



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:30 PM GMT

PDB ID : 4V87
Title : Crystal structure analysis of ribosomal decoding.
Authors : Demeshkina, N.; Jenner, L.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-09-20
Resolution : 3.10 Å(reported)

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

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

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

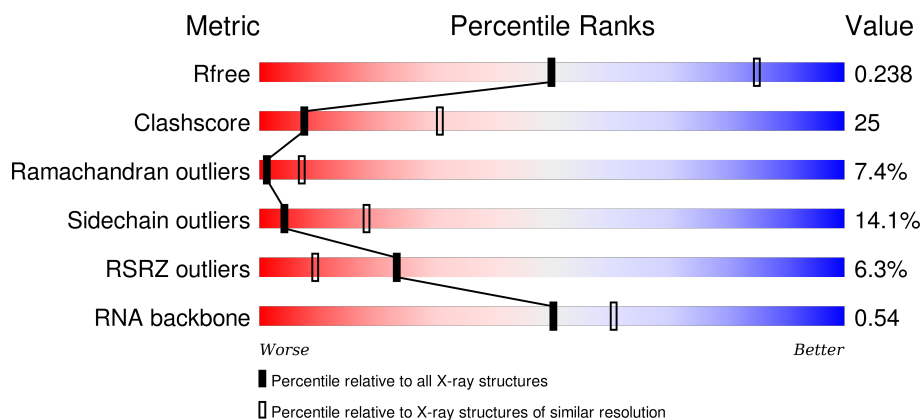
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.








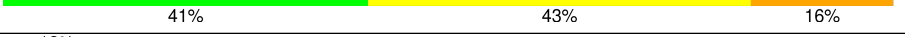
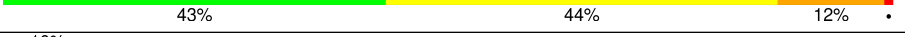

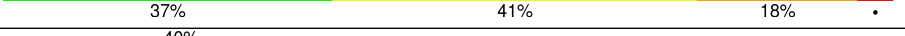

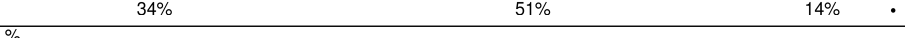
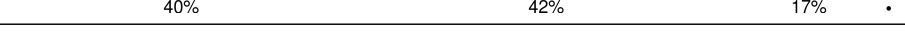

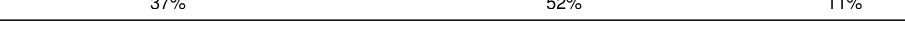


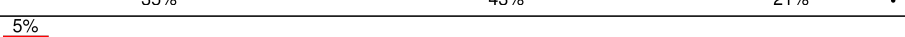
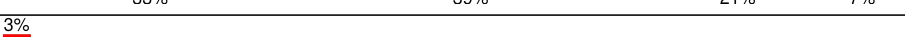
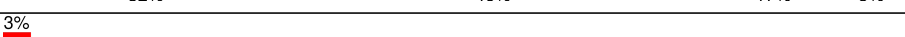




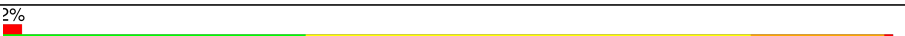

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)
RNA backbone	2183	1010 (3.52-2.68)

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

Mol	Chain	Length	Quality of chain
1	AA	2912	<div> <div>4%</div> <div>41%</div> <div>45%</div> <div>14%</div> </div>
1	DA	2912	<div> <div>5%</div> <div>41%</div> <div>43%</div> <div>16%</div> </div>
2	AB	122	<div> <div>37%</div> <div>45%</div> <div>16%</div> <div>•</div> </div>
2	DB	122	<div> <div>3%</div> <div>33%</div> <div>48%</div> <div>19%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AD	272	
3	DD	272	
4	AE	205	
4	DE	205	
5	AF	208	
5	DF	208	
6	AG	181	
6	DG	181	
7	AH	170	
7	DH	170	
8	AK	146	
8	DK	146	
9	AM	138	
9	DM	138	
10	AN	122	
10	DN	122	
11	AO	150	
11	DO	150	
12	AP	141	
12	DP	141	
13	A0	118	
13	D0	118	
14	AQ	111	
14	DQ	111	
15	AR	137	

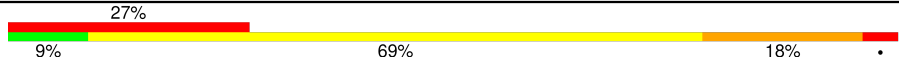
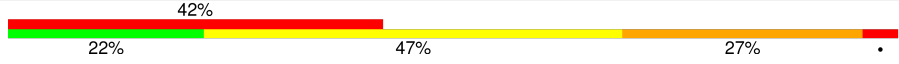
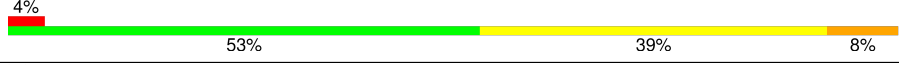

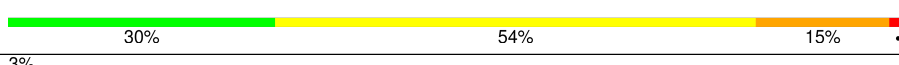
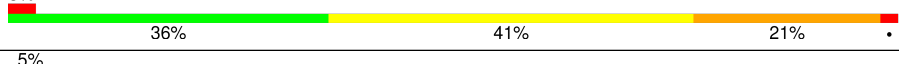
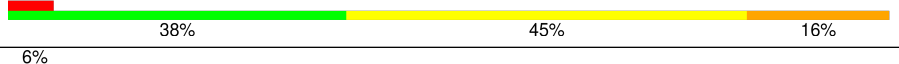
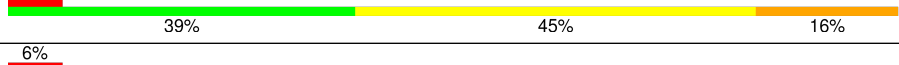
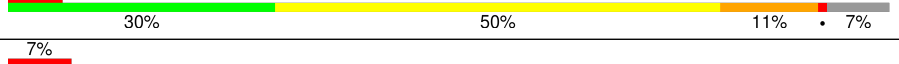
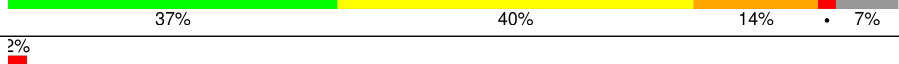
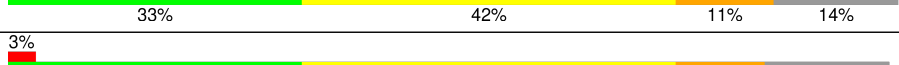

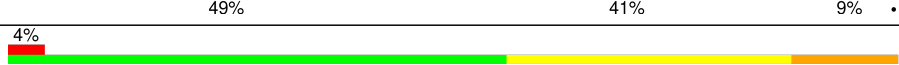
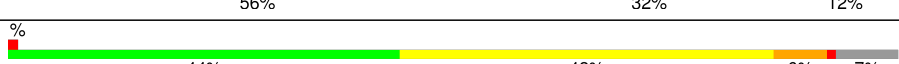
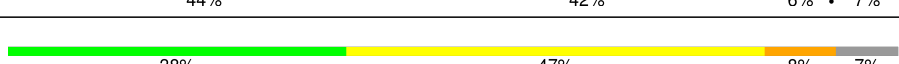

