3214	1/1	0.86	0.17	-0.68	73,73,73,73	0
57	MG	BA	3641	1/1	0.75	0.21	-0.68	68,68,68,68	0
57	MG	DE	302	1/1	0.96	0.17	-0.69	33,33,33,33	0
57	MG	BD	307	1/1	0.99	0.21	-0.72	40,40,40,40	0
57	MG	BA	3449	1/1	0.98	0.21	-0.72	35,35,35,35	0
57	MG	AA	3085	1/1	0.93	0.18	-0.75	48,48,48,48	0
57	MG	BA	3529	1/1	0.96	0.20	-0.76	56,56,56,56	0
59	ZN	BY	501	1/1	0.98	0.15	-0.77	58,58,58,58	0
57	MG	BA	3286	1/1	0.98	0.21	-0.79	34,34,34,34	0
57	MG	AA	3065	1/1	0.86	0.20	-0.80	63,63,63,63	0
57	MG	BA	3388	1/1	0.92	0.19	-0.81	48,48,48,48	0
57	MG	CA	3070	1/1	0.61	0.15	-0.81	63,63,63,63	0
57	MG	DA	3308	1/1	0.82	0.15	-0.82	61,61,61,61	0
59	ZN	DY	501	1/1	0.90	0.15	-0.82	96,96,96,96	0
57	MG	DA	3118	1/1	0.81	0.15	-0.82	77,77,77,77	0
57	MG	BA	3011	1/1	0.97	0.19	-0.86	35,35,35,35	0
57	MG	CA	3065	1/1	0.98	0.17	-0.87	49,49,49,49	0
57	MG	BA	3023	1/1	0.89	0.22	-0.90	36,36,36,36	0
57	MG	BA	3426	1/1	0.87	0.20	-0.91	37,37,37,37	0
57	MG	AA	3014	1/1	0.94	0.21	-0.91	32,32,32,32	0
57	MG	DA	3540	1/1	0.93	0.17	-0.92	42,42,42,42	0
57	MG	DA	3191	1/1	0.97	0.17	-0.93	37,37,37,37	0
57	MG	BB	215	1/1	0.59	0.18	-0.95	73,73,73,73	0
57	MG	BA	3144	1/1	0.97	0.19	-0.95	41,41,41,41	0
57	MG	BP	202	1/1	0.93	0.21	-0.97	36,36,36,36	0
57	MG	DA	3675	1/1	0.94	0.13	-0.99	52,52,52,52	0
57	MG	DA	3586	1/1	0.92	0.16	-0.99	60,60,60,60	0
57	MG	CA	3048	1/1	0.96	0.12	-1.00	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
57	MG	DX	101	1/1	0.89	0.12	-1.04	51,51,51,51	0
57	MG	BU	203	1/1	0.98	0.21	-1.04	47,47,47,47	0
57	MG	DA	3145	1/1	0.96	0.17	-1.05	43,43,43,43	0
57	MG	BA	3158	1/1	0.97	0.20	-1.05	41,41,41,41	0
57	MG	AA	3004	1/1	0.63	0.15	-1.07	67,67,67,67	0
57	MG	DA	3367	1/1	0.88	0.14	-1.07	61,61,61,61	0
57	MG	DA	3206	1/1	0.89	0.13	-1.09	50,50,50,50	0
57	MG	AX	3005	1/1	0.97	0.14	-1.09	47,47,47,47	0
57	MG	BU	208	1/1	0.94	0.21	-1.09	40,40,40,40	0
57	MG	AX	3015	1/1	0.95	0.21	-1.09	42,42,42,42	0
58	SF4	AD	501	8/8	0.98	0.16	-1.11	62,68,73,86	0
57	MG	BA	3427	1/1	0.41	0.20	-1.12	61,61,61,61	0
57	MG	CE	3001	1/1	0.86	0.10	-1.13	79,79,79,79	0
57	MG	BA	3202	1/1	0.97	0.19	-1.13	60,60,60,60	0
57	MG	AE	203	1/1	0.93	0.18	-1.15	63,63,63,63	0
57	MG	DA	3673	1/1	0.60	0.14	-1.15	69,69,69,69	0
57	MG	BA	3190	1/1	0.93	0.20	-1.18	52,52,52,52	0
57	MG	BA	3798	1/1	0.95	0.20	-1.19	28,28,28,28	0
57	MG	BA	3060	1/1	0.98	0.20	-1.20	30,30,30,30	0
57	MG	DA	3607	1/1	0.79	0.14	-1.21	65,65,65,65	0
57	MG	CA	3164	1/1	0.93	0.16	-1.25	60,60,60,60	0
57	MG	CV	101	1/1	0.84	0.13	-1.25	72,72,72,72	0
57	MG	DA	3099	1/1	0.97	0.17	-1.26	32,32,32,32	0
57	MG	DA	3375	1/1	0.95	0.16	-1.26	39,39,39,39	0
57	MG	DA	3435	1/1	0.97	0.15	-1.28	50,50,50,50	0
57	MG	BA	3030	1/1	0.88	0.18	-1.29	46,46,46,46	0
57	MG	BA	3333	1/1	0.88	0.20	-1.30	38,38,38,38	0
57	MG	BN	3003	1/1	0.97	0.19	-1.30	48,48,48,48	0
57	MG	BA	3531	1/1	0.93	0.21	-1.32	26,26,26,26	0
57	MG	BA	3405	1/1	0.91	0.19	-1.34	63,63,63,63	0
57	MG	BA	3781	1/1	0.80	0.20	-1.35	41,41,41,41	0
57	MG	DA	3433	1/1	0.95	0.18	-1.36	46,46,46,46	0
57	MG	BA	3810	1/1	0.89	0.19	-1.36	41,41,41,41	0
57	MG	CX	3004	1/1	0.95	0.18	-1.38	63,63,63,63	0
57	MG	CA	3034	1/1	0.97	0.13	-1.42	59,59,59,59	0
57	MG	CA	3147	1/1	0.98	0.12	-1.42	64,64,64,64	0
57	MG	CA	3166	1/1	0.80	0.14	-1.42	66,66,66,66	0
59	ZN	B9	501	1/1	0.99	0.18	-1.42	38,38,38,38	0
57	MG	AM	201	1/1	0.89	0.16	-1.43	51,51,51,51	0
57	MG	CA	3037	1/1	0.95	0.14	-1.44	73,73,73,73	0
57	MG	AA	3015	1/1	0.95	0.15	-1.44	65,65,65,65	0
58	SF4	CD	302	8/8	0.98	0.16	-1.44	60,68,83,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BV	203	1/1	0.89	0.19	-1.46	38,38,38,38	0
57	MG	DA	3004	1/1	0.91	0.17	-1.46	40,40,40,40	0
57	MG	BA	3677	1/1	0.97	0.17	-1.48	60,60,60,60	0
57	MG	AA	3032	1/1	0.94	0.19	-1.50	67,67,67,67	0
57	MG	CA	3071	1/1	0.97	0.15	-1.52	68,68,68,68	0
57	MG	BQ	3001	1/1	0.95	0.22	-1.52	45,45,45,45	0
57	MG	BA	3806	1/1	0.96	0.16	-1.53	30,30,30,30	0
57	MG	DA	3037	1/1	0.94	0.16	-1.54	43,43,43,43	0
57	MG	DA	3514	1/1	0.93	0.13	-1.54	42,42,42,42	0
57	MG	DA	3672	1/1	0.93	0.16	-1.55	71,71,71,71	0
57	MG	B6	101	1/1	0.98	0.17	-1.57	48,48,48,48	0
57	MG	DA	3042	1/1	0.97	0.17	-1.57	38,38,38,38	0
57	MG	BA	3295	1/1	0.93	0.19	-1.58	38,38,38,38	0
57	MG	AN	503	1/1	0.93	0.15	-1.58	54,54,54,54	0
57	MG	CA	3033	1/1	0.86	0.19	-1.59	71,71,71,71	0
57	MG	DA	3613	1/1	0.97	0.15	-1.59	54,54,54,54	0
57	MG	BA	3049	1/1	0.98	0.21	-1.62	36,36,36,36	0
57	MG	DA	3173	1/1	0.92	0.12	-1.62	53,53,53,53	0
57	MG	DA	3575	1/1	0.87	0.14	-1.62	64,64,64,64	0
57	MG	BA	3465	1/1	0.90	0.18	-1.62	43,43,43,43	0
57	MG	AA	3133	1/1	0.92	0.16	-1.63	56,56,56,56	0
57	MG	BA	3320	1/1	0.93	0.22	-1.63	48,48,48,48	0
57	MG	DA	3281	1/1	0.98	0.16	-1.63	53,53,53,53	0
57	MG	BA	3713	1/1	0.93	0.18	-1.64	33,33,33,33	0
57	MG	AA	3001	1/1	0.85	0.14	-1.64	61,61,61,61	0
59	ZN	D4	501	1/1	0.79	0.07	-1.65	144,144,144,144	0
57	MG	BA	3807	1/1	0.93	0.17	-1.68	47,47,47,47	0
57	MG	B0	101	1/1	0.98	0.17	-1.69	36,36,36,36	0
57	MG	BN	3006	1/1	0.93	0.20	-1.69	49,49,49,49	0
57	MG	BA	3509	1/1	0.94	0.21	-1.69	31,31,31,31	0
57	MG	DA	3271	1/1	0.90	0.15	-1.70	48,48,48,48	0
57	MG	DA	3313	1/1	0.89	0.16	-1.70	47,47,47,47	0
57	MG	BA	3057	1/1	0.88	0.19	-1.70	34,34,34,34	0
57	MG	DA	3205	1/1	0.77	0.10	-1.72	56,56,56,56	0
57	MG	DA	3183	1/1	0.95	0.15	-1.73	38,38,38,38	0
57	MG	DA	3663	1/1	0.96	0.13	-1.73	60,60,60,60	0
59	ZN	D9	501	1/1	0.97	0.12	-1.74	68,68,68,68	0
59	ZN	CN	501	1/1	0.98	0.08	-1.76	93,93,93,93	0
57	MG	DW	3002	1/1	0.96	0.15	-1.78	45,45,45,45	0
57	MG	BA	3722	1/1	0.92	0.19	-1.78	47,47,47,47	0
57	MG	BA	3740	1/1	0.88	0.16	-1.78	28,28,28,28	0
57	MG	CA	3099	1/1	0.98	0.15	-1.79	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
57	MG	AA	3137	1/1	0.97	0.15	-1.81	51,51,51,51	0
57	MG	DA	3174	1/1	0.95	0.13	-1.85	44,44,44,44	0
57	MG	DA	3388	1/1	0.88	0.15	-1.85	53,53,53,53	0
57	MG	BA	3433	1/1	0.91	0.20	-1.88	32,32,32,32	0
57	MG	DB	3004	1/1	0.90	0.15	-1.88	55,55,55,55	0
57	MG	BA	3456	1/1	0.85	0.18	-1.89	49,49,49,49	0
57	MG	DA	3237	1/1	0.93	0.14	-1.90	56,56,56,56	0
57	MG	CA	3040	1/1	0.93	0.11	-1.90	51,51,51,51	0
57	MG	BA	3587	1/1	0.83	0.17	-1.95	36,36,36,36	0
57	MG	DA	3366	1/1	0.96	0.14	-1.96	42,42,42,42	0
57	MG	BN	3002	1/1	0.91	0.16	-1.97	39,39,39,39	0
57	MG	BA	3763	1/1	0.96	0.19	-2.00	24,24,24,24	0
57	MG	CA	3053	1/1	0.94	0.15	-2.05	41,41,41,41	0
57	MG	BA	3539	1/1	0.95	0.20	-2.06	52,52,52,52	0
57	MG	DA	3127	1/1	0.93	0.15	-2.06	35,35,35,35	0
57	MG	DA	3492	1/1	0.89	0.12	-2.07	55,55,55,55	0
57	MG	BA	3009	1/1	0.94	0.17	-2.07	28,28,28,28	0
57	MG	AA	3002	1/1	0.83	0.15	-2.08	71,71,71,71	0
57	MG	BA	3510	1/1	0.95	0.16	-2.10	46,46,46,46	0
57	MG	DA	3344	1/1	0.99	0.16	-2.11	31,31,31,31	0
57	MG	CA	3009	1/1	0.83	0.11	-2.12	64,64,64,64	0
57	MG	BA	3463	1/1	0.81	0.20	-2.12	48,48,48,48	0
57	MG	AA	3030	1/1	0.91	0.18	-2.14	60,60,60,60	0
57	MG	CA	3109	1/1	0.82	0.13	-2.16	67,67,67,67	0
57	MG	BA	3541	1/1	0.90	0.16	-2.16	38,38,38,38	0
57	MG	AA	3212	1/1	0.96	0.13	-2.16	42,42,42,42	0
57	MG	BV	202	1/1	0.96	0.17	-2.17	50,50,50,50	0
57	MG	BA	3133	1/1	0.95	0.19	-2.17	45,45,45,45	0
57	MG	BE	304	1/1	0.96	0.19	-2.17	42,42,42,42	0
57	MG	CT	3001	1/1	0.58	0.12	-2.18	56,56,56,56	0
57	MG	DA	3101	1/1	0.96	0.16	-2.20	49,49,49,49	0
57	MG	DA	3261	1/1	0.97	0.12	-2.21	49,49,49,49	0
57	MG	DA	3285	1/1	0.99	0.13	-2.22	32,32,32,32	0
57	MG	DE	303	1/1	0.85	0.12	-2.24	54,54,54,54	0
57	MG	DA	3177	1/1	0.98	0.15	-2.24	42,42,42,42	0
57	MG	DA	3545	1/1	0.93	0.13	-2.24	35,35,35,35	0
57	MG	DB	3003	1/1	0.88	0.12	-2.26	57,57,57,57	0
57	MG	DA	3592	1/1	0.86	0.08	-2.26	51,51,51,51	0
57	MG	DA	3424	1/1	0.90	0.09	-2.27	61,61,61,61	0
57	MG	DA	3061	1/1	0.87	0.13	-2.28	48,48,48,48	0
57	MG	CA	3083	1/1	0.94	0.10	-2.33	79,79,79,79	0
57	MG	BA	3565	1/1	0.97	0.17	-2.33	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
57	MG	BA	3219	1/1	0.94	0.17	-2.35	36,36,36,36	0
57	MG	BA	3646	1/1	0.93	0.17	-2.37	42,42,42,42	0
57	MG	DA	3353	1/1	0.96	0.16	-2.38	42,42,42,42	0
57	MG	CA	3028	1/1	0.91	0.13	-2.40	41,41,41,41	0
57	MG	BF	302	1/1	0.92	0.18	-2.42	46,46,46,46	0
57	MG	AA	3094	1/1	0.88	0.16	-2.44	59,59,59,59	0
57	MG	BA	3797	1/1	0.92	0.17	-2.44	53,53,53,53	0
57	MG	BE	308	1/1	0.93	0.17	-2.45	40,40,40,40	0
57	MG	CA	3038	1/1	0.90	0.14	-2.45	58,58,58,58	0
57	MG	BA	3458	1/1	0.99	0.18	-2.46	18,18,18,18	0
57	MG	DQ	3001	1/1	0.98	0.13	-2.49	47,47,47,47	0
57	MG	DA	3201	1/1	0.93	0.14	-2.49	61,61,61,61	0
57	MG	AA	3009	1/1	0.94	0.18	-2.52	57,57,57,57	0
57	MG	DA	3043	1/1	0.94	0.15	-2.53	38,38,38,38	0
57	MG	CA	3124	1/1	0.87	0.12	-2.53	59,59,59,59	0
57	MG	AA	3117	1/1	0.90	0.12	-2.58	79,79,79,79	0
57	MG	DA	3171	1/1	0.97	0.12	-2.58	31,31,31,31	0
57	MG	BA	3430	1/1	0.88	0.16	-2.60	37,37,37,37	0
57	MG	AA	3211	1/1	0.90	0.12	-2.61	47,47,47,47	0
57	MG	BA	3730	1/1	0.31	0.19	-2.61	71,71,71,71	0
57	MG	AA	3139	1/1	0.83	0.14	-2.63	59,59,59,59	0
57	MG	DA	3030	1/1	0.95	0.14	-2.63	39,39,39,39	0
57	MG	CA	3046	1/1	0.91	0.09	-2.64	69,69,69,69	0
57	MG	AA	3091	1/1	0.81	0.14	-2.65	60,60,60,60	0
57	MG	CA	3112	1/1	0.93	0.15	-2.65	69,69,69,69	0
57	MG	BA	3366	1/1	0.91	0.12	-2.67	57,57,57,57	0
57	MG	DA	3310	1/1	0.97	0.13	-2.68	38,38,38,38	0
57	MG	DA	3537	1/1	0.96	0.08	-2.69	44,44,44,44	0
57	MG	DA	3270	1/1	0.90	0.10	-2.69	46,46,46,46	0
57	MG	BA	3332	1/1	0.98	0.18	-2.69	38,38,38,38	0
57	MG	BA	3563	1/1	0.98	0.17	-2.71	36,36,36,36	0
57	MG	DA	3135	1/1	0.92	0.12	-2.71	38,38,38,38	0
57	MG	AA	3023	1/1	0.83	0.13	-2.74	74,74,74,74	0
57	MG	BA	3236	1/1	0.94	0.20	-2.75	49,49,49,49	0
57	MG	BB	204	1/1	0.97	0.18	-2.76	41,41,41,41	0
57	MG	DA	3501	1/1	0.95	0.15	-2.77	37,37,37,37	0
57	MG	BA	3211	1/1	0.96	0.16	-2.78	55,55,55,55	0
57	MG	BA	3319	1/1	0.93	0.19	-2.82	46,46,46,46	0
57	MG	BA	3214	1/1	0.97	0.17	-2.82	41,41,41,41	0
57	MG	DA	3425	1/1	0.85	0.12	-2.82	61,61,61,61	0
57	MG	BD	303	1/1	0.97	0.14	-2.84	39,39,39,39	0
57	MG	BA	3351	1/1	0.90	0.17	-2.85	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3671	1/1	0.99	0.13	-2.86	74,74,74,74	0
57	MG	B7	102	1/1	0.93	0.16	-2.87	47,47,47,47	0
57	MG	BA	3423	1/1	0.91	0.18	-2.90	44,44,44,44	0
57	MG	CA	3123	1/1	0.97	0.14	-2.91	58,58,58,58	0
57	MG	B7	103	1/1	0.97	0.16	-2.92	42,42,42,42	0
57	MG	BA	3480	1/1	0.84	0.20	-2.93	35,35,35,35	0
57	MG	BA	3526	1/1	0.88	0.17	-2.95	44,44,44,44	0
57	MG	CA	3043	1/1	0.98	0.11	-2.97	47,47,47,47	0
57	MG	BA	3459	1/1	0.92	0.19	-2.98	48,48,48,48	0
57	MG	AA	3182	1/1	0.97	0.14	-2.98	49,49,49,49	0
57	MG	DA	3472	1/1	0.94	0.16	-3.04	44,44,44,44	0
57	MG	BA	3788	1/1	0.83	0.15	-3.06	51,51,51,51	0
57	MG	DA	3363	1/1	0.98	0.15	-3.06	29,29,29,29	0
57	MG	DA	3122	1/1	0.84	0.11	-3.06	49,49,49,49	0
57	MG	BA	3792	1/1	0.98	0.14	-3.07	54,54,54,54	0
57	MG	BA	3415	1/1	0.94	0.16	-3.10	28,28,28,28	0
57	MG	DA	3326	1/1	0.97	0.16	-3.12	43,43,43,43	0
57	MG	DA	3667	1/1	0.86	0.12	-3.12	50,50,50,50	0
57	MG	BA	3334	1/1	0.97	0.14	-3.13	37,37,37,37	0
57	MG	DA	3464	1/1	0.96	0.10	-3.13	46,46,46,46	0
57	MG	BA	3790	1/1	0.89	0.18	-3.17	34,34,34,34	0
57	MG	DD	305	1/1	0.98	0.12	-3.17	36,36,36,36	0
57	MG	DA	3003	1/1	0.98	0.15	-3.18	27,27,27,27	0
