



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:06 PM GMT

PDB ID : 4V63  
Title : Structural basis for translation termination on the 70S ribosome.  
Authors : Laurberg, M.; Asahara, H.; Korostelev, A.; Zhu, J.; Trakhanov, S.; Noller, H.F.  
Deposited on : 2008-05-16  
Resolution : 3.21 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](mailto: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

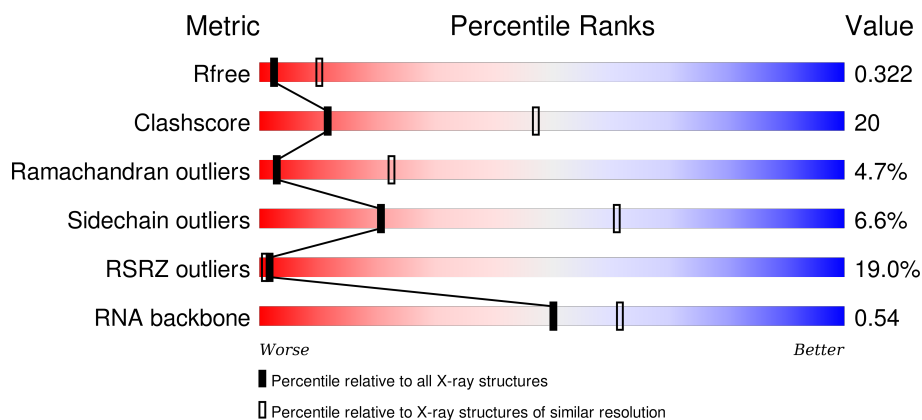
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.21 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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  $\geq 3$ , 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	1525	<div> <div>5%</div> <div>41%</div> <div>48%</div> <div>9%</div> <div>..</div> </div>
1	CA	1525	<div> <div>9%</div> <div>42%</div> <div>47%</div> <div>9%</div> <div>..</div> </div>
2	AY	77	<div> <div>47%</div> <div>44%</div> <div>8%</div> <div>.</div> </div>
2	AZ	77	<div> <div>14%</div> <div>43%</div> <div>49%</div> <div>8%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	CY	77	
2	CZ	77	
3	AV	27	
3	CV	27	
4	AB	256	
4	CB	256	
5	AC	239	
5	CC	239	
6	AD	209	
6	CD	209	
7	AE	162	
7	CE	162	
8	AF	101	
8	CF	101	
9	AG	156	
9	CG	156	
10	AH	138	
10	CH	138	
11	AI	128	
11	CI	128	
12	AJ	105	
12	CJ	105	
13	AK	129	
13	CK	129	
14	AL	134	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	CL	134	
15	AM	126	
15	CM	126	
16	AN	61	
16	CN	61	
17	AO	89	
17	CO	89	
18	AP	88	
18	CP	88	
19	AQ	105	
19	CQ	105	
20	AR	88	
20	CR	88	
21	AS	93	
21	CS	93	
22	AT	106	
22	CT	106	
23	AU	27	
23	CU	27	
24	AX	354	
24	CX	354	
25	BA	2894	
25	DA	2894	
26	BB	124	
26	DB	124	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BI	148	
32	DI	148	
33	BJ	173	
33	DJ	173	
34	BN	163	
34	DN	163	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	DS	112	
40	BT	146	
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	97	
51	D4	97	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	AA	1645	-	-	-	X
56	MG	AA	1756	-	-	-	X
56	MG	AA	1802	-	-	-	X
56	MG	AA	1834	-	-	-	X
56	MG	AA	1844	-	-	-	X
56	MG	AA	1861	-	-	-	X
56	MG	AD	304	-	-	-	X
56	MG	AY	105	-	-	-	X
56	MG	BA	3011	-	-	-	X
56	MG	BA	3169	-	-	-	X
56	MG	BA	3380	-	-	-	X
56	MG	BA	3481	-	-	-	X
56	MG	BA	3597	-	-	-	X
56	MG	BA	3708	-	-	-	X
56	MG	BA	3762	-	-	-	X
56	MG	BA	3775	-	-	-	X
56	MG	BA	3796	-	-	-	X
56	MG	BR	202	-	-	-	X
56	MG	CA	1615	-	-	-	X
56	MG	CA	1624	-	-	-	X
56	MG	CA	1800	-	-	-	X
56	MG	CA	1930	-	-	-	X
56	MG	CA	1941	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	1963	-	-	-	X
56	MG	CA	1982	-	-	-	X
56	MG	CA	1983	-	-	-	X
56	MG	CA	2008	-	-	-	X
56	MG	CX	406	-	-	-	X
56	MG	CY	113	-	-	-	X
56	MG	DA	3254	-	-	-	X
56	MG	DA	3256	-	-	-	X
56	MG	DA	3283	-	-	-	X
56	MG	DA	3417	-	-	-	X
56	MG	DA	3430	-	-	-	X
56	MG	DA	3637	-	-	-	X
56	MG	DA	3661	-	-	-	X
56	MG	DA	3673	-	-	-	X
56	MG	DA	3679	-	-	-	X
56	MG	DA	3688	-	-	-	X
56	MG	DA	3721	-	-	-	X
56	MG	DA	3726	-	-	-	X
56	MG	DA	3729	-	-	-	X

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 299961 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32332	14391	5994	10444	1503			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	466	G	C	CONFLICT	GB 155076
CA	466	G	C	CONFLICT	GB 155076

- Molecule 2 is a RNA chain called P and E-site tRNA(fMet).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AZ	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	AY	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	CZ	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
2	CY	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AV	12	Total	C	N	O	P	0	0	0
			258	118	54	75	11			
3	CV	12	Total	C	N	O	P	0	0	0
			258	118	54	75	11			

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			
4	CB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
5	CC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
6	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
7	CE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
8	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
10	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AI	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				
11	CI	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			
12	CJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
13	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			
14	CL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	ALA	-	INSERTION	UNP P61941
AL	3	LEU	-	INSERTION	UNP P61941
CL	2	ALA	-	INSERTION	UNP P61941
CL	3	LEU	-	INSERTION	UNP P61941

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AM	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
15	CM	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 16 is a protein called 30S ribosomal protein S14.

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

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
17	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
18	CP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AQ	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			
19	CQ	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AR	70	Total	C	N	O		0	0	0
			574	367	112	95				
20	CR	70	Total	C	N	O		0	0	0
			574	367	112	95				

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
21	CS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
22	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 23 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AU	24	Total	C	N	O		0	0	0
			208	128	50	30				
23	CU	24	Total	C	N	O		0	0	0
			208	128	50	30				

- Molecule 24 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	354	Total	C	N	O	S	0	0	0
			2813	1743	509	549	12			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	CX	354	Total	C	N	O	S	0	0	0
			2813	1743	509	549	12			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			
25	DA	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
26	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	INSERTION	GB 48271
BB	120	U	-	INSERTION	GB 48271
BB	121	U	-	INSERTION	GB 48271
DB	-1	A	-	INSERTION	GB 48271
DB	120	U	-	INSERTION	GB 48271
DB	121	U	-	INSERTION	GB 48271

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			
27	DD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	DE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			
29	DF	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	1	MET	-	INSERTION	UNP Q72I05
BF	2	LYS	-	INSERTION	UNP Q72I05
BF	3	GLU	-	INSERTION	UNP Q72I05
BF	4	VAL	-	INSERTION	UNP Q72I05
BF	5	ALA	-	INSERTION	UNP Q72I05
DF	1	MET	-	INSERTION	UNP Q72I05
DF	2	LYS	-	INSERTION	UNP Q72I05
DF	3	GLU	-	INSERTION	UNP Q72I05
DF	4	VAL	-	INSERTION	UNP Q72I05
DF	5	ALA	-	INSERTION	UNP Q72I05

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			
30	DG	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			
31	DH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			
32	DI	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	BJ	32	Total	C	N	O	0	0	0
			253	157	49	47			
33	DJ	32	Total	C	N	O	0	0	0
			253	157	49	47			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			
34	DN	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BN	2	VAL	-	INSERTION	UNP Q72IN1
BN	3	LYS	-	INSERTION	UNP Q72IN1
BN	4	SER	-	INSERTION	UNP Q72IN1
BN	5	SER	-	INSERTION	UNP Q72IN1
BN	6	LEU	-	INSERTION	UNP Q72IN1
BN	7	ALA	-	INSERTION	UNP Q72IN1
BN	8	PHE	-	INSERTION	UNP Q72IN1
BN	9	LEU	-	INSERTION	UNP Q72IN1
BN	10	ARG	-	INSERTION	UNP Q72IN1
BN	11	GLY	-	INSERTION	UNP Q72IN1
BN	12	PRO	-	INSERTION	UNP Q72IN1
BN	13	PRO	-	INSERTION	UNP Q72IN1
BN	14	ILE	-	INSERTION	UNP Q72IN1
BN	15	PRO	-	INSERTION	UNP Q72IN1
BN	16	ARG	-	INSERTION	UNP Q72IN1
BN	17	GLN	-	INSERTION	UNP Q72IN1
BN	18	GLU	-	INSERTION	UNP Q72IN1
BN	19	GLN	-	INSERTION	UNP Q72IN1
BN	20	ARG	-	INSERTION	UNP Q72IN1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
BN	21	ARG	-	INSERTION	UNP Q72IN1
BN	22	ALA	-	INSERTION	UNP Q72IN1
BN	23	LEU	-	INSERTION	UNP Q72IN1
BN	24	VAL	-	INSERTION	UNP Q72IN1
DN	2	VAL	-	INSERTION	UNP Q72IN1
DN	3	LYS	-	INSERTION	UNP Q72IN1
DN	4	SER	-	INSERTION	UNP Q72IN1
DN	5	SER	-	INSERTION	UNP Q72IN1
DN	6	LEU	-	INSERTION	UNP Q72IN1
DN	7	ALA	-	INSERTION	UNP Q72IN1
DN	8	PHE	-	INSERTION	UNP Q72IN1
DN	9	LEU	-	INSERTION	UNP Q72IN1
DN	10	ARG	-	INSERTION	UNP Q72IN1
DN	11	GLY	-	INSERTION	UNP Q72IN1
DN	12	PRO	-	INSERTION	UNP Q72IN1
DN	13	PRO	-	INSERTION	UNP Q72IN1
DN	14	ILE	-	INSERTION	UNP Q72IN1
DN	15	PRO	-	INSERTION	UNP Q72IN1
DN	16	ARG	-	INSERTION	UNP Q72IN1
DN	17	GLN	-	INSERTION	UNP Q72IN1
DN	18	GLU	-	INSERTION	UNP Q72IN1
DN	19	GLN	-	INSERTION	UNP Q72IN1
DN	20	ARG	-	INSERTION	UNP Q72IN1
DN	21	ARG	-	INSERTION	UNP Q72IN1
DN	22	ALA	-	INSERTION	UNP Q72IN1
DN	23	LEU	-	INSERTION	UNP Q72IN1
DN	24	VAL	-	INSERTION	UNP Q72IN1

- 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
			932	587	171	170	4			
35	DO	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			
37	DQ	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
38	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	98	Total	C	N	O		0	0	0
			770	486	154	130				
39	DS	98	Total	C	N	O		0	0	0
			770	486	154	130				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			
40	DT	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	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
			779	501	142	135	1			
42	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	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
			890	560	175	153	2			
43	DW	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BX	92	Total	C	N	O	0	0	0
			725	471	131	123			
44	DX	92	Total	C	N	O	0	0	0
			725	471	131	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
45	DY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	188	Total	C	N	O	S	0	0	0
			1491	950	265	274	2			
46	DZ	188	Total	C	N	O	S	0	0	0
			1491	950	265	274	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			
47	D0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	88	Total	C	N	O	S	0	0	0
			694	435	141	118				
48	D1	88	Total	C	N	O	S	0	0	0
			694	435	141	118				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	72	Total	C	N	O	S	0	0	0
			605	375	122	106	2			
49	D2	72	Total	C	N	O	S	0	0	0
			605	375	122	106	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	S	0	0	0
			467	298	90	78	1			
50	D3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			
51	D4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B4	2	PRO	-	INSERTION	UNP Q72JR0
B4	3	LEU	-	INSERTION	UNP Q72JR0
B4	4	GLY	-	INSERTION	UNP Q72JR0

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B4	5	VAL	-	INSERTION	UNP Q72JR0
B4	6	HIS	-	INSERTION	UNP Q72JR0
B4	7	PRO	-	INSERTION	UNP Q72JR0
B4	8	LEU	-	INSERTION	UNP Q72JR0
B4	9	TYR	-	INSERTION	UNP Q72JR0
B4	10	THR	-	INSERTION	UNP Q72JR0
B4	11	LYS	-	INSERTION	UNP Q72JR0
B4	12	ARG	-	INSERTION	UNP Q72JR0
B4	13	TRP	-	INSERTION	UNP Q72JR0
B4	14	LEU	-	INSERTION	UNP Q72JR0
B4	15	ALA	-	INSERTION	UNP Q72JR0
B4	16	HIS	-	INSERTION	UNP Q72JR0
B4	17	GLY	-	INSERTION	UNP Q72JR0
B4	18	GLN	-	INSERTION	UNP Q72JR0
B4	19	ASP	-	INSERTION	UNP Q72JR0
B4	20	ARG	-	INSERTION	UNP Q72JR0
B4	21	ALA	-	INSERTION	UNP Q72JR0
B4	22	LYS	-	INSERTION	UNP Q72JR0
B4	23	LYS	-	INSERTION	UNP Q72JR0
B4	24	GLU	-	INSERTION	UNP Q72JR0
B4	25	ALA	-	INSERTION	UNP Q72JR0
B4	26	ASN	-	INSERTION	UNP Q72JR0
B4	27	VAL	-	INSERTION	UNP Q72JR0
D4	2	PRO	-	INSERTION	UNP Q72JR0
D4	3	LEU	-	INSERTION	UNP Q72JR0
D4	4	GLY	-	INSERTION	UNP Q72JR0
D4	5	VAL	-	INSERTION	UNP Q72JR0
D4	6	HIS	-	INSERTION	UNP Q72JR0
D4	7	PRO	-	INSERTION	UNP Q72JR0
D4	8	LEU	-	INSERTION	UNP Q72JR0
D4	9	TYR	-	INSERTION	UNP Q72JR0
D4	10	THR	-	INSERTION	UNP Q72JR0
D4	11	LYS	-	INSERTION	UNP Q72JR0
D4	12	ARG	-	INSERTION	UNP Q72JR0
D4	13	TRP	-	INSERTION	UNP Q72JR0
D4	14	LEU	-	INSERTION	UNP Q72JR0
D4	15	ALA	-	INSERTION	UNP Q72JR0
D4	16	HIS	-	INSERTION	UNP Q72JR0
D4	17	GLY	-	INSERTION	UNP Q72JR0
D4	18	GLN	-	INSERTION	UNP Q72JR0
D4	19	ASP	-	INSERTION	UNP Q72JR0
D4	20	ARG	-	INSERTION	UNP Q72JR0

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D4	21	ALA	-	INSERTION	UNP Q72JR0
D4	22	LYS	-	INSERTION	UNP Q72JR0
D4	23	LYS	-	INSERTION	UNP Q72JR0
D4	24	GLU	-	INSERTION	UNP Q72JR0
D4	25	ALA	-	INSERTION	UNP Q72JR0
D4	26	ASN	-	INSERTION	UNP Q72JR0
D4	27	VAL	-	INSERTION	UNP Q72JR0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			
52	D5	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			
53	D6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	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	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
55	D8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	AP	1	Total 1 Mg 1	0	0
56	CZ	19	Total 19 Mg 19	0	0
56	BA	806	Total 806 Mg 806	0	0
56	AK	1	Total 1 Mg 1	0	0
56	DQ	1	Total 1 Mg 1	0	0
56	AB	2	Total 2 Mg 2	0	0
56	DF	1	Total 1 Mg 1	0	0
56	CV	4	Total 4 Mg 4	0	0
56	CI	2	Total 2 Mg 2	0	0
56	BE	1	Total 1 Mg 1	0	0
56	D8	1	Total 1 Mg 1	0	0
56	B1	2	Total 2 Mg 2	0	0
56	CD	2	Total 2 Mg 2	0	0
56	BP	1	Total 1 Mg 1	0	0
56	AX	6	Total 6 Mg 6	0	0
56	DN	1	Total 1 Mg 1	0	0
56	BI	3	Total 3 Mg 3	0	0
56	CY	21	Total 21 Mg 21	0	0
56	CA	414	Total 414 Mg 414	0	0
56	B5	1	Total 1 Mg 1	0	0
56	BB	26	Total 26 Mg 26	0	0
56	AJ	1	Total 1 Mg 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BT	2	Total 2	Mg 2	0	0
56	DO	2	Total 2	Mg 2	0	0
56	AE	1	Total 1	Mg 1	0	0
56	DG	1	Total 1	Mg 1	0	0
56	CF	1	Total 1	Mg 1	0	0
56	DT	1	Total 1	Mg 1	0	0
56	D3	1	Total 1	Mg 1	0	0
56	BF	5	Total 5	Mg 5	0	0
56	AV	1	Total 1	Mg 1	0	0
56	DR	1	Total 1	Mg 1	0	0
56	B2	3	Total 3	Mg 3	0	0
56	AA	310	Total 310	Mg 310	0	0
56	BQ	3	Total 3	Mg 3	0	0
56	D7	2	Total 2	Mg 2	0	0
56	BJ	1	Total 1	Mg 1	0	0
56	CX	9	Total 9	Mg 9	0	0
56	DV	1	Total 1	Mg 1	0	0
56	CH	1	Total 1	Mg 1	0	0
56	DI	2	Total 2	Mg 2	0	0
56	AM	1	Total 1	Mg 1	0	0
56	BU	1	Total 1	Mg 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	CC	7	Total 7	Mg 7	0	0
56	AD	8	Total 8	Mg 8	0	0
56	BN	2	Total 2	Mg 2	0	0
56	DH	4	Total 4	Mg 4	0	0
56	CG	1	Total 1	Mg 1	0	0
56	BG	3	Total 3	Mg 3	0	0
56	AI	2	Total 2	Mg 2	0	0
56	BY	1	Total 1	Mg 1	0	0
56	CJ	1	Total 1	Mg 1	0	0
56	BR	3	Total 3	Mg 3	0	0
56	AZ	6	Total 6	Mg 6	0	0
56	D4	3	Total 3	Mg 3	0	0
56	DA	758	Total 758	Mg 758	0	0
56	CE	1	Total 1	Mg 1	0	0
56	DW	3	Total 3	Mg 3	0	0
56	B7	3	Total 3	Mg 3	0	0
56	D2	2	Total 2	Mg 2	0	0
56	AL	2	Total 2	Mg 2	0	0
56	BV	1	Total 1	Mg 1	0	0
56	AG	1	Total 1	Mg 1	0	0
56	BO	3	Total 3	Mg 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AQ	1	Total 1	Mg 1	0	0
56	DX	1	Total 1	Mg 1	0	0
56	AH	2	Total 2	Mg 2	0	0
56	BZ	1	Total 1	Mg 1	0	0
56	CO	2	Total 2	Mg 2	0	0
56	DZ	4	Total 4	Mg 4	0	0
56	AC	6	Total 6	Mg 6	0	0
56	DB	28	Total 28	Mg 28	0	0
56	CB	2	Total 2	Mg 2	0	0
56	D5	1	Total 1	Mg 1	0	0
56	BD	2	Total 2	Mg 2	0	0
56	CL	1	Total 1	Mg 1	0	0
56	DP	6	Total 6	Mg 6	0	0
56	CP	1	Total 1	Mg 1	0	0
56	AO	3	Total 3	Mg 3	0	0
56	BW	2	Total 2	Mg 2	0	0
56	AY	25	Total 25	Mg 25	0	0
56	DD	1	Total 1	Mg 1	0	0
56	CK	2	Total 2	Mg 2	0	0
56	AF	2	Total 2	Mg 2	0	0
56	BH	2	Total 2	Mg 2	0	0

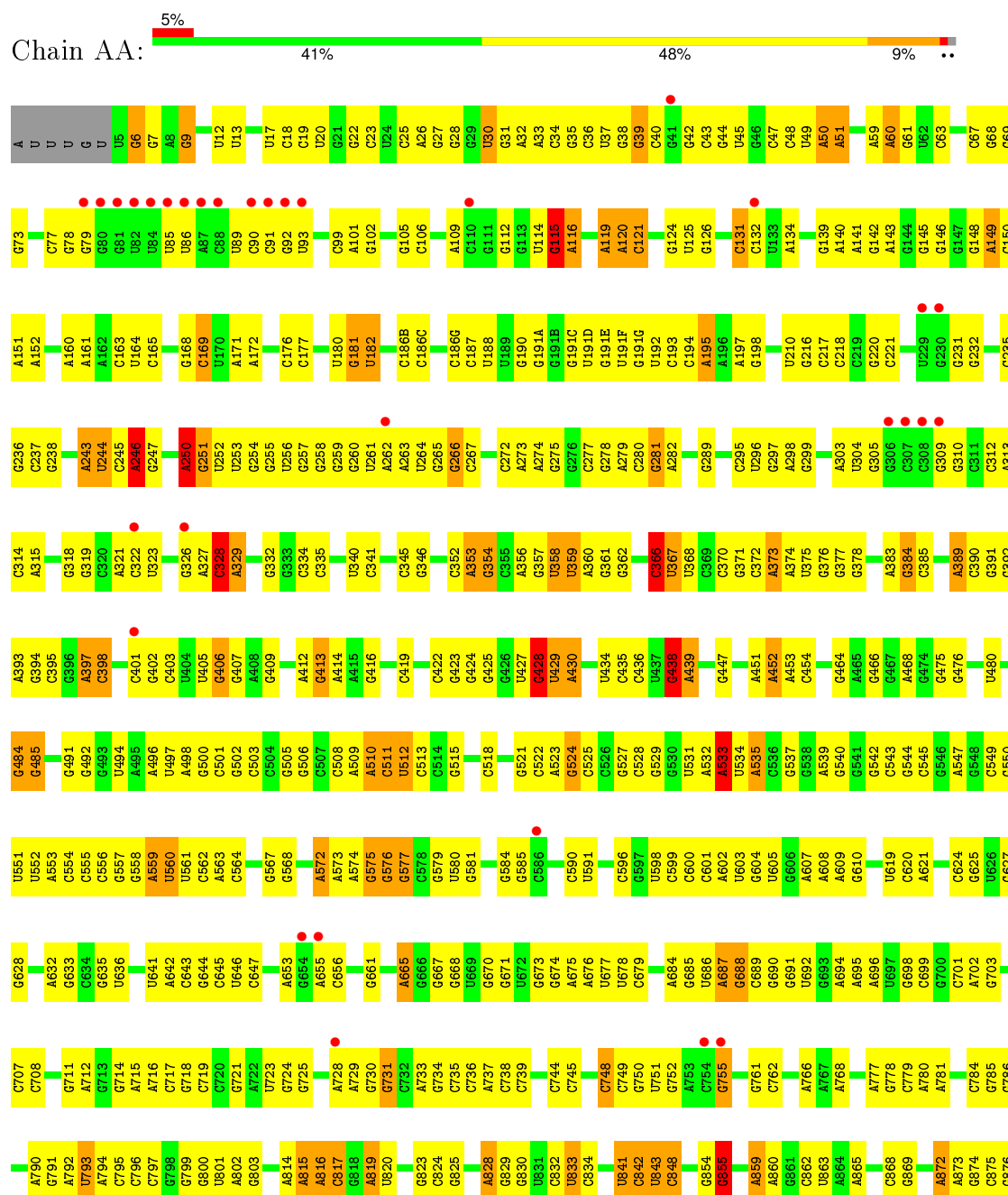
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CN	1	Total 1	Zn 1	0	0
57	AD	1	Total 1	Zn 1	0	0
57	CD	1	Total 1	Zn 1	0	0
57	AN	1	Total 1	Zn 1	0	0

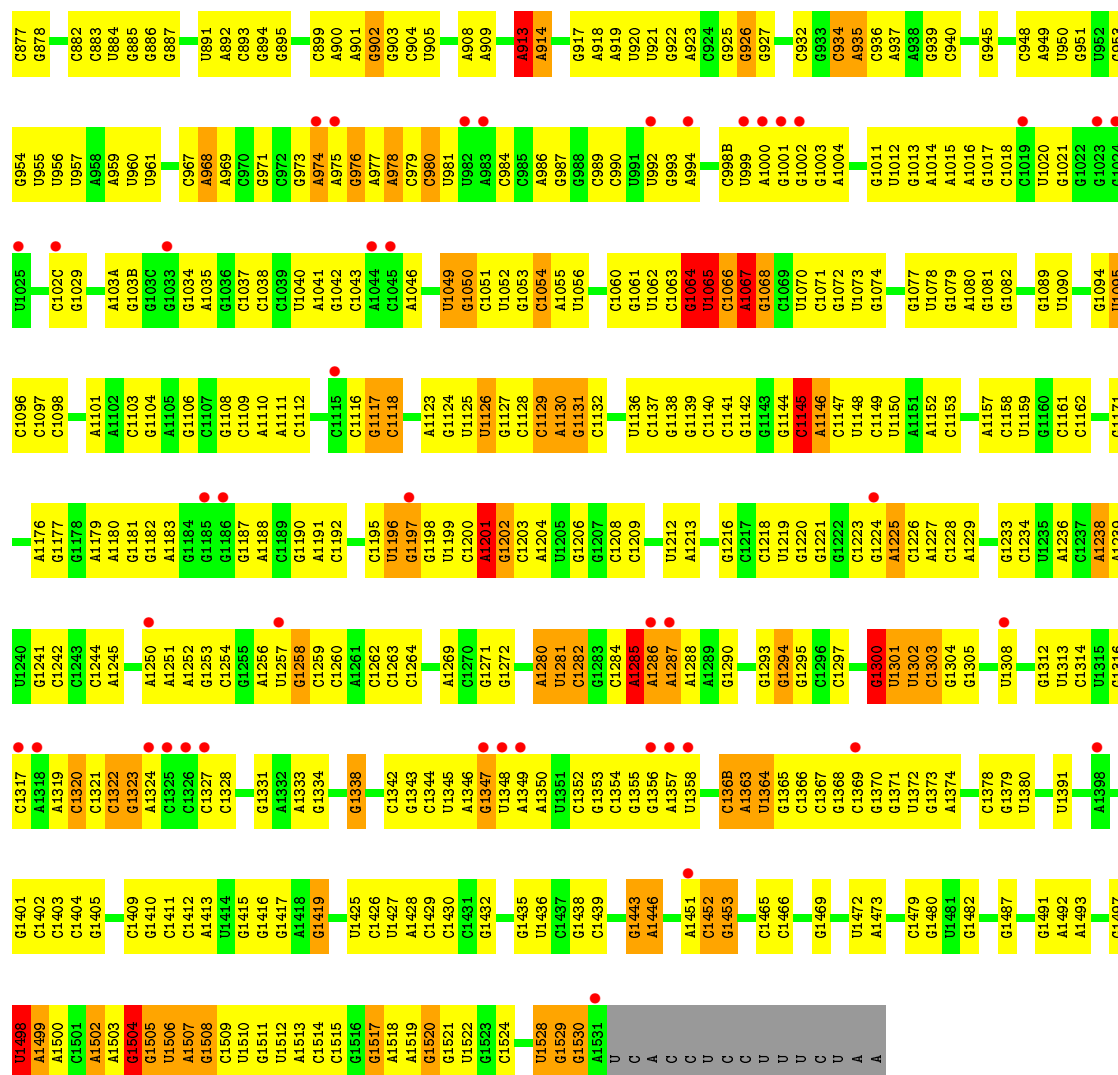
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

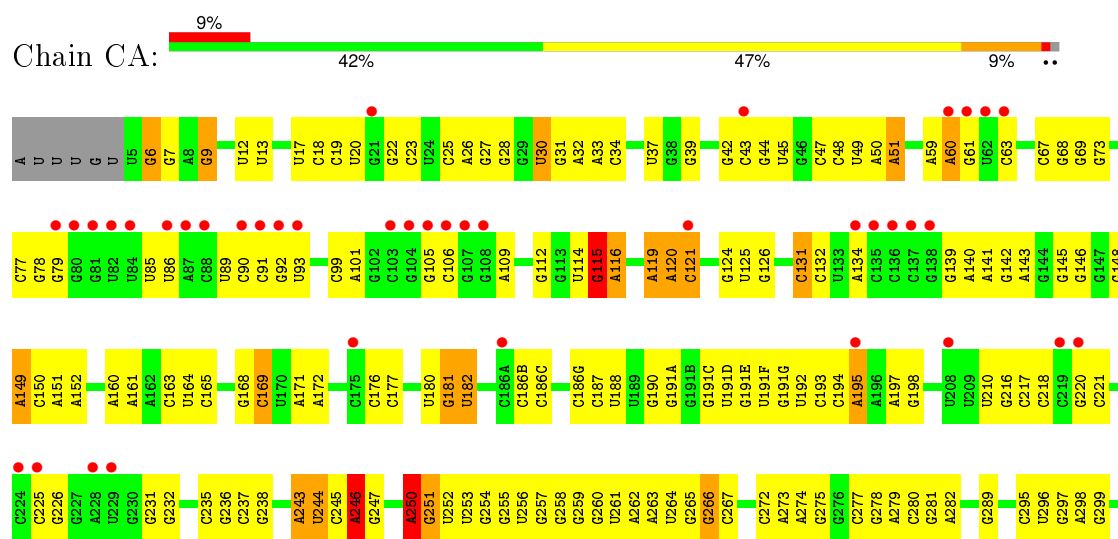
#### • Molecule 1: 16S rRNA

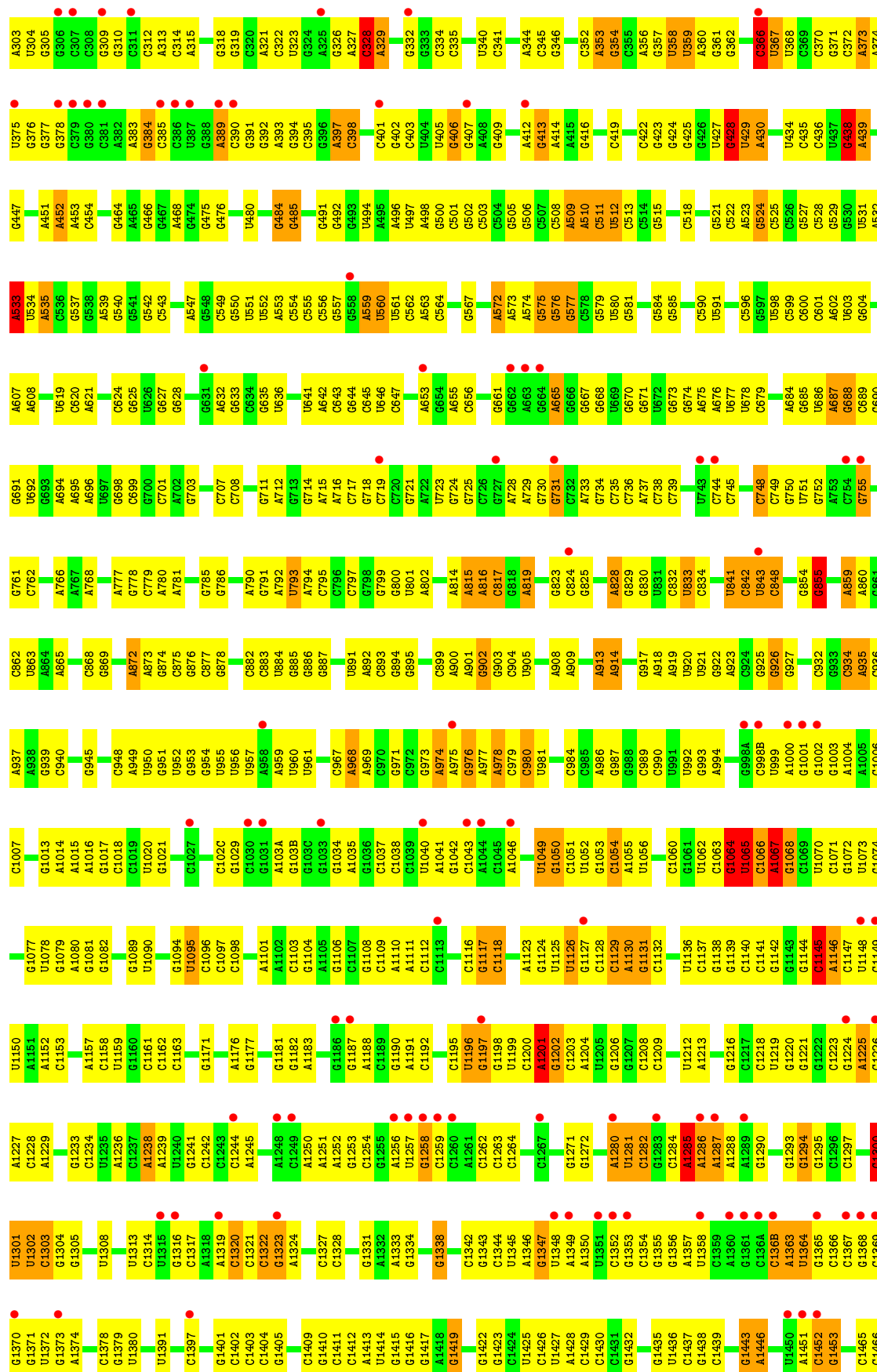


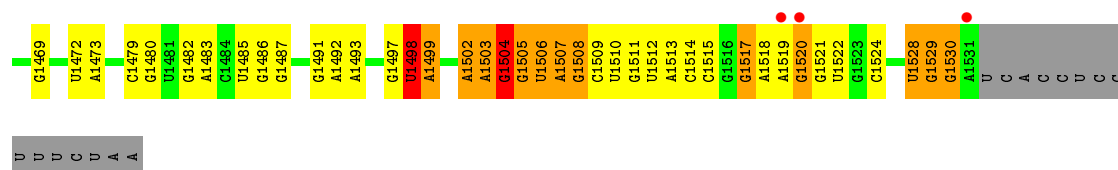




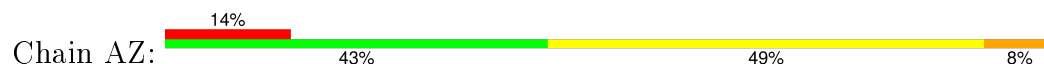
• Molecule 1: 16S rRNA







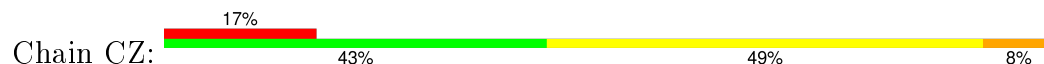
- Molecule 2: P and E-site tRNA(fMet)



- Molecule 2: P and E-site tRNA(fMet)



- Molecule 2: P and E-site tRNA(fMet)



- Molecule 2: P and E-site tRNA(fMet)



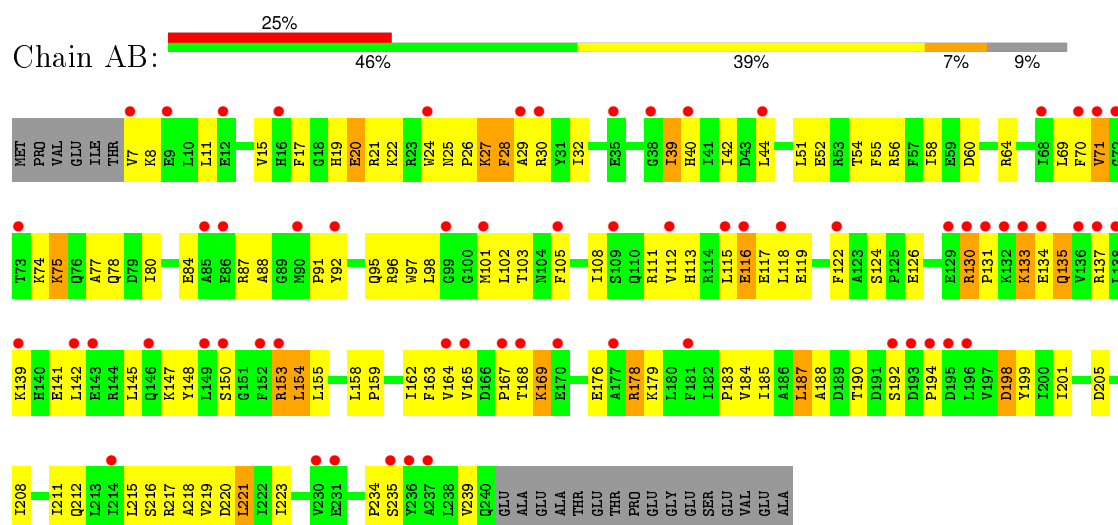
- Molecule 3: mRNA



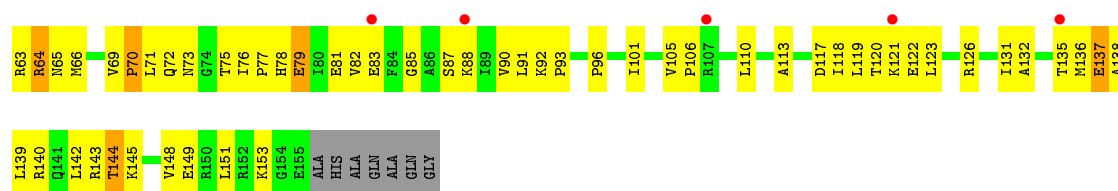
- Molecule 3: mRNA



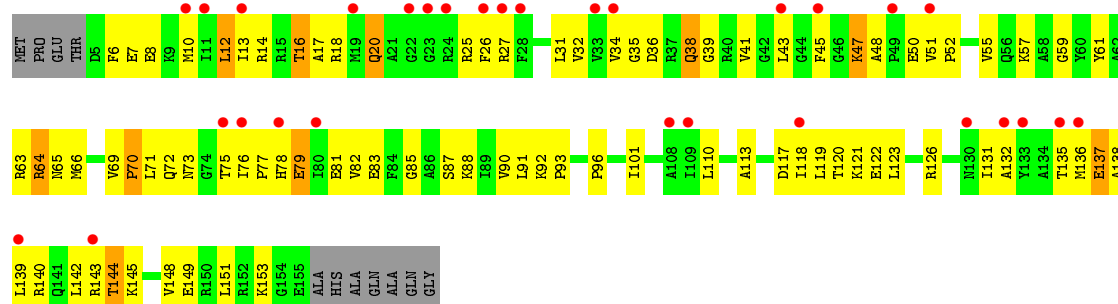
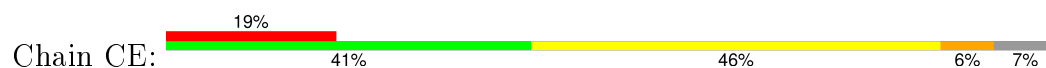
- Molecule 4: 30S ribosomal protein S2



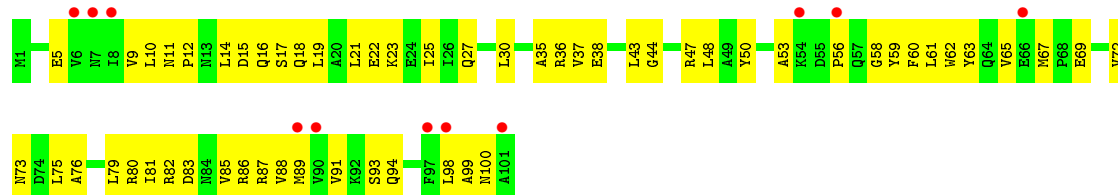




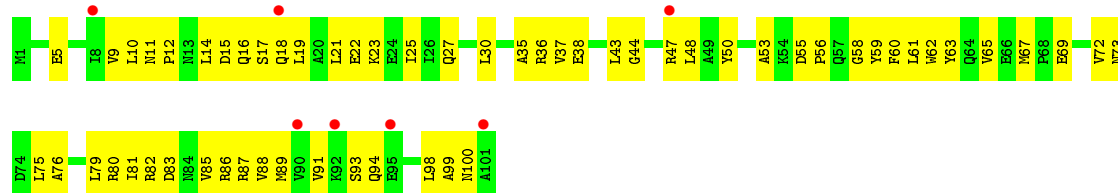
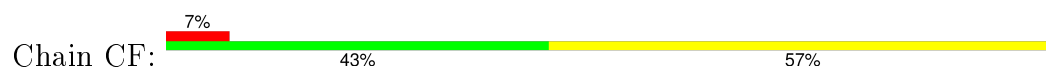
• Molecule 7: 30S ribosomal protein S5



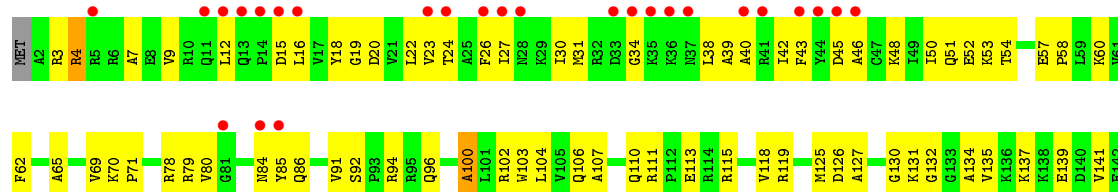
• Molecule 8: 30S ribosomal protein S6



• Molecule 8: 30S ribosomal protein S6



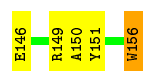
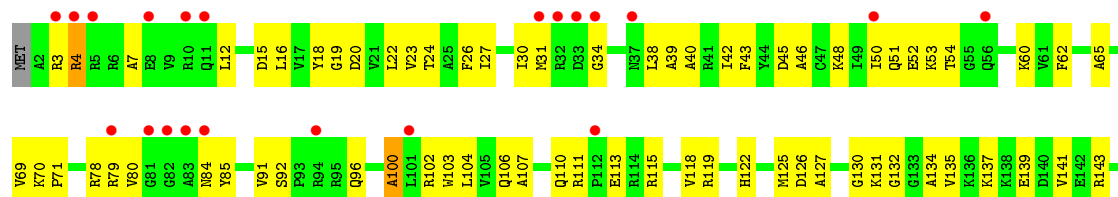
• Molecule 9: 30S ribosomal protein S7





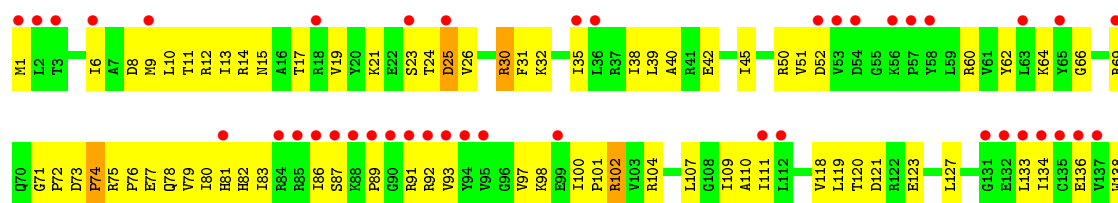
• Molecule 9: 30S ribosomal protein S7

Chain CG: 13% 52% 46%



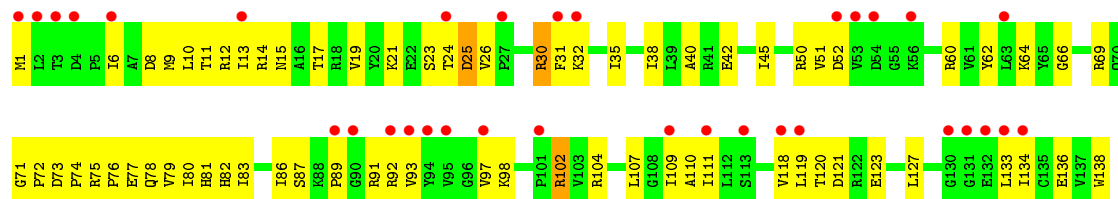
• Molecule 10: 30S ribosomal protein S8

Chain AH: 30% 47% 50%



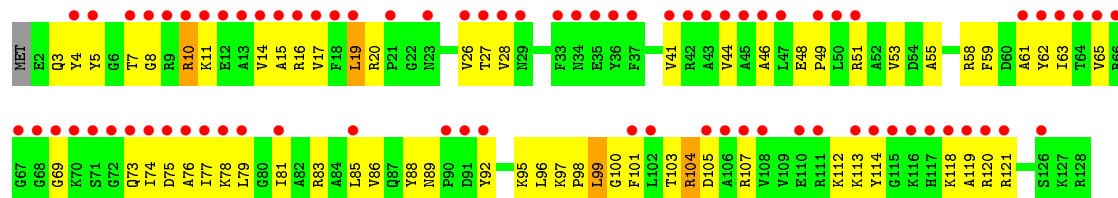
• Molecule 10: 30S ribosomal protein S8

Chain CH: 24% 49% 49%

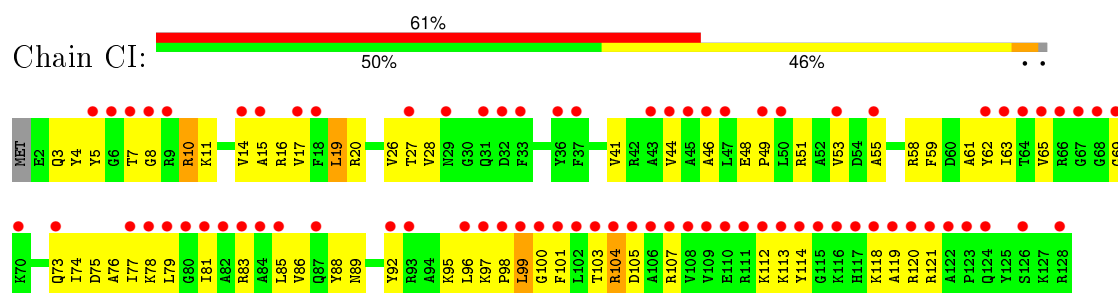


• Molecule 11: 30S ribosomal protein S9

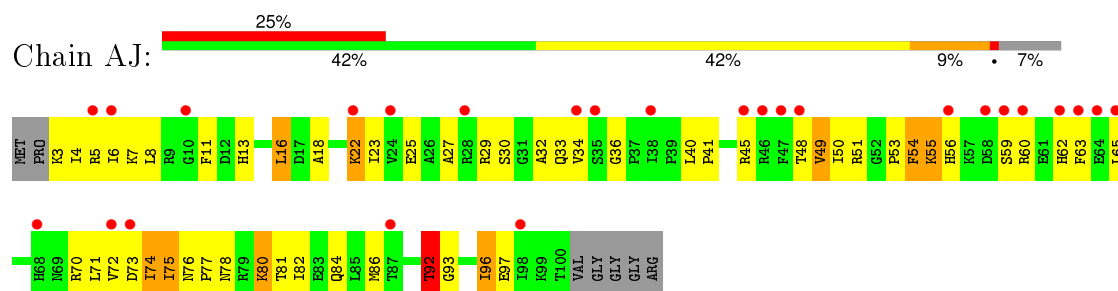
Chain AI: 61% 50% 46%



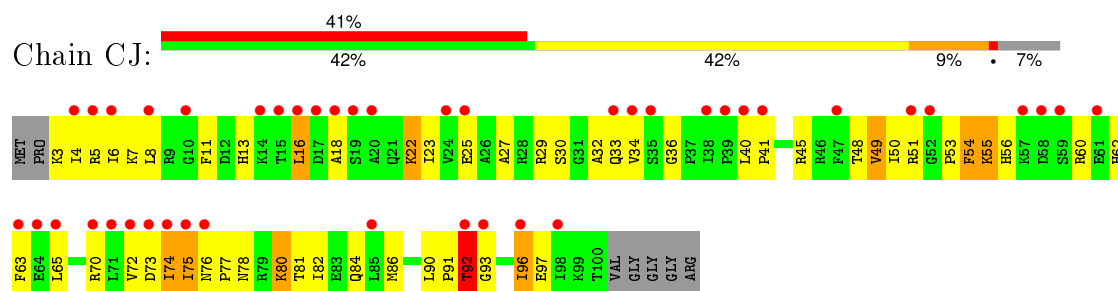
• Molecule 11: 30S ribosomal protein S9



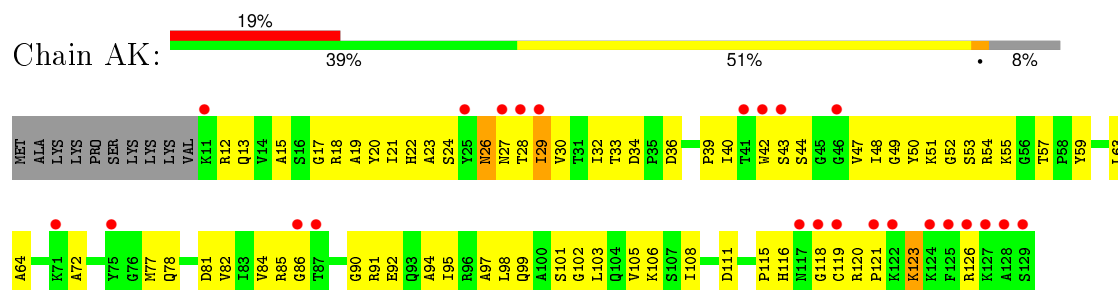
- Molecule 12: 30S ribosomal protein S10



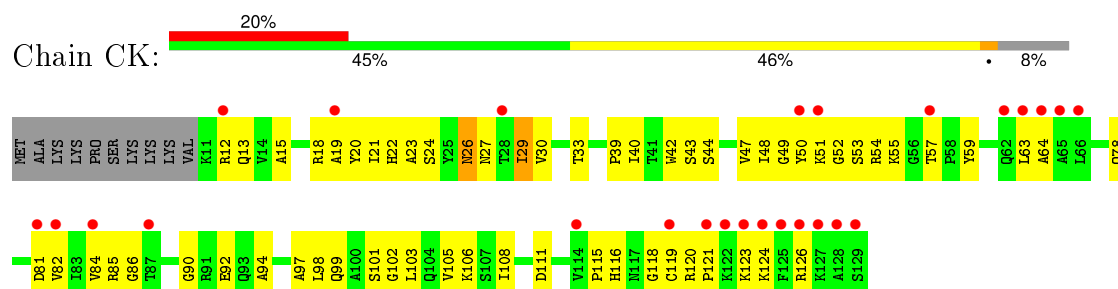
- Molecule 12: 30S ribosomal protein S10