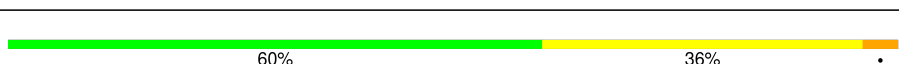

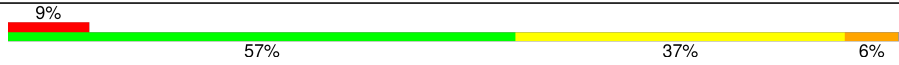


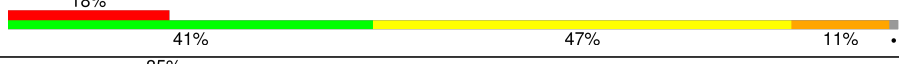

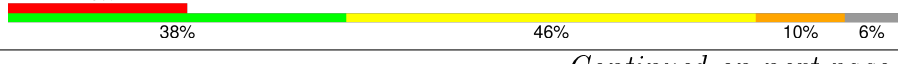

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	DR	137	
16	A1	117	
16	D1	117	
17	A2	101	
17	D2	101	
18	AS	113	
18	DS	113	
19	AT	92	
19	DT	92	
20	AU	102	
20	DU	102	
21	AV	179	
21	DV	179	
22	A3	77	
22	D3	77	
23	AZ	97	
23	DZ	97	
24	AW	69	
24	DW	69	
25	AX	59	
25	DX	59	
26	A4	66	
26	D4	66	
27	A5	59	
27	D5	59	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	A6	45	
28	D6	45	
29	A7	49	
29	D7	49	
30	A8	61	
30	D8	61	
31	BA	1506	
31	CA	1506	
32	BE	256	
32	CE	256	
33	BF	239	
33	CF	239	
34	BG	208	
34	CG	208	
35	BH	162	
35	CH	162	
36	BI	101	
36	CI	101	
37	BJ	156	
37	CJ	156	
38	BK	138	
38	CK	138	
39	BL	128	
39	CL	128	
40	BM	105	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	CM	105	
41	BN	129	
41	CN	129	
42	BO	132	
42	CO	132	
43	BP	126	
43	CP	126	
44	BQ	61	
44	CQ	61	
45	BR	89	
45	CR	89	
46	BS	88	
46	CS	88	
47	BT	105	
47	CT	105	
48	BU	88	
48	CU	88	
49	BV	93	
49	CV	93	
50	BW	106	
50	CW	106	
51	BX	27	
51	CX	27	
52	BB	87	
52	CB	87	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	BC	77	
53	BD	77	
53	CC	77	
53	CD	77	
54	B1	10	
54	C1	10	