57	MG	BA	3550	1/1	0.90	0.19	-3.20	36,36,36,36	0
57	MG	BA	3381	1/1	0.95	0.15	-3.21	46,46,46,46	0
57	MG	DA	3419	1/1	0.94	0.11	-3.21	32,32,32,32	0
57	MG	BA	3102	1/1	0.97	0.18	-3.22	44,44,44,44	0
57	MG	BA	3350	1/1	0.94	0.20	-3.25	28,28,28,28	0
57	MG	BA	3581	1/1	0.90	0.19	-3.31	30,30,30,30	0
57	MG	AA	3045	1/1	0.87	0.12	-3.33	58,58,58,58	0
57	MG	BD	305	1/1	0.97	0.15	-3.33	35,35,35,35	0
57	MG	DA	3319	1/1	0.96	0.12	-3.33	41,41,41,41	0
57	MG	DA	3539	1/1	0.95	0.12	-3.34	53,53,53,53	0
57	MG	CA	3089	1/1	0.98	0.12	-3.35	47,47,47,47	0
57	MG	DA	3666	1/1	0.89	0.14	-3.36	35,35,35,35	0
57	MG	DA	3337	1/1	0.90	0.13	-3.37	41,41,41,41	0
57	MG	CA	3132	1/1	0.95	0.13	-3.38	66,66,66,66	0
57	MG	BA	3477	1/1	0.92	0.18	-3.38	61,61,61,61	0
57	MG	BA	3411	1/1	0.90	0.19	-3.39	33,33,33,33	0
57	MG	BF	301	1/1	0.97	0.16	-3.41	35,35,35,35	0
57	MG	DA	3198	1/1	0.98	0.13	-3.45	40,40,40,40	0
57	MG	DA	3324	1/1	0.94	0.11	-3.45	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DG	3001	1/1	0.81	0.09	-3.46	55,55,55,55	0
57	MG	BA	3398	1/1	0.95	0.21	-3.47	32,32,32,32	0
57	MG	DA	3422	1/1	0.83	0.08	-3.48	46,46,46,46	0
57	MG	BA	3425	1/1	0.97	0.15	-3.48	40,40,40,40	0
57	MG	BA	3379	1/1	0.97	0.18	-3.51	31,31,31,31	0
57	MG	DA	3284	1/1	0.93	0.12	-3.53	47,47,47,47	0
57	MG	BA	3789	1/1	0.97	0.18	-3.58	12,12,12,12	0
57	MG	DA	3306	1/1	0.96	0.13	-3.59	55,55,55,55	0
57	MG	DA	3486	1/1	0.95	0.09	-3.61	47,47,47,47	0
57	MG	BA	3067	1/1	0.97	0.15	-3.65	41,41,41,41	0
57	MG	BA	3407	1/1	0.92	0.15	-3.66	47,47,47,47	0
57	MG	BA	3752	1/1	0.97	0.19	-3.66	32,32,32,32	0
57	MG	D0	101	1/1	0.85	0.08	-3.68	71,71,71,71	0
57	MG	AA	3033	1/1	0.85	0.14	-3.68	59,59,59,59	0
57	MG	BA	3630	1/1	0.97	0.14	-3.68	58,58,58,58	0
57	MG	BA	3791	1/1	0.98	0.18	-3.69	28,28,28,28	0
57	MG	DA	3465	1/1	0.90	0.12	-3.70	46,46,46,46	0
57	MG	BA	3570	1/1	0.95	0.16	-3.72	42,42,42,42	0
57	MG	DA	3074	1/1	0.93	0.12	-3.72	37,37,37,37	0
57	MG	AW	3004	1/1	0.57	0.14	-3.73	49,49,49,49	0
57	MG	BA	3755	1/1	0.85	0.15	-3.74	55,55,55,55	0
57	MG	DA	3192	1/1	0.97	0.10	-3.74	60,60,60,60	0
57	MG	CA	3003	1/1	0.88	0.12	-3.74	57,57,57,57	0
57	MG	DA	3632	1/1	0.87	0.15	-3.78	36,36,36,36	0
57	MG	BA	3274	1/1	0.86	0.14	-3.78	49,49,49,49	0
57	MG	BA	3636	1/1	0.57	0.14	-3.85	64,64,64,64	0
57	MG	DA	3434	1/1	0.94	0.10	-3.85	39,39,39,39	0
57	MG	AA	3146	1/1	0.90	0.13	-3.94	66,66,66,66	0
57	MG	AA	3121	1/1	0.87	0.12	-3.95	70,70,70,70	0
57	MG	DA	3530	1/1	0.51	0.13	-3.95	74,74,74,74	0
57	MG	BA	3629	1/1	0.96	0.16	-3.97	43,43,43,43	0
57	MG	BU	207	1/1	0.95	0.17	-3.98	38,38,38,38	0
57	MG	BA	3365	1/1	0.94	0.13	-4.00	62,62,62,62	0
57	MG	BA	3420	1/1	0.97	0.16	-4.01	40,40,40,40	0
57	MG	CF	3001	1/1	0.94	0.11	-4.02	46,46,46,46	0
57	MG	DA	3246	1/1	0.93	0.14	-4.02	43,43,43,43	0
57	MG	BU	201	1/1	0.89	0.15	-4.03	43,43,43,43	0
57	MG	BA	3249	1/1	0.95	0.13	-4.07	49,49,49,49	0
57	MG	DA	3286	1/1	0.95	0.14	-4.08	42,42,42,42	0
57	MG	BA	3013	1/1	0.99	0.14	-4.10	32,32,32,32	0
57	MG	DA	3053	1/1	0.94	0.10	-4.10	47,47,47,47	0
57	MG	BA	3538	1/1	0.75	0.15	-4.14	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
57	MG	BA	3605	1/1	0.98	0.17	-4.16	43,43,43,43	0
57	MG	DA	3609	1/1	0.88	0.10	-4.18	46,46,46,46	0
57	MG	DA	3455	1/1	0.97	0.10	-4.19	47,47,47,47	0
57	MG	AA	3145	1/1	0.88	0.12	-4.19	66,66,66,66	0
57	MG	BA	3542	1/1	0.92	0.18	-4.19	45,45,45,45	0
57	MG	CA	3157	1/1	0.88	0.11	-4.24	58,58,58,58	0
57	MG	BB	208	1/1	0.97	0.14	-4.28	45,45,45,45	0
57	MG	BA	3369	1/1	0.92	0.15	-4.29	44,44,44,44	0
57	MG	DA	3325	1/1	0.92	0.12	-4.31	35,35,35,35	0
57	MG	BA	3701	1/1	0.96	0.15	-4.31	43,43,43,43	0
57	MG	DA	3103	1/1	0.91	0.10	-4.33	58,58,58,58	0
57	MG	DA	3373	1/1	0.97	0.15	-4.34	44,44,44,44	0
57	MG	AA	3020	1/1	0.83	0.13	-4.36	76,76,76,76	0
57	MG	CA	3020	1/1	0.89	0.11	-4.36	56,56,56,56	0
57	MG	BA	3436	1/1	0.94	0.14	-4.36	40,40,40,40	0
57	MG	AA	3152	1/1	0.93	0.10	-4.37	62,62,62,62	0
57	MG	BA	3736	1/1	0.98	0.16	-4.37	42,42,42,42	0
57	MG	DA	3509	1/1	0.96	0.12	-4.37	59,59,59,59	0
57	MG	DA	3342	1/1	0.82	0.11	-4.42	42,42,42,42	0
57	MG	BA	3793	1/1	0.89	0.13	-4.42	40,40,40,40	0
57	MG	BR	202	1/1	0.98	0.14	-4.43	31,31,31,31	0
57	MG	DA	3157	1/1	0.98	0.11	-4.46	47,47,47,47	0
57	MG	DA	3365	1/1	0.96	0.08	-4.46	36,36,36,36	0
57	MG	BA	3562	1/1	0.91	0.14	-4.52	37,37,37,37	0
57	MG	DA	3498	1/1	0.85	0.08	-4.52	51,51,51,51	0
57	MG	BX	3003	1/1	0.92	0.17	-4.55	35,35,35,35	0
57	MG	BA	3247	1/1	0.98	0.16	-4.58	25,25,25,25	0
57	MG	BA	3183	1/1	0.94	0.18	-4.60	42,42,42,42	0
57	MG	AA	3054	1/1	0.86	0.13	-4.60	53,53,53,53	0
57	MG	DA	3430	1/1	0.84	0.11	-4.61	37,37,37,37	0
57	MG	DA	3596	1/1	0.96	0.10	-4.64	56,56,56,56	0
57	MG	BA	3175	1/1	0.95	0.20	-4.65	20,20,20,20	0
57	MG	DA	3648	1/1	0.96	0.14	-4.65	57,57,57,57	0
57	MG	DA	3006	1/1	0.93	0.10	-4.66	38,38,38,38	0
57	MG	DA	3580	1/1	0.96	0.16	-4.66	36,36,36,36	0
57	MG	BU	204	1/1	0.95	0.16	-4.73	35,35,35,35	0
57	MG	AA	3115	1/1	0.92	0.08	-4.75	79,79,79,79	0
57	MG	DA	3635	1/1	0.76	0.11	-4.76	38,38,38,38	0
57	MG	BB	217	1/1	0.98	0.18	-4.76	29,29,29,29	0
57	MG	DA	3447	1/1	0.93	0.15	-4.77	58,58,58,58	0
57	MG	BA	3222	1/1	0.97	0.18	-4.80	37,37,37,37	0
57	MG	CA	3023	1/1	0.96	0.14	-4.81	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
57	MG	BA	3387	1/1	0.92	0.15	-4.84	54,54,54,54	0
57	MG	DA	3334	1/1	0.88	0.15	-4.86	52,52,52,52	0
57	MG	DA	3039	1/1	0.94	0.10	-4.86	43,43,43,43	0
57	MG	BA	3051	1/1	0.92	0.19	-4.87	43,43,43,43	0
57	MG	DA	3515	1/1	0.96	0.15	-4.96	45,45,45,45	0
57	MG	AA	3158	1/1	0.97	0.13	-4.98	45,45,45,45	0
57	MG	AA	3042	1/1	0.89	0.09	-4.98	57,57,57,57	0
57	MG	BA	3418	1/1	0.82	0.17	-5.00	30,30,30,30	0
57	MG	BE	301	1/1	0.89	0.14	-5.04	35,35,35,35	0
57	MG	BA	3772	1/1	0.98	0.19	-5.05	33,33,33,33	0
57	MG	CA	3096	1/1	0.94	0.10	-5.07	44,44,44,44	0
57	MG	BA	3299	1/1	0.97	0.16	-5.08	25,25,25,25	0
57	MG	DA	3417	1/1	0.79	0.11	-5.10	52,52,52,52	0
57	MG	AA	3019	1/1	0.88	0.11	-5.11	66,66,66,66	0
57	MG	BA	3354	1/1	0.95	0.10	-5.11	48,48,48,48	0
57	MG	BA	3025	1/1	0.98	0.16	-5.12	27,27,27,27	0
57	MG	DA	3529	1/1	0.97	0.08	-5.14	38,38,38,38	0
57	MG	BA	3326	1/1	0.97	0.19	-5.16	20,20,20,20	0
57	MG	BA	3472	1/1	0.98	0.16	-5.17	20,20,20,20	0
57	MG	DA	3562	1/1	0.95	0.12	-5.18	64,64,64,64	0
57	MG	BA	3409	1/1	0.88	0.16	-5.20	30,30,30,30	0
57	MG	DA	3345	1/1	0.97	0.09	-5.22	44,44,44,44	0
57	MG	BA	3402	1/1	0.89	0.14	-5.23	40,40,40,40	0
57	MG	DA	3011	1/1	0.91	0.08	-5.25	48,48,48,48	0
57	MG	DA	3500	1/1	0.98	0.10	-5.27	49,49,49,49	0
57	MG	DA	3318	1/1	0.95	0.14	-5.27	40,40,40,40	0
57	MG	DA	3440	1/1	0.87	0.09	-5.30	61,61,61,61	0
57	MG	DA	3330	1/1	0.98	0.11	-5.32	45,45,45,45	0
57	MG	DA	3148	1/1	0.88	0.12	-5.36	54,54,54,54	0
57	MG	DA	3296	1/1	0.96	0.12	-5.36	28,28,28,28	0
57	MG	CA	3077	1/1	0.94	0.08	-5.41	66,66,66,66	0
57	MG	DA	3369	1/1	0.97	0.15	-5.41	28,28,28,28	0
57	MG	AA	3178	1/1	0.93	0.15	-5.42	59,59,59,59	0
57	MG	DA	3358	1/1	0.93	0.14	-5.42	45,45,45,45	0
57	MG	BQ	3005	1/1	0.89	0.13	-5.43	49,49,49,49	0
57	MG	BA	3532	1/1	0.89	0.15	-5.46	52,52,52,52	0
57	MG	BA	3441	1/1	0.96	0.13	-5.49	35,35,35,35	0
57	MG	BA	3048	1/1	0.97	0.13	-5.50	47,47,47,47	0
57	MG	BA	3486	1/1	0.85	0.13	-5.51	57,57,57,57	0
57	MG	BA	3353	1/1	0.76	0.12	-5.56	50,50,50,50	0
57	MG	BV	205	1/1	0.96	0.09	-5.57	38,38,38,38	0
57	MG	B3	3001	1/1	0.95	0.12	-5.59	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3008	1/1	0.98	0.09	-5.63	36,36,36,36	0
57	MG	BA	3269	1/1	0.91	0.16	-5.69	53,53,53,53	0
57	MG	CA	3068	1/1	0.94	0.15	-5.69	48,48,48,48	0
57	MG	BA	3234	1/1	0.98	0.15	-5.73	38,38,38,38	0
57	MG	BA	3715	1/1	0.81	0.14	-5.74	63,63,63,63	0
57	MG	BA	3750	1/1	0.91	0.17	-5.74	27,27,27,27	0
57	MG	DA	3287	1/1	0.95	0.10	-5.74	41,41,41,41	0
57	MG	BA	3343	1/1	0.97	0.15	-5.76	53,53,53,53	0
57	MG	BA	3517	1/1	0.96	0.14	-5.77	45,45,45,45	0
57	MG	CA	3041	1/1	0.89	0.13	-5.79	59,59,59,59	0
57	MG	BA	3555	1/1	0.93	0.14	-5.81	29,29,29,29	0
57	MG	AA	3074	1/1	0.96	0.09	-5.89	50,50,50,50	0
57	MG	DA	3618	1/1	0.88	0.12	-5.89	53,53,53,53	0
57	MG	BA	3483	1/1	0.97	0.15	-5.92	28,28,28,28	0
57	MG	BA	3132	1/1	0.96	0.14	-5.93	40,40,40,40	0
57	MG	BA	3558	1/1	0.98	0.14	-5.93	32,32,32,32	0
57	MG	DA	3341	1/1	0.96	0.13	-5.93	51,51,51,51	0
57	MG	BA	3692	1/1	0.96	0.15	-5.95	40,40,40,40	0
57	MG	BA	3167	1/1	0.98	0.12	-5.98	41,41,41,41	0
57	MG	BA	3119	1/1	0.93	0.13	-6.01	45,45,45,45	0
57	MG	BA	3598	1/1	0.86	0.14	-6.03	63,63,63,63	0
57	MG	BA	3217	1/1	0.94	0.16	-6.06	37,37,37,37	0
57	MG	DA	3351	1/1	0.93	0.12	-6.06	48,48,48,48	0
57	MG	BA	3027	1/1	0.95	0.11	-6.09	26,26,26,26	0
57	MG	BA	3309	1/1	0.97	0.18	-6.10	41,41,41,41	0
57	MG	BN	3004	1/1	0.90	0.12	-6.10	60,60,60,60	0
57	MG	AA	3164	1/1	0.97	0.10	-6.13	61,61,61,61	0
57	MG	DA	3414	1/1	0.84	0.13	-6.14	43,43,43,43	0
57	MG	BA	3487	1/1	0.98	0.14	-6.32	50,50,50,50	0
57	MG	DA	3040	1/1	0.96	0.12	-6.33	31,31,31,31	0
57	MG	AA	3093	1/1	0.89	0.12	-6.47	66,66,66,66	0
57	MG	BA	3410	1/1	0.97	0.16	-6.48	27,27,27,27	0
57	MG	DA	3272	1/1	0.95	0.10	-6.49	41,41,41,41	0
57	MG	BA	3764	1/1	0.84	0.17	-6.50	51,51,51,51	0
57	MG	BA	3620	1/1	0.95	0.15	-6.55	40,40,40,40	0
57	MG	DA	3612	1/1	0.94	0.09	-6.62	62,62,62,62	0
57	MG	BA	3768	1/1	0.93	0.12	-6.63	47,47,47,47	0
57	MG	DA	3579	1/1	0.97	0.10	-6.65	48,48,48,48	0
57	MG	DA	3502	1/1	0.90	0.10	-6.73	55,55,55,55	0
57	MG	DA	3401	1/1	0.90	0.10	-6.74	38,38,38,38	0
57	MG	DA	3356	1/1	0.87	0.10	-6.77	36,36,36,36	0
57	MG	BA	3511	1/1	0.94	0.14	-6.95	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3100	1/1	0.90	0.12	-7.08	65,65,65,65	0
57	MG	DA	3021	1/1	0.98	0.09	-7.08	31,31,31,31	0
57	MG	DA	3446	1/1	0.83	0.11	-7.10	45,45,45,45	0
57	MG	BA	3043	1/1	0.92	0.15	-7.24	48,48,48,48	0
57	MG	DA	3387	1/1	0.96	0.10	-7.31	42,42,42,42	0
57	MG	CA	3117	1/1	0.93	0.10	-7.31	71,71,71,71	0
57	MG	BA	3008	1/1	0.89	0.17	-7.35	47,47,47,47	0
57	MG	BA	3318	1/1	0.87	0.12	-7.36	41,41,41,41	0
57	MG	AA	3063	1/1	0.91	0.10	-7.38	35,35,35,35	0
57	MG	DA	3265	1/1	0.97	0.12	-7.40	30,30,30,30	0
57	MG	DA	3549	1/1	0.93	0.10	-7.43	57,57,57,57	0
57	MG	DA	3377	1/1	0.95	0.09	-7.48	38,38,38,38	0
57	MG	BA	3395	1/1	0.95	0.17	-7.49	38,38,38,38	0
57	MG	AA	3200	1/1	0.88	0.08	-7.51	73,73,73,73	0
57	MG	CA	3110	1/1	0.94	0.09	-7.53	65,65,65,65	0
57	MG	DA	3321	1/1	0.81	0.08	-7.54	48,48,48,48	0
57	MG	BA	3010	1/1	0.98	0.16	-7.54	39,39,39,39	0
57	MG	BA	3649	1/1	0.94	0.11	-7.56	40,40,40,40	0
57	MG	DA	3460	1/1	0.97	0.13	-7.57	41,41,41,41	0
57	MG	DA	3570	1/1	0.95	0.13	-7.70	31,31,31,31	0
57	MG	BA	3548	1/1	0.87	0.17	-7.71	40,40,40,40	0
57	MG	CA	3081	1/1	0.89	0.09	-7.74	46,46,46,46	0
57	MG	BA	3661	1/1	0.96	0.09	-7.80	44,44,44,44	0
57	MG	CA	3086	1/1	0.93	0.13	-7.83	64,64,64,64	0
57	MG	BA	3609	1/1	0.98	0.11	-7.87	39,39,39,39	0
57	MG	BA	3535	1/1	0.92	0.19	-7.94	31,31,31,31	0
57	MG	AA	3081	1/1	0.95	0.11	-7.95	48,48,48,48	0
57	MG	AA	3130	1/1	0.93	0.08	-8.00	56,56,56,56	0
57	MG	DA	3328	1/1	0.90	0.08	-8.09	47,47,47,47	0
57	MG	BA	3650	1/1	0.91	0.12	-8.20	52,52,52,52	0
57	MG	BA	3371	1/1	0.97	0.14	-8.21	35,35,35,35	0