- Molecule 13: 30S ribosomal protein S11

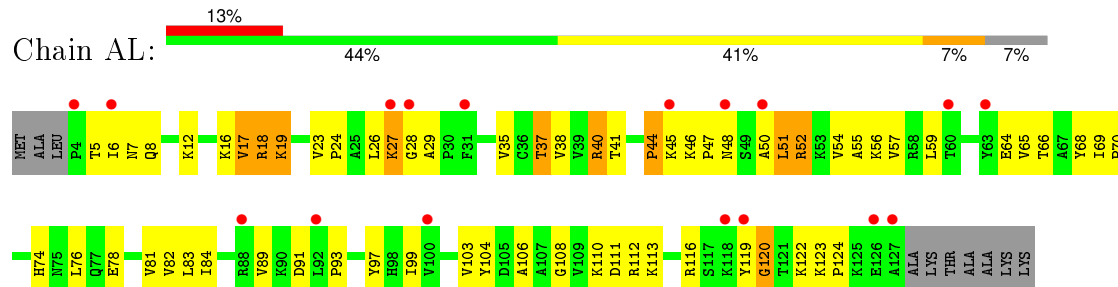


- Molecule 13: 30S ribosomal protein S11

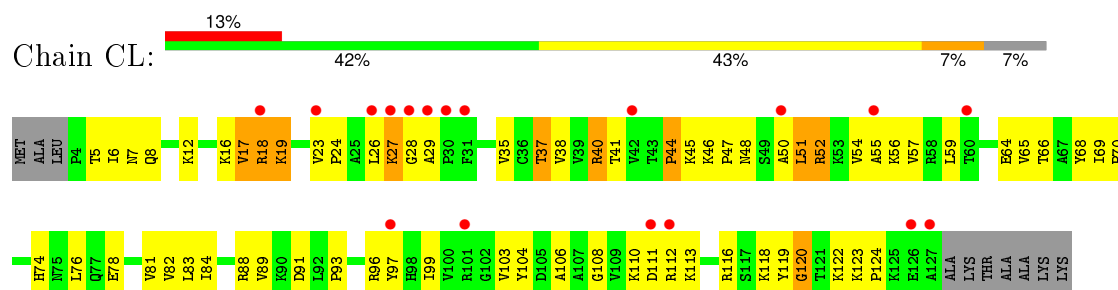




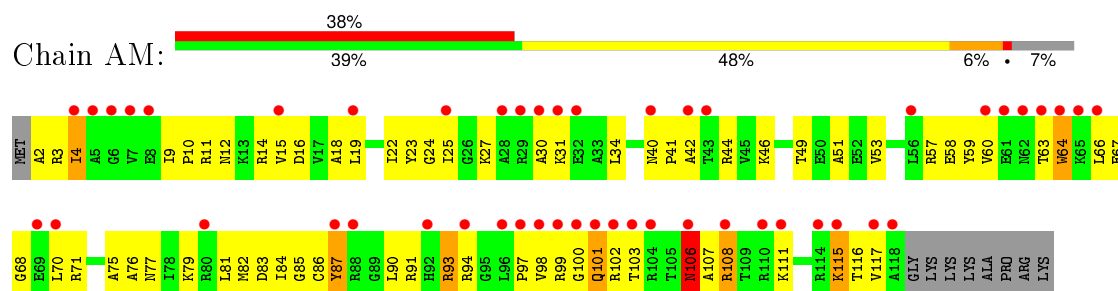
- Molecule 14: 30S ribosomal protein S12



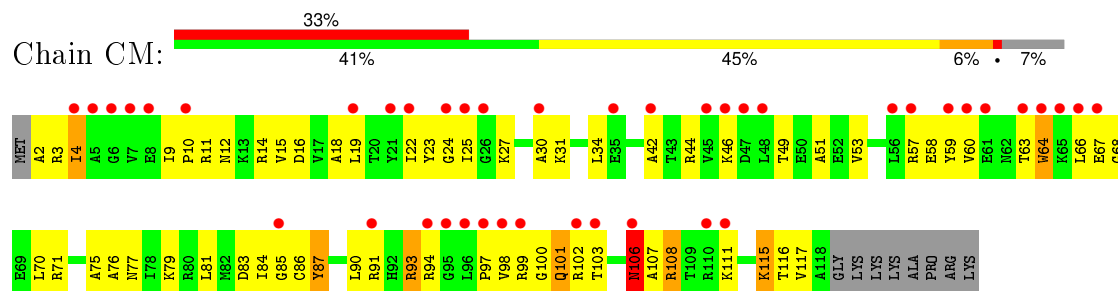
- Molecule 14: 30S ribosomal protein S12



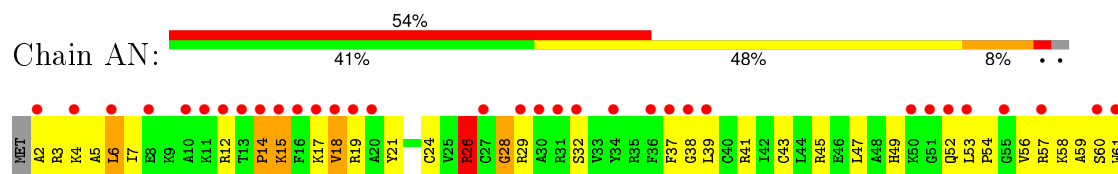
- Molecule 15: 30S ribosomal protein S13



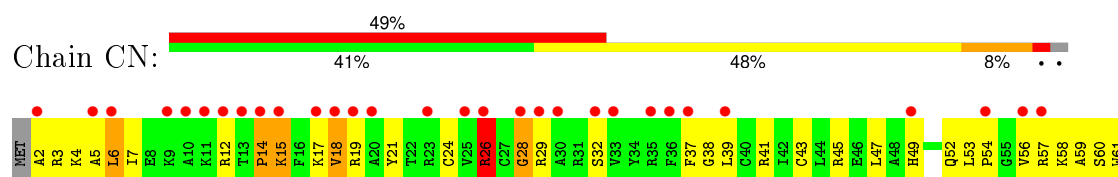
- Molecule 15: 30S ribosomal protein S13



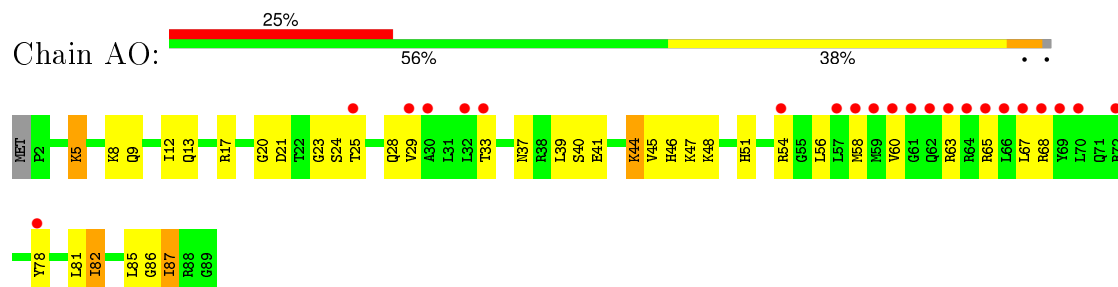
- Molecule 16: 30S ribosomal protein S14



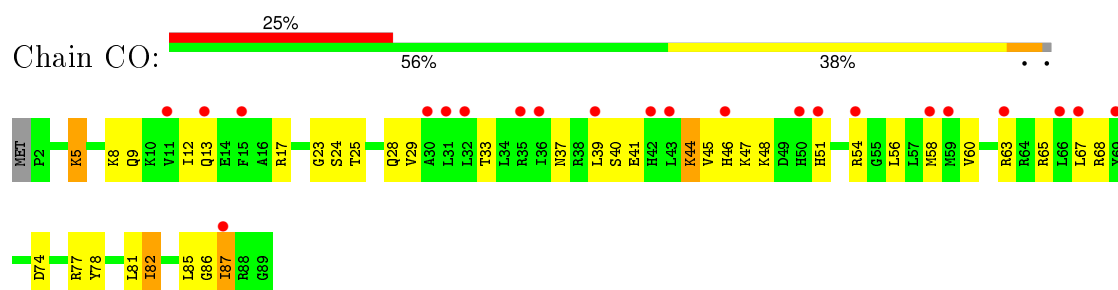
- Molecule 16: 30S ribosomal protein S14



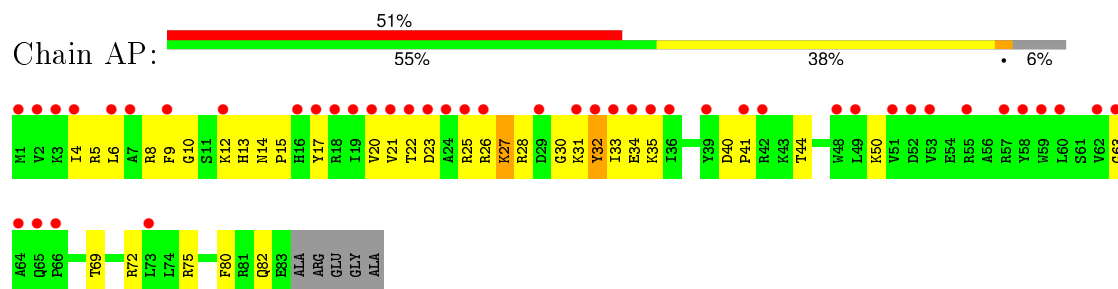
- Molecule 17: 30S ribosomal protein S15



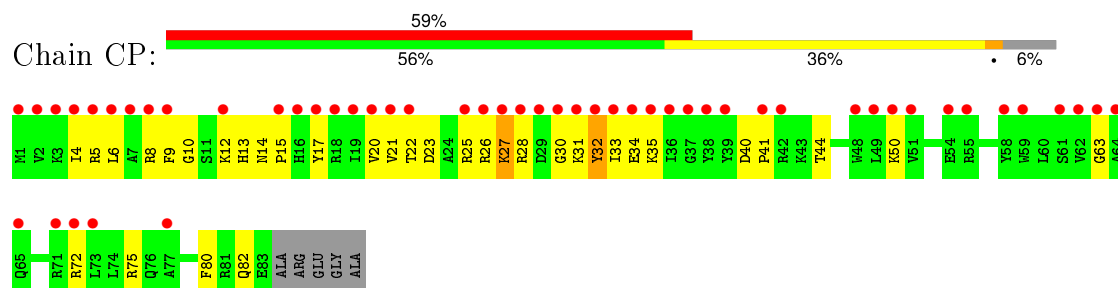
- Molecule 17: 30S ribosomal protein S15



- Molecule 18: 30S ribosomal protein S16

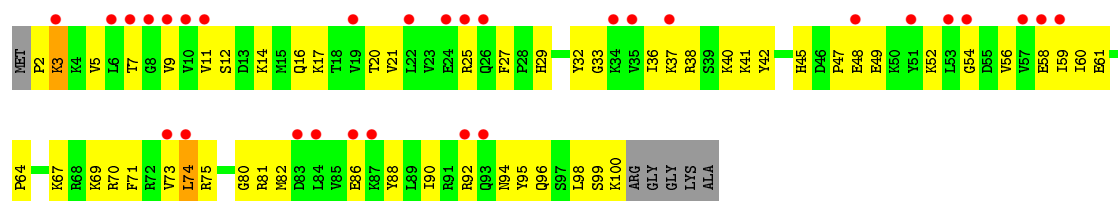


- Molecule 18: 30S ribosomal protein S16

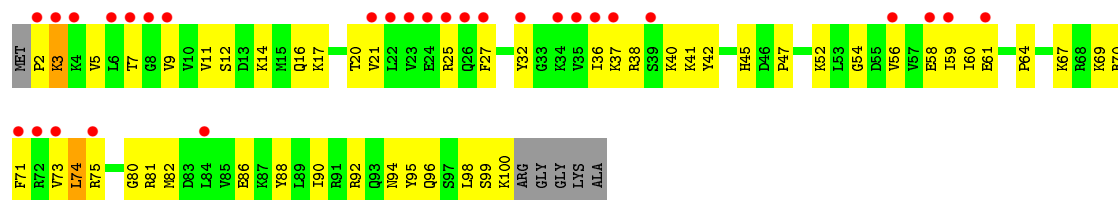


- Molecule 19: 30S ribosomal protein S17

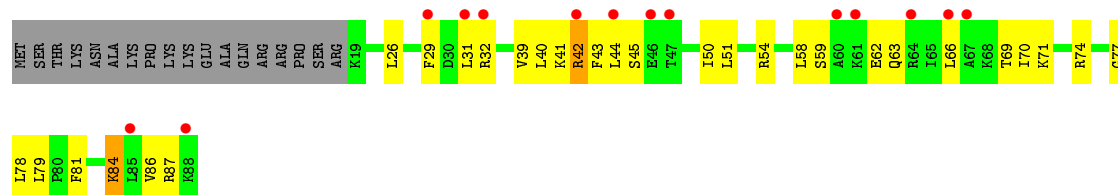




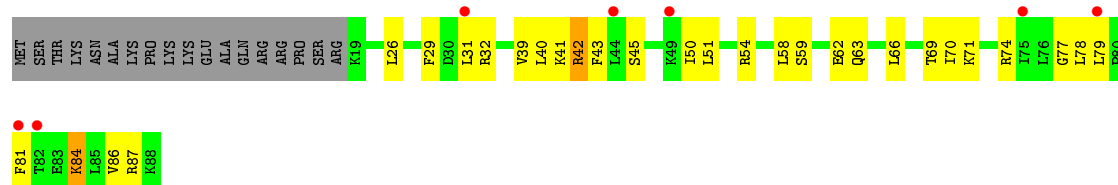
- Molecule 19: 30S ribosomal protein S17



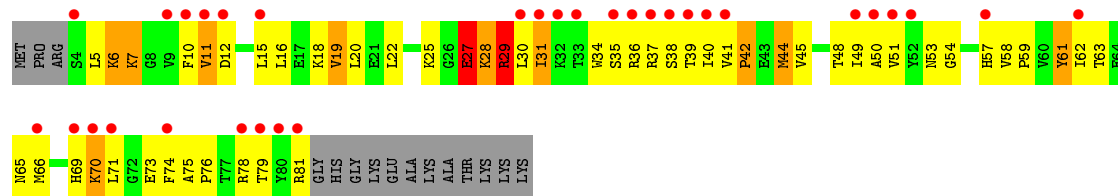
- Molecule 20: 30S ribosomal protein S18



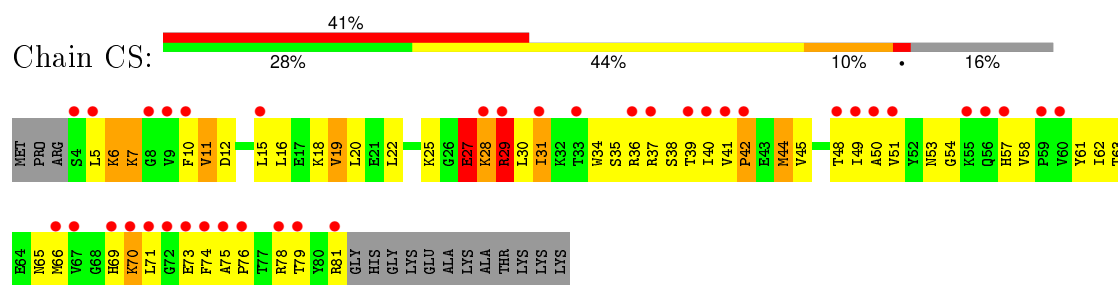
- Molecule 20: 30S ribosomal protein S18



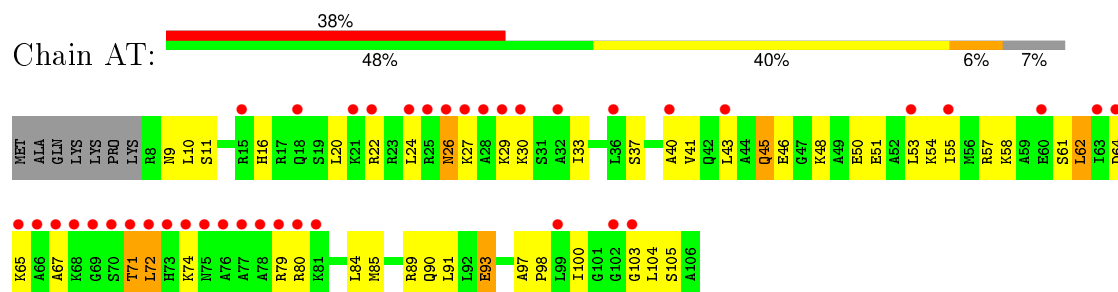
- Molecule 21: 30S ribosomal protein S19



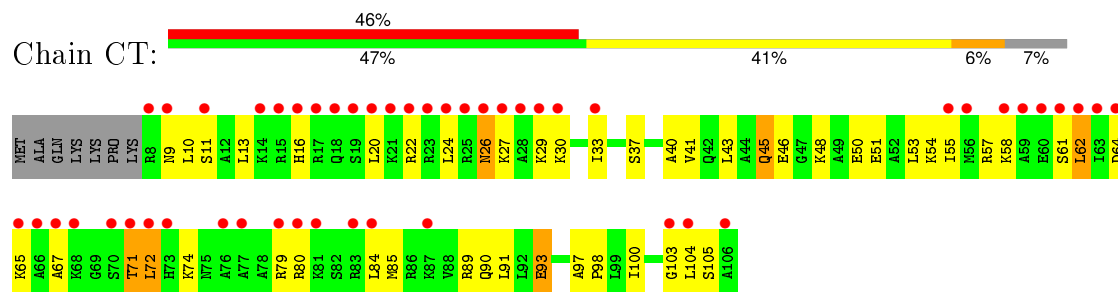
- Molecule 21: 30S ribosomal protein S19



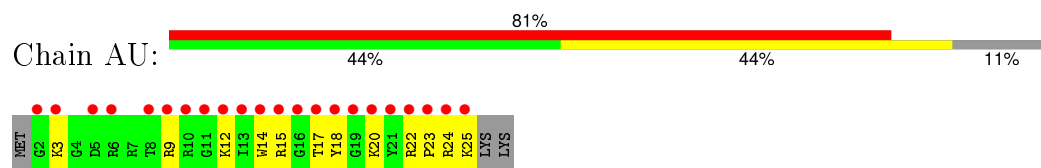
- Molecule 22: 30S ribosomal protein S20



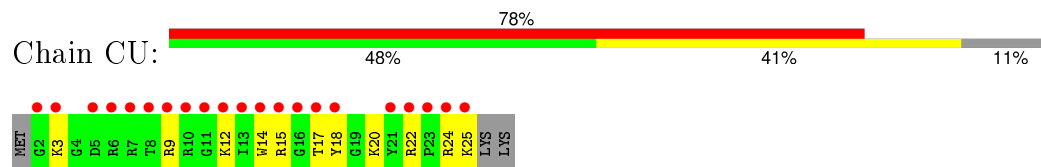
- Molecule 22: 30S ribosomal protein S20



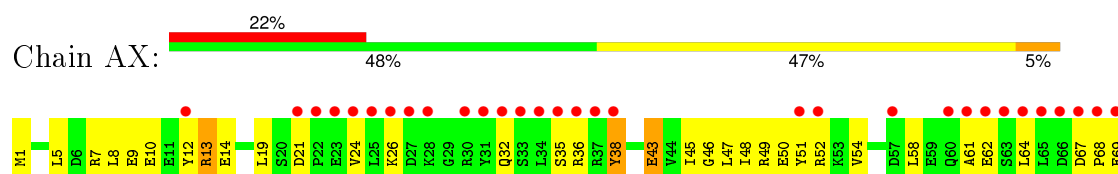
- Molecule 23: 30S ribosomal protein Thx

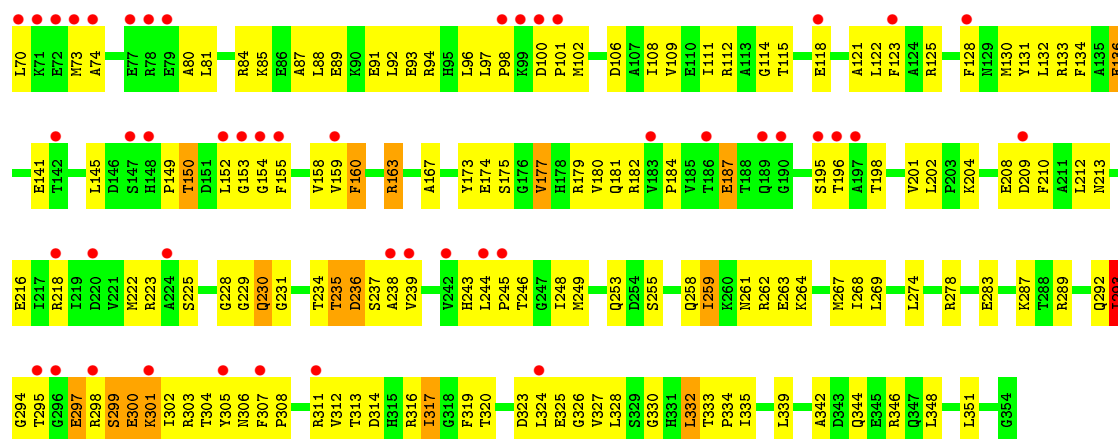


- Molecule 23: 30S ribosomal protein Thx

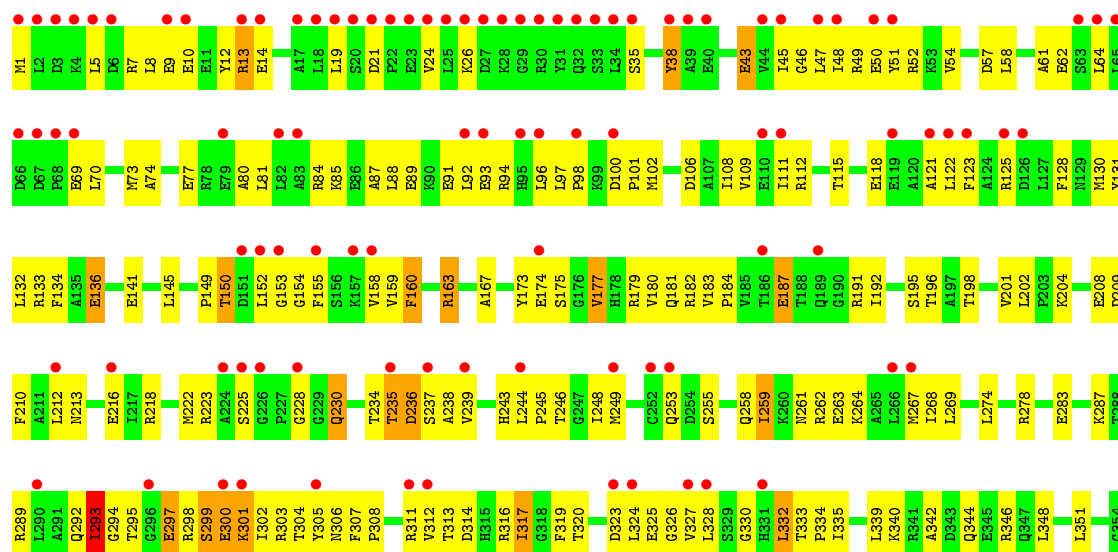


- Molecule 24: Peptide chain release factor 1

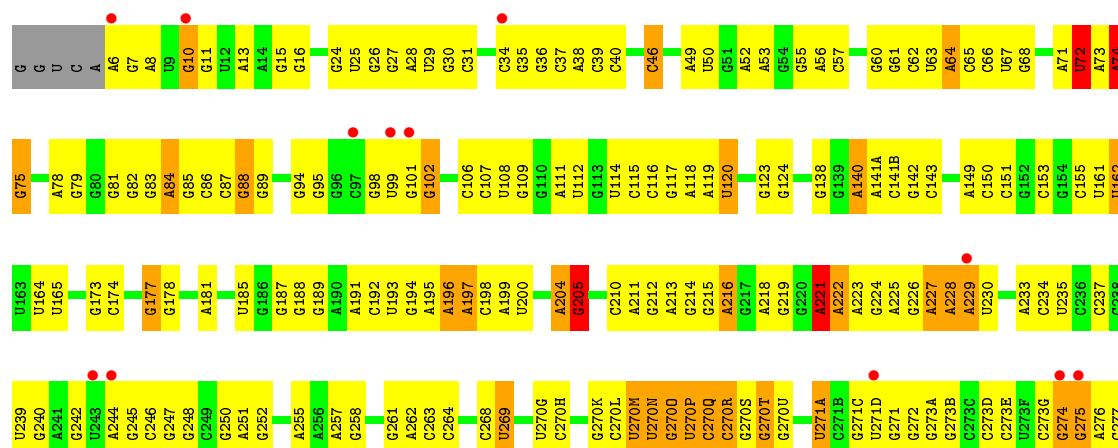




• Molecule 24: Peptide chain release factor 1

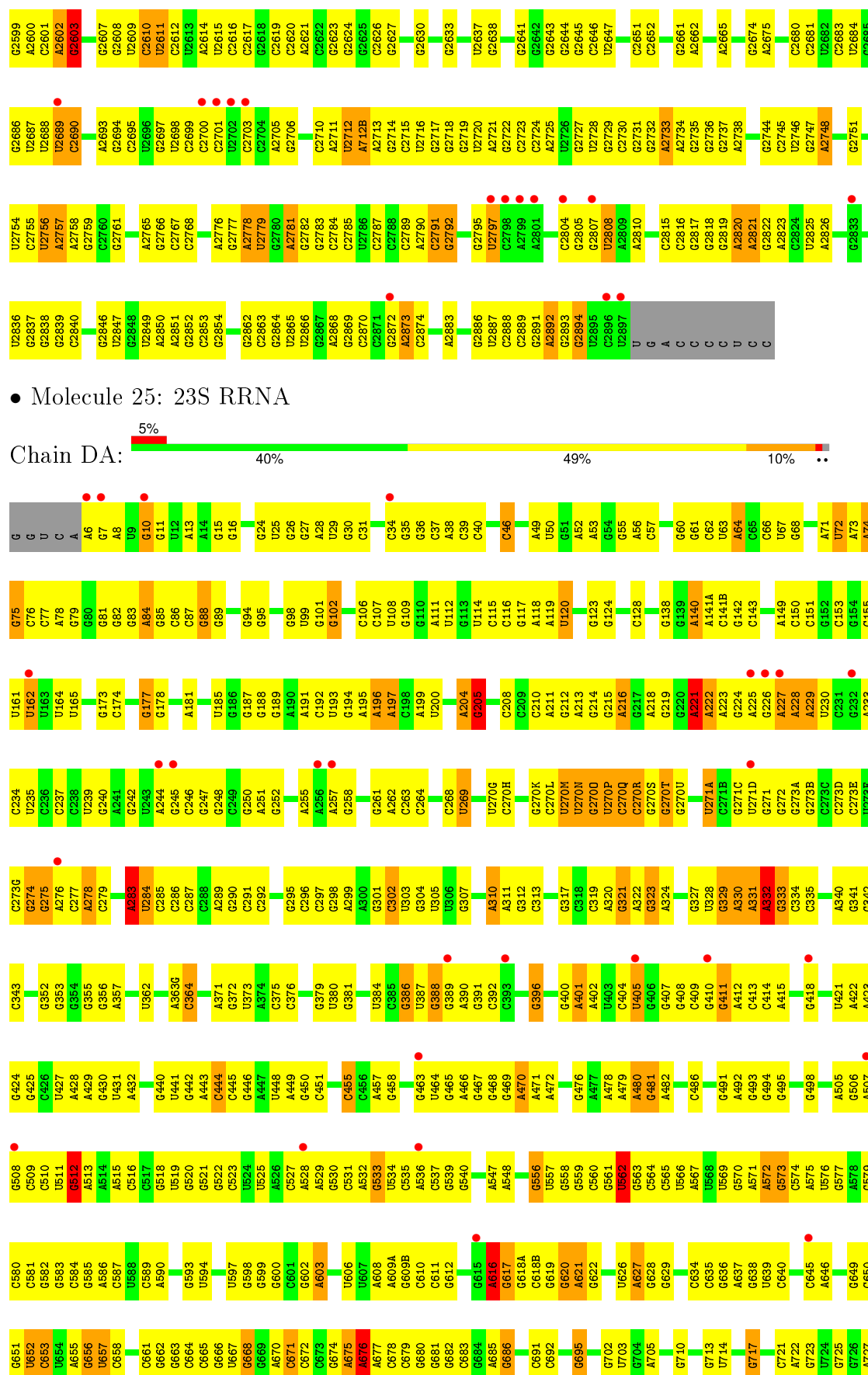


• Molecule 25: 23S RRNA



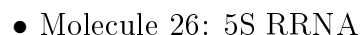
G1332	C1333	A1336	G1337	G1338	G1339	G1340	U1341	G1342	A1343	G1348	A1349	A1353	A1354	G1355	G1356	U1357	G1283	A1286	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	A1300	A1301	G1385	G1386	C1387	U1394	A1395	U1396	U1397	C1398	G1404	U1405	U1406	C1407	C1408	C1411	A1412	G1416	G1417	A1418	G1419	A1420											
U1263	G1264	A1265	G1266	G1267	A1268	G1269	G1270	A1271	A1272	U1273	A1274	A1275	G1276	G1277	A1278	G1279	U1282	U1283	U1286	G1289	G1290	G1291	G1292	G1293	G1294	G1295	G1296	G1297	G1298	G1299	A1300	A1301	G1385	G1386	C1387	U1394	A1395	U1396	U1397	C1398	G1404	U1405	U1406	C1407	C1408	C1411	A1412	G1416	G1417	A1418	G1419	A1420										
G1187	U1188	A1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	U1197	U1198	U1199	G1200	G1201	G1202	G1203	A1204	U1205	A1210	G1215	G1216	G1217	G1218	G1219	A1220	G1221	G1222	G1223	G1224	G1225	G1227	G1230	G1231	U1234	A1241	G1244	G1245	A1246	A1247	G1248	G1252	G1253	A1254	U1255	G1256	G1257	G1258	G1259	G1260	G1261	A1262											
U1105	G1106	U1107	U1108	A1111	U1112	U1113	G1114	G1115	G1120	G1121	G1122	G1125	A1126	A1127	A1128	A1129	U1130	U1131	U1132	G1135	G1136	G1137	U1138	U1139	U1140	U1141	U1142	U1143	A1144	G1145	G1151	C1152	G1153	G1154	A1155	C1161	G1162	U1165	C1166	U1167	G1168	G1173	A1174	U1175	U1176	A1177	C1178	G1183	G1184	C1185	A1186											
G1044	U1045	A1046	G1047	A1050	G1051	A1054	G1055	G1056	G1057	G1058	G1059	U1060	U1061	G1062	U1063	G1064	U1065	U1066	A1067	G1068	U1069	U1070	G1071	G1072	A1073	G1074	U1075	G1076	U1077	U1078	U1079	C1080	U1081	U1082	U1083	A1084	A1085	U1086	U1087	U1088	G1089	U1090	A1091	G1092	U1093	U1094	A1095	A1096	U1097	U1098	G1099	C1100	U1101	G1102	A1103							
G968	U969	C970	C971	G972	A973	G974	G975	G976	G977	G978	G979	G982	G983	G984	G985	G986	G987	G988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	G1002	G1003	G1004	C1005	G1006	G1007	G1008	A1009	U1010	G1011	U1012	C1013	U1014	G1015	U1019	A1020	A1021	G1022	U1023	G1024	G1025	U1026	U1027	A1028	A1029	G1030	U1033	G1034	U1035	G1039	C1040
G892	G893	U894	U895	A896	C897	G904	U905	G906	U907	C908	U909	A910	A911	G914	C915	G916	A917	A918	G919	G920	C923	C924	G929	U930	G931	G932	G933	G934	U937	U938	G939	C940	U941	U942	U943	G944	A945	G946	G950	C951	G952	A953	U954	C955	G956	U957	U958	A959	A960	C961	G962	U963										
U813	C814	C815	C816	A819	G823	A824	C825	U826	U827	U828	A829	G830	G831	G832	U833	C834	A835	G836	U839	C840	G845	G846	U847	G848	A849	G850	U851	G852	G853	G854	G855	C856	U857	C858	U859	A860	G861	G862	A863	G864	G865	G866	U867	U868	U869	A870	U871	C876	U877	C886	A887	C888	C889	A890								
G739	U740	G741	G742	G743	A746	U747	G755	G756	U757	U762	U763	A764	G765	G766	U767	G768	G769	G770	G771	G772	U773	A774	G775	G776	A777	A782	A783	A784	G785	A788	A789	G790	C791	G792	G793	G794	G795	G796	G797	G798	A800	G801	A802	U803	A804	G805	C806	U807	G808	G809	U810	U811	C812									
G662	G663	G664	G665	G666	U667	G668	G669	A670	G671	G672	G673	A675	A676	G677	G678	G679	G680	G681	G682	G683	G684	A685	G686	C691	G692	G695	G702	U703	A705	A706	G710	G713	U714	G715	A716	G717	C721	A722	G723	U724	G725	A726	G727	G728	U729	C730	G733	G738														
G585	A586	C587	U588	G589	A590	G593	U597	G598	G599	G600	A603	U606	U607	G608	A609	G609B	C610	C611	G612	G615	A616	G617	G618	G618B	G619	G620	A621	G622	U626	A627	C634	G635	G636	A637	G638	U639	C640	C645	A646	G649	C650	G651	U652	G653	U654	A655	G656	C657	G658	C659	C660											
A513	A514	C516	G517	G518	U519	G520	G521	G522	C523	U524	U525	A526	C527	A528	A529	C531	A532	G533	U534	C535	A536	C537	G538	G539	G540	A547	A548	G556	U557	G558	G559	C560	G561	U562	G563	C564	C565	U566	A567	U568	U569	G570	A571	A572	G573	C574	A575	U576	G577	A578	G579	C580	C581	G582	U583	C584						
G430	U431	A432	G440	U441	G442	A443	C444	G445	G446	U447	U448	A449	A450	C451	U455	G456	A457	G458	G463	U464	G465	A466	G467	G468	G469	A470	A471	G473	G476	A477	A478	A479	A480	G481	A482	C486	G491	A492	C493	A494	G495	G498	A505	G506	A507	G508	C509	C510	U511	G512												
A278	C279	A282	A283	U284	C285	C286	C287	C288	A289	C290	C291	C292	G295	C296	C297	G298	A299	A300	G301	C302	U303	G304	U305	U306	G307	A310	A311	G312	C313	G317	G318	G319	A320	G321	A322	G323	A324	G329	A330	A331	A332	G333	G334	G335	A340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354			

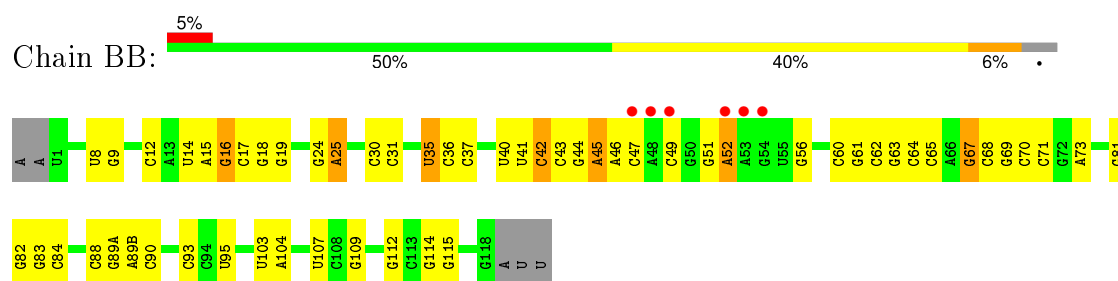
G1421	G1422	C1506	C1508	C1509	A1510	A1511	U1516	U1517	U1518	C1588	C1589	C1590	C1591	G1594	G1595	C1598	C1599	C1600	C1601	C1602	A1603	C1607	C1608	C1609	A1610	G1613	C1614	C1615	C1616	C1617	A1618	C1619	C1620	G1630	C1631	A1632	A1633	G1639	C1640	C1641	C1642	G1646	C1647	G1478	G1479	G1483	G1484	G1485	A1486	A1490	G1491	G1492	C1493	A1494	A1495	A1496	U1497	C1498	C1499	C1504	C1505
A1427	C1428	U1775	C1782	A1783	A1784	A1785	A1786	A1787	C1788	A1789	C1790	C1791	C1792	C1793	U1794	U1795	C1796	C1797	U1798	C1799	C1800	C1801	C1802	A1803	A1809	A1810	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	A1821	G1824	C1825	C1826	C1827	C1828	A1829	C1830	C1831	C1832	C1833	U1834	C1837	C1838	C1839	U1840	C1841	C1842	C1843	C1844						
A1847	A1848	U1938	U1939	G1945	U1946	G1949	G1950	U1951	C1952	C1953	C1954	U1955	C1961	C1962	C1963	C1964	C1965	A1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1975	C1976	C1977	C1978	C1979	C1980	C1981	C1982	C1983	C1984	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	G2002	C2007	C2008	C2009	C2010	C2011	C2012	A2013	A2014					
A2015	G2018	A2019	A2020	C2021	U2022	G2023	C2026	C2027	C2028	C2029	A2030	A2031	C2032	C2033	U2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041	A2042	C2043	C2046	C2050	C2051	C2052	C2053	A2054	C2055	C2056	C2057	A2058	C2059	A2060	G2061	C2062	C2065	U2068	C2069	C2070	A2071	C2072	C2073	C2074	U2075	C2076	A2077	C2078	C2079	C2080	C2081								
G2087	U2088	G2090	U2091	U2092	C2093	C2094	C2095	U2096	C2097	C2098	U2099	G2100	G2101	U2102	C2103	C2104	C2105	C2107	C2108	U2109	C2110	C2111	C2112	C2113	C2114	C2115	C2116	C2117	C2118	C2119	C2120	C2121	U2122	C2123	C2124	C2125	A2126	C2127	C2128	C2129	U2130	C2131	C2132	C2133	C2134	A2135	C2136	C2137	C2138	C2139	C2140	C2141	C2142	U2143	C2144	C2145					
C2146	C2147	C2148	C2149	U2150	C2151	C2154	C2155	C2156	C2157	C2158	C2159	C2160	C2164	C2165	C2166	C2167	C2168	A2169	C2170	C2171	C2172	C2173	C2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184	C2185	C2186	U2189	C2190	C2193	C2194	C2195	C2196	U2197	C2198	A2199	C2200	C2201	C2202	C2203	C2204	C2205	C2206	C2207	C2210	C2211	C2212	U2213	C2215	C2219			
G2224	A2225	C2226	C2227	C2228	C2229	C2230	C2238	C2239	C2240	A2241	C2242	U2243	U2244	U2245	U2246	C2250	C2251	C2258	C2259	C2260	C2261	U2262	C2263	C2264	A2268	C2271	U2272	C2273	C2274	C2275	C2276	C2277	C2282	C2283	C2284	C2285	C2286	A2287	C2288	C2289	C2290	U2291	C2292	C2293	C2294	C2295	C2298	C2299	C2300	C2301	C2302	C2303									
C2304	C2305	C2306	C2307	C2311	C2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	C2320	C2321	C2322	C2325	C2326	C2327	C2328	C2331	C2332	C2333	C2334	C2335	C2336	C2337	C2338	C2339	C2340	C2341	C2342	C2343	C2344	C2345	C2346	C2347	C2350	C2351	U2357	C2358	C2359	A2360	C2364	C2365	C2370	C2371	C2372	C2373	C2374	C2375	C2376	C2377									
C2378	C2379	C2380	C2381	C2382	C2383	C2384	C2385	C2389	U2390	C2391	C2392	C2393	C2394	C2395	C2396	C2399	C2400	C2401	C2402	U2406	C2407	C2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	A2430	U2431	C2435	C2436	U2437	C2438	C2439	C2440	C2441	C2442	C2443	C2444								
C2445	C2446	C2447	C2448	U2449	C2452	C2453	C2454	C2455	C2456	C2457	C2458	C2459	C2460	C2461	C2462	C2467	C2468	C2469	C2470	C2471	C2472	C2476	C2477	C2478	C2479	C2480	C2481	C2484	C2485	C2486	C2487	C2488	C2489	C2490	C2491	C2492	C2493	C2494	C2495	C2496	C2497	C2498	C2502	C2503	U2504	C2505	C2506	C2507	C2508	C2509	C2513	C2514	C2515	C2516	C2517	C2518					
C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	C2530	C2531	C2532	C2533	C2534	C2535	C2536	C2537	C2538	C2542	C2543	C2544	C2550	C2551	C2552	C2553	C2554	C2555	C2556	C2557	C2558	C2561	C2562	C2563	C2564	C2565	C2566	C2567	C2572	C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2585	C2588	C2589	C2591	C2592	C2593	C2594	C2595	C2596	C2597	C2598		



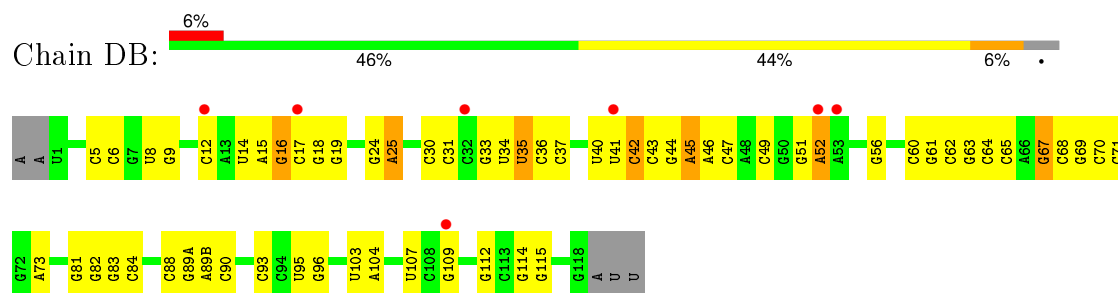




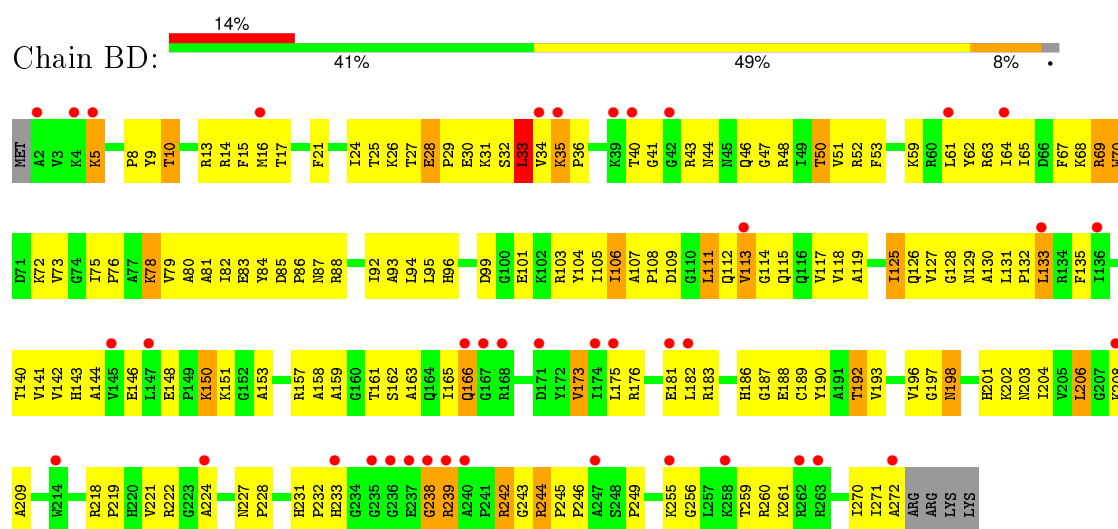




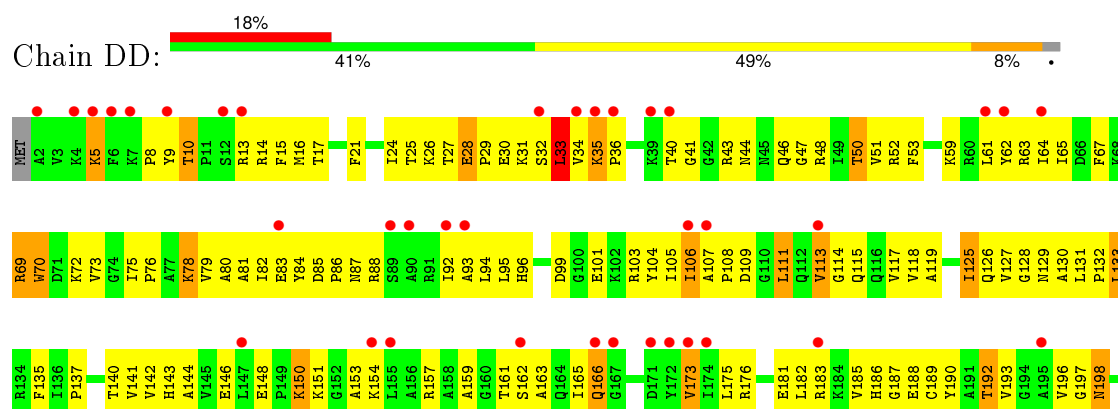
• Molecule 26: 5S rRNA



• Molecule 27: 50S ribosomal protein L2

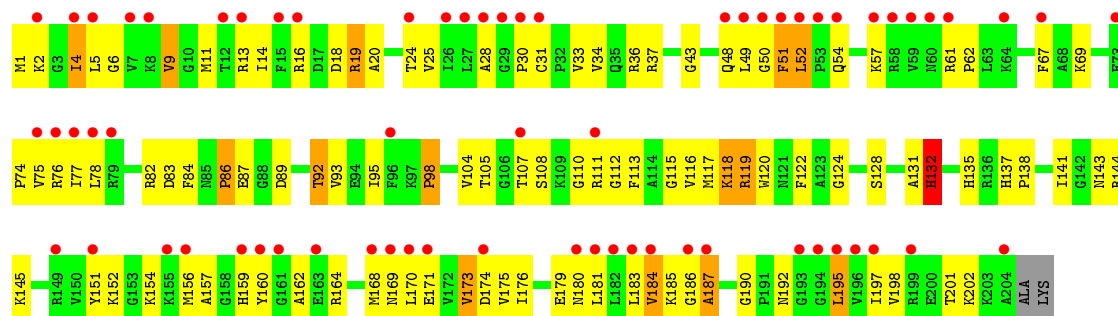


• Molecule 27: 50S ribosomal protein L2

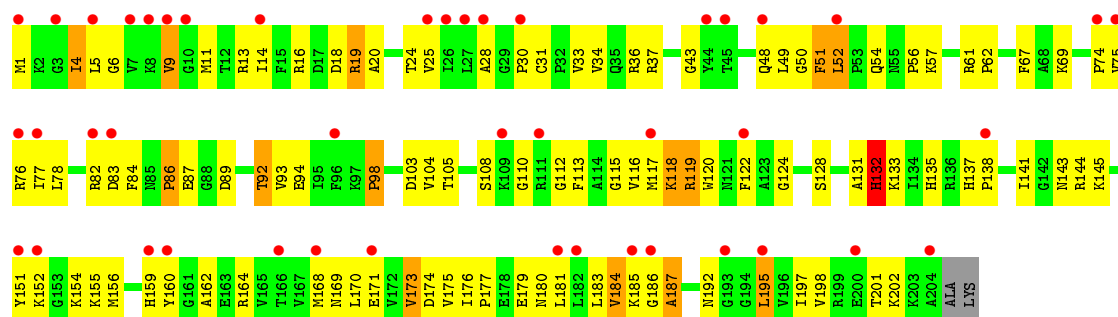




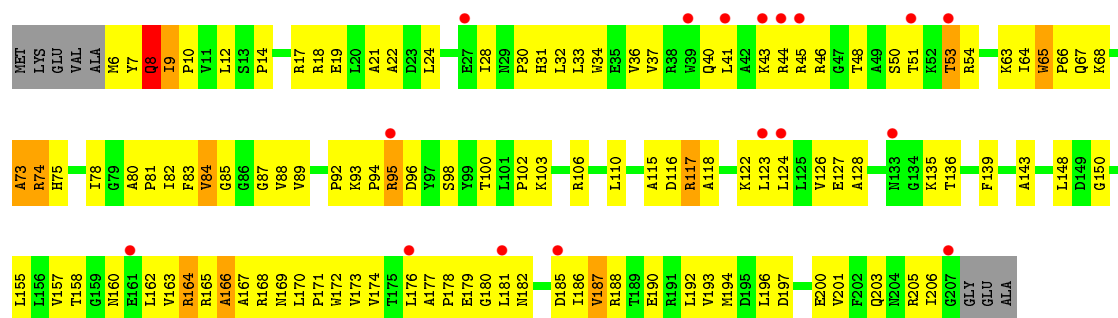
• Molecule 28: 50S ribosomal protein L3



• Molecule 28: 50S ribosomal protein L3

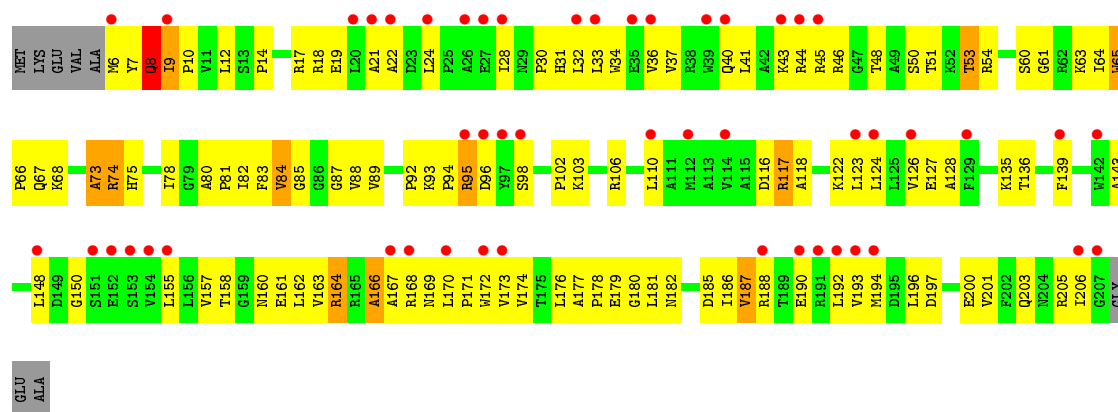


• Molecule 29: 50S ribosomal protein L4

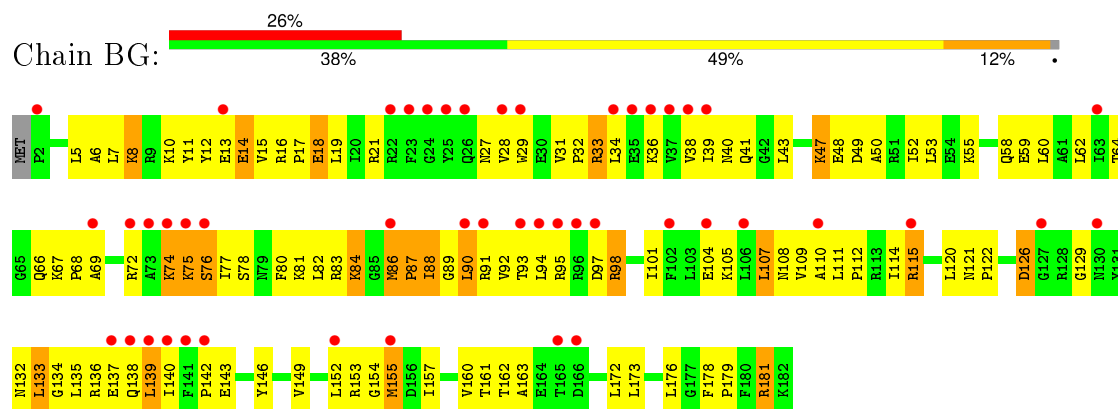


• Molecule 29: 50S ribosomal protein L4

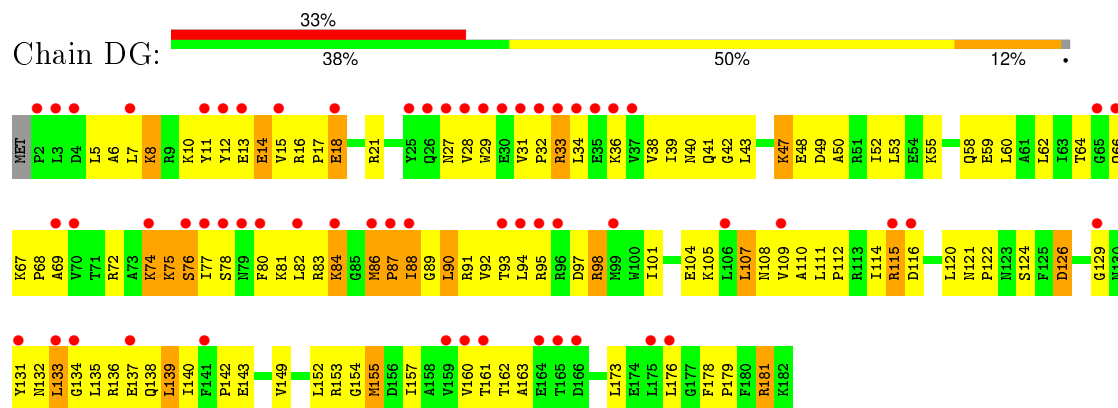




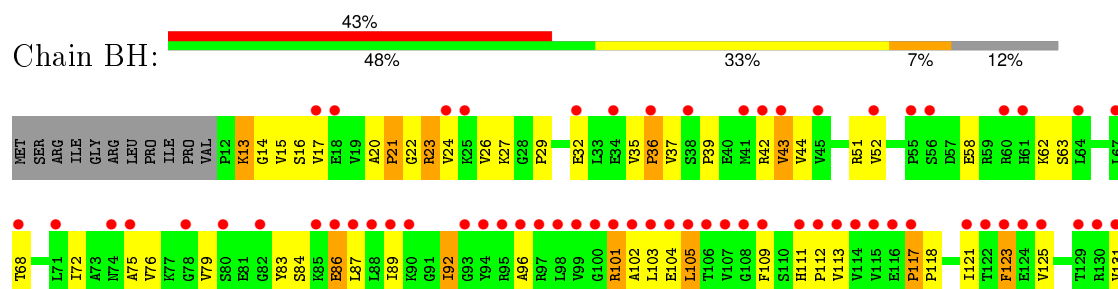
• Molecule 30: 50S ribosomal protein L5

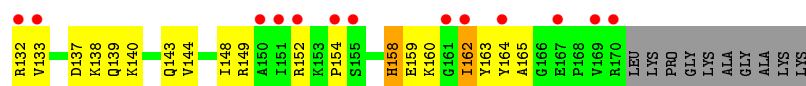


• Molecule 30: 50S ribosomal protein L5

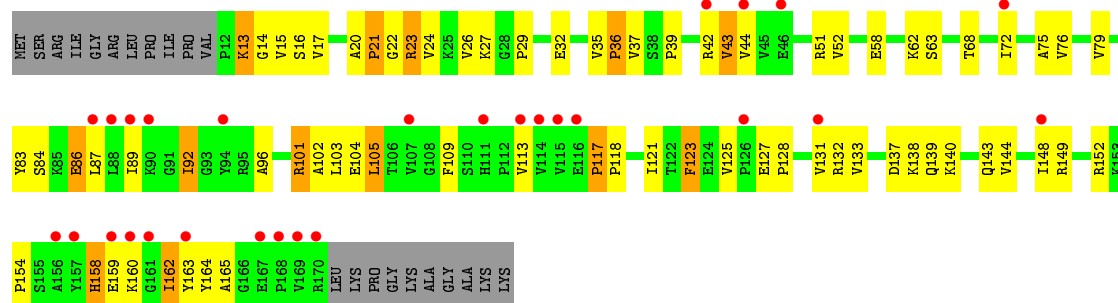


• Molecule 31: 50S ribosomal protein L6

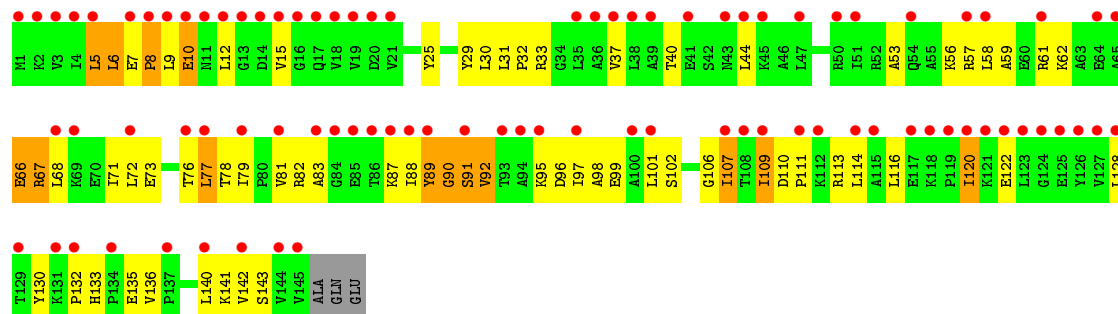




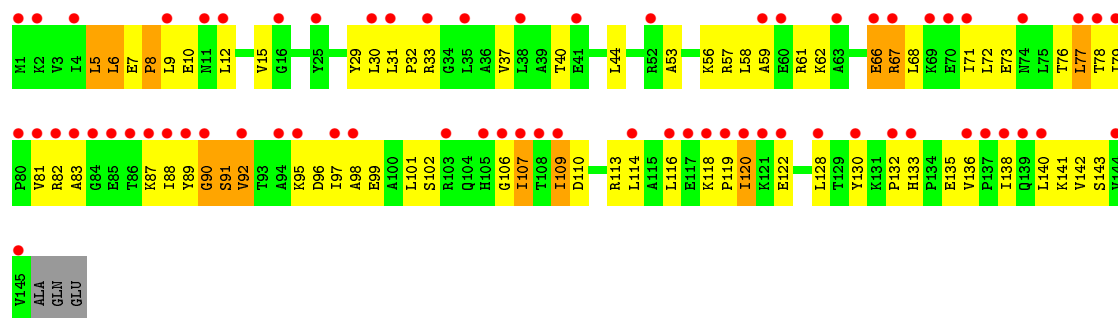
• Molecule 31: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L9