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
55	MG	A1	201	-	-	-	X
55	MG	A6	101	-	-	-	X
55	MG	AA	3001	-	-	-	X
55	MG	AA	3002	-	-	-	X
55	MG	AA	3004	-	-	-	X
55	MG	AA	3006	-	-	-	X
55	MG	AA	3010	-	-	-	X
55	MG	AA	3012	-	-	-	X
55	MG	AA	3014	-	-	-	X
55	MG	AA	3016	-	-	-	X
55	MG	AA	3018	-	-	-	X
55	MG	AA	3020	-	-	-	X
55	MG	AA	3021	-	-	-	X
55	MG	AA	3024	-	-	-	X
55	MG	AA	3026	-	-	-	X
55	MG	AA	3027	-	-	-	X
55	MG	AA	3031	-	-	-	X
55	MG	AA	3034	-	-	-	X
55	MG	AA	3045	-	-	-	X
55	MG	AA	3050	-	-	-	X
55	MG	AA	3051	-	-	-	X
55	MG	AA	3052	-	-	-	X
55	MG	AA	3053	-	-	-	X
55	MG	AA	3054	-	-	-	X
55	MG	AA	3057	-	-	-	X
55	MG	AA	3073	-	-	-	X
55	MG	AA	3080	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	3081	-	-	-	X
55	MG	AA	3084	-	-	-	X
55	MG	AA	3085	-	-	-	X
55	MG	AA	3092	-	-	-	X
55	MG	AA	3107	-	-	-	X
55	MG	AA	3112	-	-	-	X
55	MG	AA	3113	-	-	-	X
55	MG	AA	3122	-	-	-	X
55	MG	AA	3123	-	-	-	X
55	MG	AA	3124	-	-	-	X
55	MG	AA	3125	-	-	-	X
55	MG	AA	3128	-	-	-	X
55	MG	AA	3132	-	-	-	X
55	MG	AA	3135	-	-	-	X
55	MG	AA	3138	-	-	-	X
55	MG	AA	3139	-	-	-	X
55	MG	AA	3141	-	-	-	X
55	MG	AA	3144	-	-	-	X
55	MG	AA	3153	-	-	-	X
55	MG	AA	3154	-	-	-	X
55	MG	AA	3159	-	-	-	X
55	MG	AA	3160	-	-	-	X
55	MG	AA	3162	-	-	-	X
55	MG	AA	3174	-	-	-	X
55	MG	AA	3176	-	-	-	X
55	MG	AA	3178	-	-	-	X
55	MG	AA	3196	-	-	-	X
55	MG	AA	3205	-	-	-	X
55	MG	AA	3213	-	-	-	X
55	MG	AA	3221	-	-	-	X
55	MG	AA	3227	-	-	-	X
55	MG	AA	3232	-	-	-	X
55	MG	AA	3246	-	-	-	X
55	MG	AA	3248	-	-	-	X
55	MG	AA	3254	-	-	-	X
55	MG	AA	3261	-	-	-	X
55	MG	AA	3263	-	-	-	X
55	MG	AA	3265	-	-	-	X
55	MG	AA	3268	-	-	-	X
55	MG	AA	3276	-	-	-	X
55	MG	AA	3306	-	-	-	X
55	MG	AA	3307	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	3308	-	-	-	X
55	MG	AA	3311	-	-	-	X
55	MG	AA	3313	-	-	-	X
55	MG	AA	3321	-	-	-	X
55	MG	AA	3345	-	-	-	X
55	MG	AA	3376	-	-	-	X
55	MG	AA	3388	-	-	-	X
55	MG	AA	3397	-	-	-	X
55	MG	AA	3405	-	-	-	X
55	MG	AA	3412	-	-	-	X
55	MG	AA	3431	-	-	-	X
55	MG	AA	3442	-	-	-	X
55	MG	AA	3453	-	-	-	X
55	MG	AA	3483	-	-	-	X
55	MG	AA	3500	-	-	-	X
55	MG	AA	3509	-	-	-	X
55	MG	AA	3514	-	-	-	X
55	MG	AA	3522	-	-	-	X
55	MG	AA	3529	-	-	-	X
55	MG	AA	3537	-	-	-	X
55	MG	AA	3539	-	-	-	X
55	MG	AA	3540	-	-	-	X
55	MG	AA	3546	-	-	-	X
55	MG	AA	3547	-	-	-	X
55	MG	AA	3548	-	-	-	X
55	MG	AA	3549	-	-	-	X
55	MG	AA	3556	-	-	-	X
55	MG	AA	3567	-	-	-	X
55	MG	AA	3569	-	-	-	X
55	MG	AA	3573	-	-	-	X
55	MG	AA	3575	-	-	-	X
55	MG	AA	3578	-	-	-	X
55	MG	AA	3579	-	-	-	X
55	MG	AA	3582	-	-	-	X
55	MG	AA	3591	-	-	-	X
55	MG	AA	3592	-	-	-	X
55	MG	AA	3593	-	-	-	X
55	MG	AA	3604	-	-	-	X
55	MG	AA	3605	-	-	-	X
55	MG	AA	3610	-	-	-	X
55	MG	AA	3626	-	-	-	X
55	MG	AA	3628	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AB	215	-	-	-	X
55	MG	AB	217	-	-	-	X
55	MG	AD	302	-	-	-	X
55	MG	BA	1601	-	-	-	X
55	MG	BA	1606	-	-	-	X
55	MG	BA	1608	-	-	-	X
55	MG	BA	1610	-	-	-	X
55	MG	BA	1645	-	-	-	X
55	MG	BA	1651	-	-	-	X
55	MG	BA	1658	-	-	-	X
55	MG	BA	1661	-	-	-	X
55	MG	BA	1679	-	-	-	X
55	MG	BA	1682	-	-	-	X
55	MG	BA	1691	-	-	-	X
55	MG	BA	1699	-	-	-	X
55	MG	BA	1700	-	-	-	X
55	MG	BA	1710	-	-	-	X
55	MG	BA	1715	-	-	-	X
55	MG	BA	1720	-	-	-	X
55	MG	BA	1766	-	-	-	X
55	MG	BA	1780	-	-	-	X
55	MG	BA	1786	-	-	-	X
55	MG	BA	1794	-	-	-	X
55	MG	BA	1822	-	-	-	X
55	MG	BA	1823	-	-	-	X
55	MG	BA	1835	-	-	-	X
55	MG	BC	101	-	-	-	X
55	MG	CA	1606	-	-	-	X
55	MG	CA	1617	-	-	-	X
55	MG	CA	1630	-	-	-	X
55	MG	CA	1633	-	-	-	X
55	MG	CA	1645	-	-	-	X
55	MG	CA	1646	-	-	-	X
55	MG	CA	1647	-	-	-	X
55	MG	CA	1668	-	-	-	X
55	MG	CA	1671	-	-	-	X
55	MG	CA	1676	-	-	-	X
55	MG	CA	1685	-	-	-	X
55	MG	CA	1686	-	-	-	X
55	MG	CA	1690	-	-	-	X
55	MG	CA	1691	-	-	-	X
55	MG	CA	1698	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	CA	1704	-	-	-	X
55	MG	CA	1720	-	-	-	X
55	MG	CA	1722	-	-	-	X
55	MG	CA	1749	-	-	-	X
55	MG	CA	1750	-	-	-	X
55	MG	CA	1754	-	-	-	X
55	MG	CA	1755	-	-	-	X
55	MG	CA	1758	-	-	-	X
55	MG	CA	1765	-	-	-	X
55	MG	CA	1770	-	-	-	X
55	MG	CA	1776	-	-	-	X
55	MG	CA	1801	-	-	-	X
55	MG	CC	102	-	-	-	X
55	MG	D1	201	-	-	-	X
55	MG	D1	202	-	-	-	X
55	MG	DA	3014	-	-	-	X
55	MG	DA	3035	-	-	-	X
55	MG	DA	3045	-	-	-	X
55	MG	DA	3050	-	-	-	X
55	MG	DA	3058	-	-	-	X
55	MG	DA	3075	-	-	-	X
55	MG	DA	3086	-	-	-	X
55	MG	DA	3088	-	-	-	X
55	MG	DA	3092	-	-	-	X
55	MG	DA	3094	-	-	-	X
55	MG	DA	3095	-	-	-	X
55	MG	DA	3096	-	-	-	X
55	MG	DA	3101	-	-	-	X
55	MG	DA	3104	-	-	-	X
55	MG	DA	3106	-	-	-	X
55	MG	DA	3114	-	-	-	X
55	MG	DA	3117	-	-	-	X
55	MG	DA	3130	-	-	-	X
55	MG	DA	3139	-	-	-	X
55	MG	DA	3140	-	-	-	X
55	MG	DA	3141	-	-	-	X
55	MG	DA	3142	-	-	-	X
55	MG	DA	3143	-	-	-	X
55	MG	DA	3145	-	-	-	X
55	MG	DA	3146	-	-	-	X
55	MG	DA	3148	-	-	-	X
55	MG	DA	3153	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3155	-	-	-	X
55	MG	DA	3156	-	-	-	X
55	MG	DA	3160	-	-	-	X
55	MG	DA	3173	-	-	-	X
55	MG	DA	3174	-	-	-	X
55	MG	DA	3178	-	-	-	X
55	MG	DA	3181	-	-	-	X
55	MG	DA	3188	-	-	-	X
55	MG	DA	3189	-	-	-	X
55	MG	DA	3190	-	-	-	X
55	MG	DA	3191	-	-	-	X