57	MG	BA	3406	1/1	0.93	0.09	-8.41	50,50,50,50	0
57	MG	BA	3585	1/1	0.93	0.09	-8.65	46,46,46,46	0
57	MG	BA	3497	1/1	0.98	0.14	-8.81	28,28,28,28	0
57	MG	BA	3744	1/1	0.98	0.14	-8.82	39,39,39,39	0
57	MG	BA	3716	1/1	0.78	0.12	-8.84	65,65,65,65	0
57	MG	BA	3363	1/1	0.97	0.15	-8.86	22,22,22,22	0
57	MG	DA	3477	1/1	0.95	0.09	-9.22	43,43,43,43	0
57	MG	BF	305	1/1	0.98	0.09	-9.40	49,49,49,49	0
57	MG	CA	3016	1/1	0.85	0.11	-9.40	57,57,57,57	0
57	MG	BA	3258	1/1	0.87	0.13	-9.41	44,44,44,44	0
57	MG	CA	3069	1/1	0.96	0.12	-9.42	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
57	MG	DA	3289	1/1	0.98	0.10	-9.53	53,53,53,53	0
57	MG	BA	3256	1/1	0.96	0.15	-9.63	40,40,40,40	0
57	MG	AA	3022	1/1	0.92	0.10	-9.64	71,71,71,71	0
57	MG	DA	3149	1/1	0.93	0.06	-9.67	56,56,56,56	0
57	MG	BA	3643	1/1	0.97	0.13	-9.84	46,46,46,46	0
57	MG	BA	3648	1/1	0.90	0.11	-9.84	65,65,65,65	0
57	MG	BA	3604	1/1	0.93	0.15	-9.86	36,36,36,36	0
57	MG	DA	3303	1/1	0.95	0.09	-9.87	48,48,48,48	0
57	MG	BA	3316	1/1	0.81	0.12	-10.12	66,66,66,66	0
57	MG	BA	3644	1/1	0.96	0.14	-10.25	35,35,35,35	0
57	MG	DA	3279	1/1	0.91	0.12	-10.44	56,56,56,56	0
57	MG	DA	3619	1/1	0.96	0.11	-10.61	69,69,69,69	0
57	MG	BA	3378	1/1	0.99	0.12	-10.77	28,28,28,28	0
57	MG	BA	3647	1/1	0.95	0.09	-11.48	56,56,56,56	0
57	MG	BA	3026	1/1	0.95	0.15	-11.57	41,41,41,41	0
57	MG	AA	3016	1/1	0.94	0.09	-11.70	63,63,63,63	0
57	MG	AA	3086	1/1	0.98	0.07	-11.88	57,57,57,57	0
57	MG	DA	3538	1/1	0.91	0.11	-12.06	58,58,58,58	0
57	MG	BA	3162	1/1	0.88	0.15	-12.29	38,38,38,38	0
57	MG	BA	3594	1/1	0.83	0.12	-12.41	40,40,40,40	0
57	MG	BA	3092	1/1	0.89	0.16	-12.53	37,37,37,37	0
57	MG	DA	3315	1/1	0.99	0.08	-12.65	42,42,42,42	0
57	MG	BA	3580	1/1	0.93	0.13	-13.63	55,55,55,55	0
57	MG	DA	3278	1/1	0.97	0.06	-14.02	43,43,43,43	0
57	MG	BA	3786	1/1	0.97	0.13	-14.14	35,35,35,35	0
57	MG	BA	3002	1/1	0.89	0.10	-16.88	50,50,50,50	0
57	MG	BA	3146	1/1	0.95	0.17	-17.32	40,40,40,40	0
57	MG	DA	3254	1/1	0.94	0.07	-19.23	52,52,52,52	0
57	MG	DA	3445	1/1	0.96	0.10	-21.95	32,32,32,32	0
57	MG	BA	3522	1/1	0.94	0.09	-25.68	52,52,52,52	0
57	MG	DA	3069	1/1	0.85	0.23	-	57,57,57,57	0
57	MG	BA	3462	1/1	0.96	0.19	-	36,36,36,36	0
57	MG	BA	3038	1/1	0.98	0.25	-	35,35,35,35	0
57	MG	BA	3568	1/1	0.63	0.10	-	59,59,59,59	0
57	MG	BA	3770	1/1	0.94	0.16	-	45,45,45,45	0
57	MG	BA	3021	1/1	0.93	0.18	-	49,49,49,49	0
57	MG	BA	3384	1/1	0.99	0.19	-	41,41,41,41	0
57	MG	BA	3091	1/1	0.96	0.39	-	56,56,56,56	0
57	MG	CA	3144	1/1	0.91	0.19	-	71,71,71,71	0
57	MG	AA	3124	1/1	0.87	0.09	-	47,47,47,47	0
57	MG	BA	3062	1/1	0.95	0.27	-	42,42,42,42	0
57	MG	BA	3385	1/1	0.92	0.16	-	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
57	MG	CA	3142	1/1	0.93	0.13	-	69,69,69,69	0
57	MG	DA	3408	1/1	0.81	0.08	-	58,58,58,58	0
57	MG	DA	3012	1/1	0.96	0.12	-	33,33,33,33	0
57	MG	B3	3002	1/1	0.96	0.12	-	66,66,66,66	0
57	MG	DR	5001	1/1	0.58	0.24	-	70,70,70,70	0
57	MG	DA	3398	1/1	0.92	0.14	-	45,45,45,45	0
57	MG	AA	3039	1/1	0.95	0.15	-	56,56,56,56	0
57	MG	BA	3536	1/1	0.94	0.27	-	49,49,49,49	0
57	MG	DA	3215	1/1	0.90	0.13	-	59,59,59,59	0
57	MG	BA	3454	1/1	0.98	0.23	-	27,27,27,27	0
57	MG	DA	3535	1/1	0.99	0.18	-	56,56,56,56	0
57	MG	CA	3090	1/1	0.87	0.10	-	67,67,67,67	0
57	MG	BA	3712	1/1	0.95	0.18	-	53,53,53,53	0
57	MG	CA	3159	1/1	0.89	0.18	-	70,70,70,70	0
57	MG	BA	3488	1/1	0.96	0.19	-	60,60,60,60	0
57	MG	DA	3599	1/1	0.97	0.20	-	36,36,36,36	0
57	MG	DA	3163	1/1	0.93	0.15	-	49,49,49,49	0
57	MG	AA	3169	1/1	0.74	0.13	-	62,62,62,62	0
57	MG	BA	3205	1/1	0.95	0.27	-	50,50,50,50	0
57	MG	BD	309	1/1	0.90	0.32	-	57,57,57,57	0
57	MG	BA	3705	1/1	0.98	0.11	-	62,62,62,62	0
57	MG	DA	3442	1/1	0.98	0.12	-	39,39,39,39	0
57	MG	DA	3476	1/1	0.84	0.14	-	62,62,62,62	0
57	MG	DA	3346	1/1	0.96	0.12	-	48,48,48,48	0
57	MG	AA	3059	1/1	0.90	0.12	-	78,78,78,78	0
57	MG	DA	3653	1/1	0.91	0.14	-	52,52,52,52	0
57	MG	BA	3377	1/1	0.94	0.14	-	44,44,44,44	0
57	MG	AA	3058	1/1	0.90	0.28	-	59,59,59,59	0
57	MG	BA	3337	1/1	0.88	0.17	-	58,58,58,58	0
57	MG	AA	3072	1/1	0.88	0.12	-	66,66,66,66	0
57	MG	DA	3178	1/1	0.85	0.22	-	50,50,50,50	0
57	MG	CA	3151	1/1	0.95	0.27	-	59,59,59,59	0
57	MG	DA	3129	1/1	0.90	0.12	-	46,46,46,46	0
57	MG	BA	3651	1/1	0.92	0.19	-	45,45,45,45	0
57	MG	BA	3514	1/1	0.88	0.23	-	48,48,48,48	0
57	MG	BA	3164	1/1	0.91	0.21	-	48,48,48,48	0
57	MG	BA	3556	1/1	0.98	0.21	-	36,36,36,36	0
57	MG	DA	3202	1/1	0.94	0.11	-	57,57,57,57	0
57	MG	CA	3140	1/1	0.84	0.15	-	67,67,67,67	0
57	MG	DA	3311	1/1	0.89	0.17	-	54,54,54,54	0
57	MG	DA	3602	1/1	0.95	0.10	-	65,65,65,65	0
57	MG	DA	3134	1/1	0.91	0.21	-	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
57	MG	BA	3554	1/1	0.92	0.13	-	51,51,51,51	0
57	MG	DA	3397	1/1	0.93	0.09	-	57,57,57,57	0
57	MG	BA	3136	1/1	0.92	0.14	-	30,30,30,30	0
57	MG	BA	3761	1/1	0.82	0.16	-	59,59,59,59	0
57	MG	BA	3323	1/1	0.94	0.20	-	30,30,30,30	0
57	MG	BA	3601	1/1	0.86	0.12	-	55,55,55,55	0
57	MG	BA	3312	1/1	0.90	0.18	-	32,32,32,32	0
57	MG	BA	3180	1/1	0.86	0.17	-	47,47,47,47	0
57	MG	BA	3681	1/1	0.85	0.08	-	66,66,66,66	0
57	MG	BY	502	1/1	0.92	0.25	-	40,40,40,40	0
57	MG	BA	3645	1/1	0.96	0.20	-	33,33,33,33	0
57	MG	DA	3123	1/1	0.96	0.20	-	56,56,56,56	0
57	MG	DA	3418	1/1	0.95	0.11	-	52,52,52,52	0
57	MG	DA	3249	1/1	0.94	0.14	-	45,45,45,45	0
57	MG	DA	3393	1/1	0.98	0.10	-	50,50,50,50	0
57	MG	BP	203	1/1	0.98	0.15	-	33,33,33,33	0
57	MG	AA	3029	1/1	0.93	0.23	-	53,53,53,53	0
57	MG	BA	3767	1/1	0.92	0.12	-	73,73,73,73	0
57	MG	BA	3084	1/1	0.94	0.22	-	38,38,38,38	0
57	MG	DA	3617	1/1	0.93	0.07	-	56,56,56,56	0
57	MG	BA	3622	1/1	0.89	0.19	-	48,48,48,48	0
57	MG	BA	3233	1/1	0.99	0.31	-	56,56,56,56	0
57	MG	DA	3421	1/1	0.84	0.13	-	50,50,50,50	0
57	MG	DA	3065	1/1	0.93	0.18	-	43,43,43,43	0
57	MG	DA	3572	1/1	0.88	0.06	-	62,62,62,62	0
57	MG	BA	3799	1/1	0.92	0.06	-	49,49,49,49	0
57	MG	BA	3593	1/1	0.95	0.22	-	38,38,38,38	0
57	MG	DA	3300	1/1	0.94	0.20	-	45,45,45,45	0
57	MG	DA	3108	1/1	0.93	0.07	-	52,52,52,52	0
57	MG	DA	3647	1/1	0.97	0.11	-	54,54,54,54	0
57	MG	BA	3221	1/1	0.97	0.17	-	37,37,37,37	0
57	MG	BA	3616	1/1	0.62	0.20	-	65,65,65,65	0
57	MG	DA	3058	1/1	0.97	0.14	-	29,29,29,29	0
57	MG	CA	3100	1/1	0.91	0.09	-	52,52,52,52	0
57	MG	BA	3200	1/1	0.93	0.15	-	67,67,67,67	0
57	MG	DA	3590	1/1	0.88	0.10	-	51,51,51,51	0
57	MG	BA	3422	1/1	0.99	0.24	-	33,33,33,33	0
57	MG	BA	3355	1/1	0.93	0.17	-	61,61,61,61	0
57	MG	BA	3432	1/1	0.85	0.14	-	58,58,58,58	0
57	MG	DA	3244	1/1	0.69	0.11	-	71,71,71,71	0
57	MG	BA	3359	1/1	0.95	0.30	-	62,62,62,62	0
57	MG	BA	3424	1/1	0.92	0.25	-	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
57	MG	DA	3438	1/1	0.93	0.20	-	47,47,47,47	0
57	MG	DA	3166	1/1	0.97	0.11	-	55,55,55,55	0
57	MG	BA	3637	1/1	0.87	0.11	-	39,39,39,39	0
57	MG	BA	3360	1/1	0.96	0.16	-	41,41,41,41	0
57	MG	DB	3002	1/1	0.88	0.17	-	65,65,65,65	0
57	MG	AA	3174	1/1	0.94	0.10	-	50,50,50,50	0
57	MG	DA	3224	1/1	0.95	0.17	-	49,49,49,49	0
57	MG	DA	3250	1/1	0.92	0.18	-	69,69,69,69	0
57	MG	DA	3625	1/1	0.93	0.07	-	69,69,69,69	0
57	MG	AA	3087	1/1	0.96	0.11	-	41,41,41,41	0
57	MG	DA	3626	1/1	0.89	0.07	-	67,67,67,67	0
57	MG	BA	3719	1/1	0.98	0.18	-	53,53,53,53	0
57	MG	AA	3062	1/1	0.98	0.28	-	51,51,51,51	0
57	MG	BA	3125	1/1	0.89	0.17	-	47,47,47,47	0
57	MG	DA	3644	1/1	0.97	0.08	-	55,55,55,55	0
57	MG	DA	3047	1/1	0.92	0.15	-	49,49,49,49	0
57	MG	BO	201	1/1	0.91	0.19	-	50,50,50,50	0
57	MG	CA	3063	1/1	0.95	0.23	-	58,58,58,58	0
57	MG	DA	3187	1/1	0.97	0.11	-	42,42,42,42	0
57	MG	BA	3017	1/1	0.92	0.25	-	48,48,48,48	0
57	MG	DA	3488	1/1	0.95	0.07	-	41,41,41,41	0
57	MG	DA	3079	1/1	0.92	0.17	-	55,55,55,55	0
57	MG	DA	3454	1/1	0.96	0.16	-	56,56,56,56	0
57	MG	DA	3144	1/1	0.98	0.11	-	38,38,38,38	0
57	MG	BA	3191	1/1	0.96	0.18	-	43,43,43,43	0
57	MG	DA	3164	1/1	0.92	0.12	-	51,51,51,51	0
57	MG	BA	3690	1/1	0.93	0.18	-	58,58,58,58	0
57	MG	BA	3186	1/1	0.93	0.45	-	45,45,45,45	0
57	MG	BA	3066	1/1	0.81	0.19	-	49,49,49,49	0
57	MG	DA	3392	1/1	0.92	0.19	-	70,70,70,70	0
57	MG	DA	3269	1/1	0.96	0.06	-	49,49,49,49	0
57	MG	DA	3297	1/1	0.99	0.11	-	39,39,39,39	0
57	MG	DA	3654	1/1	0.86	0.12	-	56,56,56,56	0
57	MG	DA	3107	1/1	0.93	0.14	-	51,51,51,51	0
57	MG	BG	203	1/1	0.96	0.16	-	42,42,42,42	0
57	MG	BA	3780	1/1	0.87	0.11	-	62,62,62,62	0
57	MG	DA	3126	1/1	0.90	0.08	-	55,55,55,55	0
57	MG	DA	3552	1/1	0.97	0.11	-	54,54,54,54	0
57	MG	BA	3403	1/1	0.93	0.08	-	54,54,54,54	0
57	MG	DA	3564	1/1	0.89	0.16	-	61,61,61,61	0
57	MG	DA	3527	1/1	0.88	0.12	-	60,60,60,60	0
57	MG	DA	3070	1/1	0.90	0.13	-	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
57	MG	DA	3262	1/1	0.77	0.10	-	65,65,65,65	0
57	MG	AW	3001	1/1	0.81	0.11	-	60,60,60,60	0
57	MG	DA	3593	1/1	0.89	0.11	-	40,40,40,40	0
57	MG	DA	3162	1/1	0.92	0.35	-	50,50,50,50	0
57	MG	DA	3360	1/1	0.86	0.16	-	46,46,46,46	0
57	MG	BA	3154	1/1	0.83	0.23	-	47,47,47,47	0
57	MG	BA	3103	1/1	0.97	0.17	-	38,38,38,38	0
57	MG	BA	3735	1/1	0.98	0.43	-	57,57,57,57	0
57	MG	BA	3229	1/1	0.91	0.22	-	54,54,54,54	0
57	MG	BA	3696	1/1	0.96	0.14	-	33,33,33,33	0
57	MG	CA	3025	1/1	0.94	0.14	-	51,51,51,51	0
57	MG	DA	3228	1/1	0.97	0.30	-	38,38,38,38	0
57	MG	DA	3546	1/1	0.73	0.11	-	71,71,71,71	0
57	MG	BZ	3001	1/1	0.89	0.29	-	55,55,55,55	0
57	MG	BA	3557	1/1	0.95	0.16	-	33,33,33,33	0
57	MG	BA	3658	1/1	0.87	0.26	-	61,61,61,61	0
57	MG	AA	3083	1/1	0.94	0.31	-	57,57,57,57	0
57	MG	DA	3536	1/1	0.93	0.10	-	48,48,48,48	0
57	MG	AX	3014	1/1	0.67	0.19	-	72,72,72,72	0
57	MG	DA	3646	1/1	0.85	0.14	-	59,59,59,59	0
57	MG	BA	3537	1/1	0.93	0.16	-	45,45,45,45	0
57	MG	BA	3627	1/1	0.96	0.17	-	56,56,56,56	0
57	MG	BA	3122	1/1	0.88	0.15	-	41,41,41,41	0
57	MG	DA	3407	1/1	0.91	0.04	-	66,66,66,66	0
57	MG	DA	3573	1/1	0.94	0.11	-	43,43,43,43	0
57	MG	BA	3624	1/1	0.88	0.10	-	68,68,68,68	0
57	MG	AA	3181	1/1	0.93	0.16	-	51,51,51,51	0
57	MG	BA	3024	1/1	0.91	0.19	-	49,49,49,49	0
57	MG	CA	3129	1/1	0.91	0.09	-	43,43,43,43	0
57	MG	BA	3039	1/1	0.98	0.20	-	32,32,32,32	0
57	MG	BA	3123	1/1	0.95	0.22	-	32,32,32,32	0
57	MG	BA	3720	1/1	0.96	0.14	-	65,65,65,65	0
57	MG	BA	3729	1/1	0.96	0.19	-	47,47,47,47	0
57	MG	BA	3090	1/1	0.95	0.31	-	53,53,53,53	0
57	MG	DA	3571	1/1	0.85	0.12	-	56,56,56,56	0
57	MG	DA	3483	1/1	0.95	0.32	-	55,55,55,55	0
57	MG	BA	3114	1/1	0.79	0.18	-	53,53,53,53	0
57	MG	AA	3082	1/1	0.98	0.13	-	46,46,46,46	0
57	MG	DA	3551	1/1	0.93	0.08	-	55,55,55,55	0
57	MG	DA	3277	1/1	0.95	0.12	-	55,55,55,55	0
57	MG	BA	3474	1/1	0.97	0.18	-	55,55,55,55	0
57	MG	CA	3019	1/1	0.95	0.10	-	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
57	MG	BA	3578	1/1	0.88	0.10	-	46,46,46,46	0
57	MG	DA	3323	1/1	0.88	0.11	-	50,50,50,50	0
57	MG	DA	3410	1/1	0.85	0.13	-	53,53,53,53	0
57	MG	DA	3252	1/1	0.76	0.08	-	37,37,37,37	0
57	MG	AA	3196	1/1	0.85	0.21	-	74,74,74,74	0
57	MG	BA	3120	1/1	0.91	0.21	-	55,55,55,55	0
57	MG	DA	3233	1/1	0.96	0.19	-	53,53,53,53	0
57	MG	CA	3108	1/1	0.94	0.31	-	68,68,68,68	0
57	MG	AA	3092	1/1	0.97	0.14	-	63,63,63,63	0
57	MG	BA	3108	1/1	0.96	0.32	-	44,44,44,44	0
57	MG	BA	3683	1/1	0.91	0.15	-	73,73,73,73	0
57	MG	BA	3018	1/1	0.84	0.20	-	56,56,56,56	0