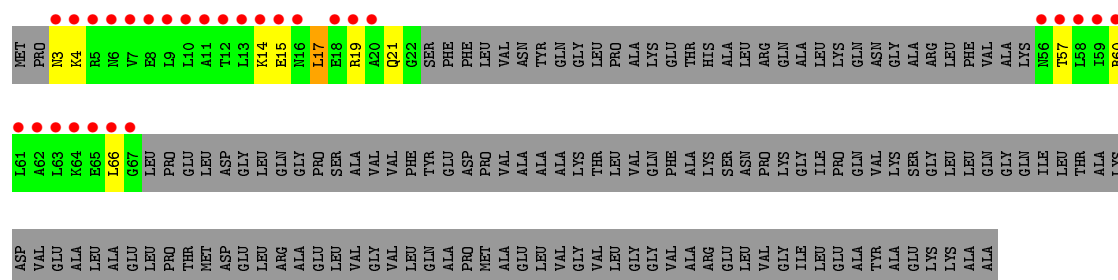


• Molecule 32: 50S ribosomal protein L9

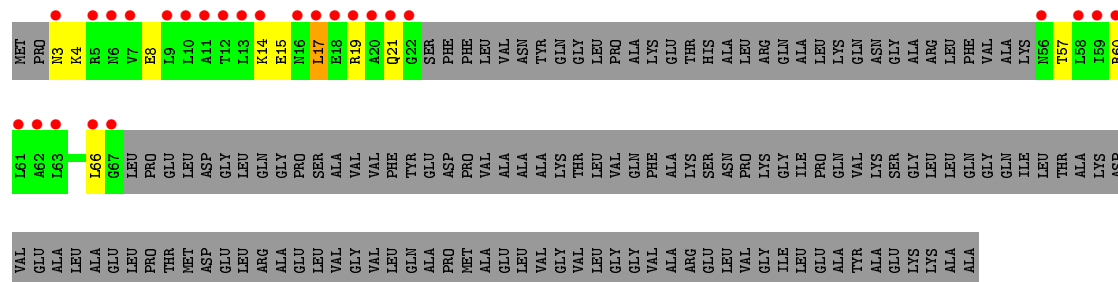


• Molecule 33: 50S ribosomal protein L10

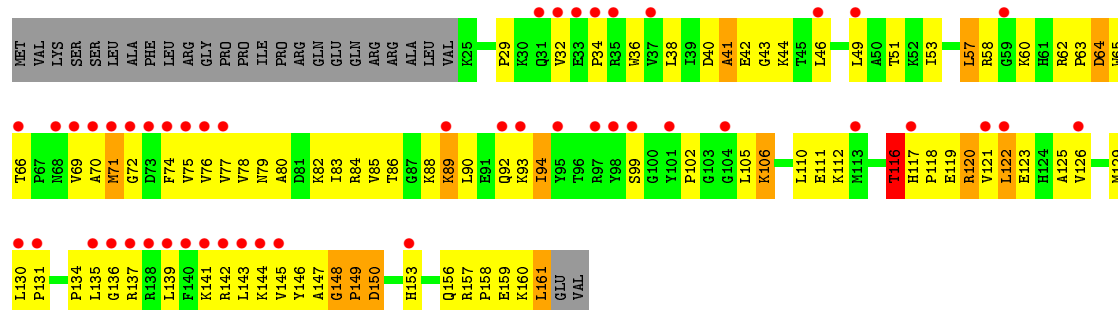




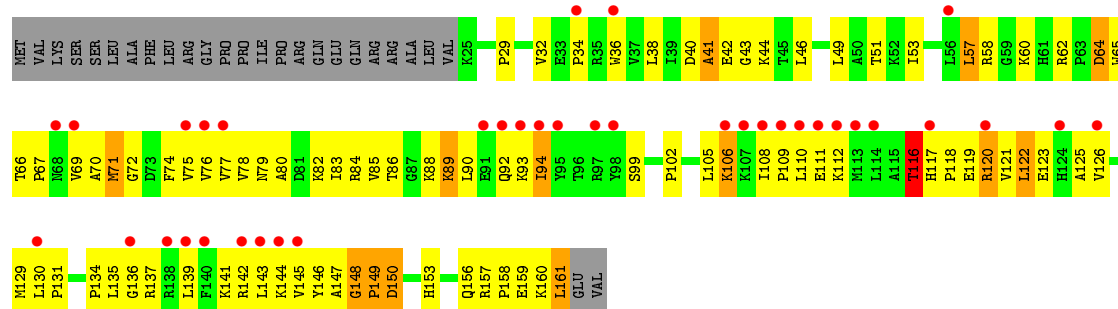
• Molecule 33: 50S ribosomal protein L10



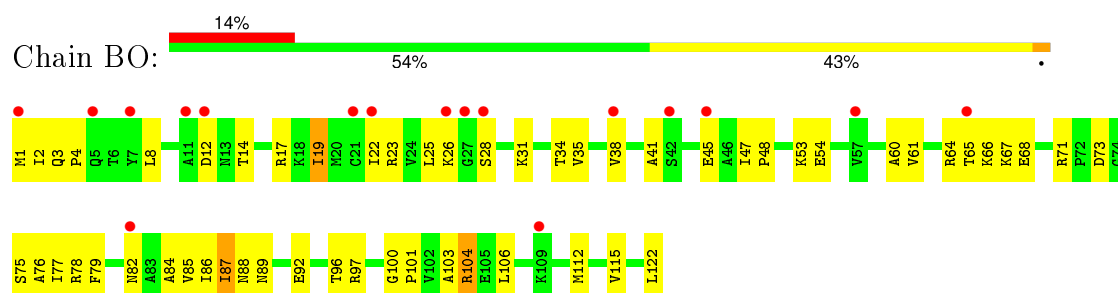
• Molecule 34: 50S ribosomal protein L13



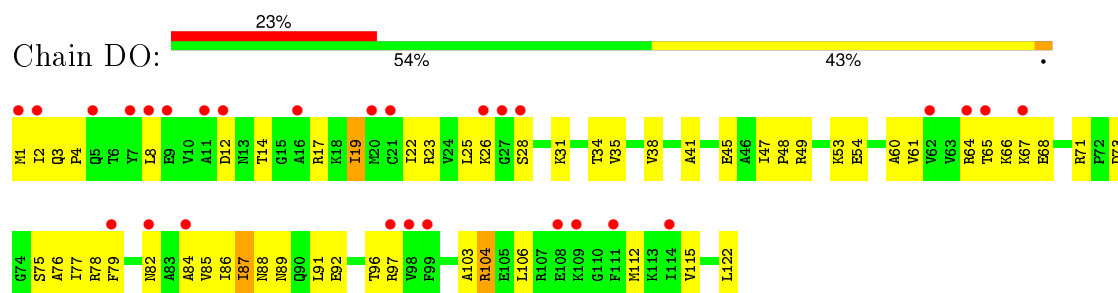
• Molecule 34: 50S ribosomal protein L13



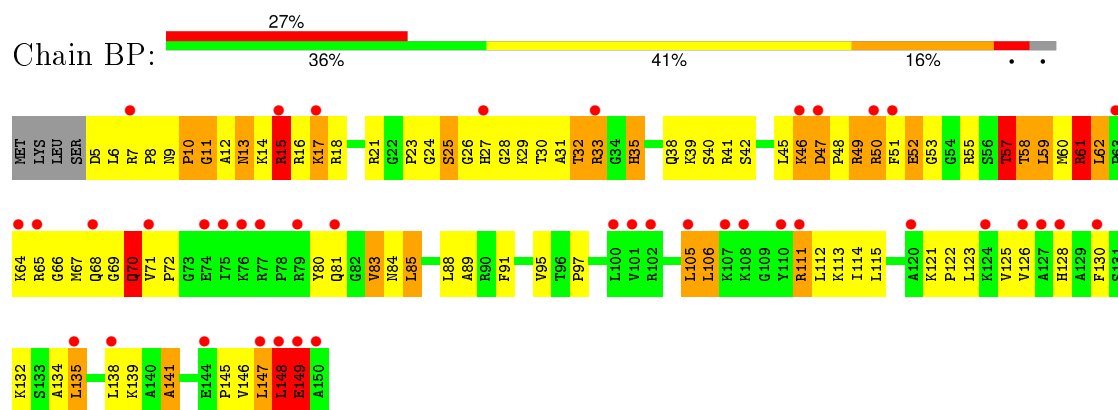
• Molecule 35: 50S ribosomal protein L14



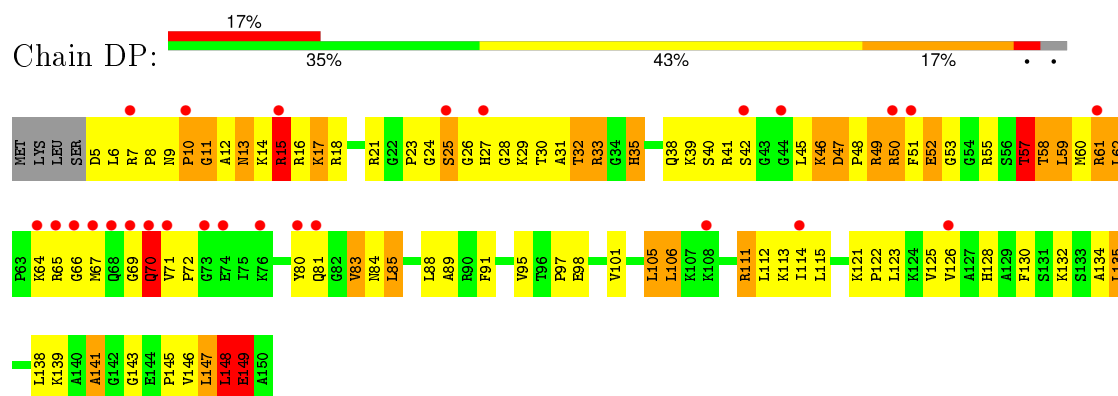
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15



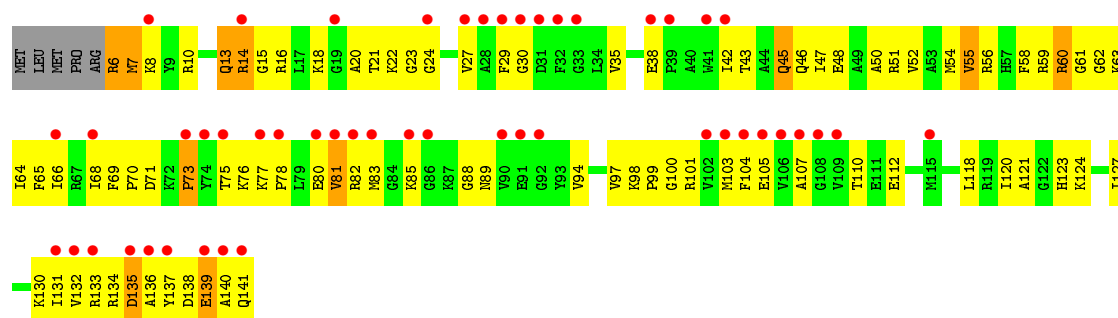
- Molecule 36: 50S ribosomal protein L15



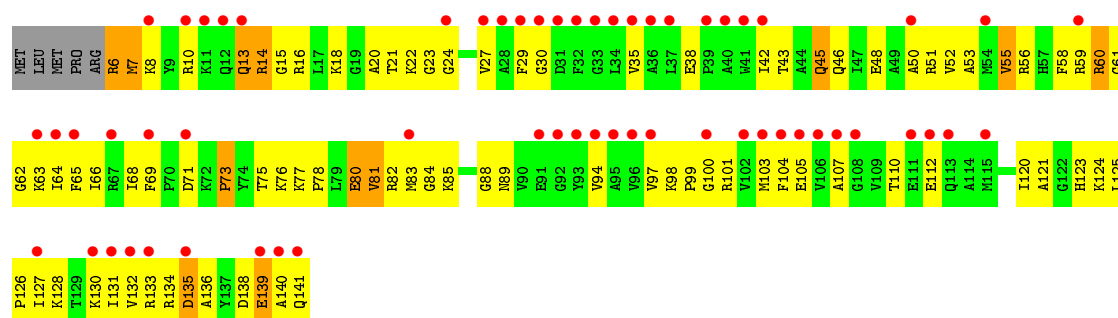
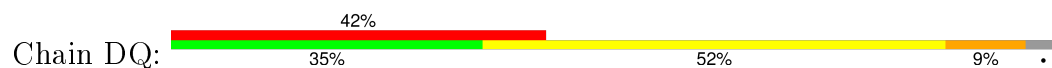
- Molecule 37: 50S ribosomal protein L16



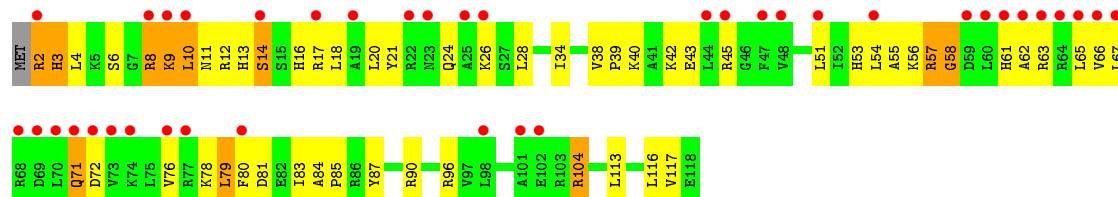




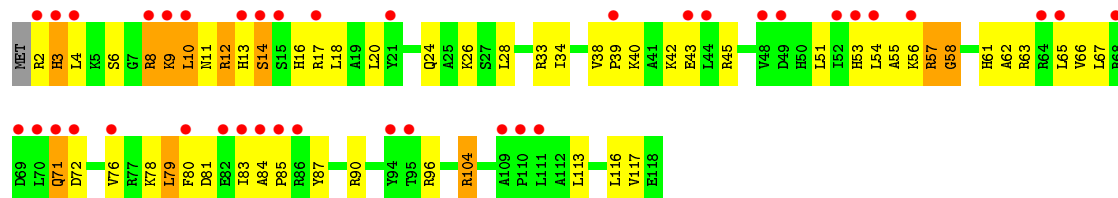
- Molecule 37: 50S ribosomal protein L16



- Molecule 38: 50S ribosomal protein L17

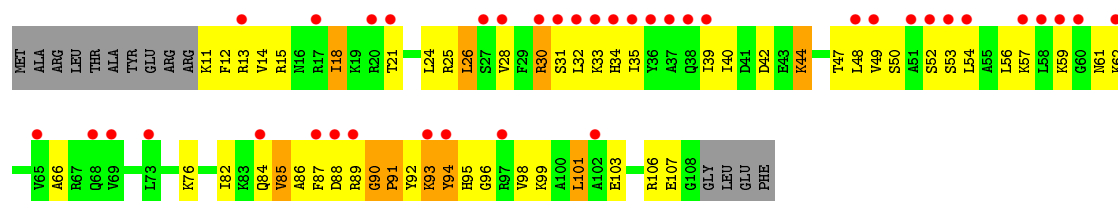


- Molecule 38: 50S ribosomal protein L17

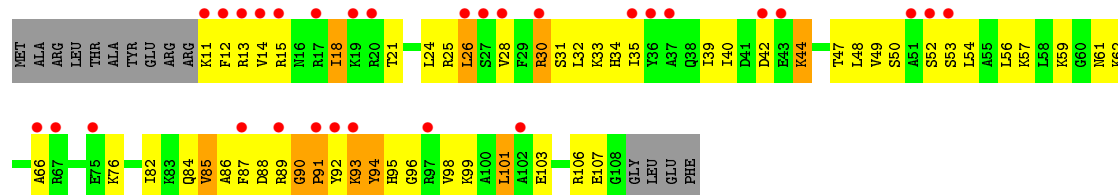


- Molecule 39: 50S ribosomal protein L18

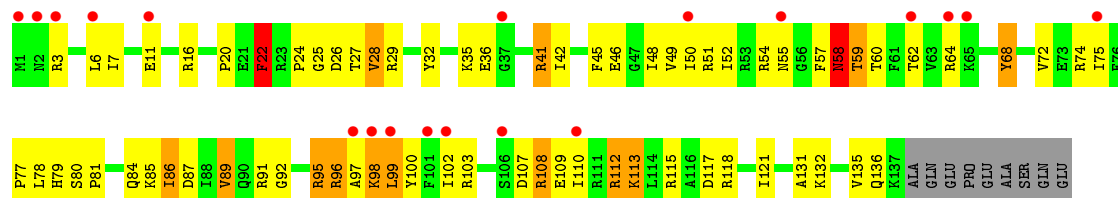




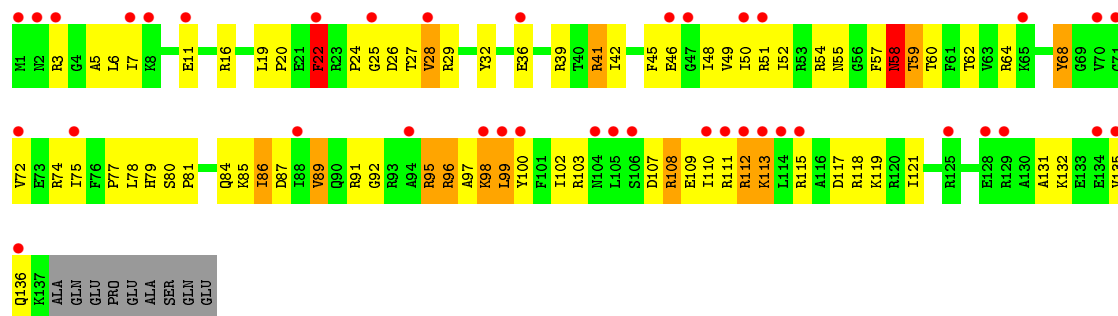
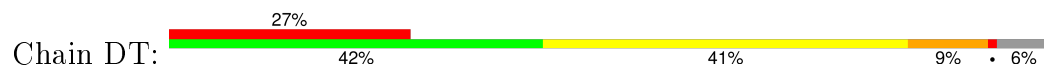
• Molecule 39: 50S ribosomal protein L18



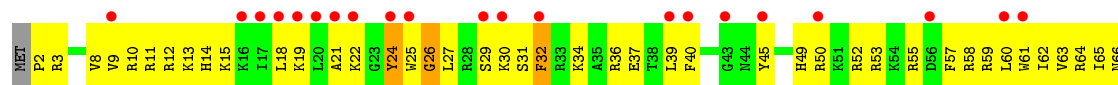
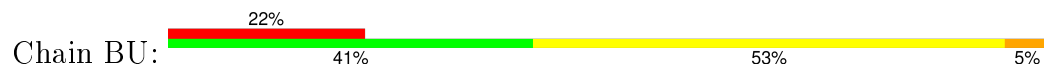
• Molecule 40: 50S ribosomal protein L19

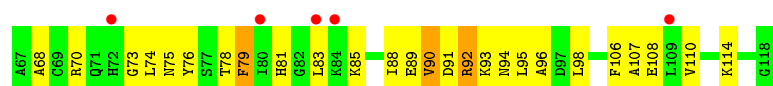


• Molecule 40: 50S ribosomal protein L19

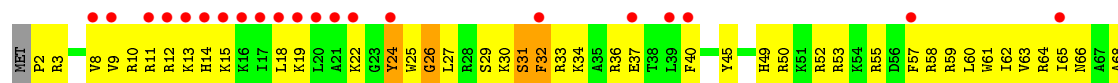
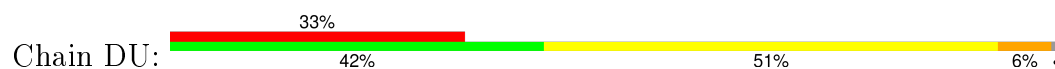


• Molecule 41: 50S ribosomal protein L20

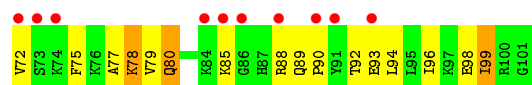
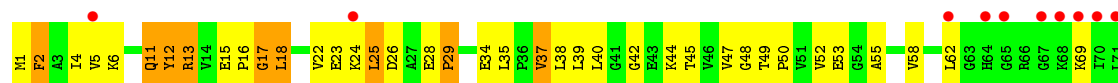




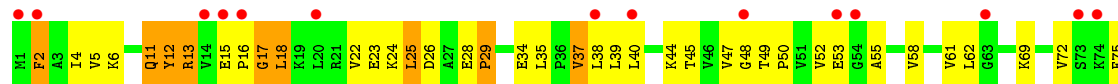
- Molecule 41: 50S ribosomal protein L20



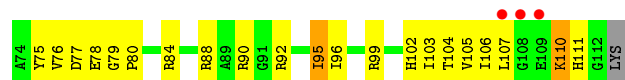
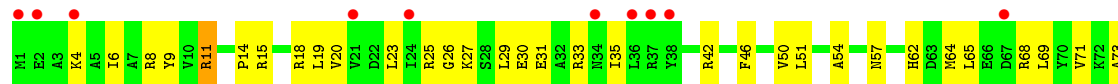
- Molecule 42: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L21

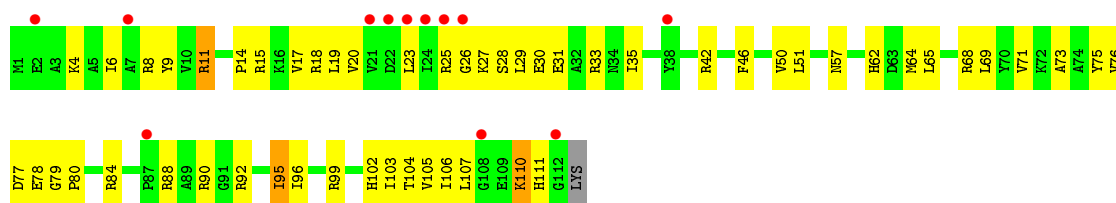


- Molecule 43: 50S ribosomal protein L22

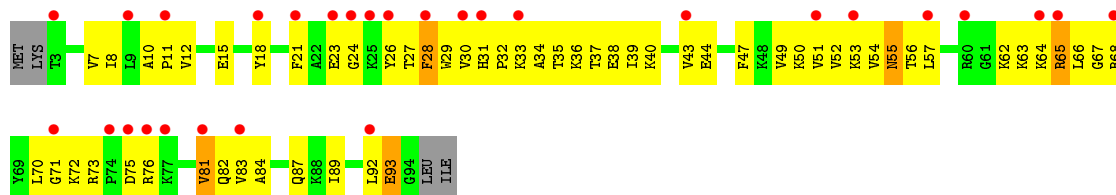


- Molecule 43: 50S ribosomal protein L22

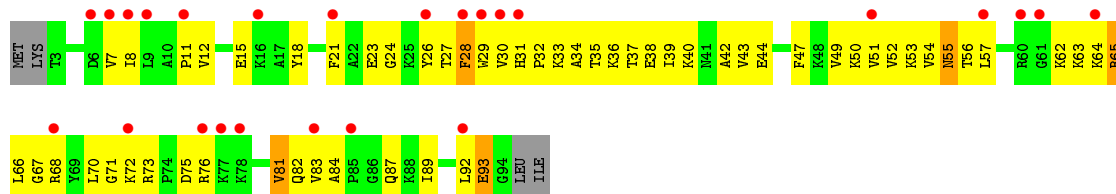




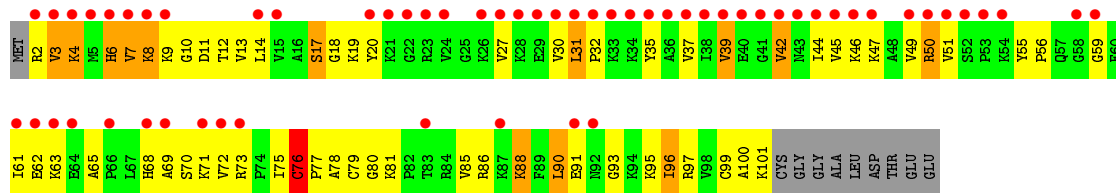
• Molecule 44: 50S ribosomal protein L23



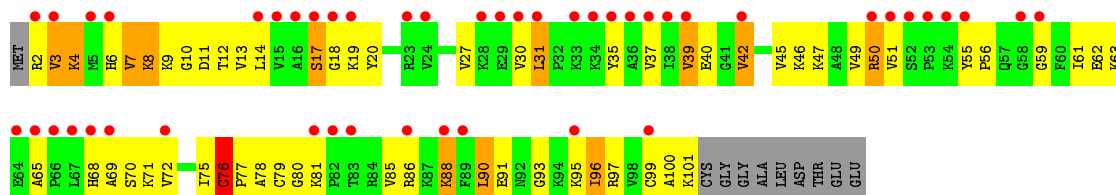
• Molecule 44: 50S ribosomal protein L23



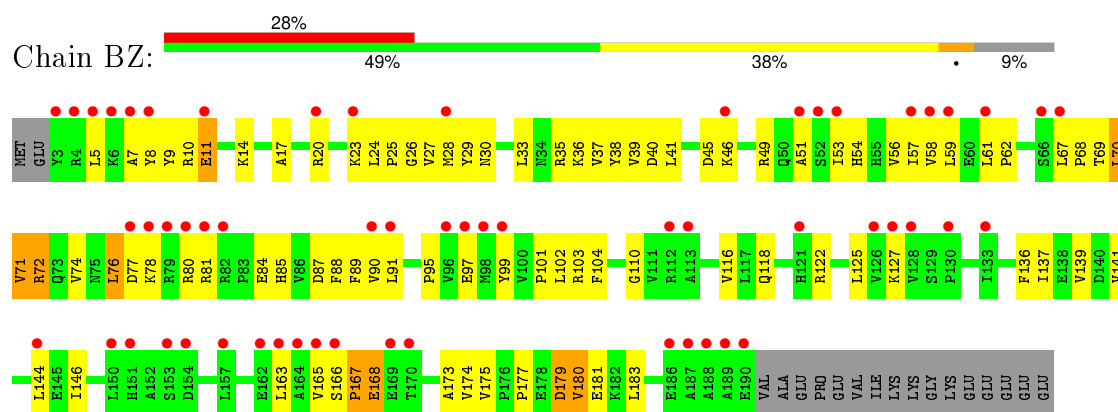
• Molecule 45: 50S ribosomal protein L24



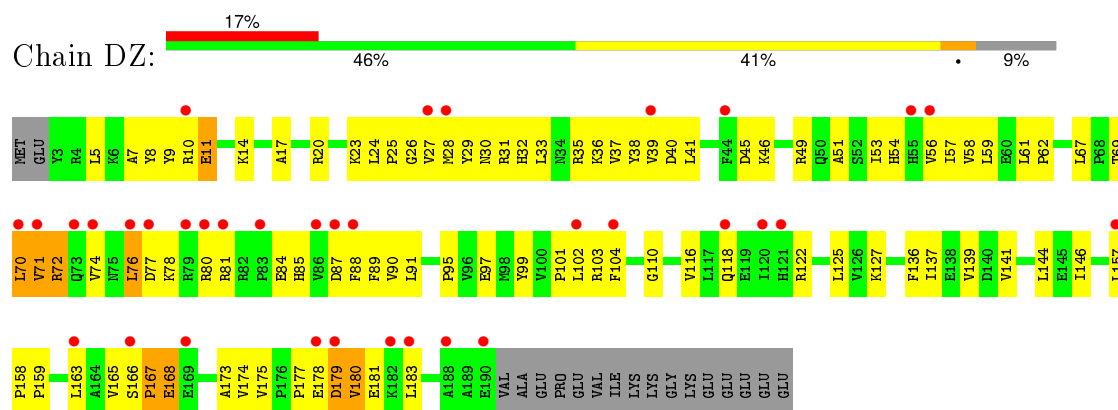
• Molecule 45: 50S ribosomal protein L24



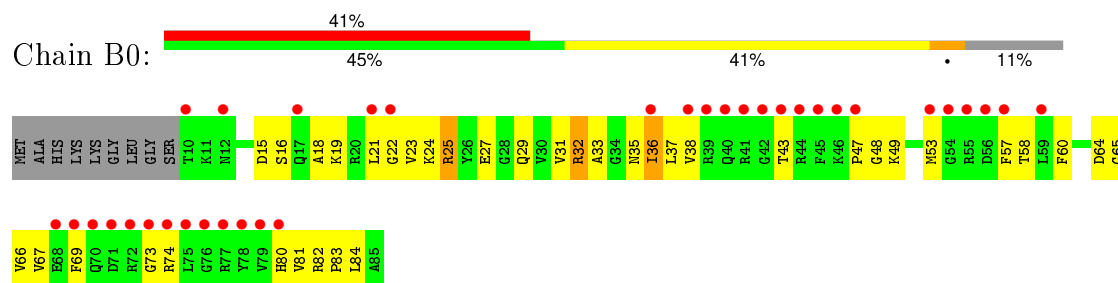
• Molecule 46: 50S ribosomal protein L25



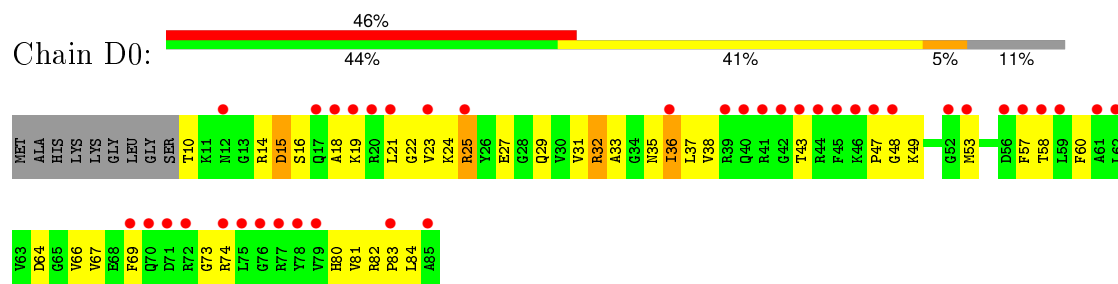
• Molecule 46: 50S ribosomal protein L25



• Molecule 47: 50S ribosomal protein L27

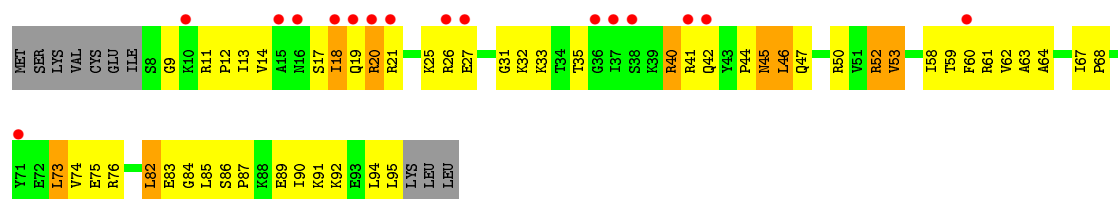


• Molecule 47: 50S ribosomal protein L27

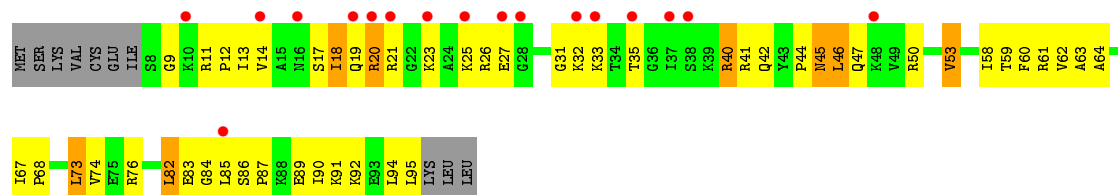
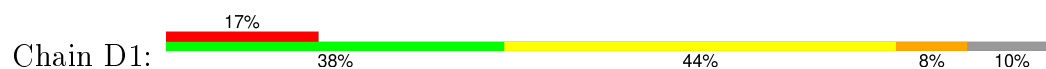


• Molecule 48: 50S ribosomal protein L28

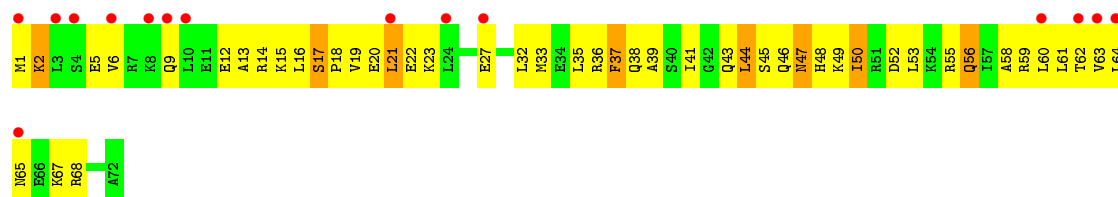




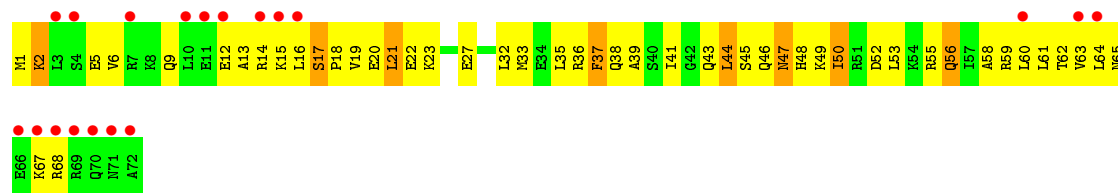
• Molecule 48: 50S ribosomal protein L28



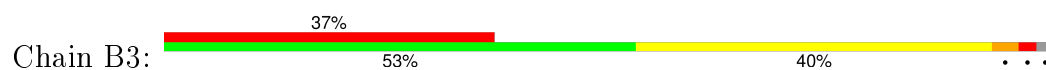
• Molecule 49: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L29

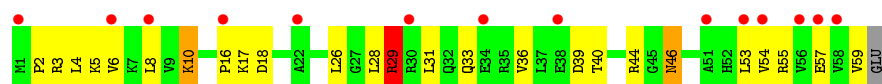


• Molecule 50: 50S ribosomal protein L30

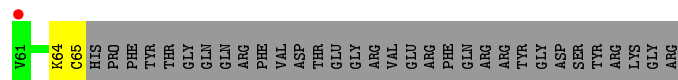
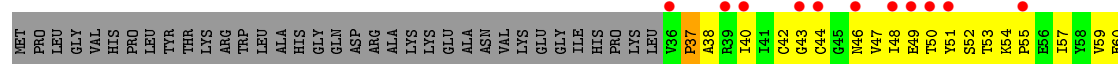


• Molecule 50: 50S ribosomal protein L30

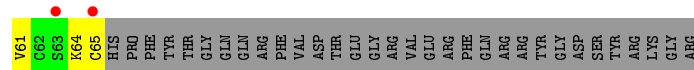
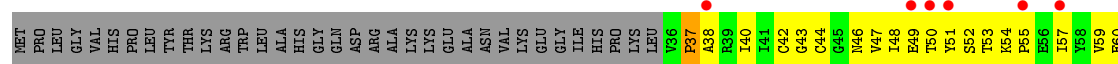




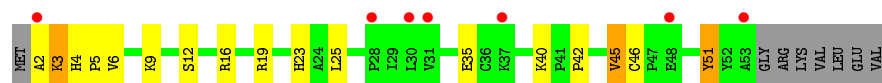
- Molecule 51: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L31



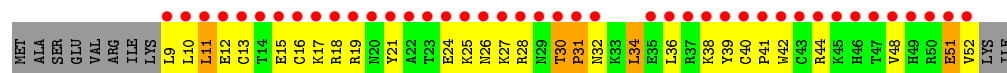
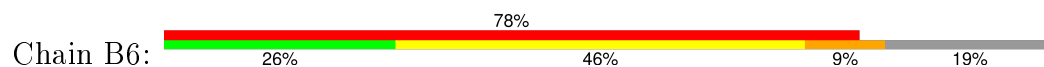
- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33

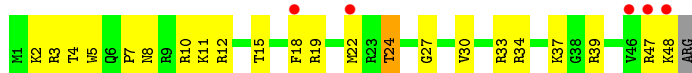


- Molecule 53: 50S ribosomal protein L33

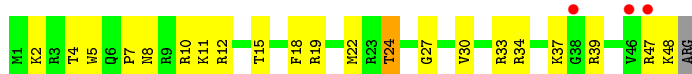




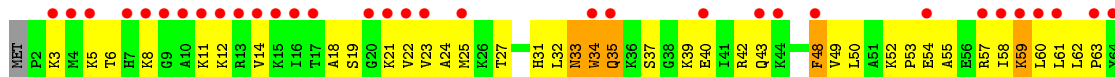
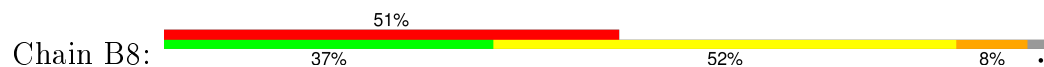
- Molecule 54: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L34

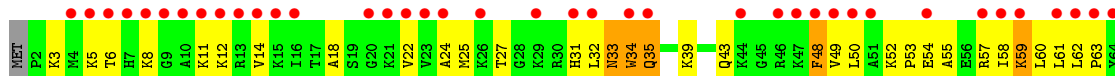


- Molecule 55: 50S ribosomal protein L35



GLU

- Molecule 55: 50S ribosomal protein L35



GLU



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.13Å 454.39Å 616.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 3.21 87.17 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.90-3.21) 95.1 (87.17-3.20)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	0.27	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.292 , 0.319 0.292 , 0.322	Depositor DCC
$R_{free}$ test set	8276 reflections (0.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.17 , 71.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.26$ , $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 952768 reflections	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	299961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	0.42	0/36194	0.85	27/56493 (0.0%)
1	CA	0.41	0/36194	0.85	24/56493 (0.0%)
2	AY	0.42	0/1832	0.81	1/2855 (0.0%)
2	AZ	0.39	0/1832	0.80	0/2855
2	CY	0.43	0/1832	0.82	1/2855 (0.0%)
2	CZ	0.40	0/1832	0.80	0/2855
3	AV	0.43	0/291	0.81	0/452
3	CV	0.42	0/291	0.82	0/452
4	AB	0.21	0/1935	0.38	0/2609
4	CB	0.21	0/1935	0.38	0/2609
5	AC	0.21	0/1636	0.36	0/2205
5	CC	0.21	0/1636	0.36	0/2205
6	AD	0.22	0/1733	0.38	0/2318
6	CD	0.22	0/1733	0.37	0/2318
7	AE	0.22	0/1171	0.39	0/1576
7	CE	0.22	0/1171	0.39	0/1576
8	AF	0.22	0/856	0.39	0/1154
8	CF	0.23	0/856	0.40	0/1154
9	AG	0.21	0/1276	0.36	0/1709
9	CG	0.21	0/1276	0.36	0/1709
10	AH	0.22	0/1136	0.40	0/1527
10	CH	0.21	0/1136	0.40	0/1527
11	AI	0.21	0/1029	0.37	0/1378
11	CI	0.21	0/1029	0.37	0/1378
12	AJ	0.21	0/807	0.39	0/1085
12	CJ	0.21	0/807	0.39	0/1085
13	AK	0.21	0/900	0.39	0/1213
13	CK	0.22	0/900	0.39	0/1213
14	AL	0.23	0/986	0.42	0/1320
14	CL	0.23	0/986	0.42	0/1320
15	AM	0.19	0/943	0.39	0/1265
15	CM	0.19	0/943	0.39	0/1265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	AN	0.22	0/501	0.36	0/664
16	CN	0.22	0/501	0.36	0/664
17	AO	0.22	0/745	0.36	0/992
17	CO	0.21	0/745	0.36	0/992
18	AP	0.22	0/716	0.40	0/963
18	CP	0.21	0/716	0.39	0/963
19	AQ	0.22	0/836	0.38	0/1117
19	CQ	0.23	0/836	0.38	0/1117
20	AR	0.22	0/579	0.39	0/768
20	CR	0.22	0/579	0.39	0/768
21	AS	0.21	0/642	0.38	0/865
21	CS	0.21	0/642	0.38	0/865
22	AT	0.22	0/764	0.36	0/1006
22	CT	0.21	0/764	0.36	0/1006
23	AU	0.20	0/212	0.36	0/277
23	CU	0.19	0/212	0.36	0/277
24	AX	0.23	0/2850	0.40	0/3829
24	CX	0.22	0/2850	0.40	0/3829
25	BA	0.44	0/69437	0.88	51/108401 (0.0%)
25	DA	0.44	0/69437	0.89	55/108401 (0.1%)
26	BB	0.41	0/2853	0.85	1/4451 (0.0%)
26	DB	0.41	0/2853	0.84	1/4451 (0.0%)
27	BD	0.25	0/2154	0.44	0/2905
27	DD	0.26	0/2154	0.44	0/2905
28	BE	0.24	0/1596	0.44	0/2153
28	DE	0.23	0/1596	0.44	0/2153
29	BF	0.23	0/1621	0.40	0/2194
29	DF	0.23	0/1621	0.40	0/2194
30	BG	0.21	0/1500	0.40	0/2017
30	DG	0.21	0/1500	0.40	0/2017
31	BH	0.20	0/1245	0.40	0/1682
31	DH	0.20	0/1245	0.40	0/1682
32	BI	0.21	0/1147	0.41	0/1552
32	DI	0.21	0/1147	0.41	0/1552
33	BJ	0.21	0/251	0.38	0/333
33	DJ	0.21	0/251	0.38	0/333
34	BN	0.22	0/1123	0.44	0/1515
34	DN	0.22	0/1123	0.44	0/1515
35	BO	0.25	0/942	0.42	0/1268
35	DO	0.24	0/942	0.42	0/1268
36	BP	0.24	0/1131	0.45	0/1504
36	DP	0.24	0/1131	0.46	0/1504
37	BQ	0.24	0/1099	0.44	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DQ	0.24	0/1099	0.44	0/1468
38	BR	0.23	0/974	0.45	1/1302 (0.1%)
38	DR	0.22	0/974	0.41	0/1302
39	BS	0.21	0/778	0.38	0/1036
39	DS	0.21	0/778	0.38	0/1036
40	BT	0.23	0/1157	0.40	0/1544
40	DT	0.22	0/1157	0.39	0/1544
41	BU	0.26	0/982	0.41	0/1306
41	DU	0.28	0/982	0.42	0/1306
42	BV	0.23	0/790	0.40	0/1057
42	DV	0.23	0/790	0.40	0/1057
43	BW	0.23	0/901	0.40	0/1209
43	DW	0.24	0/901	0.39	0/1209
44	BX	0.24	0/739	0.41	0/993
44	DX	0.24	0/739	0.41	0/993
45	BY	0.24	0/788	0.44	0/1051
45	DY	0.24	0/788	0.43	0/1051
46	BZ	0.22	0/1523	0.42	0/2068
46	DZ	0.22	0/1523	0.42	0/2068
47	B0	0.22	0/613	0.39	0/816
47	D0	0.22	0/613	0.39	0/816
48	B1	0.25	0/701	0.47	0/932
48	D1	0.25	0/701	0.47	0/932
49	B2	0.24	0/607	0.48	0/803
49	D2	0.24	0/607	0.48	0/803
50	B3	0.22	0/472	0.40	0/634
50	D3	0.22	0/472	0.40	0/634
51	B4	0.20	0/228	0.41	0/309
51	D4	0.21	0/228	0.41	0/309
52	B5	0.22	0/418	0.43	0/567
52	D5	0.22	0/418	0.43	0/567
53	B6	0.23	0/387	0.43	0/518
53	D6	0.23	0/387	0.43	0/518
54	B7	0.23	0/426	0.41	0/561
54	D7	0.25	0/426	0.41	0/561
55	B8	0.24	0/515	0.41	0/679
55	D8	0.24	0/515	0.41	0/679
All	All	0.38	0/323000	0.77	162/482646 (0.0%)

There are no bond length outliers.

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DA	1379	A	C1'-O4'-C4'	-11.90	100.38	109.90
25	BA	1379	A	C1'-O4'-C4'	-11.49	100.71	109.90
25	DA	1091	G	P-O3'-C3'	10.71	132.56	119.70
25	BA	1091	G	P-O3'-C3'	10.65	132.48	119.70
25	DA	1786	A	C1'-O4'-C4'	-9.82	102.04	109.90

There are no chirality outliers.

There are no planarity outliers.