55	MG	DA	3194	-	-	-	X
55	MG	DA	3197	-	-	-	X
55	MG	DA	3198	-	-	-	X
55	MG	DA	3200	-	-	-	X
55	MG	DA	3203	-	-	-	X
55	MG	DA	3204	-	-	-	X
55	MG	DA	3205	-	-	-	X
55	MG	DA	3206	-	-	-	X
55	MG	DA	3209	-	-	-	X
55	MG	DA	3215	-	-	-	X
55	MG	DA	3221	-	-	-	X
55	MG	DA	3233	-	-	-	X
55	MG	DA	3234	-	-	-	X
55	MG	DA	3236	-	-	-	X
55	MG	DA	3255	-	-	-	X
55	MG	DA	3258	-	-	-	X
55	MG	DA	3262	-	-	-	X
55	MG	DA	3267	-	-	-	X
55	MG	DA	3272	-	-	-	X
55	MG	DA	3291	-	-	-	X
55	MG	DA	3292	-	-	-	X
55	MG	DA	3303	-	-	-	X
55	MG	DA	3319	-	-	-	X
55	MG	DA	3324	-	-	-	X
55	MG	DA	3332	-	-	-	X
55	MG	DA	3336	-	-	-	X
55	MG	DA	3337	-	-	-	X
55	MG	DA	3339	-	-	-	X
55	MG	DA	3341	-	-	-	X
55	MG	DA	3348	-	-	-	X
55	MG	DA	3375	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3382	-	-	-	X
55	MG	DA	3387	-	-	-	X
55	MG	DA	3422	-	-	-	X
55	MG	DA	3427	-	-	-	X
55	MG	DA	3440	-	-	-	X
55	MG	DA	3457	-	-	-	X
55	MG	DA	3460	-	-	-	X
55	MG	DA	3463	-	-	-	X
55	MG	DA	3464	-	-	-	X
55	MG	DA	3465	-	-	-	X
55	MG	DA	3467	-	-	-	X
55	MG	DA	3469	-	-	-	X
55	MG	DA	3471	-	-	-	X
55	MG	DA	3481	-	-	-	X
55	MG	DA	3482	-	-	-	X
55	MG	DA	3484	-	-	-	X
55	MG	DA	3486	-	-	-	X
55	MG	DA	3489	-	-	-	X
55	MG	DA	3492	-	-	-	X
55	MG	DA	3494	-	-	-	X
55	MG	DA	3499	-	-	-	X
55	MG	DA	3509	-	-	-	X
55	MG	DA	3512	-	-	-	X
55	MG	DA	3514	-	-	-	X
55	MG	DA	3516	-	-	-	X
55	MG	DA	3517	-	-	-	X
55	MG	DE	303	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299628 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 RNA (2909-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
1	DA	2907	Total	C	N	O	P	0	0	0
			62607	27866	11712	20123	2906			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	161	U	-	INSERTION	GB AP008226.1
AA	654A	A	G	CONFLICT	GB AP008226.1
AA	654E	C	G	CONFLICT	GB AP008226.1
AA	654P	G	C	CONFLICT	GB AP008226.1
AA	654T	A	C	CONFLICT	GB AP008226.1
AA	1058	U	G	CONFLICT	GB AP008226.1
AA	1080	A	C	CONFLICT	GB AP008226.1
DA	166	U	-	EXPRESSION TAG	GB AP008226.1
DA	654A	A	G	CONFLICT	GB AP008226.1
DA	654E	C	G	CONFLICT	GB AP008226.1
DA	654P	G	C	CONFLICT	GB AP008226.1
DA	654T	A	C	CONFLICT	GB AP008226.1
DA	1058	U	G	CONFLICT	GB AP008226.1
DA	1080	A	C	CONFLICT	GB AP008226.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
2	DB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	272	Total	C	N	O	S	0	0	0
			2116	1335	420	358	3			
3	DD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			
4	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	203	Total	C	N	O	S	0	0	1
			1586	1011	298	275	2			
5	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
6	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	170	Total	C	N	O	S	0	0	0
			1308	829	245	233	1			
7	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AK	146	Total	C	N	O	S	0	0	0
			1137	726	201	209	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	DK	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AM	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			
9	DM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
11	DO	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	A0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	D0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AQ	111	Total	C	N	O	0	0	0
			882	556	176	150			
14	DQ	111	Total	C	N	O	0	0	0
			882	556	176	150			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AR	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			
15	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	A1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
16	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	A2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
17	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
18	DS	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AT	92	Total	C	N	O	0	0	0
			726	471	131	124			
19	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	102	Total	C	N	O	S	0	0	0
			786	505	150	126	5			
20	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	175	Total	C	N	O	S	0	0	0
			1397	892	251	251	3			
21	DV	179	Total	C	N	O	S	0	0	0
			1428	911	255	259	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
22	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
23	DZ	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	DW	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AX	59	Total	C	N	O		0	0	0
			469	298	90	81				
25	DX	59	Total	C	N	O		0	0	0
			469	298	90	81				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
26	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	45	Total	C	N	O	S	0	0	0
			390	241	79	66	4			
28	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			
29	D7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			
30	D8	61	Total	C	N	O	S	0	0	0
			488	312	99	75	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	1506	Total	C	N	O	P	0	0	0
			32369	14408	5997	10459	1505			
31	CA	1506	Total	C	N	O	P	0	0	0
			32372	14408	5997	10461	1506			