57	MG	CA	3111	1/1	0.91	0.16	-	64,64,64,64	0
57	MG	BW	204	1/1	0.96	0.22	-	42,42,42,42	0
57	MG	BA	3088	1/1	0.96	0.35	-	48,48,48,48	0
57	MG	DA	3128	1/1	0.92	0.15	-	58,58,58,58	0
57	MG	DA	3372	1/1	0.95	0.08	-	56,56,56,56	0
57	MG	DA	3485	1/1	0.95	0.12	-	52,52,52,52	0
57	MG	DA	3222	1/1	0.80	0.15	-	57,57,57,57	0
57	MG	BA	3288	1/1	0.95	0.20	-	56,56,56,56	0
57	MG	BA	3774	1/1	0.97	0.07	-	46,46,46,46	0
57	MG	BA	3297	1/1	0.88	0.14	-	43,43,43,43	0
57	MG	BA	3447	1/1	0.86	0.10	-	72,72,72,72	0
57	MG	AA	3051	1/1	0.87	0.23	-	73,73,73,73	0
57	MG	DA	3185	1/1	0.86	0.11	-	68,68,68,68	0
57	MG	BA	3304	1/1	0.91	0.15	-	67,67,67,67	0
57	MG	DA	3674	1/1	0.95	0.16	-	37,37,37,37	0
57	MG	CD	301	1/1	0.95	0.19	-	56,56,56,56	0
57	MG	BA	3300	1/1	0.74	0.25	-	57,57,57,57	0
57	MG	DA	3151	1/1	0.89	0.09	-	55,55,55,55	0
57	MG	CA	3084	1/1	0.97	0.13	-	60,60,60,60	0
57	MG	CA	3156	1/1	0.89	0.10	-	73,73,73,73	0
57	MG	DA	3197	1/1	0.98	0.14	-	55,55,55,55	0
57	MG	BA	3672	1/1	0.94	0.20	-	43,43,43,43	0
57	MG	DA	3041	1/1	0.93	0.09	-	38,38,38,38	0
57	MG	BB	213	1/1	0.96	0.19	-	60,60,60,60	0
57	MG	BA	3746	1/1	0.91	0.11	-	51,51,51,51	0
57	MG	DA	3060	1/1	0.74	0.15	-	64,64,64,64	0
57	MG	BA	3686	1/1	0.90	0.25	-	60,60,60,60	0
57	MG	DA	3432	1/1	0.93	0.12	-	37,37,37,37	0
57	MG	DA	3452	1/1	0.90	0.16	-	51,51,51,51	0
57	MG	BA	3470	1/1	0.65	0.13	-	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
57	MG	DA	3035	1/1	0.86	0.20	-	52,52,52,52	0
57	MG	AA	3194	1/1	0.90	0.11	-	56,56,56,56	0
57	MG	DA	3082	1/1	0.81	0.14	-	47,47,47,47	0
57	MG	BA	3500	1/1	0.95	0.15	-	56,56,56,56	0
57	MG	BA	3569	1/1	0.99	0.19	-	49,49,49,49	0
57	MG	DA	3348	1/1	0.95	0.10	-	34,34,34,34	0
57	MG	AA	3118	1/1	0.95	0.17	-	47,47,47,47	0
57	MG	AX	3008	1/1	0.92	0.19	-	70,70,70,70	0
57	MG	BA	3691	1/1	0.96	0.16	-	55,55,55,55	0
57	MG	CA	3024	1/1	0.79	0.10	-	74,74,74,74	0
57	MG	DA	3466	1/1	0.97	0.11	-	41,41,41,41	0
57	MG	BA	3527	1/1	0.95	0.16	-	54,54,54,54	0
57	MG	BA	3074	1/1	0.87	0.21	-	46,46,46,46	0
57	MG	BA	3336	1/1	0.95	0.15	-	64,64,64,64	0
57	MG	DB	3007	1/1	0.96	0.20	-	58,58,58,58	0
57	MG	BA	3490	1/1	0.97	0.10	-	54,54,54,54	0
57	MG	DA	3450	1/1	0.84	0.10	-	40,40,40,40	0
57	MG	DA	3001	1/1	0.92	0.17	-	60,60,60,60	0
57	MG	CA	3008	1/1	0.92	0.27	-	51,51,51,51	0
57	MG	DA	3212	1/1	0.80	0.15	-	45,45,45,45	0
57	MG	DA	3034	1/1	0.98	0.17	-	38,38,38,38	0
57	MG	BA	3003	1/1	0.72	0.19	-	60,60,60,60	0
57	MG	BA	3282	1/1	0.93	0.16	-	39,39,39,39	0
57	MG	DA	3584	1/1	0.94	0.18	-	53,53,53,53	0
57	MG	BA	3784	1/1	0.97	0.21	-	33,33,33,33	0
57	MG	BA	3179	1/1	0.84	0.18	-	50,50,50,50	0
57	MG	DA	3526	1/1	0.88	0.11	-	48,48,48,48	0
57	MG	AA	3031	1/1	0.87	0.23	-	70,70,70,70	0
57	MG	BA	3340	1/1	0.94	0.14	-	39,39,39,39	0
57	MG	BA	3745	1/1	0.89	0.08	-	75,75,75,75	0
57	MG	DA	3655	1/1	0.94	0.11	-	64,64,64,64	0
57	MG	BA	3287	1/1	0.98	0.14	-	42,42,42,42	0
57	MG	DA	3036	1/1	0.93	0.14	-	48,48,48,48	0
57	MG	BA	3731	1/1	0.97	0.30	-	37,37,37,37	0
57	MG	AA	3157	1/1	0.95	0.17	-	45,45,45,45	0
57	MG	B4	502	1/1	0.75	0.14	-	71,71,71,71	0
57	MG	BA	3394	1/1	0.90	0.18	-	40,40,40,40	0
57	MG	DA	3146	1/1	0.90	0.10	-	55,55,55,55	0
57	MG	AA	3163	1/1	0.92	0.18	-	56,56,56,56	0
57	MG	BA	3101	1/1	0.92	0.19	-	53,53,53,53	0
57	MG	BA	3140	1/1	0.96	0.14	-	47,47,47,47	0
57	MG	CA	3148	1/1	0.98	0.11	-	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
57	MG	BA	3036	1/1	0.97	0.17	-	40,40,40,40	0
57	MG	BA	3189	1/1	0.94	0.19	-	39,39,39,39	0
57	MG	AA	3147	1/1	0.97	0.10	-	70,70,70,70	0
57	MG	BA	3749	1/1	0.89	0.12	-	56,56,56,56	0
57	MG	BA	3275	1/1	0.88	0.18	-	58,58,58,58	0
57	MG	BA	3501	1/1	0.90	0.22	-	71,71,71,71	0
57	MG	AX	3011	1/1	0.80	0.20	-	78,78,78,78	0
57	MG	BA	3016	1/1	0.92	0.13	-	38,38,38,38	0
57	MG	DA	3114	1/1	0.94	0.15	-	55,55,55,55	0
57	MG	BA	3528	1/1	0.96	0.18	-	56,56,56,56	0
57	MG	BA	3007	1/1	0.91	0.19	-	55,55,55,55	0
57	MG	AA	3180	1/1	0.96	0.10	-	73,73,73,73	0
57	MG	BA	3064	1/1	0.94	0.13	-	43,43,43,43	0
57	MG	DA	3007	1/1	0.87	0.14	-	50,50,50,50	0
57	MG	BA	3172	1/1	0.81	0.19	-	46,46,46,46	0
57	MG	DA	3087	1/1	0.95	0.18	-	58,58,58,58	0
57	MG	BA	3223	1/1	0.93	0.13	-	41,41,41,41	0
57	MG	AA	3161	1/1	0.92	0.23	-	65,65,65,65	0
57	MG	BA	3015	1/1	0.95	0.16	-	32,32,32,32	0
57	MG	BA	3225	1/1	0.76	0.16	-	61,61,61,61	0
57	MG	BA	3466	1/1	0.91	0.17	-	49,49,49,49	0
57	MG	CA	3036	1/1	0.89	0.14	-	66,66,66,66	0
57	MG	AX	3016	1/1	0.90	0.10	-	56,56,56,56	0
57	MG	B2	3001	1/1	0.85	0.21	-	56,56,56,56	0
57	MG	CA	3127	1/1	0.95	0.18	-	62,62,62,62	0
57	MG	CA	3161	1/1	0.94	0.09	-	56,56,56,56	0
57	MG	BA	3265	1/1	0.93	0.21	-	54,54,54,54	0
57	MG	BB	211	1/1	0.87	0.10	-	51,51,51,51	0
57	MG	DA	3152	1/1	0.93	0.20	-	51,51,51,51	0
57	MG	BA	3611	1/1	0.97	0.17	-	46,46,46,46	0
57	MG	BA	3618	1/1	0.89	0.14	-	65,65,65,65	0
57	MG	BA	3612	1/1	0.90	0.14	-	21,21,21,21	0
57	MG	CA	3137	1/1	0.97	0.16	-	56,56,56,56	0
57	MG	BA	3695	1/1	0.82	0.18	-	67,67,67,67	0
57	MG	DA	3327	1/1	0.92	0.12	-	57,57,57,57	0
57	MG	AA	3175	1/1	0.94	0.18	-	63,63,63,63	0
57	MG	DA	3511	1/1	0.94	0.16	-	49,49,49,49	0
57	MG	BA	3523	1/1	0.94	0.11	-	48,48,48,48	0
57	MG	DB	3012	1/1	0.86	0.33	-	61,61,61,61	0
57	MG	DA	3338	1/1	0.97	0.15	-	61,61,61,61	0
57	MG	AA	3027	1/1	0.93	0.15	-	50,50,50,50	0
57	MG	BA	3176	1/1	0.94	0.17	-	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3476	1/1	0.97	0.15	-	55,55,55,55	0
57	MG	BB	216	1/1	0.96	0.23	-	51,51,51,51	0
57	MG	DP	202	1/1	0.89	0.11	-	53,53,53,53	0
57	MG	DA	3639	1/1	0.96	0.48	-	59,59,59,59	0
57	MG	DA	3332	1/1	0.89	0.11	-	53,53,53,53	0
57	MG	BA	3118	1/1	0.93	0.17	-	48,48,48,48	0
57	MG	BA	3503	1/1	0.75	0.12	-	49,49,49,49	0
57	MG	CA	3130	1/1	0.90	0.09	-	57,57,57,57	0
57	MG	CA	3155	1/1	0.97	0.12	-	53,53,53,53	0
57	MG	AA	3040	1/1	0.98	0.11	-	60,60,60,60	0
57	MG	AA	3150	1/1	0.95	0.19	-	57,57,57,57	0
57	MG	DA	3582	1/1	0.82	0.07	-	56,56,56,56	0
57	MG	CA	3093	1/1	0.96	0.10	-	55,55,55,55	0
57	MG	DA	3555	1/1	0.98	0.29	-	53,53,53,53	0
57	MG	CA	3107	1/1	0.82	0.20	-	80,80,80,80	0
57	MG	BA	3734	1/1	0.92	0.16	-	52,52,52,52	0
57	MG	BA	3754	1/1	0.85	0.18	-	48,48,48,48	0
57	MG	DA	3207	1/1	0.95	0.30	-	63,63,63,63	0
57	MG	BA	3400	1/1	0.91	0.21	-	33,33,33,33	0
57	MG	DA	3531	1/1	0.76	0.18	-	61,61,61,61	0
57	MG	DA	3282	1/1	0.96	0.06	-	52,52,52,52	0
57	MG	BB	214	1/1	0.77	0.17	-	49,49,49,49	0
57	MG	BA	3302	1/1	0.93	0.12	-	69,69,69,69	0
60	K	AX	3001	1/1	0.94	0.12	-	65,65,65,65	0
57	MG	DA	3097	1/1	0.91	0.21	-	33,33,33,33	0
57	MG	DA	3083	1/1	0.92	0.19	-	40,40,40,40	0
57	MG	CW	3001	1/1	0.91	0.22	-	67,67,67,67	0
57	MG	AA	3068	1/1	0.94	0.14	-	69,69,69,69	0
57	MG	AA	3176	1/1	0.89	0.10	-	67,67,67,67	0
57	MG	CA	3158	1/1	0.85	0.13	-	67,67,67,67	0
57	MG	BA	3808	1/1	0.95	0.17	-	42,42,42,42	0
57	MG	BA	3769	1/1	0.83	0.18	-	52,52,52,52	0
57	MG	BA	3113	1/1	0.97	0.25	-	53,53,53,53	0
57	MG	DA	3581	1/1	0.95	0.23	-	57,57,57,57	0
57	MG	AA	3159	1/1	0.94	0.12	-	66,66,66,66	0
57	MG	CA	3031	1/1	0.95	0.10	-	68,68,68,68	0
57	MG	BA	3668	1/1	0.91	0.17	-	53,53,53,53	0
57	MG	BA	3231	1/1	0.85	0.32	-	63,63,63,63	0
57	MG	CA	3026	1/1	0.90	0.20	-	63,63,63,63	0
57	MG	DA	3018	1/1	0.90	0.20	-	62,62,62,62	0
57	MG	DA	3448	1/1	0.43	0.21	-	70,70,70,70	0
57	MG	BA	3452	1/1	0.94	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
57	MG	AE	202	1/1	0.79	0.12	-	80,80,80,80	0
57	MG	BA	3777	1/1	0.94	0.17	-	40,40,40,40	0
57	MG	BU	202	1/1	0.93	0.28	-	40,40,40,40	0
57	MG	BA	3147	1/1	0.88	0.16	-	45,45,45,45	0
57	MG	BA	3551	1/1	0.95	0.19	-	36,36,36,36	0
57	MG	BA	3505	1/1	0.93	0.12	-	55,55,55,55	0
57	MG	DA	3238	1/1	0.94	0.26	-	44,44,44,44	0
57	MG	AA	3149	1/1	0.93	0.10	-	46,46,46,46	0
57	MG	DA	3444	1/1	0.89	0.06	-	44,44,44,44	0
57	MG	AA	3034	1/1	0.85	0.11	-	47,47,47,47	0
57	MG	DA	3051	1/1	0.90	0.11	-	48,48,48,48	0
57	MG	AA	3166	1/1	0.85	0.14	-	69,69,69,69	0
57	MG	BA	3080	1/1	0.98	0.17	-	60,60,60,60	0
57	MG	BB	207	1/1	0.96	0.22	-	54,54,54,54	0
57	MG	BA	3266	1/1	0.88	0.19	-	39,39,39,39	0
57	MG	DA	3650	1/1	0.93	0.12	-	67,67,67,67	0
57	MG	CA	3092	1/1	0.95	0.10	-	50,50,50,50	0
57	MG	DA	3595	1/1	0.92	0.17	-	59,59,59,59	0
57	MG	DA	3080	1/1	0.95	0.10	-	55,55,55,55	0
57	MG	DA	3404	1/1	0.98	0.12	-	48,48,48,48	0
57	MG	CA	3017	1/1	0.78	0.19	-	53,53,53,53	0
57	MG	BA	3625	1/1	0.98	0.18	-	39,39,39,39	0
57	MG	BA	3401	1/1	0.75	0.16	-	35,35,35,35	0
57	MG	BA	3061	1/1	0.91	0.23	-	29,29,29,29	0
57	MG	BA	3226	1/1	0.91	0.27	-	47,47,47,47	0
57	MG	CA	3054	1/1	0.90	0.30	-	69,69,69,69	0
57	MG	BA	3376	1/1	0.94	0.16	-	48,48,48,48	0
57	MG	BA	3055	1/1	0.93	0.21	-	45,45,45,45	0
57	MG	BQ	3003	1/1	0.94	0.27	-	49,49,49,49	0
57	MG	BA	3375	1/1	0.96	0.13	-	68,68,68,68	0
57	MG	DA	3458	1/1	0.94	0.05	-	52,52,52,52	0
57	MG	CA	3056	1/1	0.96	0.10	-	64,64,64,64	0
57	MG	DA	3110	1/1	0.87	0.32	-	58,58,58,58	0
57	MG	DB	3013	1/1	0.94	0.17	-	64,64,64,64	0
57	MG	AX	3012	1/1	0.96	0.17	-	59,59,59,59	0
57	MG	DA	3258	1/1	0.98	0.14	-	48,48,48,48	0
57	MG	BA	3442	1/1	0.88	0.17	-	44,44,44,44	0
57	MG	DA	3620	1/1	0.76	0.11	-	68,68,68,68	0
57	MG	DA	3553	1/1	0.82	0.10	-	49,49,49,49	0
57	MG	BA	3177	1/1	0.90	0.19	-	46,46,46,46	0
57	MG	AA	3116	1/1	0.95	0.11	-	55,55,55,55	0
57	MG	BA	3765	1/1	0.93	0.22	-	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
57	MG	BA	3434	1/1	0.83	0.13	-	55,55,55,55	0
57	MG	BA	3134	1/1	0.92	0.17	-	48,48,48,48	0
57	MG	AA	3151	1/1	0.96	0.14	-	45,45,45,45	0
57	MG	BA	3131	1/1	0.89	0.11	-	58,58,58,58	0
57	MG	BA	3688	1/1	0.93	0.16	-	46,46,46,46	0
57	MG	CA	3030	1/1	0.94	0.22	-	57,57,57,57	0
57	MG	AX	3009	1/1	0.92	0.18	-	64,64,64,64	0
57	MG	DA	3357	1/1	0.98	0.07	-	50,50,50,50	0
57	MG	BA	3519	1/1	0.93	0.08	-	55,55,55,55	0
57	MG	DA	3469	1/1	0.88	0.28	-	44,44,44,44	0
57	MG	DA	3349	1/1	0.97	0.07	-	52,52,52,52	0
57	MG	BA	3489	1/1	0.97	0.07	-	59,59,59,59	0
57	MG	DA	3247	1/1	0.84	0.09	-	45,45,45,45	0
57	MG	DA	3199	1/1	0.96	0.10	-	47,47,47,47	0
57	MG	BA	3679	1/1	0.88	0.12	-	62,62,62,62	0
57	MG	DA	3090	1/1	0.89	0.10	-	52,52,52,52	0
57	MG	BA	3621	1/1	0.91	0.17	-	53,53,53,53	0
57	MG	DA	3453	1/1	0.98	0.22	-	60,60,60,60	0
57	MG	DA	3175	1/1	0.97	0.12	-	41,41,41,41	0
57	MG	BA	3220	1/1	0.94	0.22	-	29,29,29,29	0
57	MG	BA	3811	1/1	0.90	0.14	-	65,65,65,65	0
57	MG	BA	3461	1/1	0.90	0.10	-	62,62,62,62	0
57	MG	BA	3329	1/1	0.94	0.19	-	60,60,60,60	0
57	MG	CA	3165	1/1	0.93	0.11	-	45,45,45,45	0
57	MG	BA	3065	1/1	0.94	0.19	-	60,60,60,60	0
57	MG	BA	3053	1/1	0.72	0.21	-	54,54,54,54	0
57	MG	BA	3507	1/1	0.91	0.20	-	49,49,49,49	0
57	MG	CA	3080	1/1	0.95	0.09	-	49,49,49,49	0
57	MG	BA	3553	1/1	0.97	0.10	-	59,59,59,59	0
57	MG	BA	3704	1/1	0.76	0.13	-	77,77,77,77	0
57	MG	BA	3479	1/1	0.97	0.07	-	50,50,50,50	0
57	MG	CA	3153	1/1	0.91	0.16	-	70,70,70,70	0
57	MG	BA	3152	1/1	0.97	0.30	-	43,43,43,43	0
57	MG	DA	3550	1/1	0.91	0.13	-	57,57,57,57	0
57	MG	BA	3235	1/1	0.98	0.16	-	42,42,42,42	0
57	MG	BA	3703	1/1	0.89	0.10	-	64,64,64,64	0
57	MG	AA	3135	1/1	0.90	0.24	-	65,65,65,65	0
57	MG	DA	3026	1/1	0.99	0.55	-	59,59,59,59	0
57	MG	DA	3614	1/1	0.88	0.07	-	65,65,65,65	0
57	MG	DA	3317	1/1	0.91	0.12	-	44,44,44,44	0