## 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	32332	0	16318	788	0
1	CA	32332	0	16318	782	0
2	AY	1640	0	837	31	0
2	AZ	1640	0	837	34	0
2	CY	1640	0	837	32	0
2	CZ	1640	0	837	32	0
3	AV	258	0	132	4	0
3	CV	258	0	132	6	0
4	AB	1900	0	1951	109	0
4	CB	1900	0	1951	109	0
5	AC	1612	0	1677	92	0
5	CC	1612	0	1677	88	0
6	AD	1703	0	1765	74	0
6	CD	1703	0	1765	72	0
7	AE	1155	0	1213	74	0
7	CE	1155	0	1213	70	0
8	AF	843	0	857	44	0
8	CF	843	0	857	45	0
9	AG	1257	0	1296	64	0
9	CG	1257	0	1296	59	0
10	AH	1116	0	1177	64	0
10	CH	1116	0	1177	62	0
11	AI	1011	0	1043	62	0
11	CI	1011	0	1043	60	0
12	AJ	794	0	840	61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	CJ	794	0	840	61	0
13	AK	885	0	904	60	0
13	CK	885	0	904	55	0
14	AL	970	0	1057	74	0
14	CL	970	0	1057	78	0
15	AM	933	0	992	55	0
15	CM	933	0	992	56	0
16	AN	492	0	531	42	0
16	CN	492	0	532	40	0
17	AO	734	0	771	33	0
17	CO	734	0	771	31	0
18	AP	700	0	720	36	0
18	CP	700	0	720	36	0
19	AQ	823	0	893	44	0
19	CQ	823	0	893	43	0
20	AR	574	0	644	28	0
20	CR	574	0	644	27	0
21	AS	629	0	652	61	0
21	CS	629	0	652	59	0
22	AT	762	0	859	39	0
22	CT	762	0	859	40	0
23	AU	208	0	221	8	0
23	CU	208	0	221	7	0
24	AX	2813	0	2823	159	0
24	CX	2813	0	2823	155	0
25	BA	61997	0	31250	1569	0
25	DA	61997	0	31250	1579	0
26	BB	2551	0	1295	54	0
26	DB	2551	0	1295	58	0
27	BD	2104	0	2182	166	0
27	DD	2104	0	2182	170	0
28	BE	1563	0	1629	110	0
28	DE	1563	0	1629	111	0
29	BF	1586	0	1632	128	0
29	DF	1586	0	1632	124	0
30	BG	1475	0	1537	115	0
30	DG	1475	0	1537	114	0
31	BH	1222	0	1282	59	0
31	DH	1222	0	1282	58	0
32	BI	1132	0	1220	60	0
32	DI	1132	0	1220	57	0
33	BJ	253	0	275	8	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DJ	253	0	275	10	0
34	BN	1096	0	1168	83	0
34	DN	1096	0	1168	85	0
35	BO	932	0	994	52	0
35	DO	932	0	994	56	0
36	BP	1114	0	1187	148	0
36	DP	1114	0	1187	150	0
37	BQ	1079	0	1127	85	0
37	DQ	1079	0	1127	89	0
38	BR	960	0	1021	60	0
38	DR	960	0	1021	57	0
39	BS	770	0	832	57	0
39	DS	770	0	832	57	0
40	BT	1143	0	1211	77	0
40	DT	1143	0	1211	82	0
41	BU	964	0	1022	84	0
41	DU	964	0	1022	80	0
42	BV	779	0	852	57	0
42	DV	779	0	852	57	0
43	BW	890	0	951	51	0
43	DW	890	0	951	55	0
44	BX	725	0	778	68	0
44	DX	725	0	778	68	0
45	BY	775	0	870	76	0
45	DY	775	0	870	71	0
46	BZ	1491	0	1513	79	0
46	DZ	1491	0	1513	83	0
47	B0	605	0	628	31	0
47	D0	605	0	628	34	0
48	B1	694	0	764	64	0
48	D1	694	0	764	66	0
49	B2	605	0	665	61	0
49	D2	605	0	665	62	0
50	B3	467	0	523	20	0
50	D3	467	0	523	18	0
51	B4	225	0	225	18	0
51	D4	225	0	225	20	0
52	B5	404	0	420	27	0
52	D5	404	0	420	28	0
53	B6	380	0	391	32	0
53	D6	380	0	391	28	0
54	B7	418	0	467	18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	D7	418	0	467	17	0
55	B8	507	0	576	39	0
55	D8	507	0	576	38	0
56	AA	310	0	0	0	0
56	AB	2	0	0	0	0
56	AC	6	0	0	0	0
56	AD	8	0	0	0	0
56	AE	1	0	0	0	0
56	AF	2	0	0	0	0
56	AG	1	0	0	0	0
56	AH	2	0	0	0	0
56	AI	2	0	0	0	0
56	AJ	1	0	0	0	0
56	AK	1	0	0	0	0
56	AL	2	0	0	0	0
56	AM	1	0	0	0	0
56	AO	3	0	0	0	0
56	AP	1	0	0	0	0
56	AQ	1	0	0	0	0
56	AV	1	0	0	0	0
56	AX	6	0	0	0	0
56	AY	25	0	0	0	0
56	AZ	6	0	0	0	0
56	B1	2	0	0	0	0
56	B2	3	0	0	0	0
56	B5	1	0	0	0	0
56	B7	3	0	0	0	0
56	BA	806	0	0	0	0
56	BB	26	0	0	0	0
56	BD	2	0	0	0	0
56	BE	1	0	0	0	0
56	BF	5	0	0	0	0
56	BG	3	0	0	0	0
56	BH	2	0	0	0	0
56	BI	3	0	0	0	0
56	BJ	1	0	0	0	0
56	BN	2	0	0	0	0
56	BO	3	0	0	0	0
56	BP	1	0	0	0	0
56	BQ	3	0	0	0	0
56	BR	3	0	0	0	0
56	BT	2	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BU	1	0	0	0	0
56	BV	1	0	0	0	0
56	BW	2	0	0	0	0
56	BY	1	0	0	0	0
56	BZ	1	0	0	0	0
56	CA	414	0	0	0	0
56	CB	2	0	0	0	0
56	CC	7	0	0	0	0
56	CD	2	0	0	0	0
56	CE	1	0	0	0	0
56	CF	1	0	0	0	0
56	CG	1	0	0	0	0
56	CH	1	0	0	0	0
56	CI	2	0	0	0	0
56	CJ	1	0	0	0	0
56	CK	2	0	0	0	0
56	CL	1	0	0	0	0
56	CO	2	0	0	0	0
56	CP	1	0	0	0	0
56	CV	4	0	0	0	0
56	CX	9	0	0	0	0
56	CY	21	0	0	0	0
56	CZ	19	0	0	0	0
56	D2	2	0	0	0	0
56	D3	1	0	0	0	0
56	D4	3	0	0	0	0
56	D5	1	0	0	0	0
56	D7	2	0	0	0	0
56	D8	1	0	0	0	0
56	DA	758	0	0	0	0
56	DB	28	0	0	0	0
56	DD	1	0	0	0	0
56	DF	1	0	0	0	0
56	DG	1	0	0	0	0
56	DH	4	0	0	0	0
56	DI	2	0	0	0	0
56	DN	1	0	0	0	0
56	DO	2	0	0	0	0
56	DP	6	0	0	0	0
56	DQ	1	0	0	0	0
56	DR	1	0	0	0	0
56	DT	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	DV	1	0	0	0	0
56	DW	3	0	0	0	0
56	DX	1	0	0	0	0
56	DZ	4	0	0	0	0
57	AD	1	0	0	0	0
57	AN	1	0	0	0	0
57	CD	1	0	0	0	0
57	CN	1	0	0	0	0
All	All	299961	0	202995	10201	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 20.

The worst 5 of 10201 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)
29:DF:40:GLN:HE22	29:DF:182:ASN:HB2	1.10	1.14
37:DQ:23:GLY:HA3	37:DQ:98:LYS:HG3	1.31	1.13
37:BQ:23:GLY:HA3	37:BQ:98:LYS:HG3	1.31	1.12
29:BF:40:GLN:HE22	29:BF:182:ASN:HB2	1.10	1.07
37:BQ:14:ARG:HG2	37:BQ:14:ARG:HH11	1.20	1.06

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	
4	AB	232/256 (91%)	186 (80%)	37 (16%)	9 (4%)	4	28
4	CB	232/256 (91%)	188 (81%)	37 (16%)	7 (3%)	5	35
5	AC	204/239 (85%)	156 (76%)	36 (18%)	12 (6%)	2	16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CC	204/239 (85%)	155 (76%)	38 (19%)	11 (5%)	2	19
6	AD	206/209 (99%)	163 (79%)	31 (15%)	12 (6%)	2	17
6	CD	206/209 (99%)	163 (79%)	30 (15%)	13 (6%)	2	13
7	AE	149/162 (92%)	122 (82%)	24 (16%)	3 (2%)	9	48
7	CE	149/162 (92%)	122 (82%)	24 (16%)	3 (2%)	9	48
8	AF	99/101 (98%)	85 (86%)	13 (13%)	1 (1%)	19	65
8	CF	99/101 (98%)	85 (86%)	13 (13%)	1 (1%)	19	65
9	AG	153/156 (98%)	125 (82%)	24 (16%)	4 (3%)	7	40
9	CG	153/156 (98%)	127 (83%)	22 (14%)	4 (3%)	7	40
10	AH	136/138 (99%)	118 (87%)	17 (12%)	1 (1%)	26	72
10	CH	136/138 (99%)	118 (87%)	18 (13%)	0	100	100
11	AI	125/128 (98%)	100 (80%)	23 (18%)	2 (2%)	12	54
11	CI	125/128 (98%)	101 (81%)	22 (18%)	2 (2%)	12	54
12	AJ	96/105 (91%)	73 (76%)	18 (19%)	5 (5%)	2	19
12	CJ	96/105 (91%)	73 (76%)	18 (19%)	5 (5%)	2	19
13	AK	117/129 (91%)	97 (83%)	18 (15%)	2 (2%)	11	52
13	CK	117/129 (91%)	96 (82%)	19 (16%)	2 (2%)	11	52
14	AL	122/134 (91%)	88 (72%)	26 (21%)	8 (7%)	1	12
14	CL	122/134 (91%)	88 (72%)	26 (21%)	8 (7%)	1	12
15	AM	115/126 (91%)	92 (80%)	16 (14%)	7 (6%)	2	15
15	CM	115/126 (91%)	92 (80%)	16 (14%)	7 (6%)	2	15
16	AN	58/61 (95%)	45 (78%)	8 (14%)	5 (9%)	1	6
16	CN	58/61 (95%)	45 (78%)	8 (14%)	5 (9%)	1	6
17	AO	86/89 (97%)	70 (81%)	15 (17%)	1 (1%)	16	60
17	CO	86/89 (97%)	69 (80%)	16 (19%)	1 (1%)	16	60
18	AP	81/88 (92%)	65 (80%)	14 (17%)	2 (2%)	7	41
18	CP	81/88 (92%)	65 (80%)	14 (17%)	2 (2%)	7	41
19	AQ	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	9	46
19	CQ	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	9	46
20	AR	68/88 (77%)	53 (78%)	13 (19%)	2 (3%)	6	36
20	CR	68/88 (77%)	52 (76%)	14 (21%)	2 (3%)	6	36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	AS	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1	5
21	CS	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1	5
22	AT	97/106 (92%)	79 (81%)	14 (14%)	4 (4%)	3	27
22	CT	97/106 (92%)	79 (81%)	14 (14%)	4 (4%)	3	27
23	AU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	3	24
23	CU	22/27 (82%)	18 (82%)	3 (14%)	1 (4%)	3	24
24	AX	352/354 (99%)	297 (84%)	44 (12%)	11 (3%)	5	34
24	CX	352/354 (99%)	296 (84%)	45 (13%)	11 (3%)	5	34
27	BD	269/276 (98%)	213 (79%)	40 (15%)	16 (6%)	2	16
27	DD	269/276 (98%)	213 (79%)	40 (15%)	16 (6%)	2	16
28	BE	202/206 (98%)	151 (75%)	41 (20%)	10 (5%)	3	21
28	DE	202/206 (98%)	151 (75%)	42 (21%)	9 (4%)	3	24
29	BF	200/210 (95%)	158 (79%)	35 (18%)	7 (4%)	4	31
29	DF	200/210 (95%)	158 (79%)	35 (18%)	7 (4%)	4	31
30	BG	179/182 (98%)	127 (71%)	42 (24%)	10 (6%)	2	18
30	DG	179/182 (98%)	124 (69%)	44 (25%)	11 (6%)	2	15
31	BH	157/180 (87%)	126 (80%)	24 (15%)	7 (4%)	3	24
31	DH	157/180 (87%)	126 (80%)	24 (15%)	7 (4%)	3	24
32	BI	143/148 (97%)	111 (78%)	25 (18%)	7 (5%)	3	22
32	DI	143/148 (97%)	112 (78%)	24 (17%)	7 (5%)	3	22
33	BJ	28/173 (16%)	27 (96%)	1 (4%)	0	100	100
33	DJ	28/173 (16%)	27 (96%)	1 (4%)	0	100	100
34	BN	135/163 (83%)	100 (74%)	27 (20%)	8 (6%)	2	16
34	DN	135/163 (83%)	100 (74%)	27 (20%)	8 (6%)	2	16
35	BO	120/122 (98%)	101 (84%)	18 (15%)	1 (1%)	24	69
35	DO	120/122 (98%)	101 (84%)	18 (15%)	1 (1%)	24	69
36	BP	144/150 (96%)	82 (57%)	44 (31%)	18 (12%)	0	2
36	DP	144/150 (96%)	82 (57%)	45 (31%)	17 (12%)	0	3
37	BQ	134/141 (95%)	86 (64%)	36 (27%)	12 (9%)	1	5
37	DQ	134/141 (95%)	87 (65%)	35 (26%)	12 (9%)	1	5
38	BR	115/118 (98%)	92 (80%)	18 (16%)	5 (4%)	3	25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DR	115/118 (98%)	91 (79%)	18 (16%)	6 (5%)	2	19
39	BS	96/112 (86%)	62 (65%)	24 (25%)	10 (10%)	1	4
39	DS	96/112 (86%)	61 (64%)	25 (26%)	10 (10%)	1	4
40	BT	135/146 (92%)	102 (76%)	29 (22%)	4 (3%)	5	35
40	DT	135/146 (92%)	103 (76%)	28 (21%)	4 (3%)	5	35
41	BU	115/118 (98%)	90 (78%)	21 (18%)	4 (4%)	4	31
41	DU	115/118 (98%)	89 (77%)	22 (19%)	4 (4%)	4	31
42	BV	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	1	5
42	DV	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	1	5
43	BW	110/113 (97%)	91 (83%)	17 (16%)	2 (2%)	11	51
43	DW	110/113 (97%)	91 (83%)	17 (16%)	2 (2%)	11	51
44	BX	90/96 (94%)	69 (77%)	20 (22%)	1 (1%)	17	62
44	DX	90/96 (94%)	69 (77%)	20 (22%)	1 (1%)	17	62
45	BY	98/110 (89%)	65 (66%)	21 (21%)	12 (12%)	0	2
45	DY	98/110 (89%)	65 (66%)	21 (21%)	12 (12%)	0	2
46	BZ	186/206 (90%)	142 (76%)	34 (18%)	10 (5%)	2	19
46	DZ	186/206 (90%)	142 (76%)	34 (18%)	10 (5%)	2	19
47	B0	74/85 (87%)	55 (74%)	14 (19%)	5 (7%)	1	11
47	D0	74/85 (87%)	55 (74%)	14 (19%)	5 (7%)	1	11
48	B1	86/98 (88%)	53 (62%)	27 (31%)	6 (7%)	1	10
48	D1	86/98 (88%)	53 (62%)	28 (33%)	5 (6%)	2	17
49	B2	70/72 (97%)	48 (69%)	16 (23%)	6 (9%)	1	6
49	D2	70/72 (97%)	48 (69%)	16 (23%)	6 (9%)	1	6
50	B3	57/60 (95%)	43 (75%)	13 (23%)	1 (2%)	11	51
50	D3	57/60 (95%)	44 (77%)	12 (21%)	1 (2%)	11	51
51	B4	28/97 (29%)	14 (50%)	11 (39%)	3 (11%)	0	3
51	D4	28/97 (29%)	14 (50%)	11 (39%)	3 (11%)	0	3
52	B5	50/60 (83%)	36 (72%)	12 (24%)	2 (4%)	4	27
52	D5	50/60 (83%)	36 (72%)	12 (24%)	2 (4%)	4	27
53	B6	42/54 (78%)	31 (74%)	8 (19%)	3 (7%)	1	10
53	D6	42/54 (78%)	31 (74%)	8 (19%)	3 (7%)	1	10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	B7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
54	D7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
55	B8	61/65 (94%)	42 (69%)	15 (25%)	4 (7%)	1	12
55	D8	61/65 (94%)	42 (69%)	15 (25%)	4 (7%)	1	12
All	All	11920/13210 (90%)	9191 (77%)	2165 (18%)	564 (5%)	3	22

5 of 564 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AC	47	LEU
12	AJ	75	ILE
15	AM	4	ILE
15	AM	106	ASN
15	AM	117	VAL

### 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	
4	AB	202/220 (92%)	189 (94%)	13 (6%)	22	62
4	CB	202/220 (92%)	189 (94%)	13 (6%)	22	62
5	AC	160/188 (85%)	151 (94%)	9 (6%)	26	68
5	CC	160/188 (85%)	151 (94%)	9 (6%)	26	68
6	AD	180/181 (99%)	171 (95%)	9 (5%)	30	71
6	CD	180/181 (99%)	171 (95%)	9 (5%)	30	71
7	AE	116/123 (94%)	105 (90%)	11 (10%)	11	40
7	CE	116/123 (94%)	105 (90%)	11 (10%)	11	40
8	AF	90/90 (100%)	86 (96%)	4 (4%)	35	74
8	CF	90/90 (100%)	86 (96%)	4 (4%)	35	74
9	AG	126/127 (99%)	125 (99%)	1 (1%)	86	96
9	CG	126/127 (99%)	125 (99%)	1 (1%)	86	96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AH	119/119 (100%)	114 (96%)	5 (4%)	36	75
10	CH	119/119 (100%)	114 (96%)	5 (4%)	36	75
11	AI	98/99 (99%)	92 (94%)	6 (6%)	23	64
11	CI	98/99 (99%)	92 (94%)	6 (6%)	23	64
12	AJ	88/92 (96%)	80 (91%)	8 (9%)	12	42
12	CJ	88/92 (96%)	80 (91%)	8 (9%)	12	42
13	AK	90/99 (91%)	86 (96%)	4 (4%)	35	74
13	CK	90/99 (91%)	86 (96%)	4 (4%)	35	74
14	AL	104/110 (94%)	98 (94%)	6 (6%)	25	66
14	CL	104/110 (94%)	98 (94%)	6 (6%)	25	66
15	AM	94/101 (93%)	87 (93%)	7 (7%)	17	56
15	CM	94/101 (93%)	87 (93%)	7 (7%)	17	56
16	AN	49/50 (98%)	47 (96%)	2 (4%)	37	76
16	CN	49/50 (98%)	47 (96%)	2 (4%)	37	76
17	AO	79/80 (99%)	74 (94%)	5 (6%)	22	63
17	CO	79/80 (99%)	74 (94%)	5 (6%)	22	63
18	AP	72/74 (97%)	68 (94%)	4 (6%)	26	68
18	CP	72/74 (97%)	68 (94%)	4 (6%)	26	68
19	AQ	94/97 (97%)	91 (97%)	3 (3%)	46	81
19	CQ	94/97 (97%)	91 (97%)	3 (3%)	46	81
20	AR	61/77 (79%)	59 (97%)	2 (3%)	45	81
20	CR	61/77 (79%)	59 (97%)	2 (3%)	45	81
21	AS	69/80 (86%)	59 (86%)	10 (14%)	4	19
21	CS	69/80 (86%)	59 (86%)	10 (14%)	4	19
22	AT	76/82 (93%)	71 (93%)	5 (7%)	21	61
22	CT	76/82 (93%)	71 (93%)	5 (7%)	21	61
23	AU	19/22 (86%)	19 (100%)	0	100	100
23	CU	19/22 (86%)	19 (100%)	0	100	100
24	AX	299/299 (100%)	278 (93%)	21 (7%)	19	58
24	CX	299/299 (100%)	278 (93%)	21 (7%)	19	58
27	BD	213/218 (98%)	196 (92%)	17 (8%)	15	52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	DD	213/218 (98%)	196 (92%)	17 (8%)	15	52
28	BE	165/166 (99%)	153 (93%)	12 (7%)	17	57
28	DE	165/166 (99%)	153 (93%)	12 (7%)	17	57
29	BF	161/166 (97%)	154 (96%)	7 (4%)	35	75
29	DF	161/166 (97%)	154 (96%)	7 (4%)	35	75
30	BG	155/156 (99%)	142 (92%)	13 (8%)	14	48
30	DG	155/156 (99%)	142 (92%)	13 (8%)	14	48
31	BH	132/148 (89%)	123 (93%)	9 (7%)	20	59
31	DH	132/148 (89%)	123 (93%)	9 (7%)	20	59
32	BI	122/124 (98%)	113 (93%)	9 (7%)	17	56
32	DI	122/124 (98%)	113 (93%)	9 (7%)	17	56
33	BJ	27/135 (20%)	26 (96%)	1 (4%)	41	79
33	DJ	27/135 (20%)	26 (96%)	1 (4%)	41	79
34	BN	116/139 (84%)	106 (91%)	10 (9%)	13	46
34	DN	116/139 (84%)	106 (91%)	10 (9%)	13	46
35	BO	100/100 (100%)	95 (95%)	5 (5%)	30	71
35	DO	100/100 (100%)	95 (95%)	5 (5%)	30	71
36	BP	112/116 (97%)	92 (82%)	20 (18%)	2	11
36	DP	112/116 (97%)	92 (82%)	20 (18%)	2	11
37	BQ	106/111 (96%)	95 (90%)	11 (10%)	9	35
37	DQ	106/111 (96%)	95 (90%)	11 (10%)	9	35
38	BR	100/101 (99%)	95 (95%)	5 (5%)	30	71
38	DR	100/101 (99%)	95 (95%)	5 (5%)	30	71
39	BS	77/88 (88%)	70 (91%)	7 (9%)	12	42
39	DS	77/88 (88%)	70 (91%)	7 (9%)	12	42
40	BT	121/128 (94%)	106 (88%)	15 (12%)	6	27
40	DT	121/128 (94%)	106 (88%)	15 (12%)	6	27
41	BU	93/94 (99%)	90 (97%)	3 (3%)	46	81
41	DU	93/94 (99%)	89 (96%)	4 (4%)	35	75
42	BV	82/82 (100%)	73 (89%)	9 (11%)	8	33
42	DV	82/82 (100%)	73 (89%)	9 (11%)	8	33

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	BW	91/92 (99%)	89 (98%)	2 (2%)	60	87
43	DW	91/92 (99%)	89 (98%)	2 (2%)	60	87
44	BX	74/78 (95%)	68 (92%)	6 (8%)	15	51
44	DX	74/78 (95%)	68 (92%)	6 (8%)	15	51
45	BY	84/91 (92%)	79 (94%)	5 (6%)	24	65
45	DY	84/91 (92%)	79 (94%)	5 (6%)	24	65
46	BZ	163/179 (91%)	160 (98%)	3 (2%)	66	89
46	DZ	163/179 (91%)	160 (98%)	3 (2%)	66	89
47	B0	61/67 (91%)	59 (97%)	2 (3%)	45	81
47	D0	61/67 (91%)	59 (97%)	2 (3%)	45	81
48	B1	73/83 (88%)	63 (86%)	10 (14%)	4	21
48	D1	73/83 (88%)	64 (88%)	9 (12%)	6	27
49	B2	67/67 (100%)	64 (96%)	3 (4%)	34	74
49	D2	67/67 (100%)	64 (96%)	3 (4%)	34	74
50	B3	51/52 (98%)	47 (92%)	4 (8%)	16	53
50	D3	51/52 (98%)	48 (94%)	3 (6%)	24	65
51	B4	27/84 (32%)	25 (93%)	2 (7%)	17	56
51	D4	27/84 (32%)	25 (93%)	2 (7%)	17	56
52	B5	45/52 (86%)	43 (96%)	2 (4%)	35	74
52	D5	45/52 (86%)	43 (96%)	2 (4%)	35	74
53	B6	43/52 (83%)	40 (93%)	3 (7%)	19	58
53	D6	43/52 (83%)	40 (93%)	3 (7%)	19	58
54	B7	41/42 (98%)	38 (93%)	3 (7%)	17	57
54	D7	41/42 (98%)	38 (93%)	3 (7%)	17	57
55	B8	53/55 (96%)	51 (96%)	2 (4%)	40	78
55	D8	53/55 (96%)	51 (96%)	2 (4%)	40	78
All	All	10080/10952 (92%)	9411 (93%)	669 (7%)	21	61

5 of 669 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BZ	72	ARG
7	CE	79	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
42	DV	18	LEU
48	B1	73	LEU
4	CB	75	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 231 such sidechains are listed below:

Mol	Chain	Res	Type
48	B1	56	GLN
7	CE	73	ASN
46	DZ	55	HIS
50	B3	19	GLN
4	CB	25	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1525 (98%)	211 (14%)	56 (3%)
1	CA	1503/1525 (98%)	211 (14%)	56 (3%)
2	AY	76/77 (98%)	11 (14%)	2 (2%)
2	AZ	76/77 (98%)	8 (10%)	1 (1%)
2	CY	76/77 (98%)	11 (14%)	2 (2%)
2	CZ	76/77 (98%)	8 (10%)	1 (1%)
25	BA	2878/2894 (99%)	448 (15%)	101 (3%)
25	DA	2878/2894 (99%)	445 (15%)	102 (3%)
26	BB	118/124 (95%)	12 (10%)	1 (0%)
26	DB	118/124 (95%)	12 (10%)	1 (0%)
3	AV	11/27 (40%)	2 (18%)	1 (9%)
3	CV	11/27 (40%)	2 (18%)	1 (9%)
All	All	9324/9448 (98%)	1381 (14%)	325 (3%)

5 of 1381 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	31	G
1	AA	39	G
1	AA	47	C

5 of 325 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2428	G
1	CA	429	U
25	DA	2172	U
25	BA	2542	A
1	CA	115	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2581 ligands modelled in this entry, 2581 are monoatomic - leaving 0 for Mogul analysis.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1504/1525 (98%)	0.27	76 (5%) 32 18	85, 138, 234, 323	0
1	CA	1504/1525 (98%)	0.51	140 (9%) 11 6	93, 155, 241, 322	0
2	AY	77/77 (100%)	-0.21	0 100 100	97, 129, 164, 212	0
2	AZ	77/77 (100%)	1.04	11 (14%) 4 2	216, 256, 275, 295	0
2	CY	77/77 (100%)	-0.15	0 100 100	86, 127, 171, 213	0
2	CZ	77/77 (100%)	0.92	13 (16%) 2 1	219, 254, 280, 289	0
3	AV	12/27 (44%)	1.22	3 (25%) 1 1	120, 129, 207, 226	0
3	CV	12/27 (44%)	2.09	4 (33%) 0 0	118, 127, 212, 221	0
4	AB	234/256 (91%)	1.28	64 (27%) 1 0	155, 190, 223, 247	0
4	CB	234/256 (91%)	1.37	71 (30%) 1 0	158, 188, 218, 246	0
5	AC	206/239 (86%)	0.49	21 (10%) 9 5	160, 191, 220, 245	0
5	CC	206/239 (86%)	0.95	40 (19%) 1 1	157, 174, 194, 224	0
6	AD	208/209 (99%)	1.11	47 (22%) 1 1	125, 146, 174, 188	0
6	CD	208/209 (99%)	1.44	67 (32%) 1 0	146, 177, 205, 230	0
7	AE	151/162 (93%)	0.73	21 (13%) 4 2	124, 145, 174, 198	0
7	CE	151/162 (93%)	0.96	30 (19%) 1 1	133, 154, 184, 220	0
8	AF	101/101 (100%)	0.25	11 (10%) 7 4	128, 148, 172, 192	0
8	CF	101/101 (100%)	0.35	7 (6%) 20 11	133, 151, 182, 195	0
9	AG	155/156 (99%)	0.70	26 (16%) 2 1	150, 170, 198, 213	0
9	CG	155/156 (99%)	0.55	21 (13%) 4 2	149, 171, 195, 210	0
10	AH	138/138 (100%)	1.52	42 (30%) 1 0	121, 147, 175, 193	0
10	CH	138/138 (100%)	1.26	33 (23%) 1 1	138, 162, 187, 202	0
11	AI	127/128 (99%)	3.37	78 (61%) 0 0	150, 194, 216, 233	0
11	CI	127/128 (99%)	3.28	78 (61%) 0 0	154, 183, 205, 227	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
12	AJ	98/105 (93%)	1.33	26 (26%)	1	0	161, 211, 241, 252	0
12	CJ	98/105 (93%)	2.24	43 (43%)	0	0	159, 190, 217, 226	0
13	AK	119/129 (92%)	0.87	24 (20%)	1	1	117, 147, 176, 185	0
13	CK	119/129 (92%)	1.15	26 (21%)	1	1	114, 136, 169, 204	0
14	AL	124/134 (92%)	0.64	17 (13%)	4	2	106, 118, 143, 171	0
14	CL	124/134 (92%)	0.99	18 (14%)	3	2	122, 134, 161, 208	0
15	AM	117/126 (92%)	1.96	48 (41%)	0	0	152, 182, 203, 216	0
15	CM	117/126 (92%)	1.78	42 (35%)	0	0	164, 193, 219, 240	0
16	AN	60/61 (98%)	2.58	33 (55%)	0	0	171, 185, 211, 230	0
16	CN	60/61 (98%)	2.67	30 (50%)	0	0	163, 173, 205, 214	0
17	AO	88/89 (98%)	1.06	22 (25%)	1	1	114, 134, 161, 176	0
17	CO	88/89 (98%)	1.20	22 (25%)	1	1	121, 148, 175, 193	0
18	AP	83/88 (94%)	2.35	45 (54%)	0	0	120, 133, 162, 173	0
18	CP	83/88 (94%)	3.58	52 (62%)	0	0	154, 178, 202, 235	0
19	AQ	99/105 (94%)	1.36	30 (30%)	1	0	115, 126, 154, 159	0
19	CQ	99/105 (94%)	1.78	29 (29%)	1	0	122, 151, 171, 188	0
20	AR	70/88 (79%)	0.86	14 (20%)	1	1	134, 151, 184, 198	0
20	CR	70/88 (79%)	0.67	7 (10%)	9	5	131, 147, 174, 191	0
21	AS	78/93 (83%)	2.15	32 (41%)	0	0	163, 192, 214, 226	0
21	CS	78/93 (83%)	1.96	38 (48%)	0	0	171, 196, 216, 232	0
22	AT	99/106 (93%)	1.88	40 (40%)	0	0	126, 144, 174, 200	0
22	CT	99/106 (93%)	2.47	49 (49%)	0	0	155, 177, 205, 234	0
23	AU	24/27 (88%)	6.02	22 (91%)	0	0	195, 213, 232, 241	0
23	CU	24/27 (88%)	5.73	21 (87%)	0	0	180, 201, 227, 248	0
24	AX	354/354 (100%)	1.12	78 (22%)	1	1	98, 137, 242, 255	0
24	CX	354/354 (100%)	1.56	98 (27%)	1	0	105, 134, 292, 310	0
25	BA	2879/2894 (99%)	0.19	154 (5%)	30	17	65, 112, 248, 354	0
25	DA	2879/2894 (99%)	0.17	147 (5%)	32	18	59, 110, 238, 321	0
26	BB	119/124 (95%)	0.22	6 (5%)	32	19	138, 171, 208, 265	0
26	DB	119/124 (95%)	0.20	7 (5%)	26	14	132, 181, 215, 265	0
27	BD	271/276 (98%)	0.77	40 (14%)	3	2	98, 122, 149, 167	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
27	DD	271/276 (98%)	0.88	51 (18%)	2	1	93, 115, 140, 163	0
28	BE	204/206 (99%)	1.46	66 (32%)	1	0	95, 126, 164, 180	0
28	DE	204/206 (99%)	1.10	44 (21%)	1	1	99, 141, 171, 194	0
29	BF	202/210 (96%)	0.54	17 (8%)	14	7	97, 142, 175, 194	0
29	DF	202/210 (96%)	1.17	50 (24%)	1	1	92, 132, 163, 183	0
30	BG	181/182 (99%)	1.10	47 (25%)	1	0	147, 198, 223, 252	0
30	DG	181/182 (99%)	1.60	60 (33%)	0	0	146, 197, 233, 251	0
31	BH	159/180 (88%)	2.36	77 (48%)	0	0	141, 172, 206, 222	0
31	DH	159/180 (88%)	0.85	28 (17%)	2	1	148, 172, 202, 215	0
32	BI	145/148 (97%)	3.80	87 (60%)	0	0	134, 211, 264, 286	0
32	DI	145/148 (97%)	2.50	68 (46%)	0	0	125, 203, 254, 286	0
33	BJ	32/173 (18%)	5.39	29 (90%)	0	0	203, 228, 245, 262	0
33	DJ	32/173 (18%)	4.35	26 (81%)	0	0	188, 222, 247, 258	0
34	BN	137/163 (84%)	1.69	48 (35%)	0	0	110, 142, 167, 219	0
34	DN	137/163 (84%)	1.26	37 (27%)	1	0	112, 140, 165, 184	0
35	BO	122/122 (100%)	0.74	17 (13%)	4	2	104, 113, 133, 184	0
35	DO	122/122 (100%)	1.19	28 (22%)	1	1	111, 128, 146, 175	0
36	BP	146/150 (97%)	1.40	41 (28%)	1	0	105, 145, 182, 203	0
36	DP	146/150 (97%)	0.89	26 (17%)	2	1	100, 143, 178, 198	0
37	BQ	136/141 (96%)	1.83	49 (36%)	0	0	109, 142, 172, 226	0
37	DQ	136/141 (96%)	2.54	59 (43%)	0	0	105, 140, 174, 226	0
38	BR	117/118 (99%)	1.63	39 (33%)	0	0	102, 116, 153, 180	0
38	DR	117/118 (99%)	1.68	39 (33%)	0	0	108, 129, 167, 183	0
39	BS	98/112 (87%)	2.07	39 (39%)	0	0	164, 192, 215, 232	0
39	DS	98/112 (87%)	1.38	30 (30%)	1	0	164, 197, 225, 240	0
40	BT	137/146 (93%)	0.56	19 (13%)	4	2	107, 120, 163, 190	0
40	DT	137/146 (93%)	1.20	39 (28%)	1	0	121, 145, 189, 205	0
41	BU	117/118 (99%)	1.01	26 (22%)	1	1	109, 144, 175, 196	0
41	DU	117/118 (99%)	1.49	39 (33%)	0	0	102, 136, 170, 183	0
42	BV	101/101 (100%)	0.76	20 (19%)	1	1	110, 160, 187, 202	0
42	DV	101/101 (100%)	1.02	21 (20%)	1	1	104, 150, 183, 202	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BW	112/113 (99%)	0.90	13 (11%) 6 4	95, 118, 156, 181	0
43	DW	112/113 (99%)	0.73	12 (10%) 8 4	92, 116, 145, 172	0
44	BX	92/96 (95%)	1.33	29 (31%) 1 0	111, 129, 161, 179	0
44	DX	92/96 (95%)	1.21	25 (27%) 1 0	101, 120, 145, 174	0
45	BY	100/110 (90%)	3.08	59 (59%) 0 0	131, 150, 181, 216	0
45	DY	100/110 (90%)	2.35	47 (47%) 0 0	115, 135, 172, 199	0
46	BZ	188/206 (91%)	1.51	58 (30%) 1 0	138, 180, 207, 229	0
46	DZ	188/206 (91%)	0.76	35 (18%) 2 1	134, 173, 200, 215	0
47	B0	76/85 (89%)	2.54	35 (46%) 0 0	116, 147, 174, 187	0
47	D0	76/85 (89%)	2.48	39 (51%) 0 0	115, 148, 175, 193	0
48	B1	88/98 (89%)	1.11	16 (18%) 2 1	107, 128, 162, 180	0
48	D1	88/98 (89%)	1.02	17 (19%) 2 1	102, 121, 165, 187	0
49	B2	72/72 (100%)	1.02	15 (20%) 1 1	128, 148, 181, 208	0
49	D2	72/72 (100%)	1.18	19 (26%) 1 0	115, 129, 183, 197	0
50	B3	59/60 (98%)	2.05	22 (37%) 0 0	127, 147, 180, 210	0
50	D3	59/60 (98%)	1.31	14 (23%) 1 1	121, 143, 172, 212	0
51	B4	30/97 (30%)	2.01	12 (40%) 0 0	204, 221, 244, 244	0
51	D4	30/97 (30%)	1.48	8 (26%) 1 0	208, 226, 243, 245	0
52	B5	52/60 (86%)	0.73	7 (13%) 4 2	98, 120, 159, 188	0
52	D5	52/60 (86%)	0.29	2 (3%) 44 29	96, 126, 177, 192	0
53	B6	44/54 (81%)	6.27	42 (95%) 0 0	132, 166, 195, 199	0
53	D6	44/54 (81%)	6.83	34 (77%) 0 0	134, 165, 193, 200	0
54	B7	48/49 (97%)	0.75	5 (10%) 8 5	98, 105, 132, 171	0
54	D7	48/49 (97%)	0.48	3 (6%) 23 13	92, 97, 120, 175	0
55	B8	63/65 (96%)	2.28	33 (52%) 0 0	115, 125, 158, 176	0
55	D8	63/65 (96%)	2.39	39 (61%) 0 0	109, 124, 151, 190	0
All	All	21460/22658 (94%)	0.94	4070 (18%) 2 1	59, 143, 230, 354	0

The worst 5 of 4070 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	80	G	43.6
1	AA	81	G	36.7