- Molecule 32 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			
32	CE	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 33 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BF	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
33	CF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 34 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
34	CG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 35 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
35	CH	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 36 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
36	CI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 37 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
37	CJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 38 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
38	CK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 39 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BL	127	Total	C	N	O		0	0	0
			1010	639	197	174				
39	CL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 40 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CM	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 41 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
41	CN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 42 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
42	CO	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 43 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BP	116	Total	C	N	O	S	0	0	0
			928	574	191	161	2			
43	CP	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			

- Molecule 44 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
44	CQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 45 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
45	CR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 46 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
46	CS	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 47 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
47	CT	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 48 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	BU	72	Total	C	N	O	0	0	0
			591	376	117	98			
48	CU	72	Total	C	N	O	0	0	0
			591	376	117	98			

- Molecule 49 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BV	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
49	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 50 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
50	CW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 51 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BX	25	Total	C	N	O	0	0	0
			217	134	52	31			
51	CX	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 52 is a RNA chain called TRNA-LEU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			
52	CB	87	Total	C	N	O	P	0	0	0
			1861	829	333	612	87			

- Molecule 53 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	BD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
53	CD	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	18	C	U	CONFLICT	GB AP012306.1
BD	18	C	U	CONFLICT	GB AP012306.1
CC	18	C	U	CONFLICT	GB AP012306.1
CD	18	C	U	CONFLICT	GB AP012306.1

- Molecule 54 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B1	10	Total	C	N	O	P	0	0	0
			205	92	28	75	10			
54	C1	10	Total	C	N	O	P	0	0	0
			205	92	28	75	10			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	BA	244	Total Mg 244 244	0	0
55	CA	209	Total Mg 209 209	0	0
55	AB	17	Total Mg 17 17	0	0
55	A6	1	Total Mg 1 1	0	0
55	DU	1	Total Mg 1 1	0	0
55	B1	2	Total Mg 2 2	0	0
55	A2	1	Total Mg 1 1	0	0
55	BB	8	Total Mg 8 8	0	0
55	AE	4	Total Mg 4 4	0	0
55	D3	1	Total Mg 1 1	0	0
55	AA	630	Total Mg 630 630	0	0
55	BQ	2	Total Mg 2 2	0	0
55	A5	2	Total Mg 2 2	0	0
55	CH	1	Total Mg 1 1	0	0
55	BC	9	Total Mg 9 9	0	0
55	CG	3	Total Mg 3 3	0	0
55	A1	1	Total Mg 1 1	0	0
55	AD	2	Total Mg 2 2	0	0
55	BN	2	Total Mg 2 2	0	0
55	D0	1	Total Mg 1 1	0	0
55	BG	1	Total Mg 1 1	0	0
55	CC	8	Total Mg 8 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	DA	528	Total 528	Mg 528	0	0
55	AU	1	Total 1	Mg 1	0	0
55	A0	1	Total 1	Mg 1	0	0
55	DE	3	Total 3	Mg 3	0	0
55	D1	2	Total 2	Mg 2	0	0
55	CB	5	Total 5	Mg 5	0	0
55	DP	1	Total 1	Mg 1	0	0
55	A7	1	Total 1	Mg 1	0	0
55	D5	1	Total 1	Mg 1	0	0
55	BD	1	Total 1	Mg 1	0	0
55	AO	3	Total 3	Mg 3	0	0
55	CS	1	Total 1	Mg 1	0	0
55	A3	1	Total 1	Mg 1	0	0
55	AF	3	Total 3	Mg 3	0	0
55	DB	14	Total 14	Mg 14	0	0

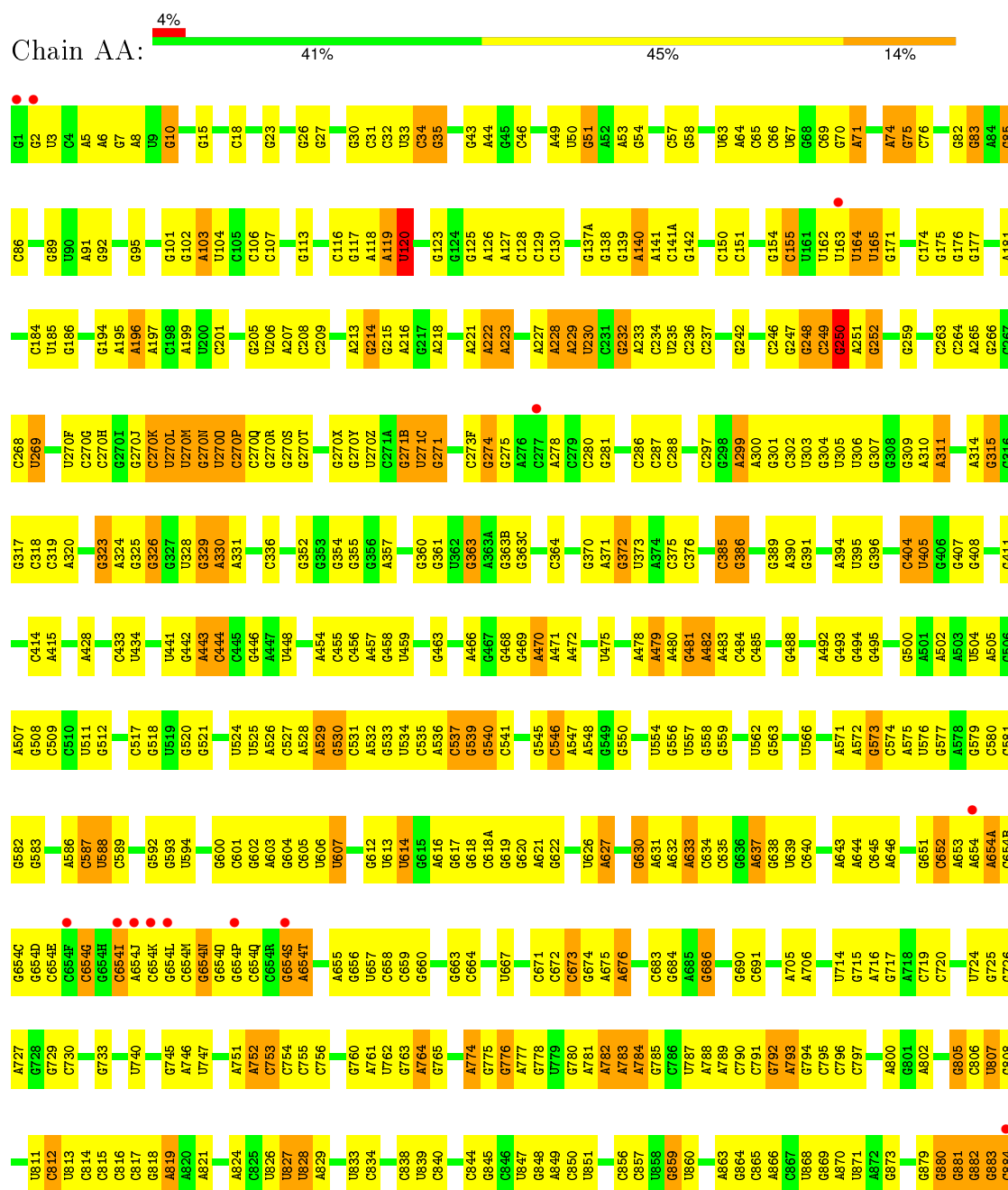
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BG	1	Total 1	Zn 1	0	0
56	BQ	1	Total 1	Zn 1	0	0
56	CQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0