57	MG	BA	3591	1/1	0.96	0.17	-	35,35,35,35	0
57	MG	DA	3402	1/1	0.81	0.10	-	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BB	205	1/1	0.96	0.20	-	60,60,60,60	0
57	MG	DA	3063	1/1	0.92	0.23	-	54,54,54,54	0
57	MG	DA	3320	1/1	0.61	0.15	-	55,55,55,55	0
57	MG	DA	3264	1/1	0.94	0.13	-	40,40,40,40	0
57	MG	DA	3160	1/1	0.96	0.10	-	56,56,56,56	0
57	MG	DA	3467	1/1	0.95	0.25	-	40,40,40,40	0
57	MG	DA	3292	1/1	0.98	0.17	-	30,30,30,30	0
57	MG	BA	3759	1/1	0.83	0.18	-	33,33,33,33	0
57	MG	CA	3018	1/1	0.72	0.16	-	69,69,69,69	0
57	MG	DA	3463	1/1	0.90	0.14	-	55,55,55,55	0
57	MG	BA	3589	1/1	0.96	0.21	-	27,27,27,27	0
57	MG	AN	502	1/1	0.91	0.29	-	63,63,63,63	0
57	MG	CA	3094	1/1	0.94	0.11	-	70,70,70,70	0
57	MG	BA	3097	1/1	0.97	0.14	-	44,44,44,44	0
57	MG	BA	3678	1/1	0.70	0.08	-	65,65,65,65	0
57	MG	DA	3054	1/1	0.94	0.23	-	48,48,48,48	0
57	MG	BA	3809	1/1	0.94	0.14	-	63,63,63,63	0
57	MG	BA	3383	1/1	0.95	0.12	-	53,53,53,53	0
57	MG	BA	3035	1/1	0.93	0.25	-	39,39,39,39	0
57	MG	DA	3094	1/1	0.98	0.22	-	50,50,50,50	0
57	MG	DA	3156	1/1	0.96	0.09	-	51,51,51,51	0
57	MG	DA	3033	1/1	0.90	0.10	-	42,42,42,42	0
57	MG	DA	3608	1/1	0.75	0.13	-	68,68,68,68	0
57	MG	DA	3395	1/1	0.96	0.12	-	47,47,47,47	0
57	MG	BA	3595	1/1	0.93	0.09	-	51,51,51,51	0
57	MG	BA	3168	1/1	0.97	0.17	-	47,47,47,47	0
57	MG	AA	3044	1/1	0.96	0.25	-	60,60,60,60	0
57	MG	BA	3244	1/1	0.96	0.22	-	53,53,53,53	0
57	MG	BA	3339	1/1	0.98	0.21	-	23,23,23,23	0
57	MG	DA	3657	1/1	0.85	0.10	-	63,63,63,63	0
57	MG	BA	3281	1/1	0.98	0.28	-	60,60,60,60	0
57	MG	DA	3263	1/1	0.92	0.13	-	41,41,41,41	0
57	MG	BA	3148	1/1	0.98	0.33	-	44,44,44,44	0
57	MG	DA	3243	1/1	0.91	0.12	-	55,55,55,55	0
57	MG	DA	3304	1/1	0.95	0.06	-	48,48,48,48	0
57	MG	CA	3044	1/1	0.89	0.23	-	62,62,62,62	0
57	MG	AA	3013	1/1	0.76	0.18	-	69,69,69,69	0
57	MG	BA	3706	1/1	0.93	0.12	-	53,53,53,53	0
57	MG	BA	3077	1/1	0.93	0.17	-	49,49,49,49	0
57	MG	BA	3165	1/1	0.86	0.17	-	45,45,45,45	0
57	MG	DA	3489	1/1	0.96	0.13	-	51,51,51,51	0
57	MG	AA	3043	1/1	0.96	0.23	-	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
57	MG	AA	3191	1/1	0.92	0.21	-	47,47,47,47	0
57	MG	BA	3610	1/1	0.94	0.09	-	61,61,61,61	0
57	MG	DA	3391	1/1	0.92	0.09	-	45,45,45,45	0
57	MG	BQ	3004	1/1	0.95	0.27	-	42,42,42,42	0
57	MG	DA	3643	1/1	0.91	0.13	-	61,61,61,61	0
57	MG	DA	3503	1/1	0.92	0.14	-	52,52,52,52	0
57	MG	AA	3024	1/1	0.97	0.11	-	54,54,54,54	0
57	MG	AA	3056	1/1	0.93	0.13	-	61,61,61,61	0
57	MG	BA	3414	1/1	0.96	0.19	-	41,41,41,41	0
57	MG	DA	3560	1/1	0.99	0.07	-	40,40,40,40	0
57	MG	BB	219	1/1	0.92	0.11	-	67,67,67,67	0
57	MG	DA	3181	1/1	0.95	0.13	-	50,50,50,50	0
57	MG	BA	3659	1/1	0.90	0.19	-	61,61,61,61	0
57	MG	AA	3202	1/1	0.92	0.14	-	57,57,57,57	0
57	MG	BA	3582	1/1	0.96	0.17	-	74,74,74,74	0
57	MG	DA	3532	1/1	0.66	0.24	-	69,69,69,69	0
57	MG	CA	3114	1/1	0.93	0.04	-	57,57,57,57	0
57	MG	DA	3556	1/1	0.90	0.11	-	67,67,67,67	0
57	MG	DA	3147	1/1	0.84	0.15	-	56,56,56,56	0
57	MG	BA	3089	1/1	0.97	0.17	-	19,19,19,19	0
57	MG	BA	3617	1/1	0.95	0.16	-	51,51,51,51	0
57	MG	BA	3469	1/1	0.96	0.14	-	49,49,49,49	0
57	MG	DA	3621	1/1	0.89	0.08	-	44,44,44,44	0
57	MG	DA	3494	1/1	0.91	0.12	-	47,47,47,47	0
57	MG	BA	3495	1/1	0.91	0.13	-	37,37,37,37	0
57	MG	BA	3110	1/1	0.95	0.17	-	41,41,41,41	0
57	MG	AA	3112	1/1	0.97	0.16	-	63,63,63,63	0
57	MG	DA	3066	1/1	0.89	0.10	-	42,42,42,42	0
57	MG	DA	3232	1/1	0.94	0.13	-	62,62,62,62	0
57	MG	DA	3194	1/1	0.92	0.10	-	56,56,56,56	0
57	MG	BA	3694	1/1	0.96	0.10	-	51,51,51,51	0
57	MG	BA	3702	1/1	0.90	0.27	-	51,51,51,51	0
57	MG	BA	3107	1/1	0.96	0.16	-	53,53,53,53	0
57	MG	DA	3102	1/1	0.94	0.19	-	40,40,40,40	0
57	MG	BA	3019	1/1	0.91	0.15	-	42,42,42,42	0
57	MG	AX	3006	1/1	0.97	0.10	-	65,65,65,65	0
57	MG	B0	102	1/1	0.92	0.22	-	48,48,48,48	0
57	MG	DA	3105	1/1	0.97	0.19	-	48,48,48,48	0
57	MG	DA	3022	1/1	0.96	0.27	-	51,51,51,51	0
57	MG	DA	3525	1/1	0.98	0.13	-	59,59,59,59	0
57	MG	CA	3095	1/1	0.92	0.14	-	64,64,64,64	0
57	MG	BA	3184	1/1	0.96	0.32	-	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3010	1/1	0.95	0.17	-	52,52,52,52	0
57	MG	DA	3451	1/1	0.81	0.16	-	55,55,55,55	0
57	MG	DA	3049	1/1	0.91	0.27	-	52,52,52,52	0
57	MG	DA	3493	1/1	0.96	0.30	-	66,66,66,66	0
57	MG	BA	3348	1/1	0.95	0.18	-	36,36,36,36	0
57	MG	DA	3223	1/1	0.89	0.14	-	50,50,50,50	0
57	MG	DA	3333	1/1	0.82	0.13	-	41,41,41,41	0
57	MG	DA	3371	1/1	0.89	0.13	-	58,58,58,58	0
57	MG	CA	3160	1/1	0.91	0.17	-	62,62,62,62	0
57	MG	BA	3349	1/1	0.96	0.09	-	56,56,56,56	0
57	MG	AA	3195	1/1	0.95	0.12	-	57,57,57,57	0
57	MG	DA	3335	1/1	0.79	0.16	-	47,47,47,47	0
57	MG	CA	3170	1/1	0.93	0.18	-	58,58,58,58	0
57	MG	DB	3006	1/1	0.95	0.14	-	57,57,57,57	0
57	MG	BA	3682	1/1	0.94	0.19	-	53,53,53,53	0
57	MG	AA	3104	1/1	0.94	0.28	-	59,59,59,59	0
57	MG	AA	3167	1/1	0.95	0.09	-	57,57,57,57	0
57	MG	BA	3795	1/1	0.95	0.15	-	35,35,35,35	0
57	MG	CA	3014	1/1	0.92	0.21	-	58,58,58,58	0
57	MG	BA	3571	1/1	0.95	0.18	-	58,58,58,58	0
57	MG	B6	102	1/1	0.92	0.12	-	68,68,68,68	0
57	MG	DA	3543	1/1	0.91	0.08	-	53,53,53,53	0
57	MG	CA	3154	1/1	0.95	0.17	-	56,56,56,56	0
57	MG	BA	3631	1/1	0.91	0.18	-	42,42,42,42	0
57	MG	AA	3126	1/1	0.98	0.09	-	49,49,49,49	0
57	MG	DA	3437	1/1	0.87	0.16	-	52,52,52,52	0
57	MG	DA	3050	1/1	0.92	0.17	-	59,59,59,59	0
57	MG	BD	308	1/1	0.96	0.23	-	46,46,46,46	0
57	MG	DA	3229	1/1	0.94	0.22	-	50,50,50,50	0
57	MG	BA	3419	1/1	0.87	0.23	-	37,37,37,37	0
57	MG	CA	3139	1/1	0.94	0.14	-	62,62,62,62	0
57	MG	DA	3314	1/1	0.90	0.12	-	43,43,43,43	0
57	MG	DA	3380	1/1	0.88	0.07	-	55,55,55,55	0
57	MG	AA	3060	1/1	0.93	0.27	-	46,46,46,46	0
57	MG	DA	3275	1/1	0.89	0.17	-	42,42,42,42	0
57	MG	DA	3259	1/1	0.58	0.21	-	43,43,43,43	0
57	MG	DA	3487	1/1	0.82	0.21	-	62,62,62,62	0
57	MG	BA	3111	1/1	0.97	0.13	-	54,54,54,54	0
57	MG	DA	3423	1/1	0.92	0.12	-	49,49,49,49	0
57	MG	BA	3739	1/1	0.94	0.23	-	40,40,40,40	0
57	MG	CA	3027	1/1	0.87	0.20	-	64,64,64,64	0
57	MG	DA	3563	1/1	0.57	0.15	-	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
57	MG	DA	3211	1/1	0.93	0.14	-	48,48,48,48	0
57	MG	CA	3035	1/1	0.94	0.09	-	59,59,59,59	0
57	MG	DA	3364	1/1	0.95	0.07	-	40,40,40,40	0
57	MG	DA	3379	1/1	0.94	0.14	-	63,63,63,63	0
57	MG	BA	3756	1/1	0.97	0.20	-	48,48,48,48	0
57	MG	BA	3327	1/1	0.98	0.18	-	38,38,38,38	0
57	MG	BA	3506	1/1	0.85	0.10	-	58,58,58,58	0
57	MG	BA	3352	1/1	0.94	0.22	-	53,53,53,53	0
57	MG	BA	3068	1/1	0.95	0.18	-	43,43,43,43	0
57	MG	DA	3288	1/1	0.88	0.14	-	52,52,52,52	0
57	MG	DA	3052	1/1	0.96	0.13	-	61,61,61,61	0
57	MG	BA	3075	1/1	0.93	0.24	-	45,45,45,45	0
57	MG	DA	3591	1/1	0.88	0.16	-	55,55,55,55	0
57	MG	AA	3198	1/1	0.91	0.12	-	61,61,61,61	0
57	MG	AA	3193	1/1	0.93	0.08	-	72,72,72,72	0
57	MG	DA	3179	1/1	0.94	0.12	-	52,52,52,52	0
57	MG	AA	3050	1/1	0.95	0.15	-	33,33,33,33	0
57	MG	BA	3596	1/1	0.89	0.10	-	64,64,64,64	0
57	MG	BA	3513	1/1	0.87	0.15	-	59,59,59,59	0
57	MG	DA	3658	1/1	0.86	0.12	-	62,62,62,62	0
57	MG	BA	3293	1/1	0.85	0.26	-	50,50,50,50	0
57	MG	AX	3003	1/1	0.92	0.13	-	71,71,71,71	0
57	MG	DA	3399	1/1	0.98	0.13	-	59,59,59,59	0
57	MG	AA	3089	1/1	0.87	0.15	-	60,60,60,60	0
57	MG	AW	3002	1/1	0.95	0.22	-	53,53,53,53	0
57	MG	BA	3642	1/1	0.93	0.12	-	48,48,48,48	0
57	MG	BA	3285	1/1	0.91	0.27	-	50,50,50,50	0
57	MG	BA	3440	1/1	0.95	0.12	-	42,42,42,42	0
57	MG	BA	3545	1/1	0.87	0.15	-	65,65,65,65	0
57	MG	AA	3037	1/1	0.92	0.22	-	55,55,55,55	0
57	MG	DA	3161	1/1	0.98	0.19	-	38,38,38,38	0
57	MG	DA	3428	1/1	0.94	0.18	-	37,37,37,37	0
57	MG	BP	204	1/1	0.96	0.06	-	46,46,46,46	0
57	MG	CA	3074	1/1	0.92	0.23	-	64,64,64,64	0
57	MG	DA	3368	1/1	0.94	0.24	-	50,50,50,50	0
57	MG	BA	3317	1/1	0.82	0.18	-	53,53,53,53	0
57	MG	DA	3420	1/1	0.89	0.24	-	60,60,60,60	0
57	MG	AE	201	1/1	0.93	0.15	-	59,59,59,59	0
57	MG	BA	3723	1/1	0.95	0.07	-	47,47,47,47	0
57	MG	BA	3310	1/1	0.92	0.24	-	58,58,58,58	0
57	MG	BA	3757	1/1	0.80	0.20	-	76,76,76,76	0
57	MG	CA	3088	1/1	0.62	0.14	-	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
57	MG	DA	3219	1/1	0.92	0.17	-	53,53,53,53	0
57	MG	BA	3253	1/1	0.84	0.23	-	55,55,55,55	0
57	MG	DA	3670	1/1	0.93	0.42	-	60,60,60,60	0
57	MG	DA	3495	1/1	0.86	0.11	-	47,47,47,47	0
57	MG	BA	3708	1/1	0.92	0.21	-	50,50,50,50	0
57	MG	DA	3189	1/1	0.97	0.20	-	41,41,41,41	0
57	MG	CA	3050	1/1	0.97	0.20	-	61,61,61,61	0
57	MG	BA	3572	1/1	0.96	0.16	-	61,61,61,61	0
57	MG	BA	3012	1/1	0.96	0.20	-	39,39,39,39	0
57	MG	BA	3194	1/1	0.95	0.18	-	47,47,47,47	0
57	MG	BA	3278	1/1	0.98	0.18	-	34,34,34,34	0
57	MG	BA	3776	1/1	0.97	0.20	-	43,43,43,43	0
57	MG	BA	3560	1/1	0.77	0.14	-	56,56,56,56	0
57	MG	BA	3301	1/1	0.85	0.13	-	60,60,60,60	0
57	MG	DA	3057	1/1	0.96	0.20	-	42,42,42,42	0
57	MG	CA	3085	1/1	0.98	0.12	-	54,54,54,54	0
57	MG	CJ	5001	1/1	0.76	0.08	-	73,73,73,73	0
57	MG	BA	3052	1/1	0.80	0.16	-	56,56,56,56	0
57	MG	BA	3037	1/1	1.00	0.24	-	34,34,34,34	0
57	MG	AA	3170	1/1	0.81	0.13	-	75,75,75,75	0
57	MG	AA	3005	1/1	0.84	0.14	-	62,62,62,62	0
57	MG	BA	3573	1/1	0.89	0.16	-	51,51,51,51	0
57	MG	BA	3492	1/1	0.96	0.14	-	46,46,46,46	0
57	MG	CA	3002	1/1	0.90	0.12	-	63,63,63,63	0
57	MG	AA	3007	1/1	0.93	0.13	-	57,57,57,57	0
57	MG	CA	3113	1/1	0.95	0.11	-	67,67,67,67	0
57	MG	BA	3308	1/1	0.86	0.19	-	43,43,43,43	0
57	MG	DA	3381	1/1	0.93	0.16	-	56,56,56,56	0
57	MG	BA	3437	1/1	0.96	0.14	-	36,36,36,36	0
57	MG	CA	3032	1/1	0.95	0.24	-	62,62,62,62	0
57	MG	DA	3095	1/1	0.89	0.15	-	58,58,58,58	0
57	MG	DA	3312	1/1	0.86	0.10	-	54,54,54,54	0
57	MG	DA	3078	1/1	0.80	0.18	-	57,57,57,57	0
57	MG	BA	3464	1/1	0.93	0.14	-	45,45,45,45	0
57	MG	BA	3272	1/1	0.96	0.61	-	48,48,48,48	0
57	MG	BA	3473	1/1	0.82	0.19	-	56,56,56,56	0
57	MG	DA	3583	1/1	0.95	0.15	-	51,51,51,51	0
57	MG	BA	3737	1/1	0.98	0.29	-	43,43,43,43	0
60	K	CX	3001	1/1	0.97	0.19	-	82,82,82,82	0
57	MG	BA	3714	1/1	0.92	0.11	-	57,57,57,57	0
57	MG	BA	3584	1/1	0.87	0.20	-	63,63,63,63	0
57	MG	BA	3448	1/1	0.95	0.24	-	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
57	MG	DA	3044	1/1	0.85	0.10	-	62,62,62,62	0
57	MG	DA	3218	1/1	0.78	0.13	-	59,59,59,59	0
57	MG	DA	3636	1/1	0.88	0.32	-	63,63,63,63	0
57	MG	DA	3217	1/1	0.87	0.14	-	38,38,38,38	0
57	MG	DA	3378	1/1	0.90	0.13	-	57,57,57,57	0
57	MG	DA	3098	1/1	0.89	0.17	-	53,53,53,53	0
57	MG	BA	3652	1/1	0.92	0.14	-	67,67,67,67	0
57	MG	AA	3038	1/1	0.87	0.33	-	68,68,68,68	0
57	MG	BA	3374	1/1	0.99	0.17	-	40,40,40,40	0
57	MG	DA	3220	1/1	0.96	0.15	-	46,46,46,46	0
57	MG	BA	3298	1/1	0.89	0.17	-	51,51,51,51	0
57	MG	BA	3491	1/1	0.96	0.15	-	45,45,45,45	0
57	MG	DA	3354	1/1	0.92	0.19	-	44,44,44,44	0
57	MG	DA	3517	1/1	0.93	0.05	-	51,51,51,51	0
57	MG	DA	3412	1/1	0.98	0.20	-	50,50,50,50	0
57	MG	BA	3031	1/1	0.95	0.19	-	52,52,52,52	0
57	MG	CA	3073	1/1	0.86	0.15	-	57,57,57,57	0
57	MG	BB	209	1/1	0.75	0.32	-	65,65,65,65	0
57	MG	AA	3197	1/1	0.87	0.27	-	70,70,70,70	0
57	MG	BA	3370	1/1	0.96	0.20	-	39,39,39,39	0
57	MG	BA	3579	1/1	0.95	0.17	-	49,49,49,49	0
57	MG	BA	3606	1/1	0.91	0.14	-	61,61,61,61	0
57	MG	BA	3243	1/1	0.94	0.17	-	53,53,53,53	0
57	MG	DA	3597	1/1	0.96	0.06	-	51,51,51,51	0
57	MG	BA	3356	1/1	0.96	0.16	-	37,37,37,37	0