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	BI	85	GLU	27.2
53	B6	13	CYS	23.0
37	DQ	140	ALA	22.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
56	MG	BA	3775	1/1	0.95	0.95	25.52	49,49,49,49	0
56	MG	DA	3673	1/1	0.70	1.03	24.28	65,65,65,65	0
56	MG	CA	1963	1/1	0.94	0.55	15.51	35,35,35,35	0
56	MG	CX	406	1/1	0.83	1.59	10.58	71,71,71,71	0
56	MG	AA	1834	1/1	0.93	0.60	8.91	36,36,36,36	0
56	MG	DA	3729	1/1	0.96	0.53	8.14	50,50,50,50	0
56	MG	DA	3417	1/1	0.93	0.33	7.75	53,53,53,53	0
56	MG	DA	3661	1/1	0.52	1.24	7.68	80,80,80,80	0
56	MG	BA	3011	1/1	0.97	0.41	7.17	33,33,33,33	0
56	MG	DA	3726	1/1	0.99	0.33	7.14	34,34,34,34	0
56	MG	CA	1930	1/1	0.76	0.59	7.07	57,57,57,57	0
56	MG	CA	1982	1/1	0.87	0.56	5.77	63,63,63,63	0
56	MG	DA	3254	1/1	0.98	0.28	5.62	35,35,35,35	0
56	MG	CA	1983	1/1	0.97	0.42	5.60	50,50,50,50	0
56	MG	AY	105	1/1	0.96	0.28	5.31	64,64,64,64	0
56	MG	CY	113	1/1	0.94	0.68	4.75	39,39,39,39	0
56	MG	BA	3380	1/1	0.86	0.28	4.60	56,56,56,56	0
56	MG	BA	3169	1/1	0.94	0.21	4.50	26,26,26,26	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3679	1/1	0.84	0.46	4.43	62,62,62,62	0
56	MG	BA	3796	1/1	0.97	0.24	3.74	27,27,27,27	0
56	MG	DA	3283	1/1	0.94	0.29	3.30	36,36,36,36	0
56	MG	BA	3708	1/1	0.78	0.32	3.10	60,60,60,60	0
56	MG	AA	1861	1/1	0.94	0.72	3.09	60,60,60,60	0
56	MG	DA	3688	1/1	0.94	0.27	3.06	63,63,63,63	0
56	MG	CA	1615	1/1	0.69	0.34	3.05	55,55,55,55	0
56	MG	AD	304	1/1	0.82	0.56	3.04	50,50,50,50	0
56	MG	DA	3256	1/1	0.94	0.26	2.95	37,37,37,37	0
56	MG	DA	3430	1/1	0.92	0.17	2.89	56,56,56,56	0
56	MG	AA	1844	1/1	0.83	0.37	2.85	38,38,38,38	0
56	MG	AA	1756	1/1	0.95	0.34	2.72	38,38,38,38	0
56	MG	BA	3481	1/1	0.95	0.34	2.67	45,45,45,45	0
56	MG	DA	3721	1/1	0.97	0.27	2.63	11,11,11,11	0
56	MG	AA	1802	1/1	0.93	0.23	2.36	56,56,56,56	0
56	MG	CA	1800	1/1	0.95	0.29	2.34	30,30,30,30	0
56	MG	CA	1624	1/1	0.97	0.36	2.27	54,54,54,54	0
56	MG	AA	1645	1/1	0.98	0.23	2.21	31,31,31,31	0
56	MG	BA	3597	1/1	0.96	0.47	2.18	40,40,40,40	0
56	MG	DA	3637	1/1	0.94	0.46	2.17	66,66,66,66	0
56	MG	BA	3606	1/1	0.95	0.36	1.97	54,54,54,54	0
56	MG	DA	3696	1/1	0.96	0.23	1.85	76,76,76,76	0
56	MG	DA	3429	1/1	0.97	0.36	1.84	48,48,48,48	0
56	MG	DA	3754	1/1	0.84	0.27	1.84	59,59,59,59	0
56	MG	BA	3024	1/1	0.99	0.27	1.72	37,37,37,37	0
56	MG	BA	3370	1/1	0.97	0.28	1.67	24,24,24,24	0
56	MG	DA	3184	1/1	0.81	0.21	1.64	22,22,22,22	0
56	MG	DA	3263	1/1	0.88	0.19	1.61	22,22,22,22	0
56	MG	DA	3452	1/1	0.96	0.35	1.49	25,25,25,25	0
56	MG	CA	1862	1/1	0.83	0.27	1.37	71,71,71,71	0
56	MG	DA	3025	1/1	0.97	0.21	1.32	24,24,24,24	0
56	MG	BA	3762	1/1	0.95	0.53	1.19	35,35,35,35	0
56	MG	BR	202	1/1	0.79	0.55	1.17	61,61,61,61	0
56	MG	AA	1666	1/1	0.97	0.30	1.12	34,34,34,34	0
56	MG	DA	3576	1/1	0.98	0.25	1.10	18,18,18,18	0
56	MG	DA	3689	1/1	0.98	0.21	1.08	45,45,45,45	0
56	MG	BA	3577	1/1	0.97	0.21	1.06	17,17,17,17	0
56	MG	AA	1883	1/1	0.98	0.22	1.06	21,21,21,21	0
56	MG	BA	3697	1/1	0.88	0.28	1.05	40,40,40,40	0
56	MG	AA	1857	1/1	0.96	0.17	0.99	41,41,41,41	0
56	MG	CA	1941	1/1	0.96	0.41	0.96	34,34,34,34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CY	106	1/1	0.97	0.17	0.89	35,35,35,35	0
56	MG	DA	3750	1/1	0.93	0.33	0.89	47,47,47,47	0
56	MG	DA	3236	1/1	0.98	0.31	0.88	14,14,14,14	0
56	MG	BA	3087	1/1	0.88	0.17	0.84	30,30,30,30	0
56	MG	DA	3279	1/1	0.96	0.18	0.76	20,20,20,20	0
56	MG	CA	2007	1/1	0.92	0.30	0.72	60,60,60,60	0
56	MG	BA	3455	1/1	0.93	0.24	0.65	46,46,46,46	0
56	MG	AA	1868	1/1	0.91	0.37	0.62	41,41,41,41	0
56	MG	DA	3234	1/1	0.97	0.27	0.59	8,8,8,8	0
56	MG	DA	3536	1/1	0.98	0.18	0.58	35,35,35,35	0
56	MG	CA	1893	1/1	0.99	0.27	0.51	23,23,23,23	0
56	MG	B7	101	1/1	0.94	0.27	0.50	24,24,24,24	0
56	MG	BA	3178	1/1	0.86	0.21	0.47	39,39,39,39	0
56	MG	CA	1696	1/1	0.96	0.25	0.46	54,54,54,54	0
56	MG	BG	203	1/1	0.89	0.35	0.41	54,54,54,54	0
56	MG	BA	3389	1/1	0.95	0.16	0.38	33,33,33,33	0
56	MG	DA	3144	1/1	0.97	0.24	0.34	11,11,11,11	0
56	MG	DA	3561	1/1	0.99	0.21	0.33	19,19,19,19	0
56	MG	CA	1861	1/1	0.97	0.20	0.27	64,64,64,64	0
56	MG	DA	3654	1/1	0.86	0.32	0.27	41,41,41,41	0
56	MG	DA	3021	1/1	0.97	0.27	0.18	2,2,2,2	0
56	MG	BA	3333	1/1	0.97	0.22	0.18	19,19,19,19	0
56	MG	CA	1686	1/1	0.97	0.29	0.17	29,29,29,29	0
56	MG	BA	3039	1/1	0.85	0.21	0.17	33,33,33,33	0
56	MG	CA	1856	1/1	0.92	0.27	0.14	78,78,78,78	0
56	MG	BA	3620	1/1	0.98	0.28	0.13	49,49,49,49	0
56	MG	CA	1885	1/1	0.92	0.19	0.13	72,72,72,72	0
56	MG	BA	3647	1/1	0.97	0.30	0.12	20,20,20,20	0
56	MG	BA	3665	1/1	0.84	0.29	0.12	46,46,46,46	0
56	MG	BA	3760	1/1	0.98	0.19	0.11	40,40,40,40	0
56	MG	DA	3302	1/1	0.88	0.25	0.10	31,31,31,31	0
56	MG	AA	1823	1/1	0.96	0.24	0.08	32,32,32,32	0
56	MG	B1	102	1/1	0.97	0.24	0.07	24,24,24,24	0
56	MG	DA	3093	1/1	0.87	0.24	0.05	23,23,23,23	0
56	MG	CA	1954	1/1	0.97	0.23	-0.00	22,22,22,22	0
56	MG	BA	3055	1/1	0.96	0.18	-0.01	27,27,27,27	0
56	MG	CC	306	1/1	0.92	0.40	-0.03	52,52,52,52	0
56	MG	BA	3192	1/1	0.97	0.23	-0.04	20,20,20,20	0
56	MG	DA	3177	1/1	0.99	0.32	-0.06	3,3,3,3	0
56	MG	BA	3028	1/1	0.97	0.21	-0.08	10,10,10,10	0
56	MG	DA	3458	1/1	0.90	0.21	-0.14	44,44,44,44	0
56	MG	BA	3263	1/1	0.96	0.18	-0.16	0,0,0,0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3554	1/1	0.95	0.22	-0.18	19,19,19,19	0
56	MG	AA	1851	1/1	0.97	0.15	-0.20	50,50,50,50	0
56	MG	DB	208	1/1	0.94	0.20	-0.22	39,39,39,39	0
56	MG	BA	3484	1/1	0.91	0.16	-0.25	23,23,23,23	0
56	MG	DA	3113	1/1	0.96	0.26	-0.26	13,13,13,13	0
56	MG	AP	101	1/1	0.94	0.25	-0.26	32,32,32,32	0
56	MG	DA	3634	1/1	0.91	0.17	-0.28	58,58,58,58	0
56	MG	DA	3273	1/1	0.98	0.19	-0.30	0,0,0,0	0
56	MG	AA	1830	1/1	0.99	0.17	-0.31	35,35,35,35	0
56	MG	BA	3049	1/1	0.95	0.15	-0.35	17,17,17,17	0
56	MG	BA	3299	1/1	0.94	0.17	-0.36	44,44,44,44	0
56	MG	DA	3251	1/1	0.96	0.23	-0.37	16,16,16,16	0
56	MG	BY	201	1/1	0.97	0.39	-0.39	36,36,36,36	0
56	MG	BA	3386	1/1	0.96	0.18	-0.40	38,38,38,38	0
56	MG	DA	3355	1/1	0.92	0.18	-0.41	39,39,39,39	0
56	MG	DA	3003	1/1	0.94	0.17	-0.42	33,33,33,33	0
56	MG	DB	225	1/1	0.92	0.17	-0.45	34,34,34,34	0
56	MG	BA	3116	1/1	0.97	0.14	-0.45	68,68,68,68	0
56	MG	CA	1967	1/1	0.89	0.21	-0.49	60,60,60,60	0
56	MG	BA	3632	1/1	0.92	0.18	-0.50	50,50,50,50	0
56	MG	BA	3624	1/1	0.94	0.25	-0.50	82,82,82,82	0
56	MG	DA	3013	1/1	0.94	0.16	-0.50	23,23,23,23	0
56	MG	DA	3731	1/1	0.91	0.14	-0.51	60,60,60,60	0
56	MG	DA	3371	1/1	0.95	0.16	-0.51	33,33,33,33	0
56	MG	AA	1637	1/1	0.97	0.20	-0.54	32,32,32,32	0
56	MG	CX	408	1/1	0.96	0.21	-0.54	44,44,44,44	0
56	MG	BF	303	1/1	0.99	0.24	-0.54	37,37,37,37	0
56	MG	CA	2008	1/1	0.97	0.44	-0.56	53,53,53,53	0
56	MG	BA	3223	1/1	0.99	0.20	-0.57	9,9,9,9	0
56	MG	DP	206	1/1	0.98	0.15	-0.58	33,33,33,33	0
56	MG	DA	3005	1/1	0.99	0.17	-0.58	1,1,1,1	0
56	MG	DA	3485	1/1	0.98	0.22	-0.62	10,10,10,10	0
56	MG	BA	3790	1/1	0.91	0.13	-0.64	75,75,75,75	0
56	MG	DA	3531	1/1	0.98	0.13	-0.65	39,39,39,39	0
56	MG	BA	3717	1/1	0.95	0.15	-0.67	40,40,40,40	0
56	MG	DA	3406	1/1	0.96	0.22	-0.67	33,33,33,33	0
56	MG	BA	3654	1/1	0.93	0.16	-0.68	40,40,40,40	0
56	MG	BB	221	1/1	0.89	0.25	-0.69	37,37,37,37	0
56	MG	AC	301	1/1	0.97	0.15	-0.69	41,41,41,41	0
56	MG	DA	3295	1/1	0.97	0.20	-0.71	37,37,37,37	0
56	MG	DA	3074	1/1	0.96	0.12	-0.71	19,19,19,19	0
56	MG	DA	3008	1/1	0.99	0.15	-0.74	9,9,9,9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DX	101	1/1	0.95	0.19	-0.75	50,50,50,50	0
56	MG	DA	3488	1/1	0.99	0.20	-0.76	10,10,10,10	0
56	MG	DA	3519	1/1	0.99	0.14	-0.76	6,6,6,6	0
56	MG	AD	305	1/1	0.96	0.21	-0.76	52,52,52,52	0
56	MG	CA	1912	1/1	0.97	0.13	-0.77	45,45,45,45	0
56	MG	AY	109	1/1	0.81	0.14	-0.78	63,63,63,63	0
56	MG	BA	3127	1/1	0.96	0.16	-0.79	38,38,38,38	0
56	MG	DA	3054	1/1	0.96	0.20	-0.80	2,2,2,2	0
56	MG	BA	3473	1/1	0.98	0.11	-0.82	35,35,35,35	0
56	MG	BA	3519	1/1	0.92	0.14	-0.82	38,38,38,38	0
56	MG	AA	1621	1/1	0.98	0.13	-0.83	15,15,15,15	0
56	MG	BA	3058	1/1	0.97	0.14	-0.85	39,39,39,39	0
56	MG	DA	3030	1/1	0.94	0.10	-0.85	17,17,17,17	0
56	MG	AA	1741	1/1	0.93	0.14	-0.89	32,32,32,32	0
56	MG	BA	3273	1/1	0.95	0.15	-0.90	17,17,17,17	0
56	MG	DA	3271	1/1	0.90	0.14	-0.91	17,17,17,17	0
56	MG	CA	1840	1/1	0.95	0.12	-0.92	54,54,54,54	0
56	MG	BA	3100	1/1	0.88	0.17	-0.92	42,42,42,42	0
56	MG	AA	1759	1/1	0.99	0.08	-0.97	6,6,6,6	0
56	MG	BA	3580	1/1	0.99	0.18	-0.97	19,19,19,19	0
56	MG	BA	3529	1/1	0.74	0.17	-0.98	32,32,32,32	0
56	MG	DA	3495	1/1	0.93	0.17	-0.98	13,13,13,13	0
56	MG	BA	3113	1/1	0.93	0.18	-0.98	10,10,10,10	0
56	MG	BA	3092	1/1	0.89	0.20	-0.98	40,40,40,40	0
56	MG	DA	3332	1/1	0.97	0.10	-0.99	50,50,50,50	0
56	MG	DA	3384	1/1	0.97	0.20	-1.01	20,20,20,20	0
56	MG	BD	302	1/1	0.99	0.14	-1.03	2,2,2,2	0
56	MG	DA	3202	1/1	0.99	0.07	-1.04	32,32,32,32	0
56	MG	DA	3057	1/1	0.92	0.14	-1.04	31,31,31,31	0
56	MG	BA	3209	1/1	0.93	0.17	-1.07	31,31,31,31	0
56	MG	BA	3711	1/1	0.90	0.21	-1.07	28,28,28,28	0
56	MG	DB	221	1/1	0.92	0.13	-1.09	49,49,49,49	0
56	MG	DA	3159	1/1	0.94	0.11	-1.10	52,52,52,52	0
56	MG	DA	3072	1/1	0.95	0.12	-1.11	29,29,29,29	0
56	MG	DA	3353	1/1	0.98	0.11	-1.12	0,0,0,0	0
56	MG	AX	403	1/1	0.93	0.06	-1.13	73,73,73,73	0
56	MG	DA	3362	1/1	0.96	0.16	-1.14	43,43,43,43	0
56	MG	AX	402	1/1	0.94	0.14	-1.19	29,29,29,29	0
56	MG	BA	3144	1/1	0.97	0.14	-1.20	34,34,34,34	0
56	MG	BA	3530	1/1	0.97	0.17	-1.20	35,35,35,35	0
56	MG	BA	3609	1/1	0.99	0.15	-1.20	10,10,10,10	0
56	MG	BA	3716	1/1	0.96	0.12	-1.20	28,28,28,28	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1817	1/1	0.98	0.12	-1.20	39,39,39,39	0
56	MG	DA	3693	1/1	0.95	0.12	-1.21	30,30,30,30	0
56	MG	DA	3197	1/1	0.95	0.14	-1.21	31,31,31,31	0
56	MG	AA	1789	1/1	0.90	0.15	-1.21	33,33,33,33	0
56	MG	BA	3132	1/1	0.99	0.15	-1.22	21,21,21,21	0
56	MG	DA	3059	1/1	0.96	0.16	-1.22	27,27,27,27	0
56	MG	BA	3595	1/1	0.67	0.12	-1.22	61,61,61,61	0
56	MG	BA	3064	1/1	0.98	0.14	-1.23	21,21,21,21	0
56	MG	DA	3022	1/1	0.95	0.08	-1.26	19,19,19,19	0
56	MG	DA	3277	1/1	0.99	0.18	-1.26	0,0,0,0	0
56	MG	CX	404	1/1	0.97	0.10	-1.26	34,34,34,34	0
56	MG	BA	3644	1/1	0.96	0.14	-1.27	32,32,32,32	0
56	MG	DA	3616	1/1	0.92	0.12	-1.27	10,10,10,10	0
56	MG	AA	1754	1/1	0.97	0.06	-1.27	21,21,21,21	0
56	MG	BA	3368	1/1	0.96	0.16	-1.29	22,22,22,22	0
56	MG	CA	1703	1/1	0.94	0.09	-1.31	34,34,34,34	0
56	MG	DW	201	1/1	0.97	0.17	-1.33	54,54,54,54	0
56	MG	BA	3213	1/1	0.98	0.15	-1.33	33,33,33,33	0
56	MG	CA	1829	1/1	0.93	0.21	-1.34	35,35,35,35	0
56	MG	BT	201	1/1	0.98	0.13	-1.35	23,23,23,23	0
56	MG	BA	3224	1/1	0.88	0.13	-1.35	52,52,52,52	0
56	MG	DA	3360	1/1	0.93	0.14	-1.36	29,29,29,29	0
56	MG	BA	3486	1/1	0.98	0.06	-1.36	41,41,41,41	0
56	MG	BA	3600	1/1	0.98	0.10	-1.37	13,13,13,13	0
56	MG	CA	1710	1/1	0.95	0.10	-1.38	29,29,29,29	0
56	MG	DA	3016	1/1	0.96	0.17	-1.38	3,3,3,3	0
56	MG	AA	1693	1/1	0.86	0.14	-1.39	45,45,45,45	0
56	MG	BA	3411	1/1	0.98	0.15	-1.40	20,20,20,20	0
56	MG	CA	1672	1/1	0.97	0.13	-1.41	33,33,33,33	0
56	MG	AA	1794	1/1	0.99	0.15	-1.42	13,13,13,13	0
56	MG	BA	3381	1/1	0.95	0.15	-1.42	2,2,2,2	0
56	MG	CA	1611	1/1	0.94	0.08	-1.43	40,40,40,40	0
56	MG	AA	1717	1/1	0.96	0.09	-1.45	28,28,28,28	0
56	MG	BA	3622	1/1	0.97	0.12	-1.45	32,32,32,32	0
56	MG	DA	3312	1/1	0.94	0.12	-1.45	24,24,24,24	0
56	MG	DA	3099	1/1	0.98	0.16	-1.48	23,23,23,23	0
56	MG	DA	3108	1/1	0.98	0.11	-1.49	1,1,1,1	0
56	MG	DA	3162	1/1	0.92	0.18	-1.51	33,33,33,33	0
56	MG	AA	1680	1/1	0.95	0.12	-1.51	26,26,26,26	0
56	MG	AA	1831	1/1	0.92	0.09	-1.51	44,44,44,44	0
57	ZN	CN	101	1/1	0.98	0.04	-1.52	82,82,82,82	0
56	MG	DP	201	1/1	0.89	0.08	-1.52	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3524	1/1	0.93	0.09	-1.52	27,27,27,27	0
56	MG	AD	306	1/1	0.97	0.16	-1.53	38,38,38,38	0
56	MG	BA	3075	1/1	0.98	0.15	-1.53	11,11,11,11	0
56	MG	BA	3291	1/1	0.98	0.18	-1.53	19,19,19,19	0
56	MG	DA	3019	1/1	0.94	0.09	-1.55	5,5,5,5	0
56	MG	CZ	103	1/1	0.93	0.06	-1.55	51,51,51,51	0
56	MG	BA	3382	1/1	0.94	0.14	-1.56	33,33,33,33	0
56	MG	DA	3343	1/1	0.90	0.11	-1.57	35,35,35,35	0
56	MG	AC	303	1/1	0.93	0.07	-1.58	51,51,51,51	0
56	MG	CA	1689	1/1	0.84	0.20	-1.60	59,59,59,59	0
56	MG	BA	3268	1/1	0.97	0.14	-1.60	6,6,6,6	0
56	MG	BA	3044	1/1	0.99	0.15	-1.60	18,18,18,18	0
56	MG	BA	3016	1/1	0.98	0.15	-1.61	0,0,0,0	0
56	MG	DA	3127	1/1	0.92	0.13	-1.61	71,71,71,71	0
56	MG	BA	3029	1/1	0.95	0.10	-1.61	1,1,1,1	0
56	MG	BB	217	1/1	0.93	0.10	-1.63	63,63,63,63	0
56	MG	AA	1633	1/1	0.91	0.12	-1.64	49,49,49,49	0
56	MG	AD	303	1/1	0.97	0.11	-1.65	17,17,17,17	0
56	MG	DA	3710	1/1	0.93	0.14	-1.66	21,21,21,21	0
56	MG	BA	3069	1/1	0.97	0.14	-1.67	11,11,11,11	0
56	MG	CA	1742	1/1	0.95	0.11	-1.68	22,22,22,22	0
56	MG	BA	3237	1/1	0.98	0.16	-1.68	28,28,28,28	0
56	MG	BA	3499	1/1	0.91	0.11	-1.69	18,18,18,18	0
56	MG	BD	301	1/1	0.97	0.08	-1.69	2,2,2,2	0
56	MG	DA	3669	1/1	0.97	0.10	-1.69	7,7,7,7	0
56	MG	AA	1639	1/1	0.99	0.04	-1.70	25,25,25,25	0
57	ZN	AN	101	1/1	0.98	0.04	-1.72	68,68,68,68	0
56	MG	BA	3137	1/1	0.96	0.11	-1.72	47,47,47,47	0
56	MG	BA	3612	1/1	0.94	0.12	-1.73	31,31,31,31	0
56	MG	BA	3203	1/1	0.93	0.14	-1.73	27,27,27,27	0
56	MG	CA	1655	1/1	0.98	0.15	-1.73	24,24,24,24	0
56	MG	CA	1626	1/1	0.96	0.10	-1.76	52,52,52,52	0
56	MG	BA	3537	1/1	0.96	0.09	-1.77	17,17,17,17	0
56	MG	DQ	201	1/1	0.87	0.10	-1.77	53,53,53,53	0
56	MG	AA	1775	1/1	0.92	0.13	-1.79	74,74,74,74	0
56	MG	DH	203	1/1	0.99	0.14	-1.79	19,19,19,19	0
56	MG	AA	1673	1/1	0.96	0.10	-1.80	21,21,21,21	0
56	MG	AA	1672	1/1	0.97	0.12	-1.81	46,46,46,46	0
56	MG	DA	3514	1/1	0.97	0.09	-1.81	44,44,44,44	0
56	MG	DA	3017	1/1	0.97	0.12	-1.83	4,4,4,4	0
56	MG	DA	3521	1/1	0.98	0.14	-1.84	7,7,7,7	0
56	MG	AA	1697	1/1	0.98	0.09	-1.85	1,1,1,1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3568	1/1	0.95	0.10	-1.86	44,44,44,44	0
56	MG	DA	3557	1/1	0.96	0.13	-1.86	13,13,13,13	0
56	MG	DD	301	1/1	0.98	0.05	-1.87	0,0,0,0	0
56	MG	BA	3085	1/1	0.94	0.12	-1.88	37,37,37,37	0
56	MG	BA	3420	1/1	0.93	0.11	-1.89	7,7,7,7	0
56	MG	BA	3269	1/1	0.95	0.10	-1.91	37,37,37,37	0
56	MG	DA	3687	1/1	0.95	0.12	-1.92	21,21,21,21	0
56	MG	BA	3423	1/1	0.91	0.16	-1.94	22,22,22,22	0
56	MG	DA	3164	1/1	0.96	0.10	-1.94	13,13,13,13	0
56	MG	BA	3480	1/1	0.94	0.20	-1.95	23,23,23,23	0
56	MG	AF	201	1/1	0.98	0.08	-1.95	30,30,30,30	0
56	MG	BF	301	1/1	0.92	0.13	-1.96	39,39,39,39	0
56	MG	DA	3571	1/1	0.96	0.10	-1.97	26,26,26,26	0
56	MG	AA	1601	1/1	0.97	0.15	-1.98	18,18,18,18	0
56	MG	AA	1765	1/1	0.97	0.08	-1.99	35,35,35,35	0
56	MG	BA	3176	1/1	0.95	0.16	-1.99	3,3,3,3	0
56	MG	CZ	112	1/1	0.96	0.13	-2.00	36,36,36,36	0
56	MG	DA	3046	1/1	0.99	0.06	-2.00	10,10,10,10	0
56	MG	DA	3549	1/1	0.96	0.07	-2.02	13,13,13,13	0
56	MG	BA	3068	1/1	0.97	0.17	-2.04	14,14,14,14	0
56	MG	DA	3682	1/1	0.98	0.14	-2.05	10,10,10,10	0
56	MG	DA	3169	1/1	0.91	0.14	-2.05	42,42,42,42	0
57	ZN	AD	301	1/1	0.99	0.21	-2.06	46,46,46,46	0
56	MG	AA	1835	1/1	0.98	0.15	-2.06	17,17,17,17	0
56	MG	BA	3355	1/1	0.96	0.16	-2.09	35,35,35,35	0
56	MG	BA	3771	1/1	0.94	0.13	-2.09	45,45,45,45	0
56	MG	BA	3032	1/1	0.97	0.10	-2.10	11,11,11,11	0
56	MG	BA	3397	1/1	0.97	0.10	-2.10	45,45,45,45	0
56	MG	DA	3106	1/1	0.95	0.13	-2.10	34,34,34,34	0
56	MG	BA	3452	1/1	0.97	0.12	-2.11	18,18,18,18	0
56	MG	CA	1760	1/1	0.96	0.07	-2.14	59,59,59,59	0
56	MG	BA	3498	1/1	0.93	0.12	-2.14	19,19,19,19	0
56	MG	DA	3139	1/1	0.98	0.12	-2.16	47,47,47,47	0
56	MG	DA	3187	1/1	0.97	0.14	-2.17	14,14,14,14	0
56	MG	DA	3063	1/1	0.98	0.07	-2.17	0,0,0,0	0
56	MG	BA	3157	1/1	0.97	0.10	-2.18	8,8,8,8	0
56	MG	BA	3217	1/1	0.98	0.12	-2.19	0,0,0,0	0
56	MG	BA	3504	1/1	0.98	0.07	-2.21	12,12,12,12	0
56	MG	DA	3131	1/1	0.99	0.10	-2.22	16,16,16,16	0
56	MG	CA	1694	1/1	0.95	0.10	-2.22	39,39,39,39	0
56	MG	BA	3560	1/1	0.96	0.15	-2.23	27,27,27,27	0
56	MG	DA	3497	1/1	0.97	0.09	-2.24	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1653	1/1	0.89	0.14	-2.24	49,49,49,49	0
56	MG	BA	3605	1/1	0.98	0.19	-2.26	41,41,41,41	0
56	MG	BA	3076	1/1	0.98	0.04	-2.26	26,26,26,26	0
56	MG	DA	3274	1/1	0.96	0.14	-2.27	6,6,6,6	0
56	MG	BF	305	1/1	0.98	0.11	-2.27	27,27,27,27	0
56	MG	DA	3318	1/1	0.98	0.12	-2.30	21,21,21,21	0
56	MG	AA	1619	1/1	0.95	0.11	-2.31	37,37,37,37	0
56	MG	D7	102	1/1	0.97	0.11	-2.31	28,28,28,28	0
56	MG	AA	1609	1/1	0.98	0.07	-2.32	28,28,28,28	0
56	MG	DA	3510	1/1	0.94	0.15	-2.33	38,38,38,38	0
56	MG	BA	3054	1/1	0.97	0.12	-2.34	6,6,6,6	0
56	MG	BA	3541	1/1	0.94	0.11	-2.35	1,1,1,1	0
56	MG	BA	3109	1/1	0.97	0.17	-2.35	25,25,25,25	0
56	MG	DA	3350	1/1	0.97	0.10	-2.36	24,24,24,24	0
56	MG	BE	301	1/1	0.95	0.09	-2.39	42,42,42,42	0
56	MG	AA	1847	1/1	0.97	0.12	-2.43	46,46,46,46	0
56	MG	DA	3272	1/1	0.96	0.10	-2.43	0,0,0,0	0
56	MG	DA	3111	1/1	0.99	0.09	-2.45	6,6,6,6	0
56	MG	B2	101	1/1	0.97	0.20	-2.46	32,32,32,32	0
56	MG	BA	3006	1/1	0.97	0.10	-2.47	9,9,9,9	0
56	MG	DO	202	1/1	0.99	0.07	-2.47	14,14,14,14	0
56	MG	BA	3436	1/1	0.97	0.10	-2.47	1,1,1,1	0
56	MG	BA	3125	1/1	0.93	0.10	-2.47	23,23,23,23	0
56	MG	AA	1838	1/1	0.97	0.13	-2.50	39,39,39,39	0
56	MG	DA	3064	1/1	0.98	0.12	-2.51	11,11,11,11	0
56	MG	BA	3464	1/1	0.97	0.13	-2.51	30,30,30,30	0
56	MG	CA	1810	1/1	0.92	0.11	-2.51	28,28,28,28	0
56	MG	AA	1698	1/1	0.97	0.10	-2.51	27,27,27,27	0
56	MG	BA	3378	1/1	0.93	0.07	-2.52	28,28,28,28	0
56	MG	DA	3426	1/1	0.94	0.10	-2.56	34,34,34,34	0
56	MG	DA	3242	1/1	0.98	0.08	-2.56	24,24,24,24	0
56	MG	DA	3103	1/1	0.94	0.10	-2.56	16,16,16,16	0
56	MG	BA	3120	1/1	0.94	0.07	-2.57	1,1,1,1	0
56	MG	BA	3045	1/1	0.92	0.12	-2.57	40,40,40,40	0
57	ZN	CD	301	1/1	0.98	0.24	-2.57	70,70,70,70	0
56	MG	BA	3074	1/1	0.97	0.06	-2.59	24,24,24,24	0
56	MG	DA	3306	1/1	0.98	0.07	-2.60	15,15,15,15	0
56	MG	BA	3283	1/1	0.95	0.10	-2.60	4,4,4,4	0
56	MG	CY	121	1/1	0.98	0.08	-2.62	0,0,0,0	0
56	MG	BA	3030	1/1	0.97	0.08	-2.62	26,26,26,26	0
56	MG	BA	3035	1/1	0.96	0.09	-2.65	38,38,38,38	0
56	MG	CA	1682	1/1	0.87	0.12	-2.66	46,46,46,46	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3023	1/1	0.94	0.11	-2.68	7,7,7,7	0
56	MG	CA	1625	1/1	0.86	0.13	-2.70	60,60,60,60	0
56	MG	CY	117	1/1	0.97	0.11	-2.70	23,23,23,23	0
56	MG	DA	3409	1/1	0.98	0.09	-2.72	24,24,24,24	0
56	MG	BA	3236	1/1	0.97	0.16	-2.73	6,6,6,6	0
56	MG	CZ	104	1/1	0.98	0.07	-2.73	42,42,42,42	0
56	MG	BA	3367	1/1	0.99	0.12	-2.73	24,24,24,24	0
56	MG	CA	1911	1/1	0.88	0.12	-2.74	62,62,62,62	0
56	MG	CA	1644	1/1	0.99	0.06	-2.76	6,6,6,6	0
56	MG	CA	1878	1/1	0.95	0.07	-2.77	31,31,31,31	0
56	MG	CA	1643	1/1	0.95	0.07	-2.77	35,35,35,35	0
56	MG	BA	3468	1/1	0.98	0.06	-2.77	1,1,1,1	0
56	MG	DA	3600	1/1	0.99	0.07	-2.77	17,17,17,17	0
56	MG	BA	3353	1/1	0.97	0.07	-2.79	40,40,40,40	0
56	MG	BA	3602	1/1	0.94	0.08	-2.80	42,42,42,42	0
56	MG	CA	1880	1/1	0.93	0.06	-2.82	51,51,51,51	0
56	MG	BA	3002	1/1	0.97	0.08	-2.83	20,20,20,20	0
56	MG	DA	3031	1/1	0.98	0.11	-2.85	21,21,21,21	0
56	MG	DA	3563	1/1	0.98	0.09	-2.85	8,8,8,8	0
56	MG	DA	3143	1/1	0.98	0.09	-2.91	31,31,31,31	0
56	MG	DA	3245	1/1	0.98	0.09	-2.92	5,5,5,5	0
56	MG	CA	1692	1/1	0.97	0.10	-2.92	6,6,6,6	0
56	MG	BB	207	1/1	0.97	0.06	-2.93	28,28,28,28	0
56	MG	BA	3235	1/1	0.96	0.07	-2.94	21,21,21,21	0
56	MG	DA	3191	1/1	0.95	0.09	-2.97	48,48,48,48	0
56	MG	AA	1642	1/1	0.96	0.13	-2.97	46,46,46,46	0
56	MG	DA	3180	1/1	0.97	0.09	-2.97	22,22,22,22	0
56	MG	DA	3598	1/1	0.98	0.08	-2.98	9,9,9,9	0
56	MG	BA	3528	1/1	0.97	0.09	-3.04	9,9,9,9	0
56	MG	BA	3018	1/1	0.99	0.07	-3.05	2,2,2,2	0
56	MG	AA	1607	1/1	0.98	0.10	-3.07	8,8,8,8	0
56	MG	BA	3493	1/1	0.99	0.05	-3.08	17,17,17,17	0
56	MG	DA	3400	1/1	0.96	0.12	-3.11	19,19,19,19	0
56	MG	AA	1730	1/1	0.97	0.10	-3.12	12,12,12,12	0
56	MG	DA	3082	1/1	0.96	0.10	-3.13	19,19,19,19	0
56	MG	BA	3366	1/1	0.99	0.06	-3.14	10,10,10,10	0
56	MG	AA	1888	1/1	0.92	0.10	-3.14	53,53,53,53	0
56	MG	AA	1803	1/1	0.90	0.15	-3.15	30,30,30,30	0
56	MG	DA	3156	1/1	0.99	0.11	-3.15	14,14,14,14	0
56	MG	AA	1787	1/1	0.95	0.09	-3.16	36,36,36,36	0
56	MG	DA	3345	1/1	0.99	0.10	-3.20	24,24,24,24	0
56	MG	DA	3502	1/1	0.98	0.08	-3.20	13,13,13,13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3611	1/1	0.99	0.07	-3.21	21,21,21,21	0
56	MG	BA	3088	1/1	0.96	0.10	-3.22	10,10,10,10	0
56	MG	BA	3146	1/1	0.99	0.04	-3.23	22,22,22,22	0
56	MG	BA	3266	1/1	0.99	0.09	-3.24	10,10,10,10	0
56	MG	BA	3497	1/1	0.99	0.07	-3.28	2,2,2,2	0
56	MG	BO	201	1/1	0.98	0.06	-3.29	17,17,17,17	0
56	MG	DA	3165	1/1	0.97	0.11	-3.30	8,8,8,8	0
56	MG	BA	3516	1/1	0.94	0.09	-3.35	25,25,25,25	0
56	MG	AA	1679	1/1	0.98	0.07	-3.37	32,32,32,32	0
56	MG	DA	3146	1/1	0.99	0.09	-3.37	20,20,20,20	0
56	MG	DA	3226	1/1	0.98	0.06	-3.38	21,21,21,21	0
56	MG	BA	3168	1/1	0.98	0.06	-3.39	4,4,4,4	0
56	MG	BA	3322	1/1	0.93	0.12	-3.41	33,33,33,33	0
56	MG	BA	3487	1/1	0.98	0.07	-3.42	16,16,16,16	0
56	MG	D2	101	1/1	0.98	0.13	-3.44	58,58,58,58	0
56	MG	CA	1622	1/1	0.95	0.07	-3.46	24,24,24,24	0
56	MG	DA	3697	1/1	0.95	0.10	-3.48	36,36,36,36	0
56	MG	BA	3105	1/1	0.97	0.10	-3.48	36,36,36,36	0
56	MG	DA	3733	1/1	0.99	0.08	-3.48	19,19,19,19	0
56	MG	BA	3314	1/1	0.98	0.09	-3.52	10,10,10,10	0
56	MG	CA	1623	1/1	0.98	0.08	-3.52	22,22,22,22	0
56	MG	BA	3042	1/1	0.98	0.07	-3.59	12,12,12,12	0
56	MG	DA	3265	1/1	0.95	0.08	-3.61	25,25,25,25	0
56	MG	BA	3503	1/1	0.99	0.08	-3.62	29,29,29,29	0
56	MG	CA	1842	1/1	0.96	0.12	-3.64	36,36,36,36	0
56	MG	BA	3428	1/1	0.97	0.07	-3.64	17,17,17,17	0
56	MG	BA	3524	1/1	0.98	0.07	-3.67	36,36,36,36	0
56	MG	BA	3298	1/1	0.99	0.11	-3.68	5,5,5,5	0
56	MG	DA	3078	1/1	0.96	0.09	-3.74	15,15,15,15	0
56	MG	AA	1769	1/1	0.99	0.04	-3.78	47,47,47,47	0
56	MG	BA	3208	1/1	0.96	0.10	-3.79	27,27,27,27	0
56	MG	BA	3067	1/1	0.99	0.06	-3.84	27,27,27,27	0
56	MG	CA	1629	1/1	0.97	0.09	-3.84	8,8,8,8	0
56	MG	AA	1757	1/1	0.91	0.06	-3.85	26,26,26,26	0
56	MG	CA	1817	1/1	0.97	0.06	-3.87	19,19,19,19	0
56	MG	CA	1969	1/1	0.89	0.10	-3.91	43,43,43,43	0
56	MG	DA	3453	1/1	0.99	0.05	-3.92	23,23,23,23	0
56	MG	BA	3316	1/1	0.97	0.09	-3.97	12,12,12,12	0
56	MG	BA	3520	1/1	0.97	0.10	-3.98	7,7,7,7	0
56	MG	DA	3150	1/1	0.98	0.09	-3.98	1,1,1,1	0
56	MG	BA	3482	1/1	1.00	0.05	-4.09	11,11,11,11	0
56	MG	DA	3397	1/1	0.98	0.07	-4.16	19,19,19,19	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3561	1/1	0.96	0.07	-4.20	30,30,30,30	0
56	MG	DA	3051	1/1	0.99	0.04	-4.20	11,11,11,11	0
56	MG	BA	3152	1/1	0.99	0.05	-4.21	7,7,7,7	0
56	MG	BA	3281	1/1	0.97	0.09	-4.23	7,7,7,7	0
56	MG	CA	1695	1/1	0.93	0.10	-4.28	59,59,59,59	0
56	MG	CA	1799	1/1	0.98	0.08	-4.31	14,14,14,14	0
56	MG	CA	1633	1/1	0.98	0.08	-4.36	12,12,12,12	0
56	MG	DA	3102	1/1	0.99	0.06	-4.41	5,5,5,5	0
56	MG	BA	3295	1/1	0.95	0.10	-4.42	1,1,1,1	0
56	MG	BA	3027	1/1	0.98	0.08	-4.43	20,20,20,20	0
56	MG	CA	1805	1/1	0.98	0.11	-4.49	9,9,9,9	0
56	MG	AA	1681	1/1	0.97	0.07	-4.55	49,49,49,49	0
56	MG	DA	3041	1/1	0.97	0.05	-4.57	12,12,12,12	0
56	MG	AA	1617	1/1	0.99	0.05	-4.62	0,0,0,0	0
56	MG	CA	1933	1/1	0.98	0.08	-4.67	36,36,36,36	0
56	MG	AA	1635	1/1	0.97	0.09	-4.81	30,30,30,30	0
56	MG	BA	3005	1/1	0.98	0.07	-4.91	2,2,2,2	0
56	MG	AA	1661	1/1	0.93	0.10	-5.01	28,28,28,28	0
56	MG	DA	3219	1/1	0.98	0.08	-5.09	12,12,12,12	0
56	MG	BA	3126	1/1	0.98	0.07	-5.29	37,37,37,37	0
56	MG	BA	3276	1/1	0.99	0.05	-5.30	0,0,0,0	0
56	MG	BA	3099	1/1	0.99	0.06	-5.34	1,1,1,1	0
56	MG	DA	3314	1/1	0.98	0.06	-5.34	25,25,25,25	0
56	MG	DA	3024	1/1	0.98	0.07	-5.48	12,12,12,12	0
56	MG	CA	1808	1/1	0.98	0.10	-5.52	13,13,13,13	0
56	MG	CA	1660	1/1	0.99	0.06	-5.70	10,10,10,10	0
56	MG	BO	203	1/1	0.99	0.04	-5.89	19,19,19,19	0
56	MG	DA	3061	1/1	0.98	0.07	-5.93	4,4,4,4	0
56	MG	BA	3026	1/1	0.94	0.08	-6.11	0,0,0,0	0
56	MG	DA	3119	1/1	0.97	0.06	-6.18	10,10,10,10	0
56	MG	DA	3264	1/1	0.98	0.08	-6.43	29,29,29,29	0
56	MG	CA	1617	1/1	0.98	0.04	-6.47	11,11,11,11	0
56	MG	BA	3300	1/1	0.99	0.04	-6.47	20,20,20,20	0
56	MG	DA	3130	1/1	0.98	0.05	-6.58	20,20,20,20	0
56	MG	BA	3084	1/1	0.99	0.04	-6.62	1,1,1,1	0
56	MG	AA	1710	1/1	0.99	0.05	-6.92	1,1,1,1	0
56	MG	BA	3458	1/1	0.97	0.09	-7.26	6,6,6,6	0
56	MG	CA	1806	1/1	0.95	0.07	-7.43	36,36,36,36	0
56	MG	DA	3285	1/1	0.99	0.06	-8.96	15,15,15,15	0
56	MG	BA	3041	1/1	0.98	0.09	-12.81	25,25,25,25	0
56	MG	DA	3471	1/1	0.98	0.08	-17.38	18,18,18,18	0
56	MG	BA	3396	1/1	0.88	0.21	-	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1729	1/1	0.98	0.08	-	12,12,12,12	0
56	MG	DA	3380	1/1	0.96	0.12	-	26,26,26,26	0
56	MG	BA	3766	1/1	0.80	0.19	-	44,44,44,44	0
56	MG	DA	3418	1/1	0.93	0.16	-	54,54,54,54	0
56	MG	CA	1818	1/1	0.80	0.19	-	64,64,64,64	0
56	MG	DA	3614	1/1	0.97	0.19	-	55,55,55,55	0
56	MG	DA	3479	1/1	0.95	0.10	-	44,44,44,44	0
56	MG	CA	1882	1/1	0.98	0.35	-	35,35,35,35	0
56	MG	DA	3132	1/1	0.99	0.14	-	11,11,11,11	0
56	MG	DA	3328	1/1	0.99	0.05	-	10,10,10,10	0
56	MG	DA	3209	1/1	0.95	0.10	-	55,55,55,55	0
56	MG	AA	1877	1/1	0.97	0.23	-	32,32,32,32	0
56	MG	CA	1641	1/1	0.97	0.08	-	14,14,14,14	0
56	MG	DA	3167	1/1	0.93	0.18	-	23,23,23,23	0
56	MG	BB	215	1/1	0.96	0.09	-	47,47,47,47	0
56	MG	BA	3655	1/1	0.87	0.17	-	47,47,47,47	0
56	MG	DA	3566	1/1	0.98	0.07	-	15,15,15,15	0
56	MG	DA	3411	1/1	0.93	0.10	-	26,26,26,26	0
56	MG	DA	3562	1/1	0.98	0.07	-	17,17,17,17	0
56	MG	CA	1939	1/1	0.96	0.25	-	55,55,55,55	0
56	MG	AA	1658	1/1	0.97	0.11	-	19,19,19,19	0
56	MG	BA	3416	1/1	0.98	0.09	-	15,15,15,15	0
56	MG	DA	3504	1/1	0.93	0.11	-	39,39,39,39	0
56	MG	DA	3450	1/1	0.98	0.48	-	29,29,29,29	0
56	MG	DA	3050	1/1	0.97	0.16	-	11,11,11,11	0
56	MG	BA	3246	1/1	0.98	0.06	-	41,41,41,41	0
56	MG	AA	1675	1/1	0.95	0.21	-	47,47,47,47	0
56	MG	D4	103	1/1	0.95	0.28	-	40,40,40,40	0
56	MG	DA	3596	1/1	0.98	0.06	-	41,41,41,41	0
56	MG	BA	3681	1/1	0.94	0.16	-	62,62,62,62	0
56	MG	DA	3543	1/1	0.95	0.12	-	20,20,20,20	0
56	MG	BA	3725	1/1	0.84	0.22	-	52,52,52,52	0
56	MG	DA	3505	1/1	0.95	0.23	-	30,30,30,30	0
56	MG	DA	3743	1/1	0.95	0.24	-	43,43,43,43	0
56	MG	CA	1767	1/1	0.98	0.08	-	22,22,22,22	0
56	MG	DA	3086	1/1	0.98	0.12	-	42,42,42,42	0
56	MG	CV	104	1/1	0.81	0.42	-	54,54,54,54	0
56	MG	AA	1700	1/1	0.98	0.20	-	46,46,46,46	0
56	MG	BA	3575	1/1	0.92	0.16	-	52,52,52,52	0
56	MG	BA	3619	1/1	0.97	0.09	-	32,32,32,32	0
56	MG	AA	1674	1/1	0.92	0.37	-	74,74,74,74	0
56	MG	BA	3476	1/1	0.91	0.27	-	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3116	1/1	0.86	0.25	-	41,41,41,41	0
56	MG	AA	1872	1/1	0.95	0.15	-	19,19,19,19	0
56	MG	BA	3466	1/1	0.98	0.08	-	22,22,22,22	0
56	MG	BA	3242	1/1	0.98	0.10	-	22,22,22,22	0
56	MG	AA	1602	1/1	0.95	0.08	-	23,23,23,23	0
56	MG	DA	3352	1/1	0.99	0.14	-	15,15,15,15	0
56	MG	CA	1757	1/1	0.93	0.23	-	27,27,27,27	0
56	MG	BA	3546	1/1	0.97	0.11	-	17,17,17,17	0
56	MG	DA	3756	1/1	0.91	0.09	-	53,53,53,53	0
56	MG	CY	101	1/1	0.98	0.13	-	12,12,12,12	0
56	MG	CA	1995	1/1	0.94	0.18	-	47,47,47,47	0
56	MG	DA	3690	1/1	0.91	0.11	-	41,41,41,41	0
56	MG	CA	2013	1/1	0.99	0.03	-	7,7,7,7	0
56	MG	BA	3408	1/1	0.98	0.10	-	12,12,12,12	0
56	MG	BA	3434	1/1	0.95	0.10	-	45,45,45,45	0
56	MG	DA	3720	1/1	0.95	0.11	-	45,45,45,45	0
56	MG	DA	3321	1/1	0.97	0.10	-	28,28,28,28	0
56	MG	BA	3769	1/1	0.94	0.07	-	65,65,65,65	0
56	MG	BA	3066	1/1	0.98	0.13	-	37,37,37,37	0
56	MG	DA	3421	1/1	0.98	0.15	-	26,26,26,26	0
56	MG	BA	3733	1/1	0.93	0.29	-	43,43,43,43	0
56	MG	BA	3204	1/1	0.97	0.11	-	41,41,41,41	0
56	MG	DA	3230	1/1	0.99	0.07	-	19,19,19,19	0
56	MG	DA	3751	1/1	0.98	0.25	-	48,48,48,48	0
56	MG	DA	3716	1/1	0.95	0.30	-	54,54,54,54	0
56	MG	BA	3705	1/1	0.96	0.16	-	47,47,47,47	0
56	MG	AL	202	1/1	0.97	0.20	-	46,46,46,46	0
56	MG	CA	1991	1/1	0.93	0.32	-	57,57,57,57	0
56	MG	DA	3284	1/1	0.95	0.14	-	7,7,7,7	0
56	MG	AA	1828	1/1	0.93	0.16	-	47,47,47,47	0
56	MG	DA	3419	1/1	0.99	0.07	-	33,33,33,33	0
56	MG	AG	201	1/1	0.95	0.10	-	23,23,23,23	0
56	MG	BA	3388	1/1	0.97	0.23	-	46,46,46,46	0
56	MG	AA	1887	1/1	0.98	0.12	-	18,18,18,18	0
56	MG	DA	3140	1/1	0.98	0.19	-	18,18,18,18	0
56	MG	AA	1663	1/1	0.96	0.13	-	35,35,35,35	0
56	MG	BA	3491	1/1	0.97	0.13	-	31,31,31,31	0
56	MG	BA	3764	1/1	0.92	0.23	-	36,36,36,36	0
56	MG	BA	3317	1/1	0.97	0.13	-	25,25,25,25	0
56	MG	BA	3700	1/1	0.89	0.27	-	67,67,67,67	0
56	MG	BO	202	1/1	0.95	0.08	-	29,29,29,29	0
56	MG	BA	3564	1/1	0.95	0.14	-	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AY	121	1/1	0.98	0.15	-	30,30,30,30	0
56	MG	CA	1965	1/1	0.94	0.09	-	54,54,54,54	0
56	MG	CZ	118	1/1	0.98	0.43	-	69,69,69,69	0
56	MG	AA	1657	1/1	0.96	0.10	-	37,37,37,37	0
56	MG	BA	3785	1/1	0.97	0.22	-	47,47,47,47	0
56	MG	B2	102	1/1	0.98	0.23	-	31,31,31,31	0
56	MG	CA	1780	1/1	0.96	0.09	-	15,15,15,15	0
56	MG	AA	1781	1/1	0.93	0.11	-	55,55,55,55	0
56	MG	CZ	114	1/1	0.95	0.12	-	46,46,46,46	0
56	MG	BA	3729	1/1	0.97	0.15	-	43,43,43,43	0
56	MG	BA	3249	1/1	0.98	0.09	-	41,41,41,41	0
56	MG	BA	3251	1/1	0.93	0.11	-	43,43,43,43	0
56	MG	BA	3111	1/1	0.99	0.06	-	10,10,10,10	0
56	MG	BA	3692	1/1	0.92	0.21	-	41,41,41,41	0
56	MG	DA	3595	1/1	0.98	0.09	-	17,17,17,17	0
56	MG	BA	3174	1/1	0.98	0.11	-	28,28,28,28	0
56	MG	AA	1632	1/1	1.00	0.08	-	5,5,5,5	0
56	MG	DA	3104	1/1	0.97	0.15	-	21,21,21,21	0
56	MG	CA	2005	1/1	0.96	0.42	-	58,58,58,58	0
56	MG	DA	3619	1/1	0.99	0.12	-	23,23,23,23	0
56	MG	BA	3472	1/1	0.91	0.21	-	44,44,44,44	0
56	MG	CA	1827	1/1	0.88	0.12	-	48,48,48,48	0
56	MG	DA	3414	1/1	0.93	0.25	-	43,43,43,43	0
56	MG	CY	109	1/1	0.78	0.20	-	68,68,68,68	0
56	MG	DB	220	1/1	0.98	0.09	-	23,23,23,23	0
56	MG	DA	3379	1/1	0.85	0.52	-	51,51,51,51	0
56	MG	BA	3547	1/1	0.96	0.08	-	26,26,26,26	0
56	MG	BA	3308	1/1	0.94	0.17	-	9,9,9,9	0
56	MG	BA	3078	1/1	0.92	0.07	-	22,22,22,22	0
56	MG	DA	3546	1/1	0.58	0.69	-	82,82,82,82	0
56	MG	CA	1903	1/1	0.99	0.13	-	31,31,31,31	0
56	MG	BA	3323	1/1	0.97	0.14	-	40,40,40,40	0
56	MG	BA	3440	1/1	0.99	0.16	-	15,15,15,15	0
56	MG	DA	3109	1/1	0.97	0.13	-	19,19,19,19	0
56	MG	CA	2001	1/1	0.96	0.07	-	36,36,36,36	0
56	MG	DA	3602	1/1	0.97	0.09	-	32,32,32,32	0
56	MG	BA	3661	1/1	0.91	0.35	-	67,67,67,67	0
56	MG	DA	3121	1/1	0.98	0.14	-	24,24,24,24	0
56	MG	AA	1726	1/1	0.92	0.12	-	44,44,44,44	0
56	MG	BA	3800	1/1	0.96	0.70	-	32,32,32,32	0
56	MG	BA	3342	1/1	0.94	0.10	-	36,36,36,36	0
56	MG	CA	1887	1/1	0.97	0.24	-	40,40,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1644	1/1	0.90	0.08	-	31,31,31,31	0
56	MG	BA	3101	1/1	0.96	0.08	-	0,0,0,0	0
56	MG	AA	1782	1/1	0.99	0.07	-	21,21,21,21	0
56	MG	CA	1926	1/1	0.91	0.15	-	61,61,61,61	0
56	MG	DA	3432	1/1	0.86	0.20	-	51,51,51,51	0
56	MG	BA	3672	1/1	0.86	0.14	-	45,45,45,45	0
56	MG	BA	3463	1/1	0.91	0.15	-	27,27,27,27	0
56	MG	CA	1777	1/1	0.92	0.14	-	34,34,34,34	0
56	MG	DA	3433	1/1	0.98	0.09	-	21,21,21,21	0