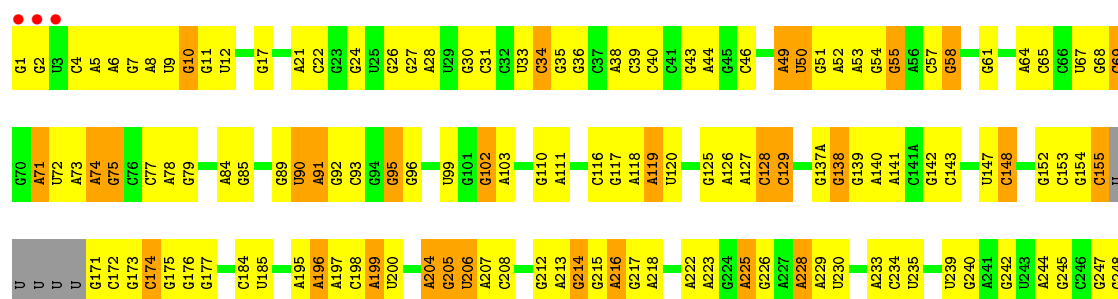
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: RNA (2909-MER)

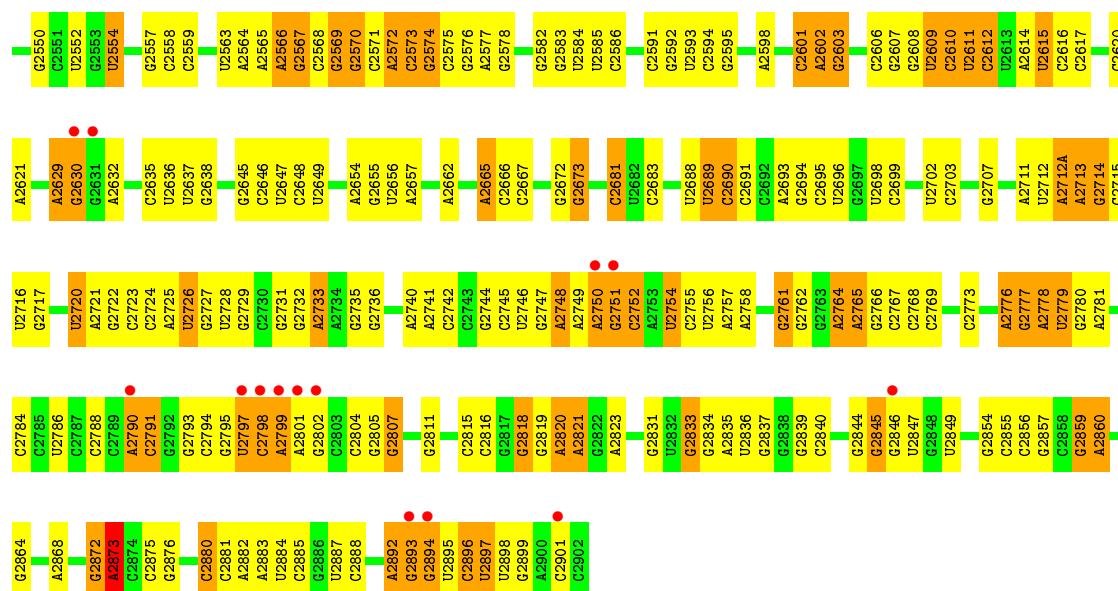


C2007	A1916	G1816	G1731	U1639	G1539	G1468	U1396	G1235	G1160	A1095	U1033	G966	C985
C2008	U1917	G1817	A1732	C1640	G1540	A1469	C1403	G1236	C1161	A1096	G1036	C967	C986
A2012	A1918	G1734	U1541	A1641	U1541	G1470	U1323	G1237	G1162	U1097	G1037	G968	A987
A2013	A1919	C1734	G1642	G1642	G1542	G1471	G1324	U1240	U1165	A1098	G1038	G969	C988
A2014	C1920	G1735	A1543	G1643	G1543	C1474	U1405	A1241	U1166	G1099	G1039	C970	C989
A2015	C1924	C1741	C1544	C1648	C1544	G1475	U1406	G1244	U1167	C1100	G1040	C971	A990
A2016	G1925	A1825	A1545	G1649	A1545	G1476	U1407	G1245	U1168	U1101	G1041	C972	G992
U2017	G1926	G1826	C1547	G1650	C1547	G1477	C1408	G1246	G1169	C1102	G1042	C973	C993
G2018	A1927	C1827	G1651	G1651	G1548	U1477	U1329	A1247	G1169	A1103	G1043	C974	C994
A2019	G1928	G1828	C1549	G1652	C1549	G1478	C1330	G1247	G1170	C1104	G1044	C975	C976
A2020	G1929	G1829	C1550	G1653	C1550	G1479	A1331	G1248	G1171	U1105	A1045	G976	A996
C2021	A1930	A1854	C1554	G1654	C1554	U1482	A1412	G1250	A1173	G1106	A1046	C977	C997
U2022	G1931	G1755	A1554	A1655	A1554	G1483	G1413	G1251	A1174	U1107	A1047	C978	C998
G2023	A1932	A1756	G1555	C1656	G1555	U1486	G1414	G1252	U1175	U1108	A1048	C979	A999
C2024	G1933	G1757	C1556	C1657	C1556	G1487	U1415	A1253	G1176	C1109	C1049	C980	A900
C2025	C1934	G1758	C1557	C1658	C1557	G1487	G1416	G1256	A1177	G1110	A1050	C981	A901
C2026	G1935	C1843	A1558	C1659	A1558	G1487	G1417	G1257	C1178	A1111	G1051	C982	C902
A2030	A1936	A1762	G1559	A1665	G1559	C1493	G1418	U1263	C1180	U1113	C1053	C983	C904
A2031	A1937	G1763	G1560	G1666	G1560	A1494	U1420	G1264	A1181	C1116	A1054	C986	U905
G2032	A1938	G1764	A1495	G1667	A1495	A1496	G1421	G1265	A1182	G1117	G1055	C987	G906
A2033	U1939	G1769	A1668	A1669	G1568	U1497	G1422	G1266	C1183	C1118	G1056	C988	U907
C2036	A1942	G1770	C1670	C1670	A1570	C1498	G1424	U1267	C1185	C1119	U1058	A990	A909
G2037	G1943	G1771	G1674	G1674	A1571	C1502	G1425	A1268	G1186	C1120	U1059	C991	A910
U1955	A1859	G1772	G1678	G1678	C1575	U1503	A1427	C1270	U1188	G1122	U1060	C992	A911
U1956	G1860	A1773	G1678	G1678	U1576	C1504	G1428	G1271	A1189	C1123	U1061	G993	C915
C2038	G1861	G1778	G1678	G1678	U1577	C1505	G1429	A1272	G1190	C1124	G1062	C994	C916
C1958	G1862	U1778	G1678	G1678	C1577	G1506	G1430	U1273	G1191	G1125	G1063	C995	A917
A2042	G1863	U1779	G1678	G1678	U1578	C1506	G1431	G1274	G1195	A1126	C1064	A996	A918
C2043	G1864	A1780	G1678	G1678	U1579	C1507	G1432	A1275	C1201	A1127	U1065	A1000	G919
G2050	G1865	C1886	G1678	G1678	A1580	A1508	U1433	A1276	C1201	U1130	U1066	A1001	C929
A2051	G1867	G1887	G1678	G1678	G1581	C1509	A1434	G1277	C1202	G1131	A1067	A1002	G929
G2052	G1868	A1688	G1678	G1678	A1582	A1510	G1435	A1278	G1203	G1132	G1068	G1003	G932
A2053	A1689	A1583	G1678	G1678	A1511	G1436	G1436	U1289	C1204	G1135	A1070	C1004	A933
G2054	A1690	C1585	G1678	G1678	G1512	G1437	U1441	U1289	U1205	G1136	G1071	C1005	G938
A1970	C1691	A1586	G1678	G1678	C1513	A1365	G1442	C1290	G1206	G1137	C1072	C1006	G938
A1971	G1692	A1587	G1678	G1678	U1514	A1365	G1443	C1291	G1207	G1138	G1073	G1007	A941
C2055	U1693	C1588	G1678	G1678	G1517	A1368	G1444	C1292	U1210	U1142	C1075	G1011	A942
G2056	G1694	C1589	G1678	G1678	G1518	G1369	G1445	U1292	U1211	U1143	C1076	G1012	G943
C1974	G1695	G1590	G1678	G1678	G1519	U1372	G1446	C1293	G1212	A1424	C1077	G1013	G944
A2059	A1698	C1591	G1678	G1678	U1520	U1373	G1448	C1297	G1215	A1425	C1078	G1014	A945
A2060	A1698	G1592	G1678	G1678	G1521	G1374	A1449	C1298	G1216	A1426	C1079	G1015	G946
C2063	G1702	G1594	G1678	G1678	G1522	G1375	G1449A	U1300	G1217	A1427	A1080	G1016	G950
G1989	G1705	G1595	G1678	G1678	G1525	G1376	U1453	A1301	G1218	C1145	U1081	G1017	G951
C1990	G1706	C1600	G1678	G1678	G1526	A1378	U1454	G1309	G1219	C1146	U1082	G1018	G952
G1991	U1709	G1601	G1678	G1678	G1527	A1379	G1455	G1310	A1220	C1147	U1083	U1019	A1020
G1992	C1800	C1601	G1678	G1678	A1528	G1380	G1456	G1311	C1221	G1148	A1084	A1021	A953
U1993	G1801	C1607	G1678	G1678	A1529	G1381	C1458	U1312	C1222	G1149	A1085	G1022	G954
C1994	G1802	A1608	G1678	G1678	G1530	G1382	G1459	U1313	G1223	C1150	A1086	A1022	G955
U1995	A1803	C1609	G1678	G1678	C1531	C1383	G1460	C1314	C1224	G1151	G1087	G1023	C956
C1996	G1906	C1610	G1678	G1678	C1532	G1384	G1461	C1315	A1227	G1152	A1088	G1024	G957
G1907	G1907	C1533	G1678	G1678	G1533	G1385	G1461	U1316	G1228	C1153	A1089	G1025	U958
C1908	G1908	G1534	G1678	G1678	G1534	G1386	G1462	U1317	G1229	G1154	U1090	U1026	A959
G2000	G1909	G1535	G1678	G1678	U1535	C1387	C1464	A1317	G1230	A1155	G1091	A1027	A960
A2002	U1727	A1618	G1678	G1678	U1536	C1388	G1465	C1318	C1231	C1158	G1092	A1028	C961
G2003	G1728	A1618	G1678	G1678	A1536	G1389	G1466	G1319	G1232	C1159	G1093	A1029	C961
G2002	A1729	C1537	G1678	G1678	C1537	G1389	C1467	C1320	G1233	U1159	U1094	A1029	C961
G2003	U1730	C1638	G1678	G1678	G1538	G1389	C1467	C1320	G1233	U1159	U1094	A1029	C961