57	MG	AA	3053	1/1	0.98	0.20	-	61,61,61,61	0
57	MG	DA	3406	1/1	0.82	0.11	-	51,51,51,51	0
57	MG	BA	3561	1/1	0.91	0.11	-	45,45,45,45	0
57	MG	DA	3519	1/1	0.95	0.18	-	63,63,63,63	0
57	MG	AA	3067	1/1	0.93	0.26	-	57,57,57,57	0
57	MG	CA	3163	1/1	0.88	0.09	-	63,63,63,63	0
57	MG	DA	3257	1/1	0.97	0.18	-	50,50,50,50	0
57	MG	DA	3370	1/1	0.97	0.14	-	51,51,51,51	0
57	MG	CA	3146	1/1	0.81	0.19	-	66,66,66,66	0
57	MG	CA	3006	1/1	0.90	0.14	-	64,64,64,64	0
57	MG	DA	3165	1/1	0.91	0.23	-	57,57,57,57	0
57	MG	DA	3521	1/1	0.87	0.13	-	58,58,58,58	0
57	MG	B0	103	1/1	0.96	0.08	-	53,53,53,53	0
57	MG	AA	3106	1/1	0.95	0.10	-	57,57,57,57	0
57	MG	DA	3628	1/1	0.82	0.24	-	76,76,76,76	0
57	MG	AA	3008	1/1	0.83	0.27	-	73,73,73,73	0
57	MG	DA	3092	1/1	0.88	0.17	-	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3273	1/1	0.92	0.11	-	47,47,47,47	0
57	MG	CA	3097	1/1	0.86	0.15	-	69,69,69,69	0
57	MG	BA	3664	1/1	0.90	0.16	-	55,55,55,55	0
57	MG	BA	3195	1/1	0.90	0.11	-	46,46,46,46	0
57	MG	BA	3104	1/1	0.90	0.13	-	42,42,42,42	0
57	MG	BA	3689	1/1	0.96	0.17	-	42,42,42,42	0
57	MG	DA	3283	1/1	0.87	0.11	-	51,51,51,51	0
57	MG	BA	3112	1/1	0.96	0.23	-	30,30,30,30	0
57	MG	BA	3261	1/1	0.93	0.11	-	61,61,61,61	0
57	MG	BA	3185	1/1	0.88	0.19	-	57,57,57,57	0
57	MG	BA	3666	1/1	0.91	0.19	-	50,50,50,50	0
57	MG	BB	201	1/1	0.93	0.17	-	55,55,55,55	0
57	MG	DA	3235	1/1	0.94	0.20	-	45,45,45,45	0
57	MG	BA	3603	1/1	0.96	0.13	-	53,53,53,53	0
57	MG	BA	3633	1/1	0.94	0.12	-	49,49,49,49	0
57	MG	AA	3143	1/1	0.90	0.08	-	60,60,60,60	0
57	MG	DA	3190	1/1	0.98	0.20	-	54,54,54,54	0
57	MG	DW	3003	1/1	0.93	0.09	-	72,72,72,72	0
57	MG	BA	3482	1/1	0.95	0.15	-	51,51,51,51	0
57	MG	BA	3178	1/1	0.95	0.13	-	46,46,46,46	0
57	MG	DA	3024	1/1	0.94	0.21	-	59,59,59,59	0
57	MG	DA	3574	1/1	0.96	0.11	-	53,53,53,53	0
57	MG	DA	3384	1/1	0.97	0.10	-	49,49,49,49	0
57	MG	BA	3450	1/1	0.98	0.13	-	48,48,48,48	0
57	MG	CA	3168	1/1	0.87	0.11	-	56,56,56,56	0
57	MG	DA	3490	1/1	0.94	0.13	-	47,47,47,47	0
57	MG	AA	3035	1/1	0.95	0.21	-	56,56,56,56	0
57	MG	DA	3139	1/1	0.85	0.17	-	53,53,53,53	0
57	MG	DA	3524	1/1	0.90	0.17	-	61,61,61,61	0
57	MG	BA	3743	1/1	0.94	0.17	-	44,44,44,44	0
57	MG	DA	3071	1/1	0.84	0.13	-	59,59,59,59	0
57	MG	CA	3004	1/1	0.89	0.25	-	66,66,66,66	0
57	MG	DA	3604	1/1	0.91	0.17	-	59,59,59,59	0
57	MG	BA	3614	1/1	0.96	0.10	-	63,63,63,63	0
57	MG	CA	3015	1/1	0.95	0.22	-	56,56,56,56	0
57	MG	DA	3002	1/1	0.87	0.10	-	48,48,48,48	0
57	MG	DA	3606	1/1	0.88	0.10	-	71,71,71,71	0
57	MG	DA	3298	1/1	0.96	0.15	-	59,59,59,59	0
57	MG	DA	3130	1/1	0.91	0.18	-	52,52,52,52	0
57	MG	DA	3561	1/1	0.97	0.04	-	57,57,57,57	0
57	MG	BA	3174	1/1	0.98	0.18	-	37,37,37,37	0
57	MG	BA	3033	1/1	0.88	0.30	-	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
57	MG	DA	3557	1/1	0.93	0.15	-	51,51,51,51	0
57	MG	DA	3009	1/1	0.93	0.15	-	48,48,48,48	0
57	MG	DQ	3003	1/1	0.94	0.15	-	51,51,51,51	0
57	MG	AA	3192	1/1	0.86	0.14	-	71,71,71,71	0
57	MG	DA	3032	1/1	0.93	0.14	-	48,48,48,48	0
57	MG	BA	3421	1/1	0.78	0.17	-	32,32,32,32	0
57	MG	DA	3396	1/1	0.93	0.10	-	40,40,40,40	0
57	MG	DA	3251	1/1	0.92	0.17	-	62,62,62,62	0
57	MG	BA	3408	1/1	0.96	0.20	-	36,36,36,36	0
57	MG	DA	3227	1/1	0.93	0.28	-	41,41,41,41	0
57	MG	DA	3605	1/1	0.89	0.12	-	58,58,58,58	0
57	MG	BA	3267	1/1	0.88	0.19	-	65,65,65,65	0
57	MG	DA	3528	1/1	0.86	0.15	-	62,62,62,62	0
57	MG	DA	3038	1/1	0.91	0.16	-	47,47,47,47	0
57	MG	DE	304	1/1	0.95	0.15	-	43,43,43,43	0
57	MG	DA	3508	1/1	0.98	0.10	-	44,44,44,44	0
57	MG	BA	3599	1/1	0.90	0.21	-	43,43,43,43	0
57	MG	CA	3102	1/1	0.93	0.08	-	68,68,68,68	0
57	MG	BA	3322	1/1	0.92	0.17	-	52,52,52,52	0
57	MG	B7	105	1/1	0.88	0.16	-	56,56,56,56	0
57	MG	CA	3062	1/1	0.89	0.17	-	64,64,64,64	0
57	MG	BA	3161	1/1	0.93	0.17	-	52,52,52,52	0
57	MG	BA	3224	1/1	0.96	0.21	-	65,65,65,65	0
57	MG	BA	3238	1/1	0.96	0.24	-	62,62,62,62	0
57	MG	DA	3245	1/1	0.91	0.12	-	54,54,54,54	0
57	MG	AA	3134	1/1	0.95	0.14	-	66,66,66,66	0
57	MG	BA	3760	1/1	0.82	0.19	-	44,44,44,44	0
57	MG	CA	3128	1/1	0.89	0.15	-	65,65,65,65	0
57	MG	DA	3076	1/1	0.69	0.14	-	58,58,58,58	0
57	MG	DA	3137	1/1	0.92	0.22	-	54,54,54,54	0
57	MG	BA	3392	1/1	0.99	0.16	-	53,53,53,53	0
57	MG	AA	3188	1/1	0.91	0.08	-	69,69,69,69	0
57	MG	BA	3654	1/1	0.91	0.20	-	57,57,57,57	0
57	MG	DA	3479	1/1	0.94	0.17	-	43,43,43,43	0
57	MG	BA	3305	1/1	0.85	0.09	-	62,62,62,62	0
57	MG	BA	3564	1/1	0.94	0.16	-	44,44,44,44	0
57	MG	DA	3159	1/1	0.96	0.15	-	58,58,58,58	0
57	MG	AA	3021	1/1	0.91	0.13	-	63,63,63,63	0
57	MG	BA	3515	1/1	0.92	0.12	-	53,53,53,53	0
57	MG	DA	3665	1/1	0.98	0.14	-	42,42,42,42	0
57	MG	CA	3029	1/1	0.94	0.17	-	63,63,63,63	0
57	MG	BA	3291	1/1	0.93	0.21	-	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3048	1/1	0.92	0.06	-	53,53,53,53	0
57	MG	BA	3109	1/1	0.89	0.18	-	51,51,51,51	0
57	MG	CA	3001	1/1	0.95	0.10	-	75,75,75,75	0
57	MG	DA	3652	1/1	0.93	0.39	-	67,67,67,67	0
57	MG	BA	3169	1/1	0.96	0.17	-	45,45,45,45	0
57	MG	BA	3373	1/1	0.95	0.17	-	48,48,48,48	0
57	MG	CA	3091	1/1	0.91	0.12	-	55,55,55,55	0
57	MG	BA	3451	1/1	0.95	0.16	-	31,31,31,31	0
57	MG	BA	3192	1/1	0.90	0.28	-	46,46,46,46	0
57	MG	BA	3460	1/1	0.96	0.10	-	62,62,62,62	0
57	MG	AA	3105	1/1	0.97	0.32	-	69,69,69,69	0
57	MG	DA	3506	1/1	0.97	0.09	-	42,42,42,42	0
57	MG	DA	3359	1/1	0.95	0.14	-	47,47,47,47	0
57	MG	DA	3507	1/1	0.95	0.14	-	43,43,43,43	0
57	MG	AA	3061	1/1	0.92	0.34	-	55,55,55,55	0
57	MG	DA	3616	1/1	0.74	0.11	-	71,71,71,71	0
57	MG	DA	3196	1/1	0.95	0.22	-	49,49,49,49	0
57	MG	DA	3299	1/1	0.96	0.20	-	55,55,55,55	0
57	MG	DA	3214	1/1	0.90	0.24	-	59,59,59,59	0
57	MG	AA	3047	1/1	0.85	0.16	-	63,63,63,63	0
57	MG	AA	3012	1/1	0.93	0.16	-	46,46,46,46	0
57	MG	BA	3546	1/1	0.85	0.19	-	40,40,40,40	0
57	MG	AY	3001	1/1	0.95	0.39	-	65,65,65,65	0
57	MG	CA	3141	1/1	0.85	0.04	-	92,92,92,92	0
57	MG	CA	3115	1/1	0.86	0.08	-	63,63,63,63	0
57	MG	BA	3779	1/1	0.92	0.29	-	66,66,66,66	0
57	MG	AX	3007	1/1	0.91	0.10	-	67,67,67,67	0
57	MG	DA	3482	1/1	0.93	0.10	-	50,50,50,50	0
57	MG	BA	3149	1/1	0.93	0.18	-	40,40,40,40	0
57	MG	AA	3077	1/1	0.98	0.25	-	56,56,56,56	0
57	MG	BA	3073	1/1	0.91	0.22	-	61,61,61,61	0
57	MG	AA	3136	1/1	0.93	0.10	-	70,70,70,70	0
57	MG	DA	3073	1/1	0.95	0.09	-	42,42,42,42	0
57	MG	BA	3669	1/1	0.83	0.09	-	62,62,62,62	0
57	MG	AA	3079	1/1	0.85	0.13	-	68,68,68,68	0
57	MG	DA	3248	1/1	0.89	0.12	-	56,56,56,56	0
57	MG	BA	3208	1/1	0.96	0.16	-	44,44,44,44	0
57	MG	DA	3339	1/1	0.87	0.15	-	61,61,61,61	0
57	MG	BA	3342	1/1	0.82	0.10	-	46,46,46,46	0
57	MG	CA	3022	1/1	0.89	0.19	-	78,78,78,78	0
57	MG	DA	3559	1/1	0.96	0.12	-	43,43,43,43	0
57	MG	DA	3461	1/1	0.96	0.11	-	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
57	MG	DA	3443	1/1	0.96	0.10	-	54,54,54,54	0
57	MG	CA	3105	1/1	0.98	0.18	-	52,52,52,52	0
57	MG	DA	3172	1/1	0.94	0.09	-	62,62,62,62	0
57	MG	DA	3361	1/1	0.87	0.12	-	44,44,44,44	0
57	MG	AA	3108	1/1	0.89	0.28	-	67,67,67,67	0
57	MG	BA	3313	1/1	0.98	0.07	-	53,53,53,53	0
57	MG	DA	3125	1/1	0.71	0.26	-	70,70,70,70	0
57	MG	AA	3052	1/1	0.94	0.29	-	65,65,65,65	0
57	MG	BA	3193	1/1	0.97	0.20	-	48,48,48,48	0
57	MG	DA	3389	1/1	0.95	0.14	-	46,46,46,46	0
57	MG	BA	3623	1/1	0.90	0.26	-	55,55,55,55	0
57	MG	BA	3187	1/1	0.98	0.25	-	29,29,29,29	0
57	MG	DA	3100	1/1	0.92	0.16	-	43,43,43,43	0
57	MG	DA	3513	1/1	0.83	0.16	-	52,52,52,52	0
57	MG	DA	3124	1/1	0.89	0.15	-	57,57,57,57	0
57	MG	BA	3207	1/1	0.92	0.24	-	54,54,54,54	0
57	MG	DA	3624	1/1	0.94	0.19	-	56,56,56,56	0
57	MG	BA	3201	1/1	0.93	0.20	-	62,62,62,62	0
57	MG	BA	3020	1/1	0.80	0.22	-	53,53,53,53	0
57	MG	BA	3093	1/1	0.97	0.26	-	56,56,56,56	0
57	MG	CA	3060	1/1	0.93	0.09	-	65,65,65,65	0
57	MG	DA	3405	1/1	0.91	0.16	-	46,46,46,46	0
57	MG	BA	3081	1/1	0.95	0.21	-	46,46,46,46	0
57	MG	BA	3296	1/1	0.85	0.18	-	53,53,53,53	0
57	MG	BA	3364	1/1	0.98	0.27	-	60,60,60,60	0
57	MG	DA	3055	1/1	0.96	0.17	-	49,49,49,49	0
57	MG	BA	3324	1/1	0.89	0.17	-	45,45,45,45	0
57	MG	DA	3520	1/1	0.96	0.11	-	57,57,57,57	0
57	MG	AA	3131	1/1	0.91	0.15	-	71,71,71,71	0
57	MG	DA	3603	1/1	0.88	0.06	-	41,41,41,41	0
57	MG	DA	3475	1/1	0.96	0.17	-	51,51,51,51	0
57	MG	BA	3372	1/1	0.83	0.16	-	28,28,28,28	0
57	MG	CA	3136	1/1	0.95	0.14	-	72,72,72,72	0
57	MG	AA	3111	1/1	0.94	0.09	-	79,79,79,79	0
57	MG	CA	3106	1/1	0.95	0.07	-	56,56,56,56	0
57	MG	DA	3468	1/1	0.84	0.27	-	66,66,66,66	0
57	MG	BA	3721	1/1	0.46	0.32	-	82,82,82,82	0
57	MG	BA	3634	1/1	0.90	0.14	-	62,62,62,62	0
57	MG	DA	3456	1/1	0.92	0.07	-	50,50,50,50	0
57	MG	DB	3001	1/1	0.91	0.17	-	64,64,64,64	0
57	MG	DA	3131	1/1	0.93	0.21	-	46,46,46,46	0
57	MG	BA	3277	1/1	0.93	0.64	-	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	3010	1/1	0.94	0.17	-	56,56,56,56	0
57	MG	DA	3253	1/1	0.96	0.13	-	45,45,45,45	0
57	MG	DA	3089	1/1	0.97	0.38	-	52,52,52,52	0
57	MG	DA	3240	1/1	0.87	0.09	-	48,48,48,48	0
57	MG	BA	3121	1/1	0.91	0.21	-	64,64,64,64	0
57	MG	AA	3073	1/1	0.85	0.10	-	56,56,56,56	0
57	MG	DA	3329	1/1	0.54	0.13	-	54,54,54,54	0
57	MG	DA	3005	1/1	0.99	0.22	-	57,57,57,57	0
57	MG	DA	3291	1/1	0.93	0.20	-	44,44,44,44	0
57	MG	DA	3231	1/1	0.97	0.10	-	62,62,62,62	0
57	MG	BR	201	1/1	0.94	0.26	-	57,57,57,57	0
57	MG	DA	3662	1/1	0.94	0.13	-	62,62,62,62	0
57	MG	BA	3389	1/1	0.94	0.13	-	55,55,55,55	0
57	MG	CA	3122	1/1	0.94	0.22	-	64,64,64,64	0
57	MG	BA	3575	1/1	0.91	0.12	-	48,48,48,48	0
57	MG	AA	3173	1/1	0.96	0.15	-	54,54,54,54	0
57	MG	DD	303	1/1	0.74	0.62	-	87,87,87,87	0
57	MG	DA	3623	1/1	0.94	0.09	-	66,66,66,66	0
57	MG	DA	3394	1/1	0.83	0.18	-	65,65,65,65	0
57	MG	DA	3234	1/1	0.77	0.21	-	63,63,63,63	0
57	MG	AA	3055	1/1	0.93	0.21	-	57,57,57,57	0
57	MG	BA	3478	1/1	0.91	0.19	-	58,58,58,58	0
57	MG	BA	3667	1/1	0.95	0.15	-	61,61,61,61	0
57	MG	AA	3162	1/1	0.91	0.07	-	66,66,66,66	0
57	MG	DA	3309	1/1	0.86	0.09	-	51,51,51,51	0
57	MG	DA	3660	1/1	0.94	0.09	-	61,61,61,61	0
57	MG	BA	3413	1/1	0.91	0.13	-	47,47,47,47	0
57	MG	DA	3473	1/1	0.92	0.11	-	50,50,50,50	0
57	MG	AA	3046	1/1	0.88	0.22	-	55,55,55,55	0
57	MG	DA	3611	1/1	0.95	0.14	-	48,48,48,48	0
57	MG	DA	3484	1/1	0.86	0.12	-	62,62,62,62	0
57	MG	DA	3109	1/1	0.96	0.15	-	40,40,40,40	0
57	MG	BA	3783	1/1	0.95	0.12	-	56,56,56,56	0
57	MG	BA	3368	1/1	0.97	0.19	-	40,40,40,40	0
57	MG	DP	201	1/1	0.79	0.30	-	70,70,70,70	0
57	MG	DA	3142	1/1	0.97	0.13	-	47,47,47,47	0
57	MG	CA	3064	1/1	0.80	0.17	-	60,60,60,60	0
57	MG	DA	3383	1/1	0.77	0.20	-	54,54,54,54	0
57	MG	CA	3101	1/1	0.95	0.11	-	49,49,49,49	0
57	MG	DA	3239	1/1	0.91	0.24	-	56,56,56,56	0
57	MG	BA	3331	1/1	0.97	0.17	-	49,49,49,49	0
57	MG	AA	3185	1/1	0.89	0.12	-	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3436	1/1	0.97	0.12	-	54,54,54,54	0
57	MG	DA	3343	1/1	0.95	0.16	-	50,50,50,50	0
57	MG	BA	3512	1/1	0.84	0.18	-	52,52,52,52	0
57	MG	DA	3280	1/1	0.90	0.16	-	33,33,33,33	0
57	MG	BA	3502	1/1	0.88	0.12	-	56,56,56,56	0
57	MG	BA	3130	1/1	0.95	0.08	-	44,44,44,44	0
57	MG	DA	3362	1/1	0.85	0.21	-	44,44,44,44	0
57	MG	BA	3341	1/1	0.93	0.12	-	51,51,51,51	0
57	MG	BB	220	1/1	0.85	0.13	-	57,57,57,57	0
57	MG	DW	3001	1/1	0.97	0.40	-	54,54,54,54	0