56	MG	CA	1774	1/1	0.92	0.10	-	31,31,31,31	0
56	MG	DA	3154	1/1	0.98	0.26	-	38,38,38,38	0
56	MG	BA	3465	1/1	0.84	0.42	-	37,37,37,37	0
56	MG	DA	3356	1/1	0.96	0.10	-	38,38,38,38	0
56	MG	DB	206	1/1	0.95	0.12	-	39,39,39,39	0
56	MG	BA	3106	1/1	0.93	0.10	-	26,26,26,26	0
56	MG	DA	3239	1/1	0.99	0.09	-	12,12,12,12	0
56	MG	BA	3358	1/1	0.94	0.33	-	44,44,44,44	0
56	MG	CA	2014	1/1	0.83	0.43	-	52,52,52,52	0
56	MG	DA	3492	1/1	0.60	0.16	-	37,37,37,37	0
56	MG	CA	1919	1/1	0.95	0.15	-	64,64,64,64	0
56	MG	BA	3304	1/1	0.92	0.14	-	42,42,42,42	0
56	MG	BA	3772	1/1	0.90	0.49	-	57,57,57,57	0
56	MG	CA	1783	1/1	0.96	0.14	-	32,32,32,32	0
56	MG	CA	1875	1/1	0.98	0.15	-	19,19,19,19	0
56	MG	DA	3545	1/1	0.86	0.08	-	50,50,50,50	0
56	MG	AA	1827	1/1	0.96	0.06	-	38,38,38,38	0
56	MG	DA	3323	1/1	0.99	0.05	-	8,8,8,8	0
56	MG	DA	3011	1/1	0.99	0.20	-	17,17,17,17	0
56	MG	BB	213	1/1	0.98	0.09	-	35,35,35,35	0
56	MG	AA	1723	1/1	0.97	0.08	-	29,29,29,29	0
56	MG	BA	3536	1/1	0.89	0.11	-	34,34,34,34	0
56	MG	DA	3603	1/1	0.97	0.22	-	32,32,32,32	0
56	MG	CA	1960	1/1	0.99	0.11	-	26,26,26,26	0
56	MG	DA	3586	1/1	0.97	0.18	-	55,55,55,55	0
56	MG	DA	3157	1/1	0.97	0.12	-	30,30,30,30	0
56	MG	CA	1796	1/1	0.92	0.07	-	27,27,27,27	0
56	MG	DA	3240	1/1	0.99	0.07	-	21,21,21,21	0
56	MG	AA	1884	1/1	0.81	0.34	-	55,55,55,55	0
56	MG	DA	3378	1/1	0.99	0.06	-	17,17,17,17	0
56	MG	AA	1899	1/1	0.97	0.17	-	42,42,42,42	0
56	MG	BA	3802	1/1	0.95	0.23	-	54,54,54,54	0
56	MG	AA	1771	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( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3571	1/1	0.99	0.04	-	40,40,40,40	0
56	MG	DA	3034	1/1	0.96	0.12	-	9,9,9,9	0
56	MG	DW	203	1/1	0.97	0.12	-	7,7,7,7	0
56	MG	AA	1822	1/1	0.90	0.16	-	39,39,39,39	0
56	MG	AA	1886	1/1	0.99	0.11	-	39,39,39,39	0
56	MG	AO	103	1/1	0.91	0.26	-	43,43,43,43	0
56	MG	BA	3379	1/1	0.98	0.09	-	25,25,25,25	0
56	MG	CA	1639	1/1	0.99	0.07	-	28,28,28,28	0
56	MG	BG	202	1/1	0.98	0.07	-	26,26,26,26	0
56	MG	DA	3424	1/1	0.99	0.08	-	22,22,22,22	0
56	MG	CA	1680	1/1	0.98	0.09	-	37,37,37,37	0
56	MG	DA	3431	1/1	0.98	0.20	-	29,29,29,29	0
56	MG	DA	3560	1/1	0.98	0.15	-	8,8,8,8	0
56	MG	DA	3588	1/1	0.96	0.11	-	14,14,14,14	0
56	MG	BI	202	1/1	0.99	0.06	-	29,29,29,29	0
56	MG	BA	3442	1/1	0.99	0.36	-	26,26,26,26	0
56	MG	AA	1628	1/1	0.96	0.10	-	34,34,34,34	0
56	MG	BA	3675	1/1	0.98	0.07	-	40,40,40,40	0
56	MG	BA	3506	1/1	0.94	0.12	-	10,10,10,10	0
56	MG	BA	3712	1/1	0.89	0.22	-	37,37,37,37	0
56	MG	CA	1884	1/1	0.95	0.09	-	39,39,39,39	0
56	MG	DA	3040	1/1	0.99	0.13	-	10,10,10,10	0
56	MG	CA	1726	1/1	0.97	0.14	-	32,32,32,32	0
56	MG	CA	1654	1/1	0.97	0.09	-	23,23,23,23	0
56	MG	BA	3592	1/1	0.96	0.22	-	58,58,58,58	0
56	MG	BA	3034	1/1	0.97	0.07	-	17,17,17,17	0
56	MG	CA	1923	1/1	0.99	0.11	-	28,28,28,28	0
56	MG	AA	1792	1/1	0.90	0.06	-	58,58,58,58	0
56	MG	DA	3538	1/1	0.98	0.12	-	34,34,34,34	0
56	MG	BA	3083	1/1	0.99	0.06	-	9,9,9,9	0
56	MG	BB	214	1/1	0.95	0.06	-	29,29,29,29	0
56	MG	DA	3584	1/1	0.96	0.07	-	35,35,35,35	0
56	MG	DA	3179	1/1	0.92	0.13	-	50,50,50,50	0
56	MG	CY	120	1/1	0.97	0.17	-	29,29,29,29	0
56	MG	DA	3253	1/1	0.91	0.19	-	48,48,48,48	0
56	MG	BA	3375	1/1	0.98	0.06	-	14,14,14,14	0
56	MG	BA	3742	1/1	0.96	0.15	-	46,46,46,46	0
56	MG	AA	1720	1/1	0.93	0.14	-	33,33,33,33	0
56	MG	BA	3079	1/1	0.96	0.11	-	29,29,29,29	0
56	MG	AA	1779	1/1	0.88	0.39	-	51,51,51,51	0
56	MG	DA	3708	1/1	0.91	0.29	-	60,60,60,60	0
56	MG	CA	1976	1/1	0.98	0.09	-	32,32,32,32	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3135	1/1	1.00	0.05	-	13,13,13,13	0
56	MG	DA	3393	1/1	0.98	0.27	-	37,37,37,37	0
56	MG	DA	3120	1/1	0.99	0.27	-	23,23,23,23	0
56	MG	BA	3216	1/1	0.96	0.11	-	33,33,33,33	0
56	MG	CA	1764	1/1	0.97	0.14	-	30,30,30,30	0
56	MG	DA	3734	1/1	0.95	0.10	-	60,60,60,60	0
56	MG	AA	1716	1/1	0.99	0.07	-	35,35,35,35	0
56	MG	BA	3780	1/1	0.69	0.25	-	56,56,56,56	0
56	MG	DA	3388	1/1	0.99	0.06	-	3,3,3,3	0
56	MG	DA	3324	1/1	0.97	0.14	-	11,11,11,11	0
56	MG	CA	1775	1/1	0.97	0.18	-	30,30,30,30	0
56	MG	AA	1753	1/1	0.96	0.19	-	31,31,31,31	0
56	MG	BA	3583	1/1	0.98	0.08	-	24,24,24,24	0
56	MG	BA	3741	1/1	0.93	0.13	-	28,28,28,28	0
56	MG	BA	3673	1/1	0.90	0.39	-	46,46,46,46	0
56	MG	DA	3609	1/1	0.87	0.29	-	62,62,62,62	0
56	MG	BA	3578	1/1	0.97	0.12	-	19,19,19,19	0
56	MG	BA	3095	1/1	0.96	0.06	-	27,27,27,27	0
56	MG	BA	3735	1/1	0.96	0.19	-	29,29,29,29	0
56	MG	AA	1889	1/1	0.98	0.22	-	20,20,20,20	0
56	MG	BA	3012	1/1	0.89	0.09	-	36,36,36,36	0
56	MG	CA	1720	1/1	0.91	0.10	-	51,51,51,51	0
56	MG	CP	101	1/1	0.85	0.45	-	57,57,57,57	0
56	MG	AA	1614	1/1	0.99	0.08	-	4,4,4,4	0
56	MG	AA	1613	1/1	0.98	0.18	-	20,20,20,20	0
56	MG	DA	3214	1/1	0.92	0.10	-	46,46,46,46	0
56	MG	BA	3326	1/1	0.92	0.24	-	46,46,46,46	0
56	MG	AA	1850	1/1	0.97	0.30	-	23,23,23,23	0
56	MG	AA	1815	1/1	0.98	0.20	-	24,24,24,24	0
56	MG	DB	218	1/1	0.95	0.10	-	46,46,46,46	0
56	MG	CA	1679	1/1	0.98	0.11	-	40,40,40,40	0
56	MG	BH	201	1/1	0.98	0.12	-	15,15,15,15	0
56	MG	CX	407	1/1	0.84	0.30	-	70,70,70,70	0
56	MG	CA	1755	1/1	0.99	0.09	-	31,31,31,31	0
56	MG	BA	3061	1/1	0.99	0.09	-	26,26,26,26	0
56	MG	BA	3462	1/1	0.91	0.27	-	39,39,39,39	0
56	MG	BA	3310	1/1	0.99	0.09	-	23,23,23,23	0
56	MG	CA	1706	1/1	0.97	0.07	-	16,16,16,16	0
56	MG	DA	3190	1/1	0.96	0.16	-	32,32,32,32	0
56	MG	CA	1904	1/1	0.96	0.06	-	42,42,42,42	0
56	MG	BA	3572	1/1	0.67	0.17	-	72,72,72,72	0
56	MG	BB	220	1/1	0.97	0.13	-	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1650	1/1	0.91	0.27	-	50,50,50,50	0
56	MG	CA	1748	1/1	0.90	0.14	-	60,60,60,60	0
56	MG	DA	3648	1/1	0.94	0.12	-	42,42,42,42	0
56	MG	BA	3226	1/1	0.99	0.12	-	24,24,24,24	0
56	MG	AA	1903	1/1	0.97	0.13	-	39,39,39,39	0
56	MG	BA	3617	1/1	0.99	0.06	-	32,32,32,32	0
56	MG	BA	3400	1/1	0.88	0.18	-	35,35,35,35	0
56	MG	DA	3601	1/1	0.91	0.12	-	45,45,45,45	0
56	MG	CA	1601	1/1	0.97	0.10	-	54,54,54,54	0
56	MG	DA	3640	1/1	0.93	0.28	-	40,40,40,40	0
56	MG	DA	3296	1/1	0.97	0.09	-	4,4,4,4	0
56	MG	BA	3656	1/1	0.87	0.39	-	52,52,52,52	0
56	MG	DA	3076	1/1	0.93	0.15	-	51,51,51,51	0
56	MG	AA	1758	1/1	0.94	0.11	-	47,47,47,47	0
56	MG	BA	3743	1/1	0.93	0.09	-	34,34,34,34	0
56	MG	CA	1758	1/1	0.93	0.07	-	37,37,37,37	0
56	MG	CA	1953	1/1	0.97	0.12	-	18,18,18,18	0
56	MG	DA	3149	1/1	0.97	0.29	-	37,37,37,37	0
56	MG	AX	404	1/1	0.59	0.18	-	68,68,68,68	0
56	MG	BA	3090	1/1	0.97	0.06	-	56,56,56,56	0
56	MG	DA	3009	1/1	0.98	0.10	-	8,8,8,8	0
56	MG	AA	1820	1/1	0.94	0.06	-	23,23,23,23	0
56	MG	AA	1746	1/1	0.98	0.10	-	14,14,14,14	0
56	MG	BA	3387	1/1	0.95	0.19	-	49,49,49,49	0
56	MG	CZ	108	1/1	0.95	0.07	-	49,49,49,49	0
56	MG	DA	3337	1/1	0.98	0.07	-	23,23,23,23	0
56	MG	CA	1662	1/1	0.99	0.04	-	12,12,12,12	0
56	MG	DA	3639	1/1	0.95	0.16	-	13,13,13,13	0
56	MG	CA	1828	1/1	0.98	0.10	-	2,2,2,2	0
56	MG	DA	3699	1/1	0.97	0.47	-	38,38,38,38	0
56	MG	AA	1776	1/1	0.97	0.08	-	11,11,11,11	0
56	MG	BB	223	1/1	0.90	0.24	-	52,52,52,52	0
56	MG	DP	203	1/1	0.92	0.19	-	43,43,43,43	0
56	MG	BA	3129	1/1	0.94	0.16	-	34,34,34,34	0
56	MG	AA	1612	1/1	0.96	0.12	-	14,14,14,14	0
56	MG	BA	3306	1/1	0.97	0.06	-	36,36,36,36	0
56	MG	CA	1944	1/1	0.96	0.23	-	42,42,42,42	0
56	MG	DB	209	1/1	0.95	0.07	-	43,43,43,43	0
56	MG	BA	3778	1/1	0.94	0.12	-	33,33,33,33	0
56	MG	DA	3677	1/1	0.97	0.22	-	27,27,27,27	0
56	MG	CA	1729	1/1	0.98	0.23	-	15,15,15,15	0
56	MG	BA	3521	1/1	0.95	0.06	-	21,21,21,21	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1958	1/1	0.96	0.14	-	51,51,51,51	0
56	MG	BA	3545	1/1	0.99	0.12	-	25,25,25,25	0
56	MG	CA	1852	1/1	0.97	0.09	-	43,43,43,43	0
56	MG	DA	3365	1/1	0.96	0.11	-	8,8,8,8	0
56	MG	DA	3730	1/1	0.95	0.19	-	33,33,33,33	0
56	MG	AA	1763	1/1	0.99	0.12	-	30,30,30,30	0
56	MG	BA	3245	1/1	0.98	0.10	-	29,29,29,29	0
56	MG	CA	1630	1/1	0.96	0.07	-	36,36,36,36	0
56	MG	DA	3261	1/1	0.99	0.06	-	33,33,33,33	0
56	MG	CA	1981	1/1	0.78	0.11	-	77,77,77,77	0
56	MG	DA	3517	1/1	0.97	0.06	-	48,48,48,48	0
56	MG	BA	3779	1/1	0.94	0.13	-	47,47,47,47	0
56	MG	DA	3058	1/1	0.99	0.06	-	15,15,15,15	0
56	MG	CA	1951	1/1	0.94	0.12	-	42,42,42,42	0
56	MG	AA	1630	1/1	0.92	0.15	-	58,58,58,58	0
56	MG	CA	1747	1/1	0.90	0.15	-	31,31,31,31	0
56	MG	CA	1607	1/1	0.90	0.08	-	38,38,38,38	0
56	MG	AA	1767	1/1	0.94	0.38	-	28,28,28,28	0
56	MG	DA	3299	1/1	0.97	0.07	-	1,1,1,1	0
56	MG	DA	3420	1/1	0.95	0.36	-	45,45,45,45	0
56	MG	AA	1747	1/1	0.95	0.13	-	40,40,40,40	0
56	MG	DA	3659	1/1	0.56	0.33	-	66,66,66,66	0
56	MG	AA	1901	1/1	0.89	0.20	-	43,43,43,43	0
56	MG	DA	3527	1/1	0.92	0.11	-	49,49,49,49	0
56	MG	CA	1835	1/1	0.93	0.26	-	46,46,46,46	0
56	MG	BA	3738	1/1	0.97	0.36	-	44,44,44,44	0
56	MG	BA	3215	1/1	0.98	0.08	-	28,28,28,28	0
56	MG	DA	3182	1/1	0.99	0.07	-	23,23,23,23	0
56	MG	BA	3112	1/1	0.98	0.08	-	26,26,26,26	0
56	MG	BI	201	1/1	0.98	0.24	-	29,29,29,29	0
56	MG	DA	3477	1/1	0.93	0.15	-	32,32,32,32	0
56	MG	DA	3626	1/1	0.98	0.15	-	46,46,46,46	0
56	MG	CA	1927	1/1	0.96	0.10	-	37,37,37,37	0
56	MG	DA	3172	1/1	0.95	0.11	-	31,31,31,31	0
56	MG	DA	3231	1/1	0.95	0.08	-	3,3,3,3	0
56	MG	DA	3382	1/1	0.98	0.07	-	39,39,39,39	0
56	MG	BA	3787	1/1	0.99	0.08	-	11,11,11,11	0
56	MG	DA	3147	1/1	0.98	0.10	-	18,18,18,18	0
56	MG	BA	3437	1/1	0.92	0.11	-	26,26,26,26	0
56	MG	BA	3460	1/1	0.99	0.09	-	10,10,10,10	0
56	MG	BA	3284	1/1	0.99	0.07	-	12,12,12,12	0
56	MG	BA	3359	1/1	0.96	0.12	-	21,21,21,21	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3385	1/1	0.99	0.06	-	18,18,18,18	0
56	MG	AA	1909	1/1	0.99	0.05	-	40,40,40,40	0
56	MG	DA	3334	1/1	0.97	0.11	-	8,8,8,8	0
56	MG	AY	120	1/1	0.97	0.12	-	47,47,47,47	0
56	MG	DA	3753	1/1	0.96	0.33	-	32,32,32,32	0
56	MG	DA	3166	1/1	0.95	0.18	-	44,44,44,44	0
56	MG	AA	1897	1/1	0.99	0.11	-	13,13,13,13	0
56	MG	DA	3575	1/1	0.83	0.27	-	53,53,53,53	0
56	MG	CA	1776	1/1	0.99	0.15	-	17,17,17,17	0
56	MG	BA	3510	1/1	0.98	0.15	-	39,39,39,39	0
56	MG	BA	3292	1/1	0.98	0.08	-	10,10,10,10	0
56	MG	DA	3315	1/1	0.99	0.15	-	39,39,39,39	0
56	MG	AA	1671	1/1	0.96	0.08	-	20,20,20,20	0
56	MG	CA	1674	1/1	0.93	0.08	-	63,63,63,63	0
56	MG	AZ	104	1/1	0.96	0.04	-	45,45,45,45	0
56	MG	BA	3744	1/1	0.97	0.35	-	21,21,21,21	0
56	MG	CA	1915	1/1	0.92	0.27	-	56,56,56,56	0
56	MG	BA	3424	1/1	0.95	0.07	-	17,17,17,17	0
56	MG	DZ	304	1/1	0.95	0.18	-	31,31,31,31	0
56	MG	DA	3676	1/1	0.95	0.45	-	25,25,25,25	0
56	MG	CA	1813	1/1	0.99	0.09	-	41,41,41,41	0
56	MG	CA	1934	1/1	0.93	0.22	-	56,56,56,56	0
56	MG	BA	3051	1/1	0.99	0.22	-	16,16,16,16	0
56	MG	BA	3444	1/1	0.98	0.05	-	33,33,33,33	0
56	MG	CA	1890	1/1	0.94	0.17	-	37,37,37,37	0
56	MG	BA	3767	1/1	0.98	0.15	-	20,20,20,20	0
56	MG	DH	202	1/1	0.83	0.16	-	64,64,64,64	0
56	MG	CA	1620	1/1	0.96	0.11	-	38,38,38,38	0
56	MG	BA	3037	1/1	0.98	0.11	-	8,8,8,8	0
56	MG	DB	219	1/1	0.90	0.09	-	55,55,55,55	0
56	MG	DA	3259	1/1	0.94	0.14	-	24,24,24,24	0
56	MG	AA	1627	1/1	0.98	0.06	-	29,29,29,29	0
56	MG	DA	3043	1/1	0.97	0.06	-	25,25,25,25	0
56	MG	BA	3669	1/1	0.90	0.40	-	33,33,33,33	0
56	MG	BA	3518	1/1	0.97	0.11	-	9,9,9,9	0
56	MG	CA	1713	1/1	0.92	0.13	-	21,21,21,21	0
56	MG	BA	3257	1/1	0.98	0.06	-	18,18,18,18	0
56	MG	DA	3300	1/1	0.99	0.04	-	16,16,16,16	0
56	MG	CY	104	1/1	0.97	0.07	-	20,20,20,20	0
56	MG	DB	210	1/1	0.86	0.15	-	44,44,44,44	0
56	MG	BA	3525	1/1	0.99	0.06	-	8,8,8,8	0
56	MG	DA	3482	1/1	0.89	0.25	-	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3758	1/1	0.86	0.51	-	63,63,63,63	0
56	MG	DA	3658	1/1	0.88	0.22	-	61,61,61,61	0
56	MG	CA	1785	1/1	0.99	0.07	-	9,9,9,9	0
56	MG	DA	3582	1/1	0.97	0.18	-	27,27,27,27	0
56	MG	BA	3331	1/1	0.99	0.06	-	10,10,10,10	0
56	MG	BA	3398	1/1	0.98	0.28	-	16,16,16,16	0
56	MG	AA	1864	1/1	0.97	0.20	-	36,36,36,36	0
56	MG	DA	3395	1/1	0.94	0.14	-	34,34,34,34	0
56	MG	DA	3705	1/1	0.95	0.19	-	39,39,39,39	0
56	MG	DA	3467	1/1	0.95	0.11	-	58,58,58,58	0
56	MG	DA	3466	1/1	0.87	0.26	-	47,47,47,47	0
56	MG	BA	3534	1/1	0.98	0.15	-	24,24,24,24	0
56	MG	CA	1604	1/1	0.97	0.24	-	37,37,37,37	0
56	MG	BA	3357	1/1	0.98	0.06	-	4,4,4,4	0
56	MG	DA	3373	1/1	0.96	0.08	-	41,41,41,41	0
56	MG	BA	3556	1/1	0.99	0.16	-	7,7,7,7	0
56	MG	DA	3398	1/1	0.99	0.13	-	26,26,26,26	0
56	MG	BA	3758	1/1	0.98	0.18	-	24,24,24,24	0
56	MG	CZ	119	1/1	0.92	0.15	-	55,55,55,55	0
56	MG	DA	3287	1/1	0.90	0.14	-	62,62,62,62	0
56	MG	DA	3664	1/1	0.91	0.25	-	39,39,39,39	0
56	MG	BA	3573	1/1	0.98	0.08	-	30,30,30,30	0
56	MG	DA	3741	1/1	0.92	0.18	-	25,25,25,25	0
56	MG	CA	1984	1/1	0.96	0.17	-	54,54,54,54	0
56	MG	BJ	201	1/1	0.88	0.10	-	59,59,59,59	0
56	MG	BA	3603	1/1	0.96	0.07	-	26,26,26,26	0
56	MG	DA	3062	1/1	0.96	0.12	-	31,31,31,31	0
56	MG	DA	3516	1/1	0.82	0.46	-	62,62,62,62	0
56	MG	AA	1783	1/1	0.98	0.18	-	50,50,50,50	0
56	MG	AA	1900	1/1	0.95	0.12	-	44,44,44,44	0
56	MG	DA	3225	1/1	0.99	0.10	-	27,27,27,27	0
56	MG	CA	2004	1/1	0.93	0.10	-	45,45,45,45	0
56	MG	BA	3492	1/1	0.97	0.08	-	47,47,47,47	0
56	MG	BA	3599	1/1	0.97	0.15	-	34,34,34,34	0
56	MG	AA	1670	1/1	0.98	0.04	-	22,22,22,22	0
56	MG	BA	3167	1/1	0.94	0.17	-	34,34,34,34	0
56	MG	CY	111	1/1	0.96	0.27	-	39,39,39,39	0
56	MG	CA	1657	1/1	0.92	0.13	-	42,42,42,42	0
56	MG	DA	3322	1/1	0.91	0.13	-	46,46,46,46	0
56	MG	DA	3555	1/1	0.98	0.10	-	24,24,24,24	0
56	MG	BA	3089	1/1	0.98	0.07	-	17,17,17,17	0
56	MG	AZ	101	1/1	0.99	0.21	-	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CV	101	1/1	0.96	0.08	-	37,37,37,37	0
56	MG	BA	3287	1/1	0.97	0.11	-	27,27,27,27	0
56	MG	CZ	102	1/1	0.92	0.12	-	67,67,67,67	0
56	MG	BA	3415	1/1	0.78	0.26	-	52,52,52,52	0
56	MG	BA	3320	1/1	0.98	0.14	-	2,2,2,2	0
56	MG	CA	1667	1/1	0.97	0.10	-	21,21,21,21	0
56	MG	DA	3702	1/1	0.94	0.29	-	42,42,42,42	0
56	MG	CA	1769	1/1	0.92	0.11	-	56,56,56,56	0
56	MG	BA	3515	1/1	0.96	0.11	-	9,9,9,9	0
56	MG	CA	1922	1/1	0.97	0.09	-	33,33,33,33	0
56	MG	BA	3036	1/1	0.92	0.19	-	32,32,32,32	0
56	MG	DA	3213	1/1	0.95	0.09	-	18,18,18,18	0
56	MG	CA	1942	1/1	0.95	0.37	-	41,41,41,41	0
56	MG	AA	1660	1/1	0.98	0.07	-	19,19,19,19	0
56	MG	DA	3518	1/1	0.95	0.12	-	13,13,13,13	0
56	MG	DA	3145	1/1	0.92	0.11	-	30,30,30,30	0
56	MG	BA	3446	1/1	0.98	0.11	-	39,39,39,39	0
56	MG	BA	3430	1/1	0.98	0.17	-	32,32,32,32	0
56	MG	AA	1750	1/1	0.92	0.12	-	50,50,50,50	0
56	MG	BA	3539	1/1	0.92	0.11	-	77,77,77,77	0
56	MG	CA	1727	1/1	0.93	0.09	-	55,55,55,55	0
56	MG	DA	3440	1/1	0.86	0.16	-	71,71,71,71	0
56	MG	DA	3551	1/1	0.99	0.16	-	17,17,17,17	0
56	MG	DA	3346	1/1	0.99	0.07	-	3,3,3,3	0
56	MG	CC	304	1/1	0.87	0.19	-	93,93,93,93	0
56	MG	BA	3098	1/1	0.96	0.09	-	28,28,28,28	0
56	MG	DA	3691	1/1	0.96	0.14	-	50,50,50,50	0
56	MG	BA	3347	1/1	0.94	0.20	-	19,19,19,19	0
56	MG	BA	3439	1/1	0.99	0.04	-	7,7,7,7	0
56	MG	BA	3535	1/1	0.94	0.12	-	43,43,43,43	0
56	MG	AY	125	1/1	0.90	0.11	-	51,51,51,51	0
56	MG	AA	1603	1/1	0.95	0.10	-	30,30,30,30	0
56	MG	BA	3238	1/1	0.99	0.17	-	14,14,14,14	0
56	MG	AA	1610	1/1	0.99	0.22	-	23,23,23,23	0
56	MG	DA	3540	1/1	0.99	0.17	-	0,0,0,0	0
56	MG	DA	3124	1/1	0.96	0.08	-	27,27,27,27	0
56	MG	CA	2010	1/1	0.97	0.09	-	35,35,35,35	0
56	MG	AA	1649	1/1	0.95	0.16	-	41,41,41,41	0
56	MG	DA	3578	1/1	0.99	0.07	-	11,11,11,11	0
56	MG	BA	3256	1/1	0.98	0.05	-	13,13,13,13	0
56	MG	AA	1772	1/1	0.99	0.06	-	17,17,17,17	0
56	MG	DA	3049	1/1	0.98	0.08	-	11,11,11,11	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1921	1/1	0.96	0.33	-	57,57,57,57	0
56	MG	DA	3612	1/1	0.97	0.19	-	41,41,41,41	0
56	MG	AA	1879	1/1	0.96	0.08	-	58,58,58,58	0
56	MG	AA	1805	1/1	0.94	0.11	-	53,53,53,53	0
56	MG	BA	3751	1/1	0.96	0.15	-	53,53,53,53	0
56	MG	BA	3280	1/1	0.97	0.20	-	26,26,26,26	0
56	MG	BA	3450	1/1	0.93	0.20	-	43,43,43,43	0
56	MG	CA	1962	1/1	0.97	0.26	-	41,41,41,41	0
56	MG	DP	202	1/1	0.93	0.19	-	44,44,44,44	0
56	MG	DA	3161	1/1	1.00	0.25	-	1,1,1,1	0
56	MG	BA	3651	1/1	0.91	0.16	-	34,34,34,34	0
56	MG	BA	3285	1/1	0.94	0.11	-	40,40,40,40	0
56	MG	CL	201	1/1	0.92	0.18	-	61,61,61,61	0
56	MG	BA	3274	1/1	0.99	0.09	-	6,6,6,6	0
56	MG	CA	1872	1/1	0.95	0.13	-	24,24,24,24	0
56	MG	AY	117	1/1	0.96	0.21	-	32,32,32,32	0
56	MG	AO	102	1/1	0.92	0.34	-	36,36,36,36	0
56	MG	DA	3192	1/1	0.70	0.11	-	67,67,67,67	0
56	MG	DA	3204	1/1	0.98	0.07	-	28,28,28,28	0
56	MG	DA	3361	1/1	0.99	0.30	-	19,19,19,19	0
56	MG	CC	302	1/1	0.89	0.14	-	56,56,56,56	0
56	MG	BA	3103	1/1	0.98	0.18	-	35,35,35,35	0
56	MG	BA	3563	1/1	0.97	0.29	-	55,55,55,55	0
56	MG	AA	1622	1/1	0.97	0.11	-	24,24,24,24	0
56	MG	DB	228	1/1	0.87	0.21	-	46,46,46,46	0
56	MG	DA	3363	1/1	0.98	0.12	-	36,36,36,36	0
56	MG	DA	3228	1/1	0.98	0.14	-	12,12,12,12	0
56	MG	DA	3599	1/1	0.95	0.18	-	39,39,39,39	0
56	MG	BA	3252	1/1	0.99	0.21	-	7,7,7,7	0
56	MG	AY	111	1/1	0.97	0.09	-	34,34,34,34	0
56	MG	AY	103	1/1	0.95	0.12	-	53,53,53,53	0
56	MG	DA	3088	1/1	0.96	0.14	-	19,19,19,19	0
56	MG	CA	1949	1/1	0.97	0.10	-	37,37,37,37	0
56	MG	DA	3280	1/1	0.99	0.04	-	3,3,3,3	0
56	MG	AA	1814	1/1	0.94	0.13	-	17,17,17,17	0
56	MG	DA	3007	1/1	0.97	0.23	-	24,24,24,24	0
56	MG	BA	3139	1/1	0.98	0.05	-	33,33,33,33	0
56	MG	DA	3646	1/1	0.84	0.16	-	55,55,55,55	0
56	MG	CA	1851	1/1	0.92	0.08	-	34,34,34,34	0
56	MG	AA	1744	1/1	0.98	0.05	-	30,30,30,30	0
56	MG	AA	1662	1/1	0.96	0.17	-	48,48,48,48	0
56	MG	DA	3174	1/1	0.95	0.16	-	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1754	1/1	0.84	0.24	-	59,59,59,59	0
56	MG	BA	3110	1/1	0.95	0.10	-	35,35,35,35	0
56	MG	AZ	103	1/1	0.96	0.09	-	34,34,34,34	0
56	MG	CY	119	1/1	0.97	0.38	-	35,35,35,35	0
56	MG	CA	1736	1/1	0.94	0.11	-	52,52,52,52	0
56	MG	BA	3230	1/1	0.97	0.17	-	0,0,0,0	0
56	MG	BA	3405	1/1	0.97	0.11	-	20,20,20,20	0
56	MG	BA	3793	1/1	0.98	0.07	-	31,31,31,31	0
56	MG	DA	3503	1/1	0.99	0.07	-	24,24,24,24	0
56	MG	BA	3007	1/1	0.98	0.07	-	34,34,34,34	0
56	MG	BA	3286	1/1	0.98	0.09	-	1,1,1,1	0
56	MG	BA	3373	1/1	0.97	0.10	-	24,24,24,24	0
56	MG	AA	1881	1/1	0.95	0.15	-	76,76,76,76	0
56	MG	AA	1611	1/1	0.99	0.07	-	6,6,6,6	0
56	MG	DA	3556	1/1	0.92	0.18	-	20,20,20,20	0
56	MG	BB	210	1/1	0.95	0.14	-	62,62,62,62	0
56	MG	DA	3366	1/1	0.96	0.19	-	21,21,21,21	0
56	MG	AB	302	1/1	0.98	0.10	-	33,33,33,33	0
56	MG	DA	3408	1/1	0.98	0.14	-	31,31,31,31	0
56	MG	BA	3737	1/1	0.98	0.26	-	22,22,22,22	0
56	MG	AA	1799	1/1	0.91	0.24	-	49,49,49,49	0
56	MG	AA	1801	1/1	0.99	0.05	-	21,21,21,21	0
56	MG	CA	1632	1/1	0.98	0.05	-	24,24,24,24	0
56	MG	DA	3248	1/1	0.99	0.15	-	19,19,19,19	0
56	MG	AA	1806	1/1	0.95	0.12	-	34,34,34,34	0
56	MG	CA	1782	1/1	0.97	0.09	-	19,19,19,19	0
56	MG	DA	3592	1/1	0.97	0.29	-	47,47,47,47	0
56	MG	BA	3685	1/1	0.96	0.33	-	37,37,37,37	0
56	MG	DA	3755	1/1	0.93	0.35	-	39,39,39,39	0
56	MG	DA	3235	1/1	0.98	0.10	-	0,0,0,0	0
56	MG	BA	3540	1/1	0.99	0.08	-	23,23,23,23	0
56	MG	DA	3434	1/1	0.94	0.13	-	29,29,29,29	0
56	MG	BA	3544	1/1	0.90	0.40	-	38,38,38,38	0
56	MG	AA	1686	1/1	0.92	0.15	-	37,37,37,37	0
56	MG	AD	309	1/1	0.96	0.33	-	36,36,36,36	0
56	MG	AA	1790	1/1	0.96	0.18	-	32,32,32,32	0
56	MG	AA	1718	1/1	0.98	0.09	-	27,27,27,27	0
56	MG	BA	3500	1/1	0.96	0.16	-	16,16,16,16	0
56	MG	BA	3591	1/1	0.94	0.10	-	50,50,50,50	0
56	MG	BA	3406	1/1	0.97	0.13	-	42,42,42,42	0
56	MG	DA	3115	1/1	0.98	0.17	-	5,5,5,5	0
56	MG	BA	3040	1/1	0.95	0.17	-	35,35,35,35	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BI	203	1/1	0.97	0.30	-	40,40,40,40	0
56	MG	AD	308	1/1	0.97	0.09	-	42,42,42,42	0
56	MG	DA	3425	1/1	0.92	0.17	-	43,43,43,43	0
56	MG	CA	1791	1/1	0.99	0.06	-	43,43,43,43	0
56	MG	CA	1857	1/1	0.94	0.19	-	33,33,33,33	0
56	MG	DA	3211	1/1	0.97	0.09	-	23,23,23,23	0
56	MG	DH	201	1/1	0.91	0.15	-	46,46,46,46	0
56	MG	BA	3265	1/1	0.97	0.19	-	0,0,0,0	0
56	MG	AY	110	1/1	0.85	0.10	-	53,53,53,53	0
56	MG	AZ	105	1/1	0.96	0.10	-	44,44,44,44	0
56	MG	CA	1968	1/1	0.98	0.21	-	25,25,25,25	0
56	MG	CA	1850	1/1	0.98	0.10	-	20,20,20,20	0
56	MG	BA	3533	1/1	0.92	0.13	-	37,37,37,37	0
56	MG	DA	3083	1/1	0.97	0.15	-	24,24,24,24	0
56	MG	BA	3443	1/1	0.97	0.28	-	29,29,29,29	0
56	MG	BB	222	1/1	0.98	0.20	-	39,39,39,39	0
56	MG	CA	1740	1/1	0.98	0.07	-	8,8,8,8	0
56	MG	DA	3186	1/1	0.98	0.06	-	47,47,47,47	0
56	MG	DA	3303	1/1	0.99	0.08	-	12,12,12,12	0
56	MG	BA	3328	1/1	0.99	0.07	-	2,2,2,2	0
56	MG	DA	3347	1/1	0.99	0.27	-	10,10,10,10	0
56	MG	DA	3657	1/1	0.95	0.27	-	38,38,38,38	0
56	MG	DA	3026	1/1	0.95	0.05	-	16,16,16,16	0
56	MG	BA	3001	1/1	0.97	0.11	-	26,26,26,26	0
56	MG	CA	1888	1/1	0.93	0.21	-	51,51,51,51	0
56	MG	CA	1938	1/1	0.96	0.40	-	48,48,48,48	0
56	MG	BA	3721	1/1	0.96	0.17	-	34,34,34,34	0
56	MG	BA	3369	1/1	0.93	0.42	-	48,48,48,48	0
56	MG	BA	3562	1/1	0.86	0.20	-	29,29,29,29	0
56	MG	AQ	201	1/1	0.97	0.50	-	47,47,47,47	0
56	MG	D4	101	1/1	0.96	0.05	-	23,23,23,23	0
56	MG	AA	1858	1/1	0.99	0.05	-	15,15,15,15	0
56	MG	BA	3341	1/1	0.97	0.13	-	26,26,26,26	0
56	MG	AA	1667	1/1	0.96	0.15	-	38,38,38,38	0
56	MG	DA	3176	1/1	0.83	0.20	-	46,46,46,46	0
56	MG	CA	1636	1/1	0.94	0.09	-	40,40,40,40	0
56	MG	BA	3507	1/1	0.99	0.11	-	29,29,29,29	0
56	MG	CA	1605	1/1	0.96	0.13	-	27,27,27,27	0
56	MG	BA	3475	1/1	0.96	0.14	-	15,15,15,15	0
56	MG	DA	3444	1/1	0.94	0.16	-	11,11,11,11	0
56	MG	BA	3346	1/1	0.94	0.15	-	18,18,18,18	0
56	MG	AY	107	1/1	0.98	0.09	-	18,18,18,18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3414	1/1	0.99	0.09	-	24,24,24,24	0
56	MG	BA	3177	1/1	0.98	0.10	-	0,0,0,0	0
56	MG	DA	3475	1/1	0.95	0.13	-	34,34,34,34	0
56	MG	AA	1829	1/1	0.91	0.24	-	68,68,68,68	0
56	MG	BA	3179	1/1	0.95	0.15	-	26,26,26,26	0
56	MG	CA	1974	1/1	0.74	0.21	-	54,54,54,54	0
56	MG	DA	3170	1/1	0.97	0.12	-	8,8,8,8	0
56	MG	CH	201	1/1	0.80	0.72	-	51,51,51,51	0
56	MG	DA	3613	1/1	0.98	0.18	-	26,26,26,26	0
56	MG	BA	3194	1/1	0.99	0.07	-	21,21,21,21	0
56	MG	AA	1728	1/1	0.96	0.10	-	14,14,14,14	0
56	MG	DA	3389	1/1	0.94	0.17	-	55,55,55,55	0
56	MG	CA	1681	1/1	0.92	0.28	-	43,43,43,43	0
56	MG	CV	103	1/1	0.99	0.12	-	29,29,29,29	0
56	MG	CA	1786	1/1	0.96	0.38	-	19,19,19,19	0
56	MG	CA	1841	1/1	0.91	0.06	-	63,63,63,63	0
56	MG	DA	3153	1/1	0.98	0.07	-	10,10,10,10	0
56	MG	DA	3250	1/1	0.97	0.17	-	32,32,32,32	0
56	MG	DA	3392	1/1	0.99	0.06	-	4,4,4,4	0
56	MG	BA	3467	1/1	0.91	0.23	-	35,35,35,35	0
56	MG	DA	3643	1/1	0.99	0.07	-	28,28,28,28	0
56	MG	DA	3678	1/1	0.97	0.09	-	20,20,20,20	0
56	MG	DA	3205	1/1	0.94	0.20	-	24,24,24,24	0
56	MG	CA	1811	1/1	0.98	0.10	-	43,43,43,43	0
56	MG	CA	1901	1/1	0.97	0.12	-	7,7,7,7	0
56	MG	DI	202	1/1	0.98	0.08	-	18,18,18,18	0
56	MG	CA	1677	1/1	0.95	0.10	-	27,27,27,27	0
56	MG	CA	1743	1/1	0.96	0.20	-	30,30,30,30	0
56	MG	CA	1772	1/1	0.93	0.28	-	40,40,40,40	0
56	MG	BA	3699	1/1	0.98	0.55	-	35,35,35,35	0
56	MG	BA	3143	1/1	0.97	0.15	-	40,40,40,40	0
56	MG	BA	3220	1/1	0.91	0.31	-	55,55,55,55	0
56	MG	BA	3723	1/1	0.93	0.15	-	18,18,18,18	0
56	MG	DA	3060	1/1	0.97	0.06	-	19,19,19,19	0
56	MG	DA	3573	1/1	0.97	0.10	-	25,25,25,25	0
56	MG	DA	3628	1/1	0.95	0.15	-	38,38,38,38	0
56	MG	BA	3010	1/1	0.97	0.13	-	2,2,2,2	0
56	MG	CA	1943	1/1	0.95	0.37	-	48,48,48,48	0
56	MG	CA	1877	1/1	0.93	0.59	-	60,60,60,60	0
56	MG	BA	3114	1/1	0.94	0.39	-	47,47,47,47	0
56	MG	BA	3050	1/1	0.98	0.07	-	4,4,4,4	0
56	MG	CA	1898	1/1	0.98	0.21	-	14,14,14,14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3633	1/1	0.92	0.18	-	20,20,20,20	0
56	MG	CA	1663	1/1	0.98	0.05	-	8,8,8,8	0
56	MG	BA	3806	1/1	0.83	0.15	-	54,54,54,54	0
56	MG	B7	102	1/1	0.98	0.09	-	13,13,13,13	0
56	MG	BA	3352	1/1	0.96	0.10	-	36,36,36,36	0
56	MG	BU	201	1/1	0.94	0.51	-	35,35,35,35	0
56	MG	DA	3015	1/1	0.96	0.11	-	11,11,11,11	0
56	MG	BA	3642	1/1	0.93	0.17	-	68,68,68,68	0
56	MG	AA	1777	1/1	0.95	0.26	-	36,36,36,36	0
56	MG	DA	3247	1/1	0.93	0.08	-	21,21,21,21	0
56	MG	BT	202	1/1	0.97	0.10	-	42,42,42,42	0
56	MG	DA	3407	1/1	0.98	0.07	-	32,32,32,32	0
56	MG	CA	1812	1/1	0.94	0.11	-	51,51,51,51	0
56	MG	DA	3649	1/1	0.98	0.08	-	19,19,19,19	0
56	MG	AA	1721	1/1	0.99	0.04	-	0,0,0,0	0
56	MG	BA	3196	1/1	0.95	0.09	-	44,44,44,44	0
56	MG	BG	201	1/1	0.96	0.15	-	47,47,47,47	0
56	MG	AA	1664	1/1	0.99	0.10	-	6,6,6,6	0
56	MG	CA	1864	1/1	0.97	0.23	-	40,40,40,40	0
56	MG	BA	3470	1/1	0.96	0.23	-	51,51,51,51	0
56	MG	CA	1907	1/1	0.97	0.08	-	31,31,31,31	0
56	MG	BA	3759	1/1	0.98	0.09	-	41,41,41,41	0
56	MG	AA	1665	1/1	0.98	0.07	-	6,6,6,6	0
56	MG	DA	3439	1/1	0.99	0.26	-	17,17,17,17	0
56	MG	CA	1900	1/1	0.97	0.10	-	56,56,56,56	0
56	MG	CI	201	1/1	0.96	0.16	-	45,45,45,45	0
56	MG	BA	3131	1/1	0.98	0.12	-	30,30,30,30	0
56	MG	BA	3124	1/1	0.98	0.16	-	33,33,33,33	0
56	MG	D5	101	1/1	0.99	0.06	-	2,2,2,2	0
56	MG	DA	3416	1/1	0.99	0.08	-	26,26,26,26	0
56	MG	AA	1766	1/1	0.99	0.09	-	18,18,18,18	0
56	MG	CA	1905	1/1	0.79	0.41	-	64,64,64,64	0
56	MG	BA	3303	1/1	0.98	0.05	-	22,22,22,22	0
56	MG	CA	1638	1/1	0.93	0.11	-	26,26,26,26	0
56	MG	BA	3569	1/1	0.99	0.06	-	0,0,0,0	0
56	MG	DA	3210	1/1	0.96	0.11	-	27,27,27,27	0
56	MG	DA	3641	1/1	0.99	0.18	-	13,13,13,13	0
56	MG	BA	3183	1/1	0.98	0.09	-	15,15,15,15	0
56	MG	BA	3107	1/1	0.98	0.08	-	21,21,21,21	0
56	MG	BA	3532	1/1	0.96	0.23	-	56,56,56,56	0
56	MG	BA	3130	1/1	0.91	0.11	-	36,36,36,36	0
56	MG	DA	3692	1/1	0.91	0.18	-	46,46,46,46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3224	1/1	0.98	0.07	-	9,9,9,9	0
56	MG	D4	102	1/1	0.97	0.22	-	40,40,40,40	0
56	MG	BA	3635	1/1	0.97	0.13	-	32,32,32,32	0
56	MG	DA	3044	1/1	0.99	0.16	-	5,5,5,5	0
56	MG	BA	3570	1/1	0.98	0.14	-	21,21,21,21	0
56	MG	AL	201	1/1	0.93	0.09	-	29,29,29,29	0
56	MG	DA	3567	1/1	0.88	0.12	-	74,74,74,74	0
56	MG	BA	3017	1/1	0.98	0.12	-	18,18,18,18	0
56	MG	BA	3272	1/1	0.94	0.10	-	15,15,15,15	0
56	MG	BA	3371	1/1	0.96	0.22	-	29,29,29,29	0
56	MG	BA	3774	1/1	0.97	0.12	-	44,44,44,44	0
56	MG	BA	3403	1/1	0.96	0.15	-	41,41,41,41	0
56	MG	BA	3614	1/1	0.98	0.22	-	32,32,32,32	0
56	MG	DA	3152	1/1	0.98	0.11	-	28,28,28,28	0
56	MG	BA	3782	1/1	0.93	0.18	-	19,19,19,19	0
56	MG	DA	3391	1/1	0.98	0.09	-	17,17,17,17	0
56	MG	AA	1821	1/1	0.98	0.08	-	27,27,27,27	0
56	MG	DA	3390	1/1	0.88	0.23	-	36,36,36,36	0
56	MG	DA	3468	1/1	0.86	0.12	-	30,30,30,30	0
56	MG	AY	102	1/1	0.99	0.10	-	32,32,32,32	0
56	MG	AA	1705	1/1	0.96	0.14	-	29,29,29,29	0
56	MG	BQ	203	1/1	0.99	0.11	-	43,43,43,43	0
56	MG	CA	1821	1/1	0.97	0.09	-	22,22,22,22	0
56	MG	DA	3607	1/1	0.93	0.22	-	44,44,44,44	0
56	MG	CA	1702	1/1	0.89	0.06	-	56,56,56,56	0
56	MG	BA	3271	1/1	0.99	0.11	-	0,0,0,0	0
56	MG	CA	1891	1/1	0.92	0.10	-	30,30,30,30	0
56	MG	BA	3625	1/1	0.98	0.07	-	25,25,25,25	0
56	MG	DB	203	1/1	0.97	0.07	-	21,21,21,21	0
56	MG	BA	3555	1/1	0.81	0.11	-	54,54,54,54	0
56	MG	DA	3569	1/1	0.95	0.24	-	39,39,39,39	0
56	MG	BA	3421	1/1	0.97	0.20	-	45,45,45,45	0
56	MG	DA	3374	1/1	0.97	0.13	-	24,24,24,24	0
56	MG	BA	3422	1/1	0.95	0.14	-	24,24,24,24	0
56	MG	DA	3351	1/1	0.78	0.20	-	38,38,38,38	0
56	MG	BA	3703	1/1	0.91	0.10	-	29,29,29,29	0
56	MG	CV	102	1/1	0.97	0.13	-	25,25,25,25	0
56	MG	BA	3019	1/1	0.99	0.14	-	5,5,5,5	0
56	MG	BA	3427	1/1	0.97	0.14	-	10,10,10,10	0
56	MG	CA	1838	1/1	0.98	0.14	-	28,28,28,28	0
56	MG	DA	3331	1/1	0.99	0.11	-	0,0,0,0	0
56	MG	AD	302	1/1	0.99	0.04	-	13,13,13,13	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1908	1/1	0.98	0.06	-	5,5,5,5	0
56	MG	BA	3315	1/1	0.83	0.38	-	64,64,64,64	0
56	MG	BA	3649	1/1	0.92	0.12	-	29,29,29,29	0
56	MG	CX	403	1/1	0.95	0.09	-	48,48,48,48	0
56	MG	BW	202	1/1	0.93	0.25	-	33,33,33,33	0
56	MG	AA	1689	1/1	0.97	0.08	-	39,39,39,39	0
56	MG	BA	3709	1/1	0.94	0.19	-	31,31,31,31	0
56	MG	AA	1826	1/1	0.98	0.08	-	35,35,35,35	0
56	MG	BA	3730	1/1	0.89	0.21	-	40,40,40,40	0
56	MG	AA	1745	1/1	0.96	0.13	-	62,62,62,62	0
56	MG	DA	3039	1/1	0.95	0.15	-	17,17,17,17	0
56	MG	BA	3594	1/1	0.96	0.14	-	46,46,46,46	0
56	MG	DP	205	1/1	0.85	0.25	-	42,42,42,42	0
56	MG	AA	1854	1/1	0.96	0.09	-	44,44,44,44	0
56	MG	DA	3270	1/1	0.96	0.08	-	35,35,35,35	0
56	MG	DA	3290	1/1	0.98	0.13	-	25,25,25,25	0
56	MG	DA	3718	1/1	0.85	0.44	-	60,60,60,60	0
56	MG	CA	1937	1/1	0.88	0.50	-	56,56,56,56	0
56	MG	DA	3359	1/1	0.95	0.28	-	19,19,19,19	0
56	MG	AA	1690	1/1	0.97	0.09	-	47,47,47,47	0
56	MG	DA	3684	1/1	0.93	0.16	-	50,50,50,50	0
56	MG	DA	3307	1/1	0.97	0.12	-	47,47,47,47	0
56	MG	DA	3221	1/1	0.98	0.14	-	11,11,11,11	0
56	MG	CA	1950	1/1	0.83	0.24	-	67,67,67,67	0
56	MG	AA	1638	1/1	0.92	0.14	-	22,22,22,22	0
56	MG	AA	1652	1/1	0.97	0.07	-	17,17,17,17	0
56	MG	CA	1973	1/1	0.97	0.11	-	37,37,37,37	0
56	MG	DA	3206	1/1	0.98	0.16	-	20,20,20,20	0
56	MG	CK	202	1/1	0.95	0.09	-	40,40,40,40	0
56	MG	BA	3604	1/1	0.98	0.16	-	36,36,36,36	0
56	MG	BA	3568	1/1	0.99	0.06	-	13,13,13,13	0
56	MG	AA	1873	1/1	0.97	0.10	-	36,36,36,36	0
56	MG	DA	3445	1/1	0.93	0.10	-	31,31,31,31	0
56	MG	BA	3634	1/1	0.99	0.16	-	18,18,18,18	0
56	MG	DA	3698	1/1	0.81	0.65	-	73,73,73,73	0
56	MG	DA	3752	1/1	0.94	0.23	-	55,55,55,55	0
56	MG	DA	3160	1/1	0.98	0.04	-	35,35,35,35	0
56	MG	CA	2000	1/1	0.88	0.12	-	45,45,45,45	0
56	MG	DA	3725	1/1	0.97	0.13	-	44,44,44,44	0
56	MG	BA	3155	1/1	0.99	0.12	-	15,15,15,15	0
56	MG	BA	3148	1/1	0.99	0.05	-	17,17,17,17	0
56	MG	DA	3590	1/1	0.94	0.18	-	37,37,37,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1910	1/1	0.99	0.08	-	15,15,15,15	0
56	MG	BA	3489	1/1	0.89	0.12	-	46,46,46,46	0
56	MG	BA	3330	1/1	0.86	0.10	-	45,45,45,45	0
56	MG	BA	3435	1/1	0.99	0.32	-	43,43,43,43	0
56	MG	BA	3574	1/1	0.93	0.16	-	35,35,35,35	0
56	MG	DA	3469	1/1	0.98	0.17	-	19,19,19,19	0
56	MG	CA	1866	1/1	0.96	0.18	-	22,22,22,22	0
56	MG	BA	3706	1/1	0.89	0.08	-	38,38,38,38	0
56	MG	CA	1669	1/1	0.95	0.14	-	52,52,52,52	0
56	MG	AA	1816	1/1	0.98	0.12	-	23,23,23,23	0
56	MG	AC	305	1/1	0.96	0.27	-	45,45,45,45	0
56	MG	DA	3735	1/1	0.94	0.46	-	51,51,51,51	0
56	MG	BA	3190	1/1	0.96	0.26	-	36,36,36,36	0
56	MG	CA	1671	1/1	0.91	0.13	-	40,40,40,40	0
56	MG	D3	101	1/1	0.96	0.10	-	43,43,43,43	0
56	MG	BB	209	1/1	0.99	0.06	-	26,26,26,26	0
56	MG	DA	3249	1/1	0.99	0.32	-	32,32,32,32	0
56	MG	CA	1980	1/1	0.98	0.10	-	40,40,40,40	0
56	MG	BA	3305	1/1	1.00	0.09	-	5,5,5,5	0
56	MG	BA	3630	1/1	0.98	0.30	-	41,41,41,41	0
56	MG	DA	3110	1/1	0.91	0.18	-	43,43,43,43	0
56	MG	BA	3063	1/1	0.98	0.05	-	0,0,0,0	0
56	MG	DA	3461	1/1	0.98	0.13	-	8,8,8,8	0
56	MG	DA	3499	1/1	0.94	0.15	-	25,25,25,25	0
56	MG	AA	1786	1/1	0.94	0.27	-	76,76,76,76	0
56	MG	AA	1768	1/1	0.93	0.10	-	32,32,32,32	0
56	MG	CA	1826	1/1	0.67	0.24	-	65,65,65,65	0
56	MG	BA	3598	1/1	0.94	0.19	-	33,33,33,33	0
56	MG	AA	1626	1/1	0.93	0.07	-	47,47,47,47	0
56	MG	CA	1762	1/1	0.94	0.15	-	30,30,30,30	0
56	MG	BA	3123	1/1	0.98	0.11	-	34,34,34,34	0
56	MG	CA	1759	1/1	0.98	0.07	-	25,25,25,25	0
56	MG	CA	1897	1/1	0.97	0.27	-	23,23,23,23	0
56	MG	CA	1916	1/1	0.94	0.17	-	62,62,62,62	0
56	MG	BA	3678	1/1	0.97	0.13	-	42,42,42,42	0
56	MG	DA	3301	1/1	0.98	0.07	-	31,31,31,31	0