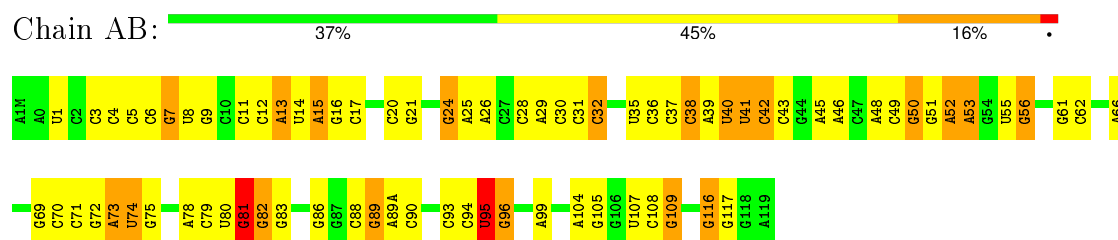




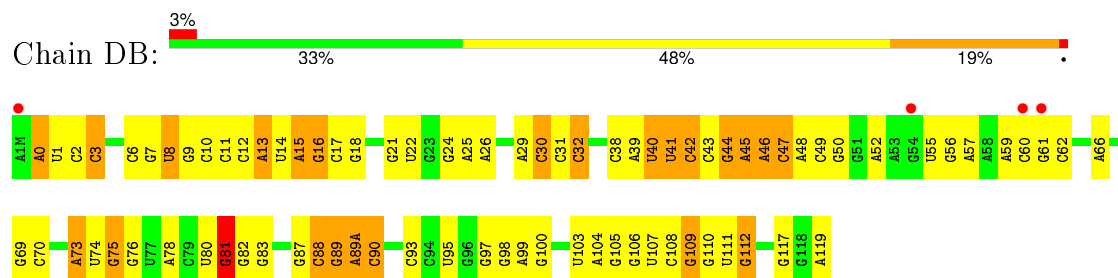




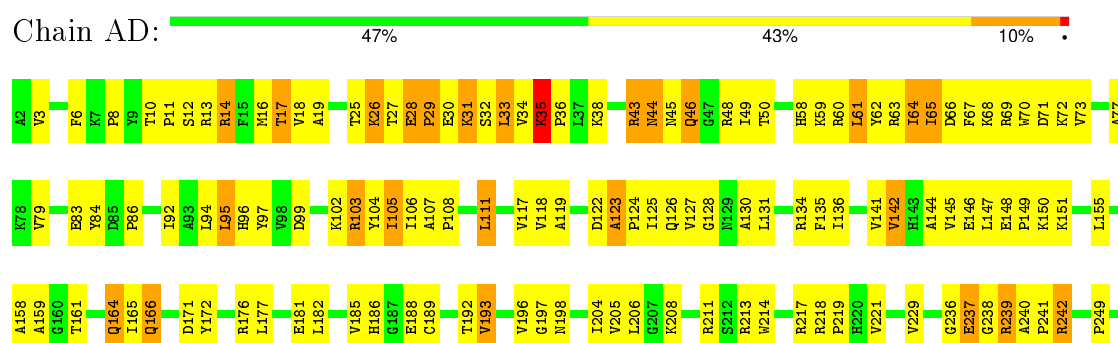
• Molecule 2: 5S RIBOSOMAL RNA

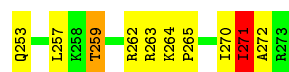


• Molecule 2: 5S RIBOSOMAL RNA



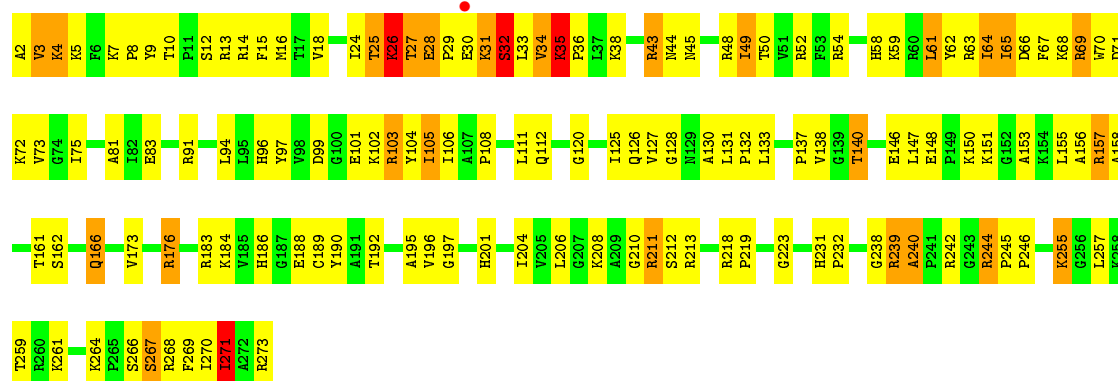
• Molecule 3: 50S ribosomal protein L2





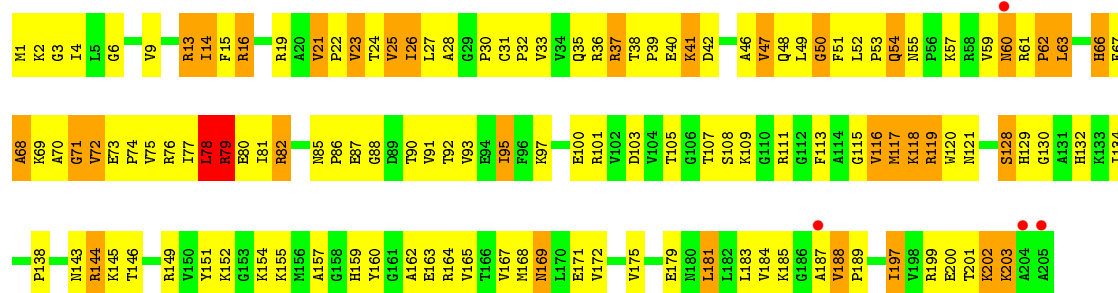
• Molecule 3: 50S ribosomal protein L2

Chain DD: 50% 40% 9%



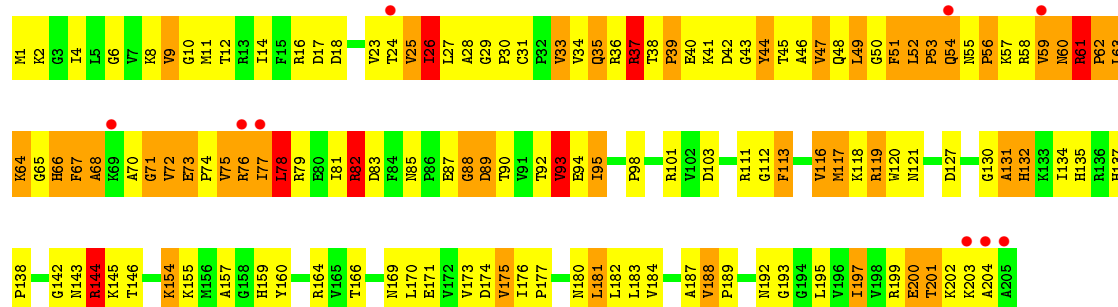
• Molecule 4: 50S ribosomal protein L3

Chain AE: 2% 36% 47% 16%



• Molecule 4: 50S ribosomal protein L3

Chain DE: 4% 33% 43% 21%

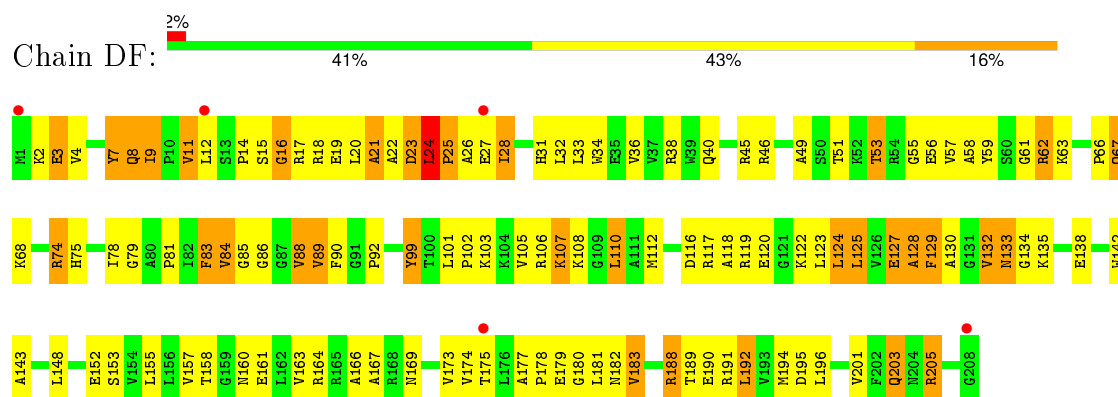


• Molecule 5: 50S ribosomal protein L4

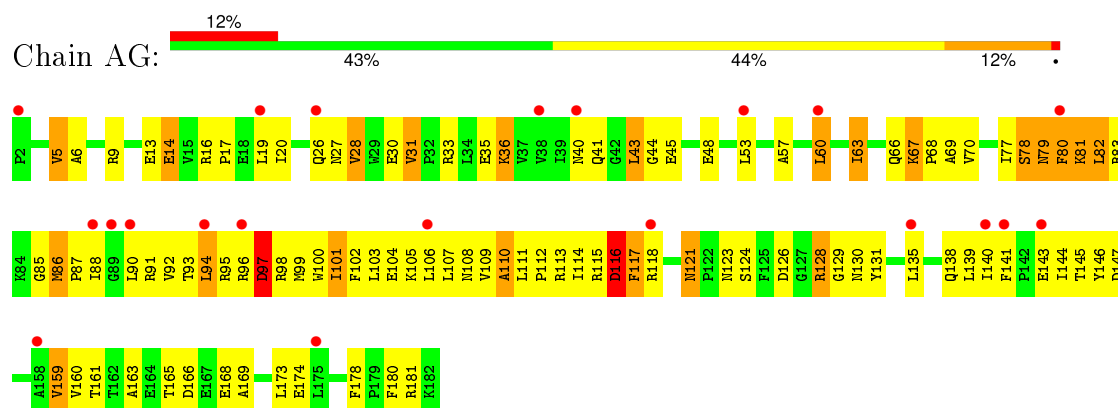
Chain AF: 49% 38% 10%



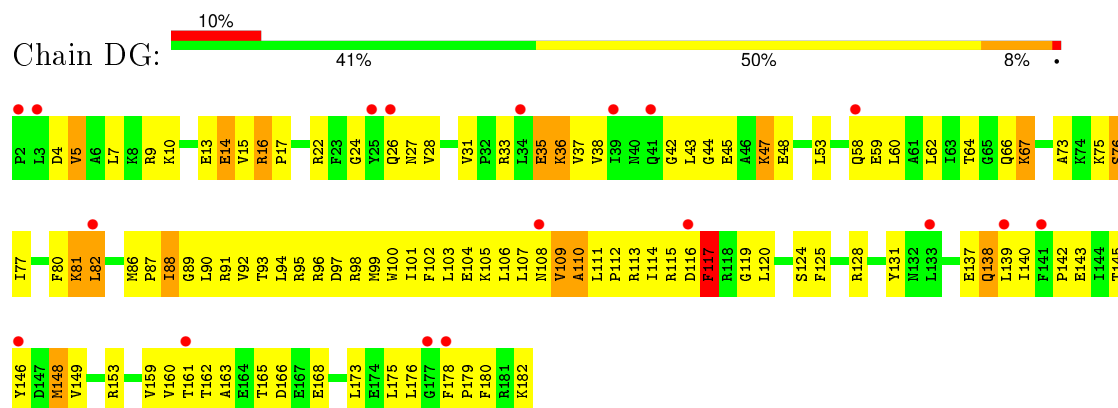
• Molecule 5: 50S ribosomal protein L4



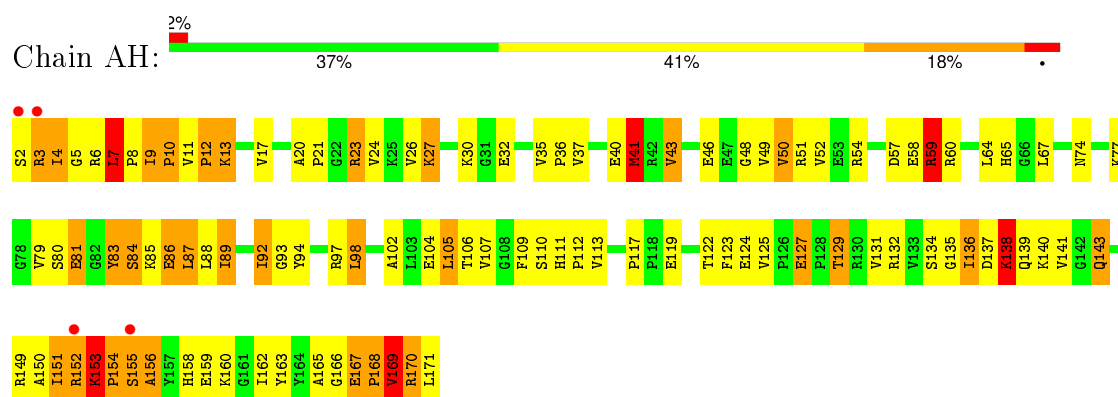
• Molecule 6: 50S ribosomal protein L5