57	MG	BA	3230	1/1	0.98	0.20	-	53,53,53,53	0
57	MG	BA	3687	1/1	0.95	0.21	-	22,22,22,22	0
57	MG	BA	3001	1/1	0.87	0.14	-	53,53,53,53	0
57	MG	AX	3013	1/1	0.96	0.13	-	58,58,58,58	0
57	MG	DQ	3002	1/1	0.95	0.10	-	51,51,51,51	0
57	MG	BA	3386	1/1	0.87	0.16	-	53,53,53,53	0
57	MG	AA	3103	1/1	0.73	0.23	-	73,73,73,73	0
57	MG	AA	3006	1/1	0.96	0.12	-	52,52,52,52	0
57	MG	AA	3110	1/1	0.96	0.13	-	48,48,48,48	0
57	MG	BA	3632	1/1	0.95	0.07	-	50,50,50,50	0
57	MG	BA	3534	1/1	0.97	0.21	-	44,44,44,44	0
57	MG	BA	3307	1/1	0.92	0.17	-	29,29,29,29	0
57	MG	BA	3635	1/1	0.95	0.13	-	58,58,58,58	0
57	MG	BA	3198	1/1	0.99	0.24	-	37,37,37,37	0
57	MG	BA	3382	1/1	0.96	0.08	-	63,63,63,63	0
57	MG	BA	3493	1/1	0.92	0.16	-	58,58,58,58	0
57	MG	BA	3071	1/1	0.87	0.35	-	59,59,59,59	0
57	MG	DA	3522	1/1	0.95	0.12	-	71,71,71,71	0
57	MG	BE	307	1/1	0.92	0.16	-	62,62,62,62	0
57	MG	AA	3128	1/1	0.88	0.08	-	57,57,57,57	0
57	MG	BA	3199	1/1	0.90	0.15	-	46,46,46,46	0
57	MG	DA	3255	1/1	0.93	0.09	-	51,51,51,51	0
57	MG	CA	3039	1/1	0.88	0.11	-	68,68,68,68	0
57	MG	BA	3435	1/1	0.97	0.27	-	45,45,45,45	0
57	MG	BA	3170	1/1	0.94	0.16	-	38,38,38,38	0
57	MG	CA	3098	1/1	0.84	0.09	-	65,65,65,65	0
57	MG	DB	3010	1/1	0.97	0.17	-	57,57,57,57	0
57	MG	BA	3773	1/1	0.93	0.25	-	52,52,52,52	0
57	MG	BA	3257	1/1	0.73	0.23	-	53,53,53,53	0
57	MG	BA	3171	1/1	0.95	0.25	-	31,31,31,31	0
57	MG	BA	3741	1/1	0.89	0.74	-	64,64,64,64	0
57	MG	DA	3403	1/1	0.45	0.14	-	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
57	MG	CX	3003	1/1	0.81	0.22	-	54,54,54,54	0
57	MG	BA	3738	1/1	0.94	0.15	-	43,43,43,43	0
57	MG	BA	3775	1/1	0.95	0.16	-	33,33,33,33	0
57	MG	AA	3209	1/1	0.89	0.08	-	59,59,59,59	0
57	MG	BA	3753	1/1	0.96	0.15	-	33,33,33,33	0
57	MG	BB	206	1/1	0.91	0.30	-	47,47,47,47	0
57	MG	DA	3209	1/1	0.90	0.24	-	53,53,53,53	0
57	MG	DA	3548	1/1	0.95	0.06	-	60,60,60,60	0
57	MG	DA	3386	1/1	0.95	0.11	-	35,35,35,35	0
57	MG	BA	3390	1/1	0.97	0.26	-	38,38,38,38	0
57	MG	DA	3091	1/1	0.92	0.10	-	48,48,48,48	0
57	MG	BA	3126	1/1	0.91	0.16	-	54,54,54,54	0
57	MG	BA	3099	1/1	0.92	0.22	-	41,41,41,41	0
57	MG	DA	3631	1/1	0.93	0.12	-	57,57,57,57	0
57	MG	BF	308	1/1	0.76	0.20	-	46,46,46,46	0
57	MG	DA	3677	1/1	0.90	0.47	-	52,52,52,52	0
57	MG	BA	3428	1/1	0.97	0.19	-	46,46,46,46	0
57	MG	AA	3129	1/1	0.95	0.11	-	47,47,47,47	0
57	MG	BA	3524	1/1	0.93	0.13	-	42,42,42,42	0
57	MG	AA	3165	1/1	0.95	0.19	-	54,54,54,54	0
57	MG	DA	3225	1/1	0.95	0.07	-	49,49,49,49	0
57	MG	BA	3592	1/1	0.95	0.20	-	28,28,28,28	0
57	MG	DA	3062	1/1	0.86	0.20	-	63,63,63,63	0
57	MG	BA	3567	1/1	0.95	0.15	-	34,34,34,34	0
57	MG	DA	3075	1/1	0.84	0.29	-	59,59,59,59	0
57	MG	DA	3121	1/1	0.93	0.07	-	44,44,44,44	0
57	MG	BA	3762	1/1	0.98	0.20	-	46,46,46,46	0
57	MG	BA	3227	1/1	0.91	0.24	-	57,57,57,57	0
57	MG	CA	3058	1/1	0.83	0.13	-	68,68,68,68	0
57	MG	DA	3138	1/1	0.86	0.13	-	55,55,55,55	0
57	MG	DA	3565	1/1	0.95	0.08	-	59,59,59,59	0
57	MG	AA	3127	1/1	0.83	0.16	-	65,65,65,65	0
57	MG	BA	3697	1/1	0.89	0.16	-	61,61,61,61	0
57	MG	BA	3615	1/1	0.77	0.21	-	68,68,68,68	0
57	MG	BA	3494	1/1	0.96	0.09	-	49,49,49,49	0
57	MG	BA	3032	1/1	0.89	0.20	-	47,47,47,47	0
57	MG	AA	3078	1/1	0.93	0.27	-	66,66,66,66	0
57	MG	BA	3294	1/1	0.94	0.24	-	61,61,61,61	0
57	MG	AA	3140	1/1	0.93	0.15	-	53,53,53,53	0
57	MG	B5	101	1/1	0.83	0.25	-	51,51,51,51	0
57	MG	DA	3316	1/1	0.72	0.11	-	45,45,45,45	0
57	MG	BA	3034	1/1	0.96	0.25	-	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
57	MG	BA	3252	1/1	0.90	0.41	-	60,60,60,60	0
57	MG	DA	3627	1/1	0.93	0.17	-	63,63,63,63	0
57	MG	BA	3145	1/1	0.92	0.10	-	44,44,44,44	0
57	MG	CA	3135	1/1	0.92	0.15	-	63,63,63,63	0
57	MG	AA	3190	1/1	0.87	0.10	-	58,58,58,58	0
57	MG	AA	3160	1/1	0.80	0.21	-	59,59,59,59	0
57	MG	BA	3674	1/1	0.97	0.15	-	63,63,63,63	0
57	MG	BA	3748	1/1	0.94	0.14	-	29,29,29,29	0
57	MG	AA	3090	1/1	0.98	0.22	-	66,66,66,66	0
57	MG	BA	3204	1/1	0.94	0.23	-	36,36,36,36	0
57	MG	BA	3263	1/1	0.97	0.35	-	49,49,49,49	0
57	MG	BA	3676	1/1	0.96	0.21	-	33,33,33,33	0
57	MG	BA	3467	1/1	0.98	0.23	-	50,50,50,50	0
57	MG	DA	3415	1/1	0.85	0.11	-	68,68,68,68	0
57	MG	DA	3155	1/1	0.97	0.24	-	48,48,48,48	0
57	MG	BA	3718	1/1	0.85	0.11	-	71,71,71,71	0
57	MG	AA	3199	1/1	0.94	0.15	-	73,73,73,73	0
57	MG	BA	3496	1/1	0.95	0.17	-	41,41,41,41	0
57	MG	BA	3544	1/1	0.98	0.22	-	44,44,44,44	0
57	MG	AA	3098	1/1	0.94	0.18	-	55,55,55,55	0
57	MG	CA	3121	1/1	0.95	0.14	-	63,63,63,63	0
57	MG	BA	3397	1/1	0.89	0.15	-	30,30,30,30	0
57	MG	BA	3693	1/1	0.81	0.19	-	56,56,56,56	0
57	MG	BA	3344	1/1	0.94	0.12	-	66,66,66,66	0
57	MG	BP	205	1/1	0.95	0.18	-	65,65,65,65	0
57	MG	BA	3782	1/1	0.95	0.16	-	65,65,65,65	0
57	MG	BA	3439	1/1	0.93	0.13	-	33,33,33,33	0
57	MG	BA	3128	1/1	0.87	0.14	-	69,69,69,69	0
57	MG	DA	3512	1/1	0.98	0.09	-	47,47,47,47	0
57	MG	AA	3003	1/1	0.91	0.30	-	72,72,72,72	0
57	MG	DA	3416	1/1	0.96	0.12	-	50,50,50,50	0
57	MG	BB	210	1/1	0.90	0.07	-	61,61,61,61	0
57	MG	DA	3568	1/1	0.95	0.08	-	52,52,52,52	0
57	MG	DA	3150	1/1	0.96	0.08	-	56,56,56,56	0
57	MG	BA	3525	1/1	0.96	0.17	-	34,34,34,34	0
57	MG	BA	3116	1/1	0.97	0.28	-	50,50,50,50	0
57	MG	DA	3010	1/1	0.98	0.17	-	47,47,47,47	0
57	MG	DA	3355	1/1	0.89	0.12	-	58,58,58,58	0
57	MG	CA	3076	1/1	0.89	0.14	-	57,57,57,57	0
57	MG	DA	3638	1/1	0.89	0.10	-	51,51,51,51	0
57	MG	DA	3301	1/1	0.90	0.19	-	52,52,52,52	0
57	MG	BA	3218	1/1	0.95	0.20	-	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3766	1/1	0.97	0.15	-	28,28,28,28	0
57	MG	BA	3671	1/1	0.92	0.16	-	63,63,63,63	0
57	MG	AA	3201	1/1	0.93	0.13	-	52,52,52,52	0
57	MG	DA	3307	1/1	0.97	0.09	-	42,42,42,42	0
57	MG	BA	3137	1/1	0.97	0.24	-	39,39,39,39	0
57	MG	DA	3158	1/1	0.94	0.16	-	60,60,60,60	0
57	MG	DD	309	1/1	0.91	0.21	-	59,59,59,59	0
57	MG	AA	3070	1/1	0.92	0.18	-	52,52,52,52	0
57	MG	BA	3095	1/1	0.76	0.24	-	51,51,51,51	0
57	MG	CA	3119	1/1	0.94	0.16	-	64,64,64,64	0
57	MG	DA	3204	1/1	0.96	0.31	-	46,46,46,46	0
57	MG	DA	3390	1/1	0.97	0.12	-	43,43,43,43	0
57	MG	BA	3255	1/1	0.91	0.15	-	47,47,47,47	0
57	MG	AA	3107	1/1	0.88	0.18	-	64,64,64,64	0
57	MG	BA	3362	1/1	0.76	0.20	-	41,41,41,41	0
57	MG	BA	3404	1/1	0.84	0.13	-	59,59,59,59	0
57	MG	DA	3385	1/1	0.83	0.11	-	52,52,52,52	0
57	MG	AA	3183	1/1	0.81	0.15	-	65,65,65,65	0
57	MG	DA	3120	1/1	0.90	0.13	-	49,49,49,49	0
57	MG	BA	3047	1/1	0.90	0.21	-	60,60,60,60	0
57	MG	BB	212	1/1	0.97	0.13	-	55,55,55,55	0
57	MG	CA	3052	1/1	0.86	0.21	-	72,72,72,72	0
57	MG	DA	3651	1/1	0.48	0.54	-	75,75,75,75	0
57	MG	BA	3396	1/1	0.91	0.15	-	50,50,50,50	0
57	MG	BB	203	1/1	0.97	0.24	-	43,43,43,43	0
57	MG	DA	3086	1/1	0.97	0.09	-	43,43,43,43	0
57	MG	BA	3711	1/1	0.96	0.19	-	54,54,54,54	0
57	MG	CA	3103	1/1	0.98	0.13	-	46,46,46,46	0
57	MG	BE	306	1/1	0.95	0.20	-	26,26,26,26	0
57	MG	DA	3084	1/1	0.96	0.08	-	39,39,39,39	0
57	MG	BA	3619	1/1	0.88	0.20	-	58,58,58,58	0
57	MG	AA	3097	1/1	0.92	0.34	-	56,56,56,56	0
57	MG	BA	3680	1/1	0.86	0.11	-	68,68,68,68	0
57	MG	AA	3049	1/1	0.87	0.21	-	64,64,64,64	0
57	MG	DA	3195	1/1	0.94	0.09	-	43,43,43,43	0
57	MG	BA	3574	1/1	0.96	0.19	-	66,66,66,66	0
57	MG	AA	3206	1/1	0.75	0.19	-	64,64,64,64	0
57	MG	BA	3657	1/1	0.96	0.26	-	47,47,47,47	0
57	MG	AA	3123	1/1	0.94	0.26	-	51,51,51,51	0
57	MG	BA	3276	1/1	0.90	0.31	-	54,54,54,54	0
57	MG	BA	3241	1/1	0.98	0.19	-	36,36,36,36	0
57	MG	BA	3303	1/1	0.91	0.17	-	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
57	MG	CA	3145	1/1	0.94	0.14	-	66,66,66,66	0
57	MG	CA	3125	1/1	0.94	0.08	-	63,63,63,63	0
57	MG	BA	3188	1/1	0.97	0.30	-	49,49,49,49	0
57	MG	BA	3520	1/1	0.94	0.16	-	61,61,61,61	0
57	MG	AA	3101	1/1	0.93	0.16	-	43,43,43,43	0
57	MG	BA	3345	1/1	0.97	0.14	-	38,38,38,38	0
57	MG	DA	3544	1/1	0.83	0.12	-	65,65,65,65	0
57	MG	BA	3475	1/1	0.97	0.13	-	42,42,42,42	0
57	MG	BA	3727	1/1	0.96	0.13	-	51,51,51,51	0
57	MG	BA	3504	1/1	0.94	0.13	-	56,56,56,56	0
57	MG	DA	3064	1/1	0.92	0.20	-	49,49,49,49	0
57	MG	DA	3013	1/1	0.93	0.09	-	40,40,40,40	0
57	MG	CA	3075	1/1	0.91	0.18	-	59,59,59,59	0
57	MG	AA	3177	1/1	0.86	0.08	-	66,66,66,66	0
57	MG	DA	3221	1/1	0.90	0.28	-	52,52,52,52	0
57	MG	DF	3004	1/1	0.99	0.38	-	44,44,44,44	0
57	MG	DA	3622	1/1	0.91	0.21	-	61,61,61,61	0
57	MG	DD	301	1/1	0.96	0.15	-	47,47,47,47	0
57	MG	BA	3499	1/1	0.89	0.10	-	58,58,58,58	0
57	MG	BA	3655	1/1	0.94	0.14	-	50,50,50,50	0
57	MG	BA	3707	1/1	0.82	0.24	-	44,44,44,44	0
57	MG	AA	3096	1/1	0.93	0.22	-	63,63,63,63	0
57	MG	DA	3533	1/1	0.94	0.11	-	43,43,43,43	0
57	MG	AA	3011	1/1	0.96	0.34	-	57,57,57,57	0
57	MG	DA	3184	1/1	0.97	0.16	-	47,47,47,47	0
57	MG	DA	3576	1/1	0.92	0.09	-	53,53,53,53	0
57	MG	CA	3049	1/1	0.96	0.20	-	63,63,63,63	0
57	MG	DA	3266	1/1	0.97	0.09	-	57,57,57,57	0
57	MG	CA	3012	1/1	0.91	0.20	-	60,60,60,60	0
57	MG	DA	3167	1/1	0.95	0.13	-	41,41,41,41	0
57	MG	BA	3805	1/1	0.94	0.12	-	44,44,44,44	0
57	MG	BA	3181	1/1	0.98	0.25	-	43,43,43,43	0
57	MG	DA	3290	1/1	0.95	0.15	-	59,59,59,59	0
57	MG	AY	3002	1/1	0.94	0.24	-	56,56,56,56	0
57	MG	AA	3141	1/1	0.93	0.23	-	61,61,61,61	0
57	MG	BA	3576	1/1	0.93	0.07	-	57,57,57,57	0
57	MG	BA	3155	1/1	0.94	0.27	-	44,44,44,44	0
57	MG	DA	3046	1/1	0.97	0.16	-	47,47,47,47	0
57	MG	BA	3251	1/1	0.96	0.19	-	44,44,44,44	0
57	MG	BA	3292	1/1	0.92	0.15	-	48,48,48,48	0
57	MG	AA	3203	1/1	0.96	0.13	-	59,59,59,59	0
57	MG	BA	3086	1/1	0.97	0.21	-	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3638	1/1	0.79	0.14	-	63,63,63,63	0
57	MG	CA	3059	1/1	0.92	0.25	-	72,72,72,72	0
57	MG	BA	3004	1/1	0.97	0.19	-	33,33,33,33	0
57	MG	DA	3331	1/1	0.94	0.17	-	37,37,37,37	0
57	MG	BA	3516	1/1	0.94	0.19	-	52,52,52,52	0
57	MG	BA	3438	1/1	0.84	0.14	-	60,60,60,60	0
57	MG	AA	3113	1/1	0.96	0.12	-	58,58,58,58	0
57	MG	AA	3026	1/1	0.88	0.13	-	70,70,70,70	0
57	MG	DA	3242	1/1	0.87	0.11	-	52,52,52,52	0
57	MG	DA	3085	1/1	0.91	0.08	-	53,53,53,53	0
57	MG	DO	5001	1/1	0.95	0.13	-	59,59,59,59	0
57	MG	BA	3315	1/1	0.89	0.19	-	31,31,31,31	0
57	MG	AA	3057	1/1	0.90	0.22	-	64,64,64,64	0
57	MG	DA	3023	1/1	0.95	0.29	-	40,40,40,40	0
57	MG	DA	3659	1/1	0.87	0.13	-	48,48,48,48	0
57	MG	DV	3003	1/1	0.92	0.10	-	65,65,65,65	0
57	MG	BA	3100	1/1	0.92	0.17	-	39,39,39,39	0
57	MG	BA	3586	1/1	0.96	0.09	-	53,53,53,53	0
57	MG	BA	3800	1/1	0.93	0.22	-	38,38,38,38	0
57	MG	DA	3457	1/1	0.96	0.07	-	54,54,54,54	0
57	MG	CA	3013	1/1	0.80	0.13	-	69,69,69,69	0
57	MG	DA	3600	1/1	0.95	0.35	-	70,70,70,70	0
57	MG	DA	3400	1/1	0.87	0.12	-	54,54,54,54	0
57	MG	AW	3003	1/1	0.94	0.13	-	72,72,72,72	0
57	MG	BA	3358	1/1	0.97	0.21	-	49,49,49,49	0
57	MG	DA	3516	1/1	0.94	0.07	-	67,67,67,67	0
57	MG	BA	3105	1/1	0.97	0.18	-	37,37,37,37	0
57	MG	BE	303	1/1	0.94	0.20	-	51,51,51,51	0
57	MG	DA	3154	1/1	0.94	0.17	-	48,48,48,48	0
57	MG	AA	3036	1/1	0.90	0.17	-	61,61,61,61	0
57	MG	CA	3066	1/1	0.84	0.14	-	66,66,66,66	0
57	MG	CA	3126	1/1	0.94	0.11	-	67,67,67,67	0
57	MG	DA	3429	1/1	0.91	0.14	-	41,41,41,41	0
57	MG	AA	3207	1/1	0.97	0.09	-	65,65,65,65	0
57	MG	BA	3468	1/1	0.96	0.17	-	62,62,62,62	0
57	MG	AA	3171	1/1	0.92	0.10	-	51,51,51,51	0
57	MG	BA	3306	1/1	0.94	0.17	-	37,37,37,37	0
57	MG	BA	3552	1/1	0.95	0.25	-	29,29,29,29	0
57	MG	BA	3271	1/1	0.92	0.17	-	58,58,58,58	0