56	MG	CA	1790	1/1	0.94	0.09	-	38,38,38,38	0
56	MG	CA	1733	1/1	0.99	0.22	-	52,52,52,52	0
56	MG	BA	3122	1/1	0.89	0.16	-	50,50,50,50	0
56	MG	BA	3198	1/1	0.97	0.07	-	21,21,21,21	0
56	MG	CA	1802	1/1	0.95	0.12	-	31,31,31,31	0
56	MG	CA	1956	1/1	0.98	0.16	-	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3768	1/1	0.94	0.18	-	46,46,46,46	0
56	MG	BA	3350	1/1	0.96	0.14	-	32,32,32,32	0
56	MG	BB	201	1/1	0.98	0.09	-	35,35,35,35	0
56	MG	CO	101	1/1	0.99	0.05	-	25,25,25,25	0
56	MG	CA	1957	1/1	0.98	0.22	-	28,28,28,28	0
56	MG	CA	1699	1/1	0.93	0.12	-	45,45,45,45	0
56	MG	DA	3217	1/1	0.98	0.05	-	20,20,20,20	0
56	MG	CA	1815	1/1	0.91	0.12	-	12,12,12,12	0
56	MG	DA	3288	1/1	0.96	0.09	-	12,12,12,12	0
56	MG	AA	1837	1/1	0.94	0.10	-	54,54,54,54	0
56	MG	BA	3365	1/1	0.97	0.23	-	40,40,40,40	0
56	MG	DA	3067	1/1	0.97	0.07	-	17,17,17,17	0
56	MG	AI	201	1/1	0.95	0.25	-	57,57,57,57	0
56	MG	BA	3527	1/1	0.94	0.21	-	37,37,37,37	0
56	MG	AY	123	1/1	0.96	0.34	-	42,42,42,42	0
56	MG	DA	3459	1/1	0.96	0.14	-	22,22,22,22	0
56	MG	AA	1699	1/1	0.97	0.10	-	35,35,35,35	0
56	MG	BA	3329	1/1	0.93	0.10	-	49,49,49,49	0
56	MG	BA	3777	1/1	0.97	0.06	-	40,40,40,40	0
56	MG	BA	3094	1/1	0.96	0.09	-	23,23,23,23	0
56	MG	BA	3552	1/1	0.97	0.17	-	12,12,12,12	0
56	MG	CA	1894	1/1	0.98	0.06	-	19,19,19,19	0
56	MG	BA	3297	1/1	0.94	0.20	-	50,50,50,50	0
56	MG	DA	3447	1/1	0.98	0.18	-	36,36,36,36	0
56	MG	BA	3392	1/1	0.99	0.15	-	27,27,27,27	0
56	MG	AA	1761	1/1	0.98	0.08	-	26,26,26,26	0
56	MG	DA	3704	1/1	0.97	0.12	-	34,34,34,34	0
56	MG	DA	3173	1/1	0.93	0.13	-	31,31,31,31	0
56	MG	DA	3686	1/1	0.98	0.19	-	30,30,30,30	0
56	MG	CA	1698	1/1	0.97	0.15	-	28,28,28,28	0
56	MG	AA	1631	1/1	0.74	0.19	-	58,58,58,58	0
56	MG	AA	1742	1/1	0.96	0.08	-	17,17,17,17	0
56	MG	DA	3090	1/1	0.98	0.06	-	12,12,12,12	0
56	MG	AA	1694	1/1	0.98	0.25	-	45,45,45,45	0
56	MG	BA	3047	1/1	0.97	0.14	-	17,17,17,17	0
56	MG	DA	3080	1/1	0.99	0.15	-	23,23,23,23	0
56	MG	CC	305	1/1	0.93	0.11	-	46,46,46,46	0
56	MG	AD	307	1/1	0.95	0.42	-	32,32,32,32	0
56	MG	BB	224	1/1	0.99	0.24	-	25,25,25,25	0
56	MG	DA	3368	1/1	0.96	0.10	-	29,29,29,29	0
56	MG	CA	1876	1/1	0.99	0.13	-	22,22,22,22	0
56	MG	BA	3441	1/1	0.98	0.15	-	28,28,28,28	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3747	1/1	0.98	0.12	-	23,23,23,23	0
56	MG	DA	3215	1/1	0.94	0.14	-	41,41,41,41	0
56	MG	CA	1610	1/1	0.93	0.10	-	24,24,24,24	0
56	MG	BA	3336	1/1	0.92	0.14	-	38,38,38,38	0
56	MG	BA	3043	1/1	0.91	0.22	-	30,30,30,30	0
56	MG	BA	3070	1/1	0.94	0.13	-	32,32,32,32	0
56	MG	CA	1881	1/1	0.86	0.46	-	47,47,47,47	0
56	MG	DA	3199	1/1	0.98	0.14	-	12,12,12,12	0
56	MG	DA	3148	1/1	0.99	0.22	-	50,50,50,50	0
56	MG	DA	3348	1/1	0.99	0.15	-	40,40,40,40	0
56	MG	BA	3657	1/1	0.96	0.11	-	27,27,27,27	0
56	MG	CA	1952	1/1	0.97	0.18	-	37,37,37,37	0
56	MG	BA	3025	1/1	0.92	0.14	-	13,13,13,13	0
56	MG	DA	3079	1/1	0.97	0.14	-	12,12,12,12	0
56	MG	DA	3667	1/1	0.97	0.16	-	38,38,38,38	0
56	MG	DA	3181	1/1	0.98	0.13	-	26,26,26,26	0
56	MG	BA	3149	1/1	0.93	0.13	-	38,38,38,38	0
56	MG	BA	3803	1/1	0.91	0.42	-	55,55,55,55	0
56	MG	AA	1832	1/1	0.92	0.17	-	49,49,49,49	0
56	MG	DA	3533	1/1	0.98	0.12	-	12,12,12,12	0
56	MG	BA	3325	1/1	0.99	0.05	-	5,5,5,5	0
56	MG	BA	3734	1/1	0.97	0.18	-	32,32,32,32	0
56	MG	AA	1762	1/1	0.86	0.12	-	52,52,52,52	0
56	MG	DA	3655	1/1	0.96	0.17	-	41,41,41,41	0
56	MG	AZ	102	1/1	0.96	0.06	-	60,60,60,60	0
56	MG	AA	1876	1/1	0.86	0.28	-	57,57,57,57	0
56	MG	BA	3210	1/1	0.97	0.14	-	31,31,31,31	0
56	MG	BA	3745	1/1	0.93	0.15	-	39,39,39,39	0
56	MG	DA	3112	1/1	0.98	0.09	-	21,21,21,21	0
56	MG	CA	1628	1/1	0.98	0.12	-	23,23,23,23	0
56	MG	AA	1764	1/1	0.77	0.27	-	61,61,61,61	0
56	MG	DA	3738	1/1	0.88	0.21	-	58,58,58,58	0
56	MG	DA	3724	1/1	0.86	0.81	-	62,62,62,62	0
56	MG	CA	1781	1/1	0.86	0.48	-	57,57,57,57	0
56	MG	DA	3680	1/1	0.97	0.18	-	6,6,6,6	0
56	MG	BA	3008	1/1	0.97	0.23	-	5,5,5,5	0
56	MG	BA	3214	1/1	0.89	0.16	-	62,62,62,62	0
56	MG	CA	1741	1/1	0.93	0.14	-	28,28,28,28	0
56	MG	BA	3513	1/1	0.98	0.07	-	24,24,24,24	0
56	MG	CA	1640	1/1	0.94	0.37	-	56,56,56,56	0
56	MG	CA	1737	1/1	0.78	0.16	-	58,58,58,58	0
56	MG	BA	3193	1/1	0.99	0.08	-	2,2,2,2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3387	1/1	0.96	0.08	-	13,13,13,13	0
56	MG	BA	3244	1/1	0.95	0.10	-	34,34,34,34	0
56	MG	BA	3319	1/1	0.96	0.14	-	35,35,35,35	0
56	MG	DA	3092	1/1	0.92	0.18	-	32,32,32,32	0
56	MG	CA	1870	1/1	0.97	0.19	-	25,25,25,25	0
56	MG	BA	3189	1/1	0.95	0.20	-	48,48,48,48	0
56	MG	BA	3495	1/1	0.99	0.10	-	10,10,10,10	0
56	MG	DA	3523	1/1	0.94	0.11	-	44,44,44,44	0
56	MG	CA	1853	1/1	0.96	0.15	-	50,50,50,50	0
56	MG	BA	3356	1/1	0.95	0.09	-	29,29,29,29	0
56	MG	AA	1715	1/1	0.94	0.19	-	51,51,51,51	0
56	MG	DA	3472	1/1	0.93	0.26	-	39,39,39,39	0
56	MG	BA	3608	1/1	0.96	0.08	-	25,25,25,25	0
56	MG	DB	216	1/1	0.92	0.17	-	35,35,35,35	0
56	MG	DA	3216	1/1	0.99	0.05	-	24,24,24,24	0
56	MG	AA	1785	1/1	0.99	0.13	-	27,27,27,27	0
56	MG	DA	3183	1/1	0.95	0.16	-	12,12,12,12	0
56	MG	AA	1653	1/1	0.94	0.14	-	44,44,44,44	0
56	MG	DA	3442	1/1	0.98	0.10	-	32,32,32,32	0
56	MG	AA	1774	1/1	0.92	0.12	-	27,27,27,27	0
56	MG	BA	3115	1/1	0.97	0.19	-	33,33,33,33	0
56	MG	DA	3317	1/1	0.99	0.08	-	1,1,1,1	0
56	MG	BA	3715	1/1	0.94	0.09	-	42,42,42,42	0
56	MG	DA	3580	1/1	0.98	0.38	-	21,21,21,21	0
56	MG	DA	3338	1/1	0.99	0.05	-	25,25,25,25	0
56	MG	DA	3006	1/1	0.92	0.23	-	27,27,27,27	0
56	MG	DA	3042	1/1	0.98	0.08	-	7,7,7,7	0
56	MG	DA	3114	1/1	0.94	0.14	-	27,27,27,27	0
56	MG	DF	301	1/1	0.93	0.30	-	45,45,45,45	0
56	MG	DA	3460	1/1	0.95	0.23	-	41,41,41,41	0
56	MG	AZ	106	1/1	0.94	0.07	-	37,37,37,37	0
56	MG	DA	3048	1/1	0.96	0.23	-	20,20,20,20	0
56	MG	BA	3372	1/1	0.90	0.12	-	38,38,38,38	0
56	MG	DA	3237	1/1	0.95	0.11	-	31,31,31,31	0
56	MG	BA	3701	1/1	0.95	0.09	-	24,24,24,24	0
56	MG	BA	3582	1/1	0.85	0.21	-	53,53,53,53	0
56	MG	BA	3526	1/1	0.98	0.12	-	4,4,4,4	0
56	MG	BA	3494	1/1	0.97	0.16	-	25,25,25,25	0
56	MG	DA	3437	1/1	0.82	0.26	-	41,41,41,41	0
56	MG	B2	103	1/1	0.97	0.44	-	38,38,38,38	0
56	MG	CA	1673	1/1	0.96	0.07	-	48,48,48,48	0
56	MG	DA	3404	1/1	0.96	0.13	-	32,32,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3196	1/1	0.98	0.10	-	12,12,12,12	0
56	MG	CA	1868	1/1	0.88	0.25	-	54,54,54,54	0
56	MG	DA	3305	1/1	0.99	0.06	-	29,29,29,29	0
56	MG	DA	3448	1/1	0.96	0.10	-	36,36,36,36	0
56	MG	CA	1883	1/1	0.85	0.13	-	41,41,41,41	0
56	MG	BA	3340	1/1	0.90	0.13	-	49,49,49,49	0
56	MG	BA	3260	1/1	0.99	0.07	-	35,35,35,35	0
56	MG	DA	3719	1/1	0.95	0.15	-	47,47,47,47	0
56	MG	DA	3198	1/1	0.86	0.47	-	51,51,51,51	0
56	MG	DA	3354	1/1	0.81	0.28	-	43,43,43,43	0
56	MG	CA	1773	1/1	0.93	0.17	-	35,35,35,35	0
56	MG	BA	3478	1/1	0.99	0.08	-	10,10,10,10	0
56	MG	CA	1730	1/1	0.97	0.34	-	45,45,45,45	0
56	MG	CA	1846	1/1	0.95	0.08	-	69,69,69,69	0
56	MG	BA	3184	1/1	0.83	0.11	-	64,64,64,64	0
56	MG	DA	3670	1/1	0.99	0.18	-	59,59,59,59	0
56	MG	BN	202	1/1	0.94	0.21	-	49,49,49,49	0
56	MG	AA	1618	1/1	0.93	0.24	-	49,49,49,49	0
56	MG	AA	1712	1/1	0.97	0.20	-	26,26,26,26	0
56	MG	BA	3275	1/1	0.96	0.18	-	12,12,12,12	0
56	MG	BA	3013	1/1	0.99	0.06	-	0,0,0,0	0
56	MG	CA	1634	1/1	0.97	0.17	-	41,41,41,41	0
56	MG	DA	3711	1/1	0.97	0.07	-	49,49,49,49	0
56	MG	BA	3102	1/1	0.95	0.12	-	22,22,22,22	0
56	MG	BA	3502	1/1	0.97	0.06	-	38,38,38,38	0
56	MG	AA	1647	1/1	0.97	0.11	-	44,44,44,44	0
56	MG	CA	1661	1/1	0.96	0.07	-	47,47,47,47	0
56	MG	AA	1678	1/1	0.96	0.13	-	43,43,43,43	0
56	MG	BA	3313	1/1	0.98	0.06	-	25,25,25,25	0
56	MG	AA	1818	1/1	0.98	0.17	-	33,33,33,33	0
56	MG	BA	3339	1/1	0.98	0.08	-	34,34,34,34	0
56	MG	DA	3610	1/1	0.92	0.14	-	29,29,29,29	0
56	MG	BA	3163	1/1	0.99	0.10	-	25,25,25,25	0
56	MG	AA	1749	1/1	0.97	0.14	-	32,32,32,32	0
56	MG	AA	1880	1/1	0.99	0.22	-	8,8,8,8	0
56	MG	BB	203	1/1	0.99	0.07	-	22,22,22,22	0
56	MG	DA	3620	1/1	0.92	0.15	-	49,49,49,49	0
56	MG	CA	1844	1/1	0.97	0.08	-	26,26,26,26	0
56	MG	DA	3541	1/1	0.86	0.14	-	53,53,53,53	0
56	MG	DA	3330	1/1	0.98	0.21	-	36,36,36,36	0
56	MG	DA	3685	1/1	0.96	0.09	-	20,20,20,20	0
56	MG	BQ	201	1/1	0.96	0.33	-	38,38,38,38	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1918	1/1	0.94	0.12	-	44,44,44,44	0
56	MG	DA	3151	1/1	0.91	0.18	-	58,58,58,58	0
56	MG	DA	3525	1/1	0.97	0.10	-	31,31,31,31	0
56	MG	DA	3723	1/1	0.97	0.11	-	28,28,28,28	0
56	MG	BA	3611	1/1	0.99	0.06	-	11,11,11,11	0
56	MG	BA	3360	1/1	0.99	0.07	-	17,17,17,17	0
56	MG	BA	3234	1/1	0.96	0.18	-	25,25,25,25	0
56	MG	DA	3476	1/1	0.97	0.10	-	37,37,37,37	0
56	MG	BA	3761	1/1	0.98	0.17	-	15,15,15,15	0
56	MG	AA	1703	1/1	0.97	0.22	-	36,36,36,36	0
56	MG	DA	3244	1/1	0.87	0.29	-	57,57,57,57	0
56	MG	BA	3667	1/1	0.94	0.22	-	63,63,63,63	0
56	MG	CA	1768	1/1	0.83	0.11	-	39,39,39,39	0
56	MG	DA	3631	1/1	0.95	0.12	-	26,26,26,26	0
56	MG	CY	116	1/1	0.97	0.07	-	19,19,19,19	0
56	MG	DA	3163	1/1	0.99	0.04	-	21,21,21,21	0
56	MG	DZ	303	1/1	0.98	0.22	-	32,32,32,32	0
56	MG	AA	1773	1/1	0.99	0.04	-	26,26,26,26	0
56	MG	BA	3765	1/1	0.95	0.15	-	36,36,36,36	0
56	MG	DA	3629	1/1	0.98	0.27	-	22,22,22,22	0
56	MG	CA	1602	1/1	0.97	0.14	-	15,15,15,15	0
56	MG	DA	3035	1/1	0.99	0.10	-	6,6,6,6	0
56	MG	BA	3031	1/1	0.98	0.13	-	11,11,11,11	0
56	MG	BA	3636	1/1	0.97	0.09	-	47,47,47,47	0
56	MG	CA	1744	1/1	0.95	0.14	-	48,48,48,48	0
56	MG	DA	3269	1/1	0.97	0.07	-	31,31,31,31	0
56	MG	CA	1761	1/1	0.95	0.41	-	45,45,45,45	0
56	MG	DA	3513	1/1	0.94	0.08	-	41,41,41,41	0
56	MG	BA	3086	1/1	0.92	0.07	-	23,23,23,23	0
56	MG	BA	3559	1/1	0.98	0.08	-	15,15,15,15	0
56	MG	AY	115	1/1	0.98	0.09	-	18,18,18,18	0
56	MG	CZ	109	1/1	0.92	0.15	-	51,51,51,51	0
56	MG	DA	3320	1/1	0.97	0.10	-	19,19,19,19	0
56	MG	DA	3097	1/1	0.99	0.08	-	5,5,5,5	0
56	MG	BA	3567	1/1	0.95	0.07	-	11,11,11,11	0
56	MG	BA	3267	1/1	0.97	0.06	-	21,21,21,21	0
56	MG	AA	1885	1/1	0.91	0.11	-	33,33,33,33	0
56	MG	CA	1728	1/1	0.91	0.22	-	28,28,28,28	0
56	MG	BA	3687	1/1	0.97	0.08	-	19,19,19,19	0
56	MG	DA	3589	1/1	0.99	0.10	-	19,19,19,19	0
56	MG	BA	3542	1/1	0.99	0.16	-	13,13,13,13	0
56	MG	BA	3718	1/1	0.97	0.11	-	33,33,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3727	1/1	0.98	0.32	-	36,36,36,36	0
56	MG	BA	3395	1/1	0.96	0.20	-	34,34,34,34	0
56	MG	BA	3200	1/1	0.97	0.09	-	20,20,20,20	0
56	MG	BA	3753	1/1	0.99	0.36	-	28,28,28,28	0
56	MG	DA	3454	1/1	0.99	0.08	-	12,12,12,12	0
56	MG	DA	3511	1/1	0.94	0.17	-	7,7,7,7	0
56	MG	BA	3229	1/1	0.91	0.10	-	27,27,27,27	0
56	MG	BA	3390	1/1	0.95	0.06	-	33,33,33,33	0
56	MG	BA	3638	1/1	0.94	0.13	-	38,38,38,38	0
56	MG	BA	3293	1/1	0.92	0.14	-	34,34,34,34	0
56	MG	BA	3783	1/1	0.98	0.28	-	29,29,29,29	0
56	MG	DA	3203	1/1	0.97	0.11	-	38,38,38,38	0
56	MG	CA	1833	1/1	0.90	0.10	-	37,37,37,37	0
56	MG	AA	1724	1/1	0.98	0.07	-	26,26,26,26	0
56	MG	CA	1708	1/1	0.98	0.12	-	17,17,17,17	0
56	MG	BA	3307	1/1	0.97	0.07	-	26,26,26,26	0
56	MG	AA	1892	1/1	0.88	0.12	-	48,48,48,48	0
56	MG	CA	1794	1/1	0.92	0.07	-	42,42,42,42	0
56	MG	DA	3252	1/1	0.98	0.07	-	16,16,16,16	0
56	MG	DA	3666	1/1	0.98	0.06	-	23,23,23,23	0
56	MG	BA	3585	1/1	0.98	0.09	-	20,20,20,20	0
56	MG	CA	1637	1/1	0.99	0.09	-	21,21,21,21	0
56	MG	DA	3278	1/1	0.99	0.11	-	11,11,11,11	0
56	MG	AA	1797	1/1	0.99	0.05	-	30,30,30,30	0
56	MG	BF	304	1/1	0.94	0.25	-	40,40,40,40	0
56	MG	AA	1615	1/1	0.99	0.06	-	8,8,8,8	0
56	MG	AX	406	1/1	0.98	0.27	-	36,36,36,36	0
56	MG	DA	3457	1/1	0.96	0.20	-	23,23,23,23	0
56	MG	DA	3266	1/1	0.97	0.08	-	31,31,31,31	0
56	MG	BA	3181	1/1	0.91	0.17	-	51,51,51,51	0
56	MG	BA	3587	1/1	0.93	0.23	-	41,41,41,41	0
56	MG	DA	3276	1/1	0.98	0.17	-	29,29,29,29	0
56	MG	BA	3613	1/1	0.84	0.14	-	45,45,45,45	0
56	MG	CA	1652	1/1	0.98	0.07	-	40,40,40,40	0
56	MG	DA	3200	1/1	0.95	0.19	-	43,43,43,43	0
56	MG	CA	1924	1/1	0.84	0.24	-	45,45,45,45	0
56	MG	BA	3690	1/1	0.98	0.14	-	38,38,38,38	0
56	MG	BA	3393	1/1	0.96	0.14	-	32,32,32,32	0
56	MG	BA	3261	1/1	0.99	0.35	-	36,36,36,36	0
56	MG	DA	3268	1/1	0.93	0.22	-	48,48,48,48	0
56	MG	DA	3587	1/1	0.98	0.10	-	42,42,42,42	0
56	MG	DA	3014	1/1	0.99	0.05	-	9,9,9,9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3566	1/1	0.92	0.18	-	45,45,45,45	0
56	MG	AA	1875	1/1	0.99	0.05	-	16,16,16,16	0
56	MG	AA	1825	1/1	0.99	0.10	-	28,28,28,28	0
56	MG	CZ	117	1/1	0.96	0.11	-	34,34,34,34	0
56	MG	AA	1683	1/1	0.92	0.14	-	39,39,39,39	0
56	MG	DA	3294	1/1	0.97	0.07	-	29,29,29,29	0
56	MG	DA	3032	1/1	0.99	0.14	-	0,0,0,0	0
56	MG	DA	3494	1/1	0.99	0.08	-	5,5,5,5	0
56	MG	DA	3333	1/1	0.98	0.07	-	4,4,4,4	0
56	MG	BA	3134	1/1	0.96	0.51	-	61,61,61,61	0
56	MG	CC	301	1/1	0.95	0.10	-	48,48,48,48	0
56	MG	DA	3672	1/1	0.97	0.07	-	29,29,29,29	0
56	MG	CA	1751	1/1	0.96	0.38	-	19,19,19,19	0
56	MG	BA	3791	1/1	0.98	0.07	-	54,54,54,54	0
56	MG	DZ	301	1/1	0.98	0.08	-	27,27,27,27	0
56	MG	AA	1620	1/1	0.97	0.08	-	35,35,35,35	0
56	MG	DA	3208	1/1	0.91	0.34	-	42,42,42,42	0
56	MG	BA	3093	1/1	0.95	0.11	-	34,34,34,34	0
56	MG	CA	1793	1/1	0.98	0.08	-	9,9,9,9	0
56	MG	DA	3319	1/1	0.98	0.14	-	18,18,18,18	0
56	MG	AA	1636	1/1	0.94	0.12	-	64,64,64,64	0
56	MG	BZ	301	1/1	0.98	0.18	-	21,21,21,21	0
56	MG	BA	3485	1/1	0.99	0.13	-	12,12,12,12	0
56	MG	DA	3381	1/1	0.91	0.38	-	36,36,36,36	0
56	MG	BA	3141	1/1	0.95	0.12	-	39,39,39,39	0
56	MG	AA	1685	1/1	0.98	0.15	-	30,30,30,30	0
56	MG	DA	3377	1/1	0.95	0.12	-	21,21,21,21	0
56	MG	BA	3722	1/1	0.97	0.27	-	16,16,16,16	0
56	MG	CA	1979	1/1	0.89	0.15	-	59,59,59,59	0
56	MG	BA	3754	1/1	0.80	0.14	-	70,70,70,70	0
56	MG	DG	201	1/1	0.96	0.38	-	34,34,34,34	0
56	MG	CA	1683	1/1	0.99	0.13	-	16,16,16,16	0
56	MG	BA	3565	1/1	0.99	0.07	-	24,24,24,24	0
56	MG	BA	3363	1/1	0.98	0.14	-	24,24,24,24	0
56	MG	AY	112	1/1	0.98	0.10	-	39,39,39,39	0
56	MG	CA	1830	1/1	0.80	0.23	-	36,36,36,36	0
56	MG	CA	1992	1/1	0.98	0.24	-	47,47,47,47	0
56	MG	CA	1839	1/1	0.97	0.09	-	31,31,31,31	0
56	MG	BA	3402	1/1	0.94	0.08	-	39,39,39,39	0
56	MG	BA	3225	1/1	0.98	0.09	-	21,21,21,21	0
56	MG	DA	3028	1/1	0.98	0.07	-	34,34,34,34	0
56	MG	CY	107	1/1	0.97	0.27	-	38,38,38,38	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1716	1/1	0.95	0.10	-	42,42,42,42	0
56	MG	CA	2011	1/1	0.97	0.18	-	28,28,28,28	0
56	MG	DA	3559	1/1	0.87	0.23	-	44,44,44,44	0
56	MG	BA	3091	1/1	0.91	0.23	-	39,39,39,39	0
56	MG	CA	1809	1/1	0.95	0.14	-	57,57,57,57	0
56	MG	BA	3531	1/1	0.99	0.06	-	16,16,16,16	0
56	MG	DA	3617	1/1	0.97	0.05	-	47,47,47,47	0
56	MG	BA	3684	1/1	0.98	0.20	-	46,46,46,46	0
56	MG	DI	201	1/1	0.94	0.10	-	18,18,18,18	0
56	MG	DA	3722	1/1	0.92	0.20	-	54,54,54,54	0
56	MG	AA	1862	1/1	0.96	0.14	-	44,44,44,44	0
56	MG	BA	3773	1/1	0.98	0.17	-	44,44,44,44	0
56	MG	DB	207	1/1	0.98	0.11	-	37,37,37,37	0
56	MG	BA	3586	1/1	0.95	0.32	-	34,34,34,34	0
56	MG	DB	226	1/1	0.94	0.36	-	51,51,51,51	0
56	MG	BA	3399	1/1	0.98	0.19	-	17,17,17,17	0
56	MG	DA	3647	1/1	0.93	0.17	-	19,19,19,19	0
56	MG	DH	204	1/1	0.98	0.20	-	11,11,11,11	0
56	MG	AA	1902	1/1	0.94	0.07	-	42,42,42,42	0
56	MG	DA	3744	1/1	0.93	0.18	-	62,62,62,62	0
56	MG	DA	3349	1/1	0.94	0.22	-	44,44,44,44	0
56	MG	CA	1804	1/1	0.96	0.15	-	32,32,32,32	0
56	MG	BA	3789	1/1	0.94	0.23	-	35,35,35,35	0
56	MG	BA	3704	1/1	0.96	0.12	-	42,42,42,42	0
56	MG	CB	302	1/1	0.97	0.58	-	48,48,48,48	0
56	MG	DA	3095	1/1	0.97	0.15	-	24,24,24,24	0
56	MG	BA	3250	1/1	0.95	0.14	-	39,39,39,39	0
56	MG	BA	3289	1/1	0.91	0.23	-	46,46,46,46	0
56	MG	BA	3646	1/1	0.97	0.12	-	12,12,12,12	0
56	MG	BA	3449	1/1	0.97	0.10	-	31,31,31,31	0
56	MG	CA	1816	1/1	0.99	0.27	-	48,48,48,48	0
56	MG	AA	1755	1/1	0.96	0.05	-	29,29,29,29	0
56	MG	AA	1871	1/1	0.94	0.09	-	35,35,35,35	0
56	MG	BA	3150	1/1	0.96	0.16	-	35,35,35,35	0
56	MG	BA	3616	1/1	0.96	0.12	-	2,2,2,2	0
56	MG	BA	3255	1/1	0.92	0.07	-	43,43,43,43	0
56	MG	BA	3279	1/1	0.95	0.09	-	39,39,39,39	0
56	MG	BA	3014	1/1	0.99	0.08	-	11,11,11,11	0
56	MG	AA	1894	1/1	0.94	0.26	-	38,38,38,38	0
56	MG	DA	3126	1/1	0.95	0.13	-	37,37,37,37	0
56	MG	BA	3763	1/1	0.95	0.20	-	55,55,55,55	0
56	MG	CA	1860	1/1	0.97	0.11	-	31,31,31,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1843	1/1	0.95	0.10	-	21,21,21,21	0
56	MG	AA	1727	1/1	0.95	0.17	-	44,44,44,44	0
56	MG	BA	3693	1/1	0.73	0.09	-	51,51,51,51	0
56	MG	CA	1659	1/1	0.97	0.09	-	44,44,44,44	0
56	MG	AA	1878	1/1	0.93	0.29	-	37,37,37,37	0
56	MG	CA	1964	1/1	0.86	0.46	-	39,39,39,39	0
56	MG	DA	3375	1/1	0.86	0.30	-	42,42,42,42	0
56	MG	BN	201	1/1	0.99	0.04	-	20,20,20,20	0
56	MG	AY	124	1/1	0.97	0.08	-	21,21,21,21	0
56	MG	BA	3009	1/1	0.96	0.12	-	0,0,0,0	0
56	MG	AA	1812	1/1	0.94	0.23	-	33,33,33,33	0
56	MG	AA	1893	1/1	0.92	0.09	-	40,40,40,40	0
56	MG	AA	1865	1/1	0.98	0.24	-	32,32,32,32	0
56	MG	CA	1722	1/1	0.97	0.23	-	36,36,36,36	0
56	MG	DW	202	1/1	0.94	0.16	-	36,36,36,36	0
56	MG	BA	3682	1/1	0.98	0.23	-	25,25,25,25	0
56	MG	DB	213	1/1	0.97	0.07	-	20,20,20,20	0
56	MG	AA	1867	1/1	0.97	0.47	-	49,49,49,49	0
56	MG	CX	401	1/1	0.99	0.07	-	13,13,13,13	0
56	MG	BA	3062	1/1	0.98	0.09	-	24,24,24,24	0
56	MG	BA	3770	1/1	0.97	0.13	-	30,30,30,30	0
56	MG	BA	3677	1/1	0.75	0.44	-	63,63,63,63	0
56	MG	DA	3591	1/1	0.94	0.12	-	26,26,26,26	0
56	MG	BA	3631	1/1	0.91	0.18	-	34,34,34,34	0
56	MG	CA	1693	1/1	0.99	0.21	-	10,10,10,10	0
56	MG	DA	3700	1/1	0.99	0.13	-	10,10,10,10	0
56	MG	CA	1719	1/1	0.89	0.20	-	58,58,58,58	0
56	MG	DA	3615	1/1	0.90	0.19	-	40,40,40,40	0
56	MG	BA	3404	1/1	0.96	0.10	-	43,43,43,43	0
56	MG	DA	3500	1/1	0.98	0.07	-	13,13,13,13	0
56	MG	CA	1896	1/1	0.98	0.07	-	31,31,31,31	0
56	MG	AY	106	1/1	0.98	0.05	-	32,32,32,32	0
56	MG	BA	3786	1/1	0.95	0.15	-	56,56,56,56	0
56	MG	DA	3644	1/1	0.97	0.14	-	5,5,5,5	0
56	MG	CA	1631	1/1	0.97	0.13	-	27,27,27,27	0
56	MG	CA	1795	1/1	0.96	0.15	-	42,42,42,42	0
56	MG	CY	115	1/1	0.98	0.05	-	38,38,38,38	0
56	MG	DA	3412	1/1	0.88	0.29	-	50,50,50,50	0
56	MG	CA	1832	1/1	0.94	0.27	-	38,38,38,38	0
56	MG	CA	1665	1/1	0.95	0.15	-	26,26,26,26	0
56	MG	BA	3731	1/1	0.95	0.10	-	45,45,45,45	0
56	MG	BA	3383	1/1	0.98	0.07	-	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3304	1/1	0.99	0.04	-	10,10,10,10	0
56	MG	DA	3175	1/1	0.97	0.10	-	32,32,32,32	0
56	MG	BA	3222	1/1	0.98	0.08	-	13,13,13,13	0
56	MG	BA	3182	1/1	0.99	0.12	-	22,22,22,22	0
56	MG	CA	1906	1/1	0.98	0.27	-	24,24,24,24	0
56	MG	CA	1845	1/1	0.98	0.06	-	21,21,21,21	0
56	MG	AA	1687	1/1	0.97	0.07	-	11,11,11,11	0
56	MG	DA	3633	1/1	0.96	0.17	-	19,19,19,19	0
56	MG	DA	3358	1/1	0.96	0.07	-	17,17,17,17	0
56	MG	BA	3756	1/1	0.93	0.17	-	52,52,52,52	0
56	MG	CA	1797	1/1	0.91	0.16	-	60,60,60,60	0
56	MG	BA	3309	1/1	0.99	0.13	-	25,25,25,25	0
56	MG	AB	301	1/1	0.94	0.09	-	44,44,44,44	0
56	MG	CO	102	1/1	0.91	0.33	-	73,73,73,73	0
56	MG	DA	3344	1/1	0.97	0.09	-	32,32,32,32	0
56	MG	BA	3749	1/1	0.90	0.18	-	30,30,30,30	0
56	MG	BA	3227	1/1	0.94	0.23	-	36,36,36,36	0
56	MG	BA	3048	1/1	0.91	0.26	-	64,64,64,64	0
56	MG	DA	3399	1/1	0.95	0.33	-	36,36,36,36	0
56	MG	CA	1848	1/1	0.98	0.06	-	41,41,41,41	0
56	MG	AA	1659	1/1	0.99	0.11	-	33,33,33,33	0
56	MG	BA	3394	1/1	0.95	0.15	-	17,17,17,17	0
56	MG	BA	3698	1/1	0.96	0.26	-	57,57,57,57	0
56	MG	DA	3386	1/1	0.94	0.12	-	27,27,27,27	0
56	MG	BA	3548	1/1	0.94	0.20	-	39,39,39,39	0
56	MG	AA	1695	1/1	0.95	0.10	-	33,33,33,33	0
56	MG	DA	3085	1/1	0.97	0.09	-	35,35,35,35	0
56	MG	DA	3091	1/1	0.98	0.06	-	8,8,8,8	0
56	MG	DA	3694	1/1	0.95	0.09	-	46,46,46,46	0
56	MG	BA	3020	1/1	0.97	0.07	-	2,2,2,2	0
56	MG	CA	1718	1/1	0.97	0.12	-	38,38,38,38	0
56	MG	CA	1859	1/1	0.98	0.05	-	22,22,22,22	0
56	MG	CK	201	1/1	0.90	0.14	-	51,51,51,51	0
56	MG	DA	3739	1/1	0.99	0.12	-	20,20,20,20	0
56	MG	DA	3394	1/1	0.96	0.13	-	38,38,38,38	0
56	MG	AA	1807	1/1	0.97	0.11	-	22,22,22,22	0
56	MG	CA	1959	1/1	0.98	0.09	-	3,3,3,3	0
56	MG	BA	3511	1/1	0.95	0.11	-	26,26,26,26	0
56	MG	CA	1803	1/1	0.99	0.17	-	6,6,6,6	0
56	MG	CY	108	1/1	0.98	0.11	-	22,22,22,22	0
56	MG	BA	3065	1/1	0.99	0.10	-	18,18,18,18	0
56	MG	AY	108	1/1	0.96	0.12	-	33,33,33,33	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3674	1/1	0.99	0.10	-	4,4,4,4	0
56	MG	CA	1920	1/1	0.96	0.53	-	32,32,32,32	0
56	MG	CA	1789	1/1	0.88	0.54	-	53,53,53,53	0
56	MG	BA	3601	1/1	0.93	0.19	-	33,33,33,33	0
56	MG	CA	1823	1/1	0.97	0.09	-	40,40,40,40	0
56	MG	BA	3158	1/1	0.99	0.24	-	44,44,44,44	0
56	MG	DA	3370	1/1	0.97	0.14	-	23,23,23,23	0
56	MG	DA	3642	1/1	0.95	0.12	-	26,26,26,26	0
56	MG	CA	1651	1/1	0.86	0.14	-	54,54,54,54	0
56	MG	DA	3066	1/1	0.91	0.16	-	47,47,47,47	0
56	MG	AV	101	1/1	0.92	0.11	-	49,49,49,49	0
56	MG	BA	3108	1/1	0.97	0.12	-	24,24,24,24	0
56	MG	AA	1839	1/1	0.99	0.12	-	39,39,39,39	0
56	MG	DA	3327	1/1	0.99	0.12	-	13,13,13,13	0
56	MG	AA	1640	1/1	0.98	0.08	-	35,35,35,35	0
56	MG	CA	1871	1/1	0.97	0.15	-	34,34,34,34	0
56	MG	DA	3396	1/1	0.98	0.05	-	21,21,21,21	0
56	MG	BA	3680	1/1	0.96	0.21	-	44,44,44,44	0
56	MG	CA	1763	1/1	0.97	0.09	-	19,19,19,19	0
56	MG	BA	3202	1/1	0.95	0.09	-	46,46,46,46	0
56	MG	DA	3313	1/1	0.97	0.12	-	42,42,42,42	0
56	MG	DA	3624	1/1	0.91	0.18	-	39,39,39,39	0
56	MG	CX	402	1/1	0.84	0.14	-	38,38,38,38	0
56	MG	AA	1707	1/1	0.98	0.07	-	26,26,26,26	0
56	MG	CA	1709	1/1	0.99	0.26	-	39,39,39,39	0
56	MG	DA	3336	1/1	0.97	0.08	-	38,38,38,38	0
56	MG	CA	1847	1/1	0.91	0.15	-	22,22,22,22	0
56	MG	DA	3255	1/1	0.97	0.09	-	19,19,19,19	0
56	MG	CA	1988	1/1	0.88	0.17	-	48,48,48,48	0
56	MG	CA	1707	1/1	0.97	0.07	-	48,48,48,48	0
56	MG	AY	104	1/1	0.96	0.14	-	38,38,38,38	0
56	MG	AA	1891	1/1	0.87	0.36	-	68,68,68,68	0
56	MG	BA	3432	1/1	0.90	0.09	-	53,53,53,53	0
56	MG	CA	1627	1/1	0.99	0.10	-	29,29,29,29	0
56	MG	AA	1696	1/1	0.96	0.14	-	27,27,27,27	0
56	MG	BA	3626	1/1	0.94	0.11	-	29,29,29,29	0
56	MG	AA	1709	1/1	0.99	0.15	-	15,15,15,15	0
56	MG	DA	3218	1/1	0.89	0.27	-	46,46,46,46	0
56	MG	AY	122	1/1	0.97	0.07	-	17,17,17,17	0
56	MG	DA	3749	1/1	0.98	0.26	-	34,34,34,34	0
56	MG	DA	3077	1/1	0.97	0.08	-	7,7,7,7	0
56	MG	DA	3142	1/1	0.96	0.15	-	24,24,24,24	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3740	1/1	0.98	0.27	-	27,27,27,27	0
56	MG	DA	3522	1/1	0.97	0.11	-	33,33,33,33	0
56	MG	AA	1804	1/1	0.98	0.21	-	18,18,18,18	0
56	MG	CA	1648	1/1	0.99	0.09	-	28,28,28,28	0
56	MG	CZ	106	1/1	0.97	0.06	-	19,19,19,19	0
56	MG	DA	3594	1/1	0.76	0.22	-	83,83,83,83	0
56	MG	DA	3281	1/1	0.96	0.10	-	4,4,4,4	0
56	MG	DA	3422	1/1	0.96	0.15	-	22,22,22,22	0
56	MG	BA	3748	1/1	0.95	0.51	-	45,45,45,45	0
56	MG	DA	3748	1/1	0.92	0.70	-	50,50,50,50	0
56	MG	DA	3554	1/1	0.84	0.14	-	71,71,71,71	0
56	MG	CA	1745	1/1	0.96	0.22	-	42,42,42,42	0
56	MG	DA	3435	1/1	0.89	0.21	-	41,41,41,41	0
56	MG	BA	3557	1/1	0.95	0.32	-	59,59,59,59	0
56	MG	DA	3484	1/1	0.97	0.31	-	6,6,6,6	0
56	MG	BA	3512	1/1	0.91	0.12	-	16,16,16,16	0
56	MG	AA	1752	1/1	0.98	0.07	-	13,13,13,13	0
56	MG	BA	3658	1/1	0.95	0.14	-	56,56,56,56	0
56	MG	DA	3622	1/1	0.95	0.09	-	34,34,34,34	0
56	MG	DA	3029	1/1	0.94	0.12	-	25,25,25,25	0
56	MG	AX	405	1/1	0.79	0.23	-	58,58,58,58	0
56	MG	CY	103	1/1	0.98	0.07	-	49,49,49,49	0
56	MG	AA	1895	1/1	0.91	0.12	-	50,50,50,50	0
56	MG	DA	3746	1/1	0.98	0.32	-	43,43,43,43	0
56	MG	DA	3570	1/1	0.88	0.07	-	36,36,36,36	0
56	MG	DA	3004	1/1	0.89	0.80	-	42,42,42,42	0
56	MG	CA	1721	1/1	0.98	0.10	-	45,45,45,45	0
56	MG	BA	3205	1/1	0.96	0.14	-	21,21,21,21	0
56	MG	BA	3691	1/1	0.92	0.13	-	44,44,44,44	0
56	MG	BA	3324	1/1	0.95	0.28	-	33,33,33,33	0
56	MG	BA	3797	1/1	0.99	0.21	-	18,18,18,18	0
56	MG	DA	3293	1/1	0.98	0.10	-	10,10,10,10	0
56	MG	DA	3498	1/1	0.95	0.07	-	59,59,59,59	0
56	MG	AI	202	1/1	0.98	0.10	-	17,17,17,17	0
56	MG	BA	3138	1/1	0.98	0.07	-	34,34,34,34	0
56	MG	CZ	101	1/1	0.95	0.13	-	61,61,61,61	0
56	MG	CA	1831	1/1	0.86	0.12	-	66,66,66,66	0
56	MG	CZ	116	1/1	0.94	0.13	-	81,81,81,81	0
56	MG	BA	3160	1/1	0.97	0.11	-	23,23,23,23	0
56	MG	DA	3656	1/1	0.97	0.48	-	35,35,35,35	0
56	MG	BA	3164	1/1	0.94	0.16	-	51,51,51,51	0
56	MG	BA	3517	1/1	0.82	0.11	-	40,40,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3258	1/1	0.96	0.11	-	39,39,39,39	0
56	MG	AA	1810	1/1	0.99	0.09	-	24,24,24,24	0
56	MG	CA	1687	1/1	0.97	0.05	-	19,19,19,19	0
56	MG	CA	1966	1/1	0.97	0.09	-	41,41,41,41	0
56	MG	CD	302	1/1	0.98	0.07	-	41,41,41,41	0
56	MG	AY	119	1/1	0.97	0.10	-	22,22,22,22	0
56	MG	CY	114	1/1	0.97	0.13	-	16,16,16,16	0
56	MG	DA	3372	1/1	0.95	0.16	-	30,30,30,30	0
56	MG	BA	3207	1/1	0.98	0.17	-	31,31,31,31	0
56	MG	CY	110	1/1	0.97	0.08	-	17,17,17,17	0
56	MG	DA	3002	1/1	0.97	0.25	-	45,45,45,45	0
56	MG	DA	3383	1/1	0.99	0.06	-	10,10,10,10	0
56	MG	BA	3376	1/1	0.97	0.10	-	35,35,35,35	0
56	MG	BA	3188	1/1	0.97	0.13	-	3,3,3,3	0
56	MG	CA	1994	1/1	0.89	0.16	-	58,58,58,58	0
56	MG	CA	1676	1/1	0.98	0.12	-	25,25,25,25	0
56	MG	DA	3632	1/1	0.95	0.20	-	32,32,32,32	0
56	MG	AA	1780	1/1	0.97	0.14	-	34,34,34,34	0
56	MG	DA	3712	1/1	0.93	0.20	-	61,61,61,61	0
56	MG	DA	3668	1/1	0.93	0.25	-	42,42,42,42	0
56	MG	AA	1677	1/1	0.85	0.10	-	49,49,49,49	0
56	MG	BA	3750	1/1	0.95	0.13	-	24,24,24,24	0
56	MG	AA	1907	1/1	0.97	0.08	-	54,54,54,54	0
56	MG	CA	1977	1/1	0.98	0.52	-	31,31,31,31	0
56	MG	BA	3401	1/1	0.99	0.10	-	44,44,44,44	0
56	MG	BA	3218	1/1	0.98	0.09	-	20,20,20,20	0
56	MG	AA	1624	1/1	0.92	0.13	-	26,26,26,26	0
56	MG	CA	1668	1/1	0.97	0.12	-	55,55,55,55	0
56	MG	AA	1684	1/1	0.97	0.28	-	27,27,27,27	0
56	MG	CA	1753	1/1	0.97	0.14	-	23,23,23,23	0
56	MG	CA	1978	1/1	0.96	0.07	-	35,35,35,35	0
56	MG	BA	3509	1/1	0.96	0.07	-	33,33,33,33	0
56	MG	BA	3118	1/1	1.00	0.17	-	20,20,20,20	0
56	MG	BA	3073	1/1	0.96	0.15	-	23,23,23,23	0
56	MG	AA	1791	1/1	0.98	0.09	-	30,30,30,30	0
56	MG	CA	1822	1/1	0.98	0.14	-	26,26,26,26	0
56	MG	AA	1841	1/1	0.99	0.05	-	24,24,24,24	0
56	MG	BA	3162	1/1	0.98	0.16	-	41,41,41,41	0
56	MG	BA	3409	1/1	0.96	0.11	-	22,22,22,22	0
56	MG	DB	215	1/1	0.98	0.07	-	47,47,47,47	0
56	MG	BA	3433	1/1	0.99	0.15	-	40,40,40,40	0
56	MG	DA	3463	1/1	0.99	0.09	-	37,37,37,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1955	1/1	0.89	0.16	-	29,29,29,29	0
56	MG	CA	1724	1/1	0.96	0.24	-	56,56,56,56	0
56	MG	DA	3585	1/1	0.97	0.14	-	31,31,31,31	0
56	MG	BA	3195	1/1	0.93	0.22	-	46,46,46,46	0
56	MG	DB	205	1/1	0.97	0.07	-	60,60,60,60	0
56	MG	DA	3707	1/1	0.96	0.14	-	45,45,45,45	0
56	MG	DA	3329	1/1	0.98	0.07	-	42,42,42,42	0
56	MG	DA	3441	1/1	0.95	0.32	-	41,41,41,41	0
56	MG	DA	3618	1/1	0.98	0.13	-	47,47,47,47	0
56	MG	CA	1929	1/1	0.98	0.09	-	48,48,48,48	0
56	MG	DA	3098	1/1	0.99	0.06	-	1,1,1,1	0
56	MG	CA	1649	1/1	0.97	0.14	-	16,16,16,16	0
56	MG	AA	1713	1/1	0.96	0.08	-	43,43,43,43	0
56	MG	DA	3501	1/1	0.94	0.24	-	47,47,47,47	0
56	MG	BA	3505	1/1	0.99	0.05	-	1,1,1,1	0
56	MG	DA	3369	1/1	0.97	0.07	-	7,7,7,7	0
56	MG	BA	3593	1/1	0.83	0.36	-	55,55,55,55	0
56	MG	DA	3275	1/1	0.99	0.32	-	2,2,2,2	0
56	MG	BA	3021	1/1	0.99	0.05	-	11,11,11,11	0
56	MG	DA	3530	1/1	0.94	0.27	-	51,51,51,51	0
56	MG	CA	1666	1/1	0.83	0.19	-	50,50,50,50	0
56	MG	BA	3327	1/1	0.90	0.08	-	43,43,43,43	0
56	MG	AA	1691	1/1	0.90	0.21	-	52,52,52,52	0
56	MG	AA	1800	1/1	0.94	0.08	-	49,49,49,49	0
56	MG	BA	3637	1/1	0.92	0.11	-	14,14,14,14	0
56	MG	BA	3627	1/1	0.95	0.07	-	49,49,49,49	0
56	MG	BA	3185	1/1	0.98	0.07	-	5,5,5,5	0
56	MG	DA	3311	1/1	0.99	0.08	-	15,15,15,15	0
56	MG	BA	3133	1/1	0.90	0.29	-	48,48,48,48	0
56	MG	CA	1854	1/1	0.94	0.13	-	43,43,43,43	0
56	MG	BA	3713	1/1	0.97	0.23	-	28,28,28,28	0
56	MG	BA	3219	1/1	0.97	0.14	-	14,14,14,14	0
56	MG	DA	3512	1/1	0.99	0.16	-	15,15,15,15	0
56	MG	DA	3073	1/1	0.98	0.04	-	34,34,34,34	0
56	MG	DA	3728	1/1	0.93	0.17	-	33,33,33,33	0
56	MG	DA	3367	1/1	0.95	0.10	-	60,60,60,60	0
56	MG	DA	3550	1/1	0.93	0.55	-	35,35,35,35	0
56	MG	BA	3418	1/1	0.98	0.07	-	34,34,34,34	0
56	MG	BA	3211	1/1	0.98	0.10	-	27,27,27,27	0
56	MG	DA	3486	1/1	0.95	0.12	-	35,35,35,35	0
56	MG	AA	1669	1/1	0.90	0.15	-	40,40,40,40	0
56	MG	BA	3413	1/1	0.91	0.06	-	62,62,62,62	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3171	1/1	0.98	0.15	-	30,30,30,30	0
56	MG	DA	3650	1/1	0.98	0.16	-	63,63,63,63	0
56	MG	DA	3665	1/1	0.94	0.12	-	35,35,35,35	0
56	MG	AA	1833	1/1	0.97	0.30	-	52,52,52,52	0
56	MG	BA	3522	1/1	0.96	0.15	-	0,0,0,0	0
56	MG	BA	3362	1/1	0.96	0.08	-	60,60,60,60	0
56	MG	DA	3745	1/1	0.90	0.21	-	39,39,39,39	0
56	MG	AA	1882	1/1	0.98	0.35	-	30,30,30,30	0
56	MG	BA	3277	1/1	0.97	0.14	-	54,54,54,54	0
56	MG	AA	1736	1/1	0.97	0.10	-	50,50,50,50	0
56	MG	AA	1849	1/1	0.95	0.20	-	40,40,40,40	0
56	MG	BA	3374	1/1	0.91	0.15	-	25,25,25,25	0
56	MG	BA	3448	1/1	0.96	0.22	-	45,45,45,45	0
56	MG	BA	3438	1/1	0.88	0.24	-	52,52,52,52	0
56	MG	AA	1623	1/1	0.98	0.07	-	7,7,7,7	0
56	MG	DA	3757	1/1	0.81	0.41	-	43,43,43,43	0
56	MG	AA	1651	1/1	0.97	0.07	-	53,53,53,53	0
56	MG	DA	3713	1/1	0.97	0.10	-	27,27,27,27	0
56	MG	BA	3514	1/1	0.98	0.17	-	29,29,29,29	0
56	MG	CA	1899	1/1	0.90	0.25	-	49,49,49,49	0
56	MG	BA	3199	1/1	0.96	0.18	-	31,31,31,31	0
56	MG	DB	204	1/1	0.88	0.13	-	48,48,48,48	0
56	MG	AA	1870	1/1	0.95	0.43	-	28,28,28,28	0
56	MG	BA	3639	1/1	0.85	0.30	-	54,54,54,54	0
56	MG	BB	206	1/1	0.60	0.21	-	65,65,65,65	0
56	MG	DB	201	1/1	0.99	0.09	-	14,14,14,14	0
56	MG	BA	3053	1/1	0.96	0.14	-	50,50,50,50	0
56	MG	CA	1999	1/1	0.95	0.13	-	31,31,31,31	0
56	MG	DP	204	1/1	0.99	0.06	-	3,3,3,3	0
56	MG	CA	2003	1/1	0.98	0.15	-	18,18,18,18	0
56	MG	DA	3201	1/1	0.96	0.06	-	45,45,45,45	0
56	MG	AA	1634	1/1	0.95	0.09	-	32,32,32,32	0
56	MG	CA	1670	1/1	0.95	0.29	-	31,31,31,31	0
56	MG	BA	3641	1/1	0.95	0.11	-	47,47,47,47	0
56	MG	CA	1889	1/1	0.97	0.22	-	31,31,31,31	0
56	MG	BA	3003	1/1	0.98	0.11	-	44,44,44,44	0
56	MG	CA	1616	1/1	0.92	0.10	-	54,54,54,54	0
56	MG	DA	3455	1/1	0.98	0.25	-	35,35,35,35	0
56	MG	AA	1648	1/1	0.97	0.10	-	26,26,26,26	0
56	MG	CA	1678	1/1	0.90	0.18	-	65,65,65,65	0
56	MG	BA	3426	1/1	0.94	0.44	-	56,56,56,56	0
56	MG	DA	3552	1/1	0.98	0.09	-	16,16,16,16	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3004	1/1	0.92	0.49	-	57,57,57,57	0
56	MG	BA	3081	1/1	0.97	0.07	-	0,0,0,0	0
56	MG	CA	1766	1/1	0.98	0.04	-	26,26,26,26	0
56	MG	BA	3142	1/1	0.96	0.11	-	40,40,40,40	0
56	MG	CZ	107	1/1	0.98	0.06	-	36,36,36,36	0
56	MG	BA	3607	1/1	0.98	0.24	-	23,23,23,23	0
56	MG	BA	3228	1/1	0.99	0.05	-	0,0,0,0	0
56	MG	BA	3628	1/1	0.97	0.16	-	24,24,24,24	0
56	MG	AH	201	1/1	0.98	0.05	-	24,24,24,24	0
56	MG	DA	3715	1/1	0.98	0.21	-	50,50,50,50	0
56	MG	DA	3193	1/1	0.98	0.18	-	17,17,17,17	0
56	MG	DA	3572	1/1	0.93	0.08	-	36,36,36,36	0
56	MG	DA	3577	1/1	0.96	0.23	-	42,42,42,42	0
56	MG	DA	3507	1/1	0.99	0.10	-	0,0,0,0	0
56	MG	CA	1613	1/1	0.98	0.08	-	17,17,17,17	0
56	MG	BA	3166	1/1	0.98	0.09	-	28,28,28,28	0
56	MG	CA	1873	1/1	0.83	0.18	-	62,62,62,62	0
56	MG	BA	3615	1/1	0.99	0.09	-	3,3,3,3	0
56	MG	DA	3297	1/1	0.98	0.09	-	34,34,34,34	0
56	MG	BA	3755	1/1	0.93	0.12	-	64,64,64,64	0
56	MG	BA	3262	1/1	0.92	0.14	-	31,31,31,31	0
56	MG	DA	3558	1/1	0.98	0.09	-	30,30,30,30	0
56	MG	DA	3212	1/1	0.97	0.15	-	34,34,34,34	0
56	MG	BA	3469	1/1	0.88	0.11	-	28,28,28,28	0
56	MG	AA	1738	1/1	0.99	0.05	-	6,6,6,6	0
56	MG	DA	3465	1/1	0.95	0.15	-	20,20,20,20	0
56	MG	BA	3792	1/1	0.97	0.06	-	42,42,42,42	0
56	MG	DA	3136	1/1	0.97	0.16	-	11,11,11,11	0
56	MG	AA	1842	1/1	0.90	0.11	-	49,49,49,49	0
56	MG	AA	1793	1/1	0.96	0.06	-	30,30,30,30	0
56	MG	BA	3694	1/1	0.86	0.15	-	50,50,50,50	0
56	MG	BA	3082	1/1	0.97	0.08	-	48,48,48,48	0
56	MG	CA	1837	1/1	0.97	0.27	-	45,45,45,45	0
56	MG	AA	1735	1/1	0.98	0.04	-	24,24,24,24	0
56	MG	DA	3282	1/1	0.95	0.07	-	20,20,20,20	0
56	MG	CA	1820	1/1	0.96	0.18	-	55,55,55,55	0
56	MG	CA	1867	1/1	0.98	0.09	-	33,33,33,33	0
56	MG	BA	3290	1/1	0.98	0.07	-	12,12,12,12	0
56	MG	CA	1849	1/1	0.92	0.15	-	32,32,32,32	0
56	MG	CA	1619	1/1	0.93	0.17	-	66,66,66,66	0
56	MG	BP	201	1/1	0.98	0.18	-	34,34,34,34	0
56	MG	BA	3233	1/1	0.96	0.28	-	35,35,35,35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3337	1/1	0.97	0.18	-	28,28,28,28	0
56	MG	BB	216	1/1	0.99	0.07	-	51,51,51,51	0
56	MG	AA	1869	1/1	0.99	0.15	-	33,33,33,33	0
56	MG	BA	3170	1/1	0.92	0.14	-	18,18,18,18	0
56	MG	BA	3648	1/1	0.98	0.15	-	4,4,4,4	0
56	MG	CA	1738	1/1	0.97	0.19	-	20,20,20,20	0
56	MG	BA	3488	1/1	0.95	0.22	-	26,26,26,26	0
56	MG	BA	3187	1/1	0.87	0.17	-	65,65,65,65	0
56	MG	DA	3490	1/1	0.98	0.07	-	5,5,5,5	0
56	MG	BA	3343	1/1	0.96	0.12	-	32,32,32,32	0
56	MG	DA	3018	1/1	0.97	0.10	-	3,3,3,3	0
56	MG	CA	1735	1/1	0.99	0.18	-	20,20,20,20	0
56	MG	BB	204	1/1	0.98	0.08	-	46,46,46,46	0
56	MG	CA	1732	1/1	0.93	0.20	-	38,38,38,38	0
56	MG	AC	304	1/1	0.93	0.24	-	55,55,55,55	0
56	MG	BA	3746	1/1	0.86	0.40	-	65,65,65,65	0
56	MG	BA	3429	1/1	0.99	0.06	-	5,5,5,5	0
56	MG	BA	3431	1/1	0.99	0.11	-	11,11,11,11	0
56	MG	AY	101	1/1	0.99	0.11	-	26,26,26,26	0
56	MG	CA	1704	1/1	0.98	0.41	-	31,31,31,31	0
56	MG	AA	1711	1/1	0.99	0.06	-	17,17,17,17	0
56	MG	CA	1932	1/1	0.82	0.27	-	54,54,54,54	0
56	MG	DA	3428	1/1	0.90	0.11	-	61,61,61,61	0
56	MG	AA	1682	1/1	0.95	0.07	-	51,51,51,51	0
56	MG	BA	3471	1/1	0.99	0.08	-	17,17,17,17	0
56	MG	DA	3529	1/1	0.98	0.17	-	7,7,7,7	0
56	MG	BA	3154	1/1	0.95	0.12	-	26,26,26,26	0
56	MG	DZ	302	1/1	0.99	0.06	-	24,24,24,24	0
56	MG	DA	3364	1/1	0.98	0.13	-	43,43,43,43	0
56	MG	DA	3627	1/1	0.97	0.20	-	24,24,24,24	0
56	MG	DA	3227	1/1	0.89	0.13	-	37,37,37,37	0
56	MG	BA	3239	1/1	0.98	0.26	-	22,22,22,22	0
56	MG	DA	3436	1/1	0.99	0.15	-	7,7,7,7	0
56	MG	CA	1935	1/1	0.96	0.07	-	49,49,49,49	0
56	MG	AA	1605	1/1	0.99	0.07	-	15,15,15,15	0
56	MG	DA	3185	1/1	0.97	0.23	-	44,44,44,44	0
56	MG	AA	1866	1/1	0.99	0.05	-	13,13,13,13	0
56	MG	CA	1865	1/1	0.99	0.07	-	12,12,12,12	0
56	MG	AA	1852	1/1	0.96	0.12	-	45,45,45,45	0
56	MG	BA	3417	1/1	0.94	0.09	-	25,25,25,25	0
56	MG	BA	3590	1/1	0.95	0.07	-	27,27,27,27	0
56	MG	BA	3551	1/1	0.93	0.28	-	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3438	1/1	0.99	0.15	-	24,24,24,24	0
56	MG	DB	202	1/1	0.95	0.13	-	59,59,59,59	0
56	MG	BA	3057	1/1	0.99	0.07	-	3,3,3,3	0
56	MG	CA	1646	1/1	0.97	0.11	-	45,45,45,45	0
56	MG	CA	2002	1/1	0.98	0.08	-	39,39,39,39	0
56	MG	BB	205	1/1	0.98	0.28	-	36,36,36,36	0
56	MG	CA	1998	1/1	0.98	0.09	-	48,48,48,48	0
56	MG	DA	3238	1/1	0.97	0.20	-	2,2,2,2	0
56	MG	BA	3335	1/1	0.99	0.06	-	4,4,4,4	0
56	MG	DA	3662	1/1	0.99	0.09	-	24,24,24,24	0
56	MG	DA	3660	1/1	0.92	0.19	-	44,44,44,44	0
56	MG	CC	307	1/1	0.94	0.28	-	27,27,27,27	0
56	MG	DA	3574	1/1	0.96	0.07	-	45,45,45,45	0
56	MG	CA	1712	1/1	0.94	0.49	-	18,18,18,18	0
56	MG	DA	3053	1/1	0.98	0.13	-	46,46,46,46	0
56	MG	BA	3794	1/1	0.99	0.22	-	12,12,12,12	0
56	MG	DA	3564	1/1	0.99	0.06	-	7,7,7,7	0
56	MG	AA	1737	1/1	0.97	0.08	-	40,40,40,40	0
56	MG	BA	3660	1/1	0.98	0.12	-	38,38,38,38	0
56	MG	BA	3151	1/1	0.88	0.26	-	52,52,52,52	0
56	MG	DA	3449	1/1	0.97	0.08	-	16,16,16,16	0
56	MG	DR	201	1/1	0.96	0.14	-	32,32,32,32	0
56	MG	BA	3254	1/1	0.98	0.11	-	31,31,31,31	0
56	MG	BA	3668	1/1	0.92	0.12	-	50,50,50,50	0
56	MG	BA	3377	1/1	0.99	0.05	-	4,4,4,4	0
56	MG	AA	1808	1/1	0.99	0.07	-	23,23,23,23	0
56	MG	BB	219	1/1	0.97	0.42	-	52,52,52,52	0
56	MG	BA	3659	1/1	0.96	0.09	-	37,37,37,37	0
56	MG	CA	1691	1/1	0.98	0.09	-	15,15,15,15	0
56	MG	BA	3015	1/1	0.98	0.08	-	16,16,16,16	0
56	MG	DA	3653	1/1	0.92	0.11	-	55,55,55,55	0
56	MG	AA	1604	1/1	0.98	0.15	-	26,26,26,26	0
56	MG	CA	1986	1/1	0.98	0.18	-	23,23,23,23	0
56	MG	DA	3489	1/1	0.94	0.10	-	24,24,24,24	0
56	MG	BA	3686	1/1	0.96	0.10	-	30,30,30,30	0
56	MG	DA	3195	1/1	0.96	0.12	-	28,28,28,28	0
56	MG	DA	3056	1/1	0.93	0.10	-	25,25,25,25	0
56	MG	DA	3727	1/1	0.97	0.08	-	27,27,27,27	0
56	MG	BA	3728	1/1	0.91	0.17	-	28,28,28,28	0
56	MG	CA	1609	1/1	0.96	0.12	-	60,60,60,60	0
56	MG	AY	116	1/1	0.97	0.31	-	51,51,51,51	0
56	MG	CA	1874	1/1	0.93	0.18	-	52,52,52,52	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3662	1/1	0.98	0.46	-	40,40,40,40	0
56	MG	BA	3645	1/1	0.98	0.06	-	25,25,25,25	0
56	MG	BA	3321	1/1	0.98	0.13	-	51,51,51,51	0
56	MG	AA	1704	1/1	0.98	0.04	-	18,18,18,18	0
56	MG	DA	3605	1/1	0.94	0.28	-	36,36,36,36	0
56	MG	BA	3720	1/1	0.97	0.07	-	30,30,30,30	0
56	MG	DA	3286	1/1	0.99	0.09	-	6,6,6,6	0
56	MG	DA	3604	1/1	0.96	0.22	-	43,43,43,43	0
56	MG	DA	3462	1/1	0.96	0.09	-	24,24,24,24	0
56	MG	CA	1948	1/1	0.97	0.35	-	43,43,43,43	0
56	MG	CA	1642	1/1	0.97	0.10	-	29,29,29,29	0
56	MG	BA	3288	1/1	0.97	0.15	-	8,8,8,8	0
56	MG	AA	1725	1/1	0.95	0.15	-	23,23,23,23	0
56	MG	BA	3621	1/1	0.93	0.05	-	57,57,57,57	0
56	MG	BA	3653	1/1	0.97	0.13	-	38,38,38,38	0
56	MG	DA	3737	1/1	0.99	0.23	-	56,56,56,56	0
56	MG	DA	3709	1/1	0.95	0.40	-	24,24,24,24	0
56	MG	AA	1688	1/1	0.85	0.10	-	52,52,52,52	0
56	MG	DA	3001	1/1	0.94	0.19	-	37,37,37,37	0
56	MG	AA	1906	1/1	0.98	0.17	-	26,26,26,26	0
56	MG	CA	1739	1/1	0.97	0.24	-	39,39,39,39	0
56	MG	DA	3341	1/1	0.98	0.10	-	31,31,31,31	0
56	MG	DA	3638	1/1	0.97	0.19	-	37,37,37,37	0
56	MG	CX	409	1/1	0.97	0.30	-	33,33,33,33	0
56	MG	DA	3464	1/1	0.94	0.14	-	26,26,26,26	0
56	MG	AA	1824	1/1	0.92	0.14	-	78,78,78,78	0
56	MG	BA	3576	1/1	0.95	0.19	-	33,33,33,33	0
56	MG	BA	3674	1/1	0.86	0.26	-	52,52,52,52	0
56	MG	BA	3391	1/1	0.96	0.29	-	46,46,46,46	0
56	MG	BB	202	1/1	0.98	0.07	-	34,34,34,34	0
56	MG	AA	1739	1/1	0.99	0.05	-	3,3,3,3	0
56	MG	BA	3145	1/1	0.95	0.09	-	36,36,36,36	0
56	MG	DA	3012	1/1	0.96	0.10	-	16,16,16,16	0
56	MG	BA	3553	1/1	0.98	0.08	-	24,24,24,24	0
56	MG	CA	1895	1/1	0.99	0.23	-	30,30,30,30	0
56	MG	DA	3292	1/1	0.98	0.09	-	8,8,8,8	0
56	MG	AA	1853	1/1	0.99	0.06	-	12,12,12,12	0
56	MG	DA	3532	1/1	0.87	0.13	-	65,65,65,65	0
56	MG	DA	3168	1/1	0.98	0.07	-	49,49,49,49	0
56	MG	DA	3385	1/1	0.96	0.18	-	56,56,56,56	0
56	MG	AA	1740	1/1	0.96	0.08	-	53,53,53,53	0
56	MG	AA	1860	1/1	0.99	0.06	-	11,11,11,11	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1971	1/1	0.95	0.14	-	49,49,49,49	0
56	MG	DA	3232	1/1	0.99	0.10	-	6,6,6,6	0
56	MG	DA	3565	1/1	0.95	0.12	-	36,36,36,36	0
56	MG	DA	3065	1/1	0.98	0.10	-	0,0,0,0	0
56	MG	AY	113	1/1	0.81	0.13	-	41,41,41,41	0
56	MG	BA	3201	1/1	0.98	0.06	-	22,22,22,22	0
56	MG	BA	3221	1/1	0.97	0.15	-	21,21,21,21	0
56	MG	CA	1869	1/1	0.98	0.09	-	32,32,32,32	0
56	MG	AA	1641	1/1	0.98	0.06	-	8,8,8,8	0
56	MG	BA	3096	1/1	0.99	0.14	-	16,16,16,16	0
56	MG	BA	3740	1/1	0.99	0.14	-	22,22,22,22	0
56	MG	BA	3052	1/1	0.99	0.06	-	0,0,0,0	0
56	MG	AA	1751	1/1	0.99	0.12	-	20,20,20,20	0
56	MG	DN	201	1/1	0.99	0.06	-	29,29,29,29	0
56	MG	BA	3752	1/1	0.94	0.19	-	30,30,30,30	0
56	MG	AA	1655	1/1	0.98	0.05	-	26,26,26,26	0
56	MG	D8	101	1/1	0.97	0.18	-	20,20,20,20	0
56	MG	BA	3543	1/1	0.99	0.10	-	19,19,19,19	0
56	MG	BB	225	1/1	0.87	0.12	-	50,50,50,50	0
56	MG	DA	3105	1/1	0.98	0.08	-	12,12,12,12	0
56	MG	BA	3301	1/1	0.98	0.10	-	15,15,15,15	0
56	MG	BA	3689	1/1	0.93	0.13	-	44,44,44,44	0
56	MG	BA	3412	1/1	0.97	0.19	-	22,22,22,22	0
56	MG	DA	3084	1/1	0.98	0.18	-	26,26,26,26	0
56	MG	BA	3191	1/1	0.94	0.20	-	41,41,41,41	0
56	MG	CA	1749	1/1	0.83	0.15	-	41,41,41,41	0
56	MG	BA	3459	1/1	0.96	0.29	-	40,40,40,40	0
56	MG	BA	3798	1/1	0.98	0.06	-	38,38,38,38	0
56	MG	BA	3296	1/1	0.99	0.06	-	20,20,20,20	0
56	MG	DA	3033	1/1	0.97	0.09	-	10,10,10,10	0
56	MG	AA	1863	1/1	0.96	0.13	-	37,37,37,37	0
56	MG	BA	3231	1/1	0.96	0.07	-	32,32,32,32	0
56	MG	DA	3071	1/1	0.99	0.19	-	31,31,31,31	0
56	MG	AA	1714	1/1	0.93	0.18	-	28,28,28,28	0
56	MG	CA	1990	1/1	0.96	0.17	-	56,56,56,56	0
56	MG	CA	1892	1/1	0.99	0.15	-	5,5,5,5	0
56	MG	CZ	105	1/1	0.99	0.03	-	16,16,16,16	0
56	MG	DA	3158	1/1	0.98	0.14	-	15,15,15,15	0
56	MG	DA	3401	1/1	0.97	0.12	-	1,1,1,1	0
56	MG	AA	1732	1/1	0.99	0.06	-	35,35,35,35	0
56	MG	AA	1788	1/1	0.99	0.14	-	12,12,12,12	0
56	MG	BA	3348	1/1	0.95	0.18	-	9,9,9,9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BR	203	1/1	0.91	0.74	-	49,49,49,49	0
56	MG	AA	1798	1/1	0.98	0.07	-	32,32,32,32	0
56	MG	DA	3623	1/1	0.98	0.10	-	39,39,39,39	0
56	MG	CA	1836	1/1	0.97	0.19	-	14,14,14,14	0
56	MG	DA	3118	1/1	0.96	0.08	-	26,26,26,26	0
56	MG	CY	118	1/1	0.88	0.14	-	56,56,56,56	0
56	MG	BA	3474	1/1	0.95	0.32	-	48,48,48,48	0
56	MG	DA	3410	1/1	0.99	0.15	-	17,17,17,17	0
56	MG	DB	211	1/1	1.00	0.04	-	15,15,15,15	0
56	MG	BA	3804	1/1	0.98	0.11	-	29,29,29,29	0
56	MG	DB	224	1/1	0.96	0.53	-	41,41,41,41	0
56	MG	BA	3643	1/1	0.98	0.08	-	23,23,23,23	0
56	MG	BA	3451	1/1	0.97	0.18	-	51,51,51,51	0
56	MG	DA	3335	1/1	0.98	0.08	-	7,7,7,7	0
56	MG	BA	3558	1/1	0.93	0.23	-	54,54,54,54	0
56	MG	CA	1985	1/1	0.74	0.14	-	52,52,52,52	0
56	MG	CA	1914	1/1	0.97	0.17	-	29,29,29,29	0
56	MG	AA	1608	1/1	0.98	0.08	-	16,16,16,16	0
56	MG	CA	1961	1/1	0.98	0.15	-	27,27,27,27	0
56	MG	BA	3022	1/1	0.98	0.17	-	2,2,2,2	0
56	MG	BA	3121	1/1	0.98	0.08	-	40,40,40,40	0
56	MG	BA	3652	1/1	0.92	0.23	-	33,33,33,33	0
56	MG	BA	3354	1/1	0.97	0.11	-	19,19,19,19	0
56	MG	BA	3666	1/1	0.95	0.25	-	51,51,51,51	0
56	MG	CA	1879	1/1	0.96	0.11	-	28,28,28,28	0
56	MG	DA	3621	1/1	0.93	0.23	-	51,51,51,51	0
56	MG	DA	3260	1/1	0.98	0.07	-	15,15,15,15	0
56	MG	DA	3508	1/1	0.99	0.07	-	16,16,16,16	0
56	MG	DA	3267	1/1	0.94	0.09	-	40,40,40,40	0
56	MG	AA	1836	1/1	0.96	0.28	-	45,45,45,45	0
56	MG	CX	405	1/1	0.96	0.22	-	49,49,49,49	0
56	MG	DA	3509	1/1	0.99	0.09	-	33,33,33,33	0
56	MG	AA	1646	1/1	0.97	0.18	-	21,21,21,21	0
56	MG	BF	302	1/1	0.97	0.12	-	13,13,13,13	0
56	MG	CA	1788	1/1	0.95	0.15	-	40,40,40,40	0
56	MG	CA	1917	1/1	0.85	0.15	-	70,70,70,70	0
56	MG	BA	3688	1/1	0.97	0.21	-	38,38,38,38	0
56	MG	AA	1706	1/1	0.99	0.08	-	26,26,26,26	0
56	MG	B5	101	1/1	0.98	0.09	-	18,18,18,18	0
56	MG	BA	3456	1/1	0.98	0.12	-	35,35,35,35	0
56	MG	BA	3147	1/1	0.98	0.14	-	53,53,53,53	0
56	MG	BA	3259	1/1	0.97	0.16	-	27,27,27,27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1711	1/1	0.93	0.10	-	23,23,23,23	0
56	MG	BA	3640	1/1	0.95	0.11	-	34,34,34,34	0
56	MG	BA	3128	1/1	0.92	0.21	-	38,38,38,38	0
56	MG	BA	3457	1/1	0.98	0.06	-	24,24,24,24	0
56	MG	CA	1902	1/1	0.90	0.12	-	50,50,50,50	0
56	MG	DA	3446	1/1	0.97	0.15	-	20,20,20,20	0
56	MG	AA	1702	1/1	0.96	0.15	-	40,40,40,40	0
56	MG	AA	1676	1/1	0.94	0.13	-	49,49,49,49	0
56	MG	DA	3645	1/1	0.98	0.09	-	20,20,20,20	0
56	MG	DA	3403	1/1	0.90	0.29	-	42,42,42,42	0
56	MG	CZ	110	1/1	0.98	0.09	-	33,33,33,33	0
56	MG	BA	3156	1/1	0.91	0.11	-	48,48,48,48	0
56	MG	DA	3340	1/1	0.96	0.13	-	33,33,33,33	0
56	MG	DA	3123	1/1	0.98	0.06	-	1,1,1,1	0
56	MG	BA	3349	1/1	0.94	0.09	-	42,42,42,42	0
56	MG	CA	1987	1/1	0.95	0.72	-	58,58,58,58	0
56	MG	BA	3710	1/1	0.95	0.15	-	13,13,13,13	0
56	MG	BA	3629	1/1	0.87	0.09	-	53,53,53,53	0
56	MG	BB	226	1/1	0.97	0.13	-	59,59,59,59	0
56	MG	BA	3206	1/1	0.98	0.09	-	37,37,37,37	0
56	MG	BA	3719	1/1	0.83	0.33	-	51,51,51,51	0
56	MG	BW	201	1/1	0.97	0.23	-	23,23,23,23	0
56	MG	BA	3695	1/1	0.91	0.17	-	50,50,50,50	0
56	MG	CA	1606	1/1	0.95	0.12	-	27,27,27,27	0
56	MG	BA	3425	1/1	0.90	0.31	-	48,48,48,48	0
56	MG	DA	3675	1/1	0.94	0.40	-	55,55,55,55	0
56	MG	BA	3282	1/1	0.99	0.07	-	6,6,6,6	0
56	MG	DA	3706	1/1	0.95	0.47	-	42,42,42,42	0
56	MG	CA	1997	1/1	0.95	0.27	-	24,24,24,24	0
56	MG	AA	1910	1/1	0.97	0.23	-	32,32,32,32	0
56	MG	CA	1658	1/1	0.98	0.12	-	37,37,37,37	0
56	MG	CA	1814	1/1	0.95	0.09	-	31,31,31,31	0
56	MG	BA	3623	1/1	0.95	0.14	-	43,43,43,43	0
56	MG	BA	3650	1/1	0.98	0.41	-	33,33,33,33	0
56	MG	DA	3636	1/1	0.97	0.14	-	46,46,46,46	0
56	MG	CA	1913	1/1	0.94	0.10	-	41,41,41,41	0
56	MG	DA	3128	1/1	0.98	0.18	-	46,46,46,46	0
56	MG	AH	202	1/1	0.99	0.17	-	41,41,41,41	0
56	MG	DA	3045	1/1	0.99	0.03	-	7,7,7,7	0
56	MG	DA	3487	1/1	0.97	0.05	-	48,48,48,48	0
56	MG	CA	1714	1/1	0.99	0.14	-	13,13,13,13	0
56	MG	BA	3332	1/1	0.99	0.12	-	9,9,9,9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3298	1/1	0.98	0.04	-	0,0,0,0	0
56	MG	CA	1909	1/1	0.98	0.23	-	33,33,33,33	0
56	MG	CA	1807	1/1	0.99	0.26	-	14,14,14,14	0
56	MG	DA	3339	1/1	0.98	0.08	-	47,47,47,47	0
56	MG	DA	3451	1/1	0.97	0.17	-	5,5,5,5	0
56	MG	BR	201	1/1	0.97	0.07	-	24,24,24,24	0
56	MG	DA	3246	1/1	0.98	0.09	-	15,15,15,15	0
56	MG	DA	3342	1/1	0.99	0.09	-	12,12,12,12	0
56	MG	BA	3461	1/1	0.94	0.11	-	23,23,23,23	0
56	MG	DB	223	1/1	0.97	0.12	-	53,53,53,53	0
56	MG	DA	3701	1/1	0.98	0.06	-	27,27,27,27	0
56	MG	DA	3257	1/1	0.93	0.21	-	32,32,32,32	0
56	MG	CY	105	1/1	0.90	0.14	-	58,58,58,58	0
56	MG	BA	3175	1/1	0.96	0.08	-	12,12,12,12	0
56	MG	CA	1779	1/1	0.97	0.12	-	14,14,14,14	0
56	MG	CY	102	1/1	0.99	0.07	-	11,11,11,11	0
56	MG	DB	214	1/1	0.96	0.28	-	34,34,34,34	0
56	MG	AA	1811	1/1	0.94	0.16	-	16,16,16,16	0
56	MG	BA	3046	1/1	0.99	0.07	-	20,20,20,20	0
56	MG	DA	3539	1/1	0.99	0.06	-	3,3,3,3	0
56	MG	AA	1748	1/1	0.94	0.16	-	54,54,54,54	0
56	MG	DA	3491	1/1	0.98	0.07	-	44,44,44,44	0
56	MG	DA	3107	1/1	1.00	0.07	-	16,16,16,16	0
56	MG	BA	3253	1/1	0.95	0.12	-	44,44,44,44	0
56	MG	CA	1675	1/1	0.99	0.05	-	26,26,26,26	0
56	MG	AA	1722	1/1	0.97	0.08	-	35,35,35,35	0
56	MG	BA	3212	1/1	0.99	0.03	-	17,17,17,17	0
56	MG	CA	1603	1/1	0.95	0.17	-	41,41,41,41	0
56	MG	DA	3222	1/1	0.99	0.15	-	2,2,2,2	0
56	MG	DA	3010	1/1	0.98	0.17	-	2,2,2,2	0
56	MG	BA	3483	1/1	0.97	0.11	-	29,29,29,29	0
56	MG	BA	3676	1/1	0.98	0.08	-	20,20,20,20	0
56	MG	BA	3248	1/1	0.97	0.12	-	42,42,42,42	0
56	MG	BA	3714	1/1	0.94	0.13	-	61,61,61,61	0
56	MG	BA	3702	1/1	0.97	0.14	-	47,47,47,47	0
56	MG	DA	3413	1/1	0.96	0.14	-	28,28,28,28	0
56	MG	DA	3496	1/1	0.97	0.18	-	18,18,18,18	0
56	MG	BA	3799	1/1	0.95	0.18	-	34,34,34,34	0
56	MG	AA	1733	1/1	0.96	0.07	-	24,24,24,24	0
56	MG	AA	1846	1/1	0.95	0.12	-	55,55,55,55	0
56	MG	DA	3047	1/1	0.98	0.06	-	10,10,10,10	0
56	MG	BA	3453	1/1	0.83	0.40	-	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3289	1/1	0.95	0.15	-	31,31,31,31	0
56	MG	BA	3618	1/1	0.99	0.10	-	10,10,10,10	0
56	MG	DA	3474	1/1	0.93	0.29	-	34,34,34,34	0
56	MG	CA	1928	1/1	0.99	0.06	-	17,17,17,17	0
56	MG	BA	3344	1/1	0.90	0.15	-	42,42,42,42	0
56	MG	CA	1635	1/1	0.93	0.28	-	39,39,39,39	0
56	MG	DA	3037	1/1	0.98	0.07	-	57,57,57,57	0
56	MG	CA	1717	1/1	0.97	0.12	-	32,32,32,32	0
56	MG	DA	3742	1/1	0.99	0.34	-	2,2,2,2	0
56	MG	DA	3141	1/1	0.97	0.09	-	9,9,9,9	0
56	MG	CA	1656	1/1	0.97	0.12	-	48,48,48,48	0
56	MG	DA	3480	1/1	0.94	0.18	-	46,46,46,46	0
56	MG	DA	3717	1/1	0.97	0.14	-	24,24,24,24	0
56	MG	DA	3020	1/1	0.97	0.24	-	9,9,9,9	0
56	MG	DA	3732	1/1	0.97	0.16	-	29,29,29,29	0
56	MG	CA	1778	1/1	0.98	0.12	-	34,34,34,34	0
56	MG	AF	202	1/1	0.87	0.12	-	58,58,58,58	0
56	MG	BA	3294	1/1	0.97	0.15	-	43,43,43,43	0
56	MG	DA	3526	1/1	0.99	0.15	-	12,12,12,12	0
56	MG	DA	3652	1/1	0.92	0.08	-	45,45,45,45	0
56	MG	CA	1612	1/1	0.94	0.12	-	30,30,30,30	0
56	MG	CC	303	1/1	0.98	0.19	-	22,22,22,22	0
56	MG	DA	3036	1/1	0.96	0.07	-	13,13,13,13	0
56	MG	BA	3801	1/1	0.95	0.12	-	45,45,45,45	0
56	MG	AA	1654	1/1	0.80	0.22	-	80,80,80,80	0
56	MG	AA	1770	1/1	0.96	0.11	-	42,42,42,42	0
56	MG	DA	3443	1/1	0.95	0.16	-	25,25,25,25	0
56	MG	DA	3535	1/1	0.94	0.09	-	42,42,42,42	0
56	MG	DA	3070	1/1	0.97	0.07	-	20,20,20,20	0
56	MG	BA	3071	1/1	0.99	0.03	-	34,34,34,34	0
56	MG	AY	118	1/1	0.98	0.08	-	45,45,45,45	0
56	MG	AA	1813	1/1	0.97	0.06	-	23,23,23,23	0
56	MG	DA	3427	1/1	0.99	0.11	-	7,7,7,7	0
56	MG	DV	201	1/1	0.94	0.08	-	61,61,61,61	0
56	MG	CA	1618	1/1	0.95	0.25	-	27,27,27,27	0
56	MG	BA	3243	1/1	0.97	0.12	-	14,14,14,14	0
56	MG	CA	1770	1/1	0.96	0.11	-	30,30,30,30	0
56	MG	BA	3165	1/1	0.99	0.05	-	8,8,8,8	0
56	MG	BA	3550	1/1	0.99	0.04	-	13,13,13,13	0
56	MG	BA	3739	1/1	0.98	0.07	-	37,37,37,37	0
56	MG	B1	101	1/1	0.96	0.12	-	28,28,28,28	0
56	MG	CA	1647	1/1	0.96	0.06	-	25,25,25,25	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1608	1/1	0.97	0.12	-	27,27,27,27	0
56	MG	CA	1989	1/1	0.98	0.09	-	33,33,33,33	0
56	MG	DA	3415	1/1	0.97	0.08	-	27,27,27,27	0
56	MG	BB	218	1/1	0.93	0.17	-	51,51,51,51	0
56	MG	CA	1645	1/1	0.95	0.11	-	45,45,45,45	0
56	MG	BA	3447	1/1	0.99	0.04	-	16,16,16,16	0
56	MG	AA	1845	1/1	0.95	0.66	-	48,48,48,48	0
56	MG	DA	3243	1/1	0.90	0.17	-	41,41,41,41	0
56	MG	DA	3129	1/1	0.92	0.08	-	32,32,32,32	0
56	MG	DA	3456	1/1	0.92	0.16	-	37,37,37,37	0
56	MG	BA	3726	1/1	0.93	0.41	-	66,66,66,66	0
56	MG	BA	3784	1/1	0.95	0.10	-	36,36,36,36	0
56	MG	CA	1787	1/1	0.99	0.04	-	19,19,19,19	0
56	MG	B7	103	1/1	0.98	0.10	-	47,47,47,47	0
56	MG	BA	3172	1/1	0.93	0.08	-	63,63,63,63	0
56	MG	DB	212	1/1	0.87	0.20	-	45,45,45,45	0
56	MG	DA	3651	1/1	0.93	0.15	-	21,21,21,21	0
56	MG	DA	3125	1/1	0.98	0.20	-	15,15,15,15	0
56	MG	DA	3478	1/1	0.99	0.10	-	18,18,18,18	0
56	MG	BA	3080	1/1	0.96	0.12	-	19,19,19,19	0
56	MG	BB	208	1/1	0.95	0.08	-	18,18,18,18	0
56	MG	CA	1925	1/1	0.90	0.31	-	45,45,45,45	0
56	MG	DA	3055	1/1	0.85	0.14	-	26,26,26,26	0
56	MG	AA	1734	1/1	0.99	0.06	-	21,21,21,21	0
56	MG	DA	3094	1/1	0.99	0.14	-	13,13,13,13	0
56	MG	CA	1725	1/1	0.98	0.07	-	26,26,26,26	0
56	MG	DA	3134	1/1	0.81	0.11	-	61,61,61,61	0
56	MG	DA	3262	1/1	0.96	0.16	-	20,20,20,20	0
56	MG	DA	3223	1/1	0.98	0.05	-	26,26,26,26	0
56	MG	DA	3038	1/1	0.95	0.17	-	14,14,14,14	0
56	MG	CA	2009	1/1	0.91	0.30	-	41,41,41,41	0
56	MG	DA	3137	1/1	0.97	0.11	-	20,20,20,20	0
56	MG	DA	3405	1/1	0.93	0.05	-	57,57,57,57	0
56	MG	DA	3241	1/1	0.99	0.20	-	12,12,12,12	0
56	MG	BA	3410	1/1	0.95	0.17	-	37,37,37,37	0
56	MG	AO	101	1/1	0.99	0.08	-	30,30,30,30	0
56	MG	BA	3033	1/1	0.97	0.13	-	24,24,24,24	0
56	MG	DA	3583	1/1	0.81	0.38	-	43,43,43,43	0
56	MG	AA	1719	1/1	0.93	0.12	-	28,28,28,28	0
56	MG	DA	3220	1/1	0.99	0.08	-	22,22,22,22	0
56	MG	DA	3683	1/1	0.77	0.08	-	89,89,89,89	0
56	MG	CA	1688	1/1	0.95	0.10	-	26,26,26,26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3581	1/1	0.93	0.12	-	16,16,16,16	0
56	MG	DA	3470	1/1	0.95	0.13	-	47,47,47,47	0
56	MG	DA	3189	1/1	0.77	0.19	-	40,40,40,40	0
56	MG	AA	1778	1/1	0.97	0.10	-	50,50,50,50	0
56	MG	DA	3714	1/1	0.93	0.23	-	28,28,28,28	0
56	MG	BA	3581	1/1	0.94	0.24	-	39,39,39,39	0
56	MG	DA	3308	1/1	0.93	0.19	-	36,36,36,36	0
56	MG	CA	1940	1/1	0.98	0.08	-	35,35,35,35	0
56	MG	BA	3364	1/1	0.92	0.15	-	60,60,60,60	0
56	MG	AK	201	1/1	0.96	0.07	-	66,66,66,66	0
56	MG	CA	1734	1/1	0.98	0.13	-	42,42,42,42	0
56	MG	DA	3310	1/1	0.98	0.13	-	34,34,34,34	0
56	MG	BA	3407	1/1	0.93	0.08	-	15,15,15,15	0
56	MG	DA	3635	1/1	0.94	0.15	-	47,47,47,47	0
56	MG	AA	1898	1/1	0.98	0.14	-	27,27,27,27	0
56	MG	CA	1886	1/1	0.91	0.30	-	62,62,62,62	0
56	MG	AA	1819	1/1	0.99	0.07	-	1,1,1,1	0
56	MG	DT	201	1/1	0.97	0.10	-	25,25,25,25	0
56	MG	DA	3593	1/1	0.97	0.27	-	28,28,28,28	0
56	MG	BA	3361	1/1	0.99	0.07	-	33,33,33,33	0
56	MG	CA	1801	1/1	0.96	0.05	-	30,30,30,30	0
56	MG	D7	101	1/1	0.98	0.07	-	22,22,22,22	0
56	MG	BA	3097	1/1	0.98	0.09	-	16,16,16,16	0
56	MG	AA	1629	1/1	0.93	0.34	-	59,59,59,59	0
56	MG	CE	201	1/1	0.40	0.25	-	70,70,70,70	0
56	MG	CA	1614	1/1	0.62	0.35	-	39,39,39,39	0
56	MG	BA	3781	1/1	0.90	0.35	-	54,54,54,54	0
56	MG	AA	1904	1/1	0.96	0.17	-	47,47,47,47	0
56	MG	AA	1668	1/1	0.95	0.09	-	14,14,14,14	0
56	MG	AC	302	1/1	0.91	0.24	-	57,57,57,57	0
56	MG	BA	3445	1/1	0.97	0.13	-	45,45,45,45	0
56	MG	DA	3606	1/1	0.97	0.30	-	54,54,54,54	0
56	MG	BA	3589	1/1	0.93	0.13	-	62,62,62,62	0
56	MG	BA	3270	1/1	0.87	0.13	-	8,8,8,8	0
56	MG	DA	3138	1/1	0.87	0.21	-	52,52,52,52	0
56	MG	CD	303	1/1	0.94	0.13	-	21,21,21,21	0
56	MG	AA	1795	1/1	0.80	0.23	-	65,65,65,65	0
56	MG	BA	3724	1/1	0.99	0.12	-	32,32,32,32	0
56	MG	DA	3100	1/1	0.98	0.07	-	3,3,3,3	0
56	MG	CZ	111	1/1	0.99	0.10	-	49,49,49,49	0
56	MG	CA	1945	1/1	0.97	0.23	-	18,18,18,18	0
56	MG	BA	3384	1/1	0.99	0.07	-	1,1,1,1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3481	1/1	0.97	0.08	-	31,31,31,31	0
56	MG	BA	3696	1/1	0.93	0.26	-	37,37,37,37	0
56	MG	D2	102	1/1	0.90	0.57	-	49,49,49,49	0
56	MG	BH	202	1/1	0.97	0.08	-	34,34,34,34	0
56	MG	AE	201	1/1	0.72	0.37	-	60,60,60,60	0
56	MG	BA	3584	1/1	0.96	0.10	-	46,46,46,46	0
56	MG	CA	1798	1/1	0.99	0.24	-	51,51,51,51	0
56	MG	DA	3553	1/1	0.99	0.06	-	6,6,6,6	0
56	MG	BA	3232	1/1	0.98	0.07	-	25,25,25,25	0
56	MG	DA	3473	1/1	0.94	0.18	-	55,55,55,55	0
56	MG	BA	3104	1/1	0.96	0.10	-	15,15,15,15	0
56	MG	AA	1874	1/1	0.99	0.26	-	10,10,10,10	0
56	MG	CA	1705	1/1	0.93	0.16	-	31,31,31,31	0
56	MG	BA	3338	1/1	0.96	0.09	-	27,27,27,27	0
56	MG	CA	1946	1/1	0.93	0.24	-	41,41,41,41	0
56	MG	AA	1843	1/1	0.99	0.07	-	28,28,28,28	0
56	MG	BA	3077	1/1	0.99	0.13	-	8,8,8,8	0
56	MG	CA	2012	1/1	0.86	0.19	-	59,59,59,59	0
56	MG	AA	1643	1/1	0.94	0.09	-	24,24,24,24	0
56	MG	BA	3776	1/1	0.98	0.09	-	6,6,6,6	0
56	MG	DA	3087	1/1	0.99	0.18	-	27,27,27,27	0
56	MG	DA	3534	1/1	0.98	0.16	-	26,26,26,26	0
56	MG	AA	1840	1/1	0.81	0.26	-	49,49,49,49	0
56	MG	AA	1908	1/1	0.99	0.10	-	13,13,13,13	0
56	MG	DA	3671	1/1	0.98	0.11	-	6,6,6,6	0
56	MG	BA	3136	1/1	0.96	0.05	-	32,32,32,32	0
56	MG	BA	3072	1/1	0.96	0.18	-	26,26,26,26	0
56	MG	DA	3229	1/1	0.99	0.06	-	1,1,1,1	0
56	MG	CZ	115	1/1	0.95	0.22	-	40,40,40,40	0
56	MG	BA	3508	1/1	0.98	0.14	-	5,5,5,5	0
56	MG	BA	3670	1/1	0.99	0.08	-	29,29,29,29	0
56	MG	CA	1834	1/1	0.92	0.18	-	61,61,61,61	0
56	MG	BA	3023	1/1	1.00	0.11	-	2,2,2,2	0
56	MG	CF	201	1/1	0.95	0.09	-	50,50,50,50	0
56	MG	BA	3180	1/1	0.96	0.10	-	8,8,8,8	0
56	MG	DA	3542	1/1	0.95	0.14	-	48,48,48,48	0
56	MG	BA	3197	1/1	0.88	0.16	-	46,46,46,46	0
56	MG	AA	1616	1/1	0.99	0.14	-	7,7,7,7	0
56	MG	AA	1760	1/1	0.99	0.13	-	24,24,24,24	0
56	MG	DA	3188	1/1	0.98	0.10	-	9,9,9,9	0
56	MG	BA	3549	1/1	0.95	0.09	-	40,40,40,40	0
56	MG	AA	1656	1/1	0.97	0.07	-	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3707	1/1	0.98	0.31	-	31,31,31,31	0
56	MG	AX	401	1/1	0.93	0.15	-	55,55,55,55	0
56	MG	BB	211	1/1	0.97	0.08	-	16,16,16,16	0
56	MG	CA	1684	1/1	0.94	0.10	-	44,44,44,44	0
56	MG	CA	1996	1/1	0.93	0.17	-	41,41,41,41	0
56	MG	BA	3538	1/1	0.98	0.06	-	10,10,10,10	0
56	MG	AA	1796	1/1	0.98	0.11	-	15,15,15,15	0
56	MG	DA	3376	1/1	0.98	0.07	-	35,35,35,35	0
56	MG	DA	3194	1/1	0.94	0.17	-	42,42,42,42	0
56	MG	BA	3312	1/1	0.98	0.10	-	7,7,7,7	0
56	MG	CA	1947	1/1	0.88	0.31	-	44,44,44,44	0
56	MG	CI	202	1/1	0.97	0.47	-	52,52,52,52	0
56	MG	BA	3477	1/1	0.96	0.20	-	31,31,31,31	0
56	MG	CY	112	1/1	0.90	0.09	-	20,20,20,20	0
56	MG	BA	3345	1/1	0.83	0.13	-	37,37,37,37	0
56	MG	BA	3186	1/1	0.96	0.23	-	28,28,28,28	0
56	MG	DO	201	1/1	0.95	0.27	-	23,23,23,23	0
56	MG	AA	1625	1/1	0.88	0.15	-	27,27,27,27	0
56	MG	BA	3596	1/1	0.99	0.14	-	8,8,8,8	0
56	MG	AA	1855	1/1	0.99	0.11	-	23,23,23,23	0
56	MG	BA	3059	1/1	0.98	0.08	-	11,11,11,11	0
56	MG	BA	3278	1/1	0.98	0.07	-	37,37,37,37	0
56	MG	DA	3069	1/1	0.97	0.12	-	15,15,15,15	0
56	MG	DA	3402	1/1	0.96	0.12	-	19,19,19,19	0
56	MG	CA	1792	1/1	0.99	0.09	-	16,16,16,16	0
56	MG	CA	1863	1/1	0.97	0.15	-	33,33,33,33	0
56	MG	CA	1858	1/1	0.94	0.10	-	66,66,66,66	0
56	MG	AC	306	1/1	0.95	0.09	-	21,21,21,21	0
56	MG	BA	3454	1/1	0.99	0.17	-	26,26,26,26	0
56	MG	DA	3027	1/1	0.95	0.22	-	22,22,22,22	0
56	MG	CA	1756	1/1	0.98	0.18	-	32,32,32,32	0
56	MG	CA	1752	1/1	0.97	0.11	-	24,24,24,24	0
56	MG	BB	212	1/1	0.96	0.16	-	50,50,50,50	0
56	MG	BA	3490	1/1	0.97	0.11	-	22,22,22,22	0
56	MG	DA	3681	1/1	0.96	0.23	-	28,28,28,28	0
56	MG	AA	1890	1/1	0.85	0.16	-	39,39,39,39	0
56	MG	DA	3736	1/1	0.92	0.14	-	64,64,64,64	0
56	MG	DA	3122	1/1	0.94	0.10	-	46,46,46,46	0
56	MG	CZ	113	1/1	0.93	0.13	-	64,64,64,64	0
56	MG	BA	3579	1/1	0.95	0.16	-	41,41,41,41	0
56	MG	BA	3671	1/1	0.91	0.18	-	57,57,57,57	0
56	MG	BA	3610	1/1	0.96	0.09	-	34,34,34,34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3135	1/1	0.98	0.21	-	25,25,25,25	0
56	MG	CG	201	1/1	0.94	0.19	-	52,52,52,52	0
56	MG	DA	3096	1/1	0.98	0.09	-	22,22,22,22	0
56	MG	CA	1723	1/1	0.95	0.09	-	33,33,33,33	0
56	MG	CA	1993	1/1	0.97	0.30	-	48,48,48,48	0
56	MG	DA	3663	1/1	0.96	0.16	-	19,19,19,19	0
56	MG	CA	1771	1/1	0.95	0.08	-	47,47,47,47	0
56	MG	CA	1731	1/1	0.95	0.11	-	30,30,30,30	0
56	MG	AA	1743	1/1	0.98	0.07	-	33,33,33,33	0
56	MG	BA	3240	1/1	0.98	0.10	-	10,10,10,10	0
56	MG	BA	3173	1/1	0.99	0.07	-	12,12,12,12	0
56	MG	DA	3326	1/1	0.96	0.09	-	27,27,27,27	0
56	MG	BA	3119	1/1	0.91	0.20	-	39,39,39,39	0
56	MG	DA	3357	1/1	0.96	0.16	-	14,14,14,14	0
56	MG	DB	227	1/1	0.96	0.17	-	53,53,53,53	0
56	MG	BA	3302	1/1	0.98	0.12	-	21,21,21,21	0
56	MG	DB	217	1/1	0.96	0.17	-	24,24,24,24	0
56	MG	CA	1819	1/1	0.79	0.19	-	46,46,46,46	0
56	MG	BA	3056	1/1	0.98	0.09	-	1,1,1,1	0
56	MG	DA	3515	1/1	0.99	0.05	-	5,5,5,5	0
56	MG	DA	3528	1/1	0.98	0.23	-	14,14,14,14	0
56	MG	BA	3334	1/1	0.95	0.15	-	23,23,23,23	0
56	MG	DA	3068	1/1	0.98	0.08	-	0,0,0,0	0
56	MG	CA	1685	1/1	0.98	0.05	-	6,6,6,6	0
56	MG	BA	3479	1/1	0.98	0.08	-	45,45,45,45	0
56	MG	BA	3588	1/1	0.98	0.05	-	22,22,22,22	0
56	MG	BA	3161	1/1	0.97	0.09	-	25,25,25,25	0
56	MG	CA	1931	1/1	0.91	0.31	-	59,59,59,59	0
56	MG	AM	201	1/1	0.93	0.28	-	54,54,54,54	0
56	MG	AA	1856	1/1	0.94	0.12	-	49,49,49,49	0
56	MG	CA	1825	1/1	0.81	0.18	-	26,26,26,26	0
56	MG	DA	3155	1/1	0.97	0.10	-	35,35,35,35	0
56	MG	DA	3178	1/1	0.79	0.14	-	47,47,47,47	0
56	MG	AA	1848	1/1	0.88	0.09	-	45,45,45,45	0
56	MG	DA	3075	1/1	0.99	0.17	-	8,8,8,8	0
56	MG	BA	3140	1/1	0.96	0.09	-	22,22,22,22	0
56	MG	DA	3520	1/1	0.95	0.26	-	63,63,63,63	0
56	MG	BA	3311	1/1	0.91	0.14	-	43,43,43,43	0
56	MG	CA	1936	1/1	0.76	0.23	-	63,63,63,63	0
56	MG	CA	1975	1/1	0.99	0.21	-	32,32,32,32	0
56	MG	BA	3060	1/1	0.99	0.08	-	7,7,7,7	0
56	MG	AA	1859	1/1	0.95	0.12	-	29,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3496	1/1	0.96	0.12	-	39,39,39,39	0
56	MG	DA	3171	1/1	0.94	0.11	-	52,52,52,52	0
56	MG	AA	1809	1/1	0.92	0.13	-	54,54,54,54	0
56	MG	DA	3483	1/1	0.99	0.17	-	19,19,19,19	0
56	MG	CA	1700	1/1	0.99	0.06	-	14,14,14,14	0
56	MG	BA	3788	1/1	0.97	0.16	-	49,49,49,49	0
56	MG	BA	3679	1/1	0.98	0.14	-	26,26,26,26	0
56	MG	DA	3625	1/1	0.98	0.09	-	28,28,28,28	0
56	MG	AA	1692	1/1	0.94	0.14	-	45,45,45,45	0
56	MG	DA	3695	1/1	0.90	0.23	-	52,52,52,52	0
56	MG	BA	3664	1/1	0.92	0.10	-	41,41,41,41	0
56	MG	BA	3663	1/1	0.98	0.46	-	32,32,32,32	0
56	MG	BA	3264	1/1	0.92	0.17	-	11,11,11,11	0
56	MG	BA	3153	1/1	0.96	0.23	-	60,60,60,60	0
56	MG	CA	1664	1/1	0.97	0.25	-	41,41,41,41	0
56	MG	CA	2006	1/1	0.94	0.15	-	41,41,41,41	0
56	MG	BA	3038	1/1	0.97	0.09	-	37,37,37,37	0
56	MG	AA	1708	1/1	0.91	0.08	-	48,48,48,48	0
56	MG	DA	3101	1/1	0.89	0.09	-	33,33,33,33	0
56	MG	AA	1701	1/1	0.96	0.12	-	17,17,17,17	0
56	MG	DA	3309	1/1	0.98	0.11	-	30,30,30,30	0
56	MG	DA	3493	1/1	0.96	0.11	-	30,30,30,30	0
56	MG	CA	1715	1/1	0.91	0.12	-	39,39,39,39	0
56	MG	BQ	202	1/1	0.96	0.26	-	45,45,45,45	0
56	MG	DA	3052	1/1	0.98	0.14	-	38,38,38,38	0
56	MG	BA	3683	1/1	0.98	0.15	-	18,18,18,18	0
56	MG	AA	1606	1/1	0.97	0.08	-	0,0,0,0	0
56	MG	BA	3747	1/1	0.82	0.28	-	63,63,63,63	0
56	MG	AY	114	1/1	0.99	0.07	-	20,20,20,20	0
56	MG	BA	3757	1/1	0.90	0.20	-	45,45,45,45	0
56	MG	DA	3207	1/1	0.97	0.07	-	20,20,20,20	0
56	MG	DA	3548	1/1	0.82	0.17	-	26,26,26,26	0
56	MG	CA	1765	1/1	0.96	0.10	-	38,38,38,38	0
56	MG	AA	1731	1/1	0.88	0.13	-	48,48,48,48	0
56	MG	BA	3501	1/1	0.99	0.07	-	60,60,60,60	0
56	MG	DA	3133	1/1	0.98	0.12	-	21,21,21,21	0
56	MG	DA	3081	1/1	0.95	0.14	-	47,47,47,47	0
56	MG	BA	3351	1/1	0.94	0.08	-	39,39,39,39	0
56	MG	BA	3241	1/1	0.96	0.13	-	19,19,19,19	0
56	MG	BA	3732	1/1	0.98	0.24	-	41,41,41,41	0
56	MG	CB	301	1/1	0.98	0.19	-	11,11,11,11	0
56	MG	DA	3630	1/1	0.97	0.10	-	21,21,21,21	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	3247	1/1	0.97	0.13	-	39,39,39,39	0
56	MG	CA	1650	1/1	0.93	0.21	-	49,49,49,49	0
56	MG	CA	1824	1/1	0.87	0.12	-	31,31,31,31	0
56	MG	DA	3089	1/1	0.99	0.19	-	30,30,30,30	0
56	MG	BA	3523	1/1	0.99	0.08	-	0,0,0,0	0
56	MG	DA	3291	1/1	0.99	0.19	-	6,6,6,6	0
56	MG	CA	1855	1/1	0.99	0.10	-	37,37,37,37	0
56	MG	DA	3608	1/1	0.98	0.05	-	36,36,36,36	0
56	MG	BV	201	1/1	0.98	0.17	-	21,21,21,21	0
56	MG	DA	3547	1/1	0.86	0.16	-	48,48,48,48	0
56	MG	DA	3117	1/1	0.97	0.08	-	24,24,24,24	0
56	MG	BA	3419	1/1	0.95	0.23	-	29,29,29,29	0
56	MG	DA	3506	1/1	0.98	0.10	-	6,6,6,6	0
56	MG	BA	3318	1/1	0.98	0.07	-	39,39,39,39	0
56	MG	AA	1905	1/1	0.96	0.14	-	40,40,40,40	0
56	MG	CA	1746	1/1	0.95	0.10	-	30,30,30,30	0
56	MG	BA	3736	1/1	0.97	0.23	-	39,39,39,39	0
56	MG	CA	1784	1/1	0.99	0.18	-	45,45,45,45	0
56	MG	AJ	201	1/1	0.92	0.10	-	36,36,36,36	0
56	MG	DA	3316	1/1	0.98	0.25	-	31,31,31,31	0
56	MG	AA	1896	1/1	0.94	0.29	-	57,57,57,57	0
56	MG	DA	3544	1/1	0.98	0.08	-	31,31,31,31	0
56	MG	BA	3117	1/1	0.98	0.11	-	33,33,33,33	0
56	MG	CA	1697	1/1	0.97	0.09	-	10,10,10,10	0
56	MG	DA	3325	1/1	0.97	0.14	-	34,34,34,34	0
56	MG	CJ	201	1/1	0.98	0.46	-	33,33,33,33	0
56	MG	CA	1621	1/1	0.96	0.20	-	34,34,34,34	0
56	MG	DA	3579	1/1	0.97	0.14	-	24,24,24,24	0
56	MG	CA	1701	1/1	0.91	0.09	-	40,40,40,40	0
56	MG	BA	3805	1/1	0.92	0.14	-	39,39,39,39	0
56	MG	BA	3258	1/1	0.96	0.09	-	30,30,30,30	0
56	MG	CA	1690	1/1	0.89	0.17	-	30,30,30,30	0
56	MG	DA	3423	1/1	0.93	0.18	-	39,39,39,39	0
56	MG	BA	3159	1/1	0.98	0.07	-	18,18,18,18	0
56	MG	CA	1970	1/1	0.85	0.16	-	63,63,63,63	0
56	MG	DA	3703	1/1	0.94	0.39	-	38,38,38,38	0
56	MG	DA	3537	1/1	0.98	0.21	-	19,19,19,19	0
56	MG	BA	3795	1/1	0.97	0.31	-	35,35,35,35	0
56	MG	CA	1750	1/1	0.93	0.10	-	35,35,35,35	0
56	MG	DA	3597	1/1	0.94	0.18	-	40,40,40,40	0
56	MG	AA	1784	1/1	0.95	0.14	-	22,22,22,22	0
56	MG	DB	222	1/1	0.85	0.10	-	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	1972	1/1	0.96	0.52	-	33,33,33,33	0
56	MG	DA	3233	1/1	0.96	0.13	-	5,5,5,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.