57	MG	AA	3208	1/1	0.97	0.17	-	60,60,60,60	0
57	MG	DA	3106	1/1	0.89	0.13	-	52,52,52,52	0
57	MG	BA	3325	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
57	MG	BA	3785	1/1	0.94	0.23	-	59,59,59,59	0
57	MG	DA	3504	1/1	0.97	0.07	-	47,47,47,47	0
57	MG	BA	3700	1/1	0.90	0.16	-	61,61,61,61	0
57	MG	DA	3274	1/1	0.88	0.15	-	58,58,58,58	0
57	MG	AA	3069	1/1	0.80	0.19	-	68,68,68,68	0
57	MG	BA	3142	1/1	0.98	0.18	-	49,49,49,49	0
57	MG	DA	3141	1/1	0.90	0.27	-	61,61,61,61	0
57	MG	BA	3380	1/1	0.97	0.10	-	48,48,48,48	0
57	MG	DA	3230	1/1	0.94	0.22	-	73,73,73,73	0
57	MG	DA	3656	1/1	0.94	0.13	-	58,58,58,58	0
57	MG	BA	3709	1/1	0.82	0.20	-	62,62,62,62	0
57	MG	AA	3109	1/1	0.92	0.14	-	62,62,62,62	0
57	MG	BA	3717	1/1	0.92	0.16	-	50,50,50,50	0
57	MG	BA	3446	1/1	0.83	0.17	-	40,40,40,40	0
57	MG	BA	3005	1/1	0.91	0.16	-	30,30,30,30	0
57	MG	AA	3142	1/1	0.90	0.11	-	41,41,41,41	0
57	MG	BA	3311	1/1	0.97	0.27	-	48,48,48,48	0
57	MG	BG	201	1/1	0.97	0.20	-	58,58,58,58	0
57	MG	DA	3411	1/1	0.94	0.22	-	53,53,53,53	0
57	MG	DA	3645	1/1	0.95	0.07	-	45,45,45,45	0
57	MG	BA	3566	1/1	0.88	0.21	-	67,67,67,67	0
57	MG	DA	3056	1/1	0.88	0.09	-	51,51,51,51	0
57	MG	DA	3093	1/1	0.88	0.09	-	62,62,62,62	0
57	MG	CA	3120	1/1	0.92	0.18	-	64,64,64,64	0
57	MG	BA	3653	1/1	0.97	0.21	-	39,39,39,39	0
57	MG	DA	3170	1/1	0.91	0.12	-	53,53,53,53	0
57	MG	BA	3533	1/1	0.93	0.10	-	59,59,59,59	0
57	MG	AA	3076	1/1	0.93	0.26	-	77,77,77,77	0
57	MG	DA	3186	1/1	0.95	0.16	-	54,54,54,54	0
57	MG	DA	3072	1/1	0.97	0.14	-	47,47,47,47	0
57	MG	BA	3006	1/1	0.88	0.19	-	48,48,48,48	0
57	MG	DA	3661	1/1	0.85	0.16	-	62,62,62,62	0
57	MG	BA	3481	1/1	0.97	0.18	-	41,41,41,41	0
57	MG	BA	3444	1/1	0.89	0.21	-	29,29,29,29	0
57	MG	DA	3112	1/1	0.92	0.16	-	59,59,59,59	0
57	MG	BA	3346	1/1	0.93	0.10	-	27,27,27,27	0
57	MG	BA	3663	1/1	0.94	0.19	-	41,41,41,41	0
57	MG	CA	3011	1/1	0.91	0.23	-	61,61,61,61	0
57	MG	BA	3726	1/1	0.99	0.19	-	63,63,63,63	0
57	MG	BA	3429	1/1	0.90	0.10	-	65,65,65,65	0
57	MG	BV	204	1/1	0.93	0.21	-	49,49,49,49	0
57	MG	BA	3724	1/1	0.79	0.18	-	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
57	MG	DA	3577	1/1	0.86	0.14	-	58,58,58,58	0
57	MG	DA	3542	1/1	0.97	0.17	-	24,24,24,24	0
57	MG	DA	3499	1/1	0.90	0.10	-	53,53,53,53	0
57	MG	DA	3136	1/1	0.95	0.14	-	52,52,52,52	0
57	MG	BA	3347	1/1	0.92	0.15	-	44,44,44,44	0
57	MG	BA	3314	1/1	0.89	0.13	-	58,58,58,58	0
57	MG	DA	3615	1/1	0.90	0.09	-	65,65,65,65	0
57	MG	DA	3077	1/1	0.89	0.23	-	61,61,61,61	0
57	MG	CA	3118	1/1	0.91	0.19	-	68,68,68,68	0
57	MG	DA	3350	1/1	0.96	0.12	-	51,51,51,51	0
57	MG	BA	3540	1/1	0.73	0.23	-	37,37,37,37	0
57	MG	DA	3241	1/1	0.96	0.13	-	45,45,45,45	0
57	MG	AA	3122	1/1	0.92	0.11	-	56,56,56,56	0
57	MG	BA	3498	1/1	0.98	0.18	-	36,36,36,36	0
57	MG	DA	3541	1/1	0.95	0.14	-	44,44,44,44	0
57	MG	BA	3508	1/1	0.91	0.20	-	51,51,51,51	0
57	MG	AA	3132	1/1	0.94	0.19	-	55,55,55,55	0
57	MG	DA	3587	1/1	0.94	0.12	-	56,56,56,56	0
57	MG	DA	3153	1/1	0.92	0.19	-	47,47,47,47	0
57	MG	DA	3176	1/1	0.96	0.19	-	41,41,41,41	0
57	MG	BA	3022	1/1	0.92	0.20	-	60,60,60,60	0
57	MG	DD	302	1/1	0.94	0.15	-	42,42,42,42	0
57	MG	BA	3577	1/1	0.95	0.19	-	51,51,51,51	0
57	MG	BA	3656	1/1	0.93	0.27	-	53,53,53,53	0
57	MG	DA	3601	1/1	0.97	0.09	-	44,44,44,44	0
57	MG	AA	3075	1/1	0.94	0.11	-	49,49,49,49	0
57	MG	DA	3474	1/1	0.95	0.14	-	51,51,51,51	0
57	MG	DA	3305	1/1	0.97	0.19	-	50,50,50,50	0
57	MG	AA	3210	1/1	0.89	0.27	-	59,59,59,59	0
57	MG	BA	3197	1/1	0.96	0.29	-	41,41,41,41	0
57	MG	CX	3002	1/1	0.67	0.14	-	70,70,70,70	0
57	MG	BA	3260	1/1	0.97	0.30	-	39,39,39,39	0
57	MG	AA	3041	1/1	0.85	0.21	-	46,46,46,46	0
57	MG	BA	3072	1/1	0.88	0.14	-	47,47,47,47	0
57	MG	DA	3496	1/1	0.95	0.07	-	53,53,53,53	0
57	MG	BA	3117	1/1	0.88	0.20	-	59,59,59,59	0
57	MG	DA	3649	1/1	0.95	0.05	-	58,58,58,58	0
57	MG	AA	3168	1/1	0.98	0.11	-	59,59,59,59	0
57	MG	BA	3361	1/1	0.89	0.13	-	49,49,49,49	0
57	MG	AA	3102	1/1	0.89	0.24	-	59,59,59,59	0
57	MG	BA	3484	1/1	0.94	0.13	-	54,54,54,54	0
57	MG	DA	3478	1/1	0.92	0.12	-	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
57	MG	AA	3184	1/1	0.85	0.12	-	60,60,60,60	0
57	MG	DA	3523	1/1	0.86	0.10	-	59,59,59,59	0
57	MG	BW	201	1/1	0.95	0.31	-	44,44,44,44	0
57	MG	DA	3449	1/1	0.97	0.10	-	54,54,54,54	0
57	MG	DA	3203	1/1	0.94	0.57	-	50,50,50,50	0
57	MG	DA	3374	1/1	0.96	0.16	-	56,56,56,56	0
57	MG	BA	3166	1/1	0.94	0.14	-	38,38,38,38	0
57	MG	CA	3104	1/1	0.95	0.12	-	68,68,68,68	0
57	MG	DB	3005	1/1	0.93	0.08	-	59,59,59,59	0
57	MG	BA	3471	1/1	0.88	0.27	-	53,53,53,53	0
57	MG	AA	3088	1/1	0.93	0.27	-	65,65,65,65	0
57	MG	BA	3242	1/1	0.82	0.21	-	55,55,55,55	0
57	MG	AA	3064	1/1	0.89	0.24	-	60,60,60,60	0
57	MG	BA	3083	1/1	0.96	0.14	-	56,56,56,56	0
57	MG	BA	3685	1/1	0.94	0.19	-	53,53,53,53	0
57	MG	DA	3017	1/1	0.93	0.06	-	55,55,55,55	0
57	MG	DA	3340	1/1	0.80	0.18	-	58,58,58,58	0
57	MG	DA	3547	1/1	0.90	0.14	-	54,54,54,54	0
57	MG	BA	3778	1/1	0.96	0.16	-	48,48,48,48	0
57	MG	BA	3665	1/1	0.96	0.16	-	49,49,49,49	0
57	MG	DA	3585	1/1	0.78	0.12	-	43,43,43,43	0
57	MG	BA	3393	1/1	0.97	0.18	-	51,51,51,51	0
57	MG	BA	3280	1/1	0.97	0.14	-	37,37,37,37	0
57	MG	BA	3106	1/1	0.89	0.22	-	42,42,42,42	0
57	MG	AA	3066	1/1	0.91	0.31	-	60,60,60,60	0
57	MG	BA	3270	1/1	0.97	0.17	-	48,48,48,48	0
57	MG	DA	3534	1/1	0.98	0.15	-	55,55,55,55	0
57	MG	BA	3391	1/1	0.84	0.24	-	63,63,63,63	0
57	MG	DA	3068	1/1	0.96	0.10	-	58,58,58,58	0
57	MG	BA	3521	1/1	0.98	0.20	-	39,39,39,39	0
57	MG	BA	3431	1/1	0.89	0.17	-	59,59,59,59	0
57	MG	DA	3302	1/1	0.94	0.28	-	70,70,70,70	0
57	MG	BA	3063	1/1	0.93	0.15	-	59,59,59,59	0
57	MG	DA	3409	1/1	0.92	0.15	-	57,57,57,57	0
57	MG	DA	3664	1/1	0.97	0.39	-	48,48,48,48	0
57	MG	BA	3675	1/1	0.92	0.19	-	67,67,67,67	0
57	MG	BA	3157	1/1	0.94	0.24	-	45,45,45,45	0
57	MG	DA	3111	1/1	0.96	0.19	-	61,61,61,61	0
57	MG	DA	3491	1/1	0.98	0.16	-	51,51,51,51	0
57	MG	DA	3382	1/1	0.92	0.07	-	48,48,48,48	0
57	MG	BA	3547	1/1	0.96	0.23	-	39,39,39,39	0
57	MG	DA	3505	1/1	0.92	0.08	-	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
57	MG	BA	3338	1/1	0.97	0.13	-	40,40,40,40	0
57	MG	CA	3078	1/1	0.93	0.14	-	44,44,44,44	0
57	MG	CA	3042	1/1	0.95	0.12	-	59,59,59,59	0
57	MG	AA	3114	1/1	0.96	0.17	-	59,59,59,59	0
57	MG	CA	3072	1/1	0.97	0.17	-	54,54,54,54	0
57	MG	BA	3210	1/1	0.91	0.33	-	49,49,49,49	0
57	MG	DA	3480	1/1	0.99	0.10	-	40,40,40,40	0
57	MG	DA	3260	1/1	0.94	0.09	-	55,55,55,55	0
57	MG	AA	3179	1/1	0.95	0.13	-	69,69,69,69	0
57	MG	BA	3150	1/1	0.91	0.17	-	55,55,55,55	0
57	MG	BF	304	1/1	0.76	0.18	-	45,45,45,45	0
57	MG	DA	3293	1/1	0.96	0.14	-	54,54,54,54	0
57	MG	BA	3182	1/1	0.92	0.14	-	55,55,55,55	0
57	MG	AA	3154	1/1	0.97	0.11	-	69,69,69,69	0
57	MG	BE	305	1/1	0.86	0.17	-	43,43,43,43	0
57	MG	CA	3149	1/1	0.82	0.14	-	52,52,52,52	0
57	MG	BA	3127	1/1	0.92	0.29	-	57,57,57,57	0
57	MG	DN	5001	1/1	0.98	0.11	-	66,66,66,66	0
57	MG	DA	3276	1/1	0.82	0.12	-	49,49,49,49	0
57	MG	CA	3055	1/1	0.91	0.09	-	69,69,69,69	0
57	MG	BA	3608	1/1	0.95	0.31	-	62,62,62,62	0
57	MG	BA	3058	1/1	0.89	0.15	-	49,49,49,49	0
57	MG	DA	3140	1/1	0.87	0.15	-	58,58,58,58	0
57	MG	AA	3187	1/1	0.90	0.13	-	62,62,62,62	0
57	MG	CA	3143	1/1	0.96	0.10	-	64,64,64,64	0
57	MG	AA	3186	1/1	0.97	0.12	-	42,42,42,42	0
57	MG	AA	3028	1/1	0.91	0.23	-	76,76,76,76	0
57	MG	BA	3590	1/1	0.89	0.16	-	50,50,50,50	0
57	MG	BA	3725	1/1	0.97	0.14	-	44,44,44,44	0
57	MG	BA	3163	1/1	0.95	0.13	-	55,55,55,55	0
57	MG	AX	3010	1/1	0.88	0.21	-	59,59,59,59	0
57	MG	BA	3453	1/1	0.85	0.32	-	45,45,45,45	0
57	MG	DA	3088	1/1	0.84	0.18	-	47,47,47,47	0
57	MG	DA	3376	1/1	0.95	0.16	-	61,61,61,61	0
57	MG	BA	3237	1/1	0.94	0.15	-	45,45,45,45	0
57	MG	DA	3566	1/1	0.64	0.13	-	69,69,69,69	0
57	MG	BA	3070	1/1	0.72	0.37	-	59,59,59,59	0
57	MG	BA	3138	1/1	0.92	0.33	-	42,42,42,42	0
57	MG	BA	3684	1/1	0.87	0.12	-	68,68,68,68	0
57	MG	B9	502	1/1	0.93	0.19	-	48,48,48,48	0
57	MG	CA	3131	1/1	0.97	0.07	-	55,55,55,55	0
57	MG	BA	3710	1/1	0.88	0.17	-	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
57	MG	BW	202	1/1	0.95	0.22	-	54,54,54,54	0
57	MG	BN	3005	1/1	0.97	0.17	-	36,36,36,36	0
57	MG	DA	3188	1/1	0.94	0.19	-	48,48,48,48	0
57	MG	DA	3216	1/1	0.88	0.22	-	56,56,56,56	0
57	MG	DA	3441	1/1	0.95	0.11	-	45,45,45,45	0
57	MG	BA	3733	1/1	0.77	0.11	-	58,58,58,58	0
57	MG	BA	3059	1/1	0.96	0.21	-	26,26,26,26	0
57	MG	DA	3567	1/1	0.88	0.27	-	62,62,62,62	0
57	MG	BA	3417	1/1	0.94	0.23	-	38,38,38,38	0
57	MG	DA	3352	1/1	0.97	0.19	-	63,63,63,63	0
57	MG	BA	3662	1/1	0.92	0.10	-	61,61,61,61	0
57	MG	AA	3048	1/1	0.96	0.22	-	57,57,57,57	0
57	MG	BA	3076	1/1	0.96	0.17	-	43,43,43,43	0
57	MG	AA	3204	1/1	0.90	0.13	-	53,53,53,53	0
57	MG	DA	3598	1/1	0.95	0.08	-	61,61,61,61	0
57	MG	DA	3633	1/1	0.71	0.12	-	58,58,58,58	0
57	MG	CA	3021	1/1	0.84	0.14	-	61,61,61,61	0
57	MG	DB	3011	1/1	0.69	0.14	-	72,72,72,72	0
57	MG	BA	3445	1/1	0.89	0.30	-	63,63,63,63	0
57	MG	BA	3602	1/1	0.76	0.16	-	53,53,53,53	0
57	MG	BA	3457	1/1	0.93	0.19	-	32,32,32,32	0
57	MG	DA	3025	1/1	0.80	0.16	-	54,54,54,54	0
57	MG	DA	3193	1/1	0.96	0.13	-	57,57,57,57	0
57	MG	DA	3427	1/1	0.94	0.14	-	45,45,45,45	0
57	MG	AA	3017	1/1	0.83	0.18	-	71,71,71,71	0
57	MG	BF	309	1/1	0.97	0.15	-	53,53,53,53	0
57	MG	BA	3660	1/1	0.96	0.11	-	61,61,61,61	0
57	MG	DA	3294	1/1	0.98	0.16	-	43,43,43,43	0
57	MG	CA	3162	1/1	0.96	0.10	-	66,66,66,66	0
57	MG	DA	3634	1/1	0.94	0.14	-	60,60,60,60	0
57	MG	AA	3189	1/1	0.83	0.12	-	65,65,65,65	0
57	MG	CA	3082	1/1	0.93	0.15	-	79,79,79,79	0
57	MG	DA	3200	1/1	0.94	0.09	-	66,66,66,66	0
57	MG	BA	3600	1/1	0.95	0.30	-	44,44,44,44	0
57	MG	BA	3758	1/1	0.93	0.11	-	45,45,45,45	0
57	MG	BA	3262	1/1	0.95	0.14	-	41,41,41,41	0
57	MG	BA	3751	1/1	0.95	0.17	-	26,26,26,26	0
57	MG	BA	3485	1/1	0.90	0.09	-	42,42,42,42	0
57	MG	AA	3119	1/1	0.92	0.12	-	51,51,51,51	0
57	MG	BA	3673	1/1	0.88	0.17	-	55,55,55,55	0
57	MG	BA	3559	1/1	0.94	0.08	-	47,47,47,47	0
57	MG	DA	3554	1/1	0.79	0.10	-	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
57	MG	DA	3497	1/1	0.84	0.11	-	55,55,55,55	0
57	MG	BA	3160	1/1	0.96	0.32	-	55,55,55,55	0
57	MG	AA	3144	1/1	0.95	0.14	-	46,46,46,46	0
57	MG	DY	502	1/1	0.95	0.13	-	50,50,50,50	0
57	MG	DA	3133	1/1	0.90	0.22	-	50,50,50,50	0
57	MG	BA	3129	1/1	0.84	0.28	-	58,58,58,58	0
57	MG	CA	3007	1/1	0.91	0.13	-	57,57,57,57	0
57	MG	CA	3047	1/1	0.98	0.14	-	53,53,53,53	0
57	MG	AA	3172	1/1	0.94	0.10	-	72,72,72,72	0
57	MG	AA	3153	1/1	0.66	0.18	-	74,74,74,74	0
57	MG	BO	202	1/1	0.91	0.09	-	65,65,65,65	0
57	MG	B8	101	1/1	0.97	0.21	-	44,44,44,44	0
57	MG	BA	3597	1/1	0.99	0.21	-	25,25,25,25	0
57	MG	BA	3173	1/1	0.93	0.15	-	48,48,48,48	0
57	MG	DA	3589	1/1	0.81	0.07	-	68,68,68,68	0
57	MG	CA	3005	1/1	0.96	0.15	-	62,62,62,62	0
57	MG	BA	3803	1/1	0.94	0.23	-	44,44,44,44	0
57	MG	DF	3001	1/1	0.87	0.20	-	44,44,44,44	0
57	MG	AX	3004	1/1	0.94	0.15	-	64,64,64,64	0
57	MG	BA	3455	1/1	0.91	0.16	-	64,64,64,64	0
57	MG	B7	101	1/1	0.97	0.24	-	39,39,39,39	0
57	MG	BA	3640	1/1	0.89	0.17	-	53,53,53,53	0
57	MG	DA	3569	1/1	0.96	0.23	-	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.