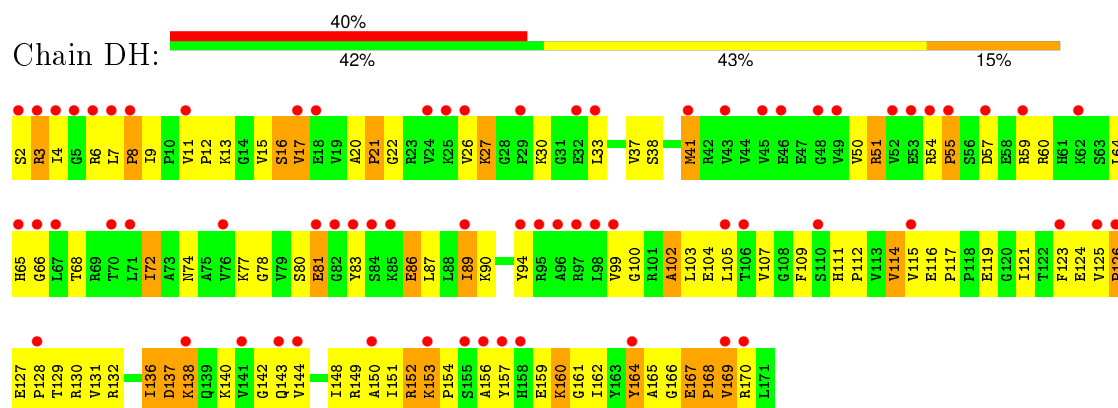
• Molecule 6: 50S ribosomal protein L5



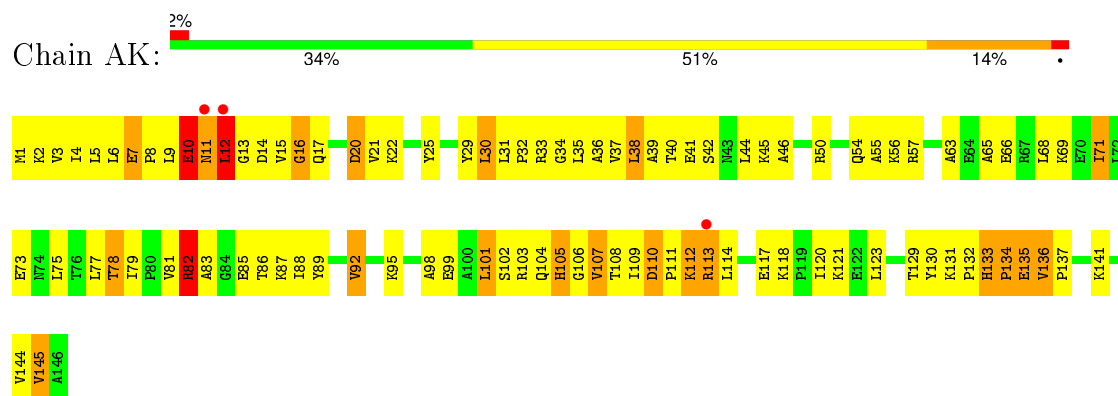
• Molecule 7: 50S ribosomal protein L6



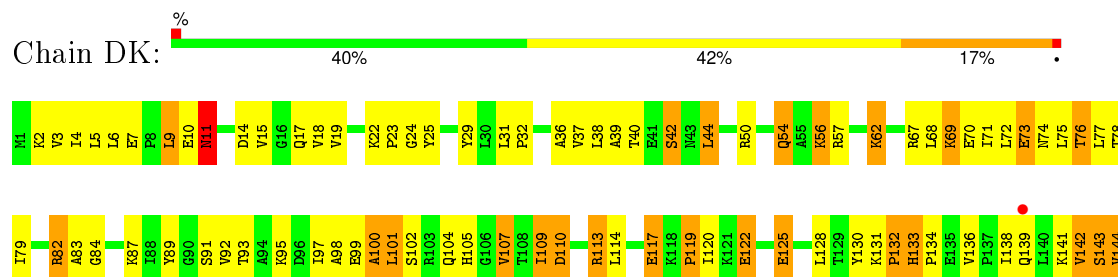
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



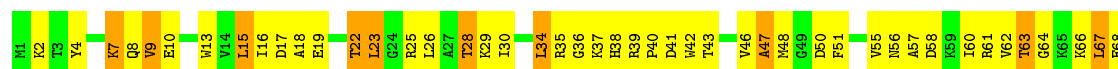
- Molecule 8: 50S ribosomal protein L9





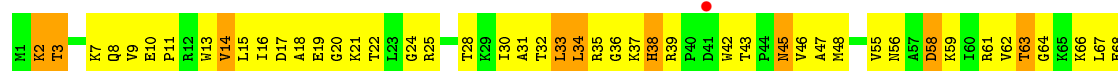
• Molecule 9: 50S ribosomal protein L13

Chain AM: 36% 51% 12%



• Molecule 9: 50S ribosomal protein L13

Chain DM: 37% 52% 11%



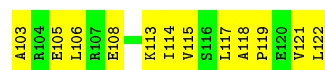
• Molecule 10: 50S ribosomal protein L14

Chain AN: 61% 33% 6%



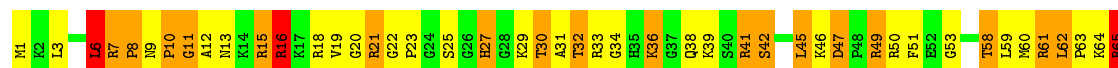
• Molecule 10: 50S ribosomal protein L14

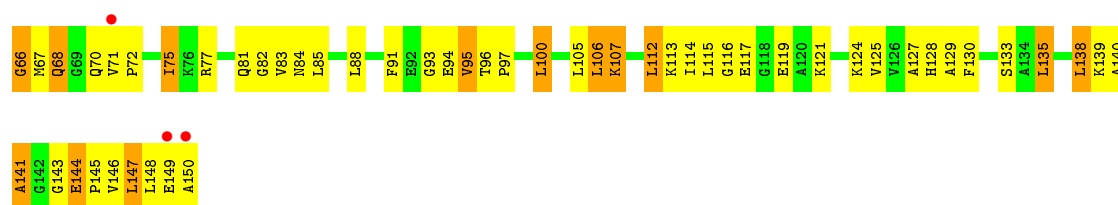
Chain DN: 57% 39% 4%



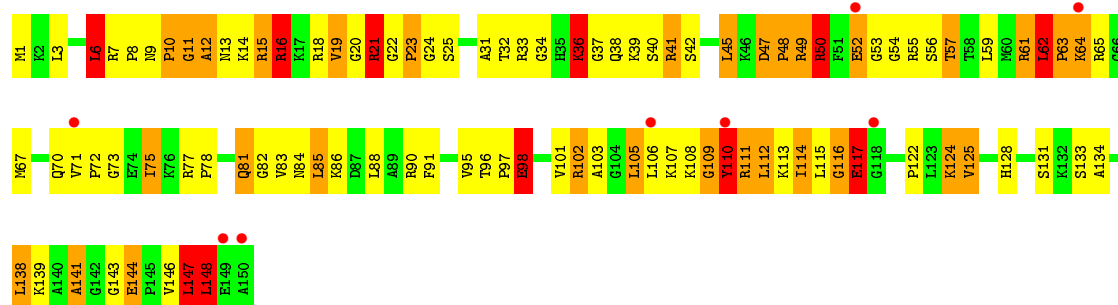
• Molecule 11: 50S ribosomal protein L15

Chain AO: 35% 43% 21% 2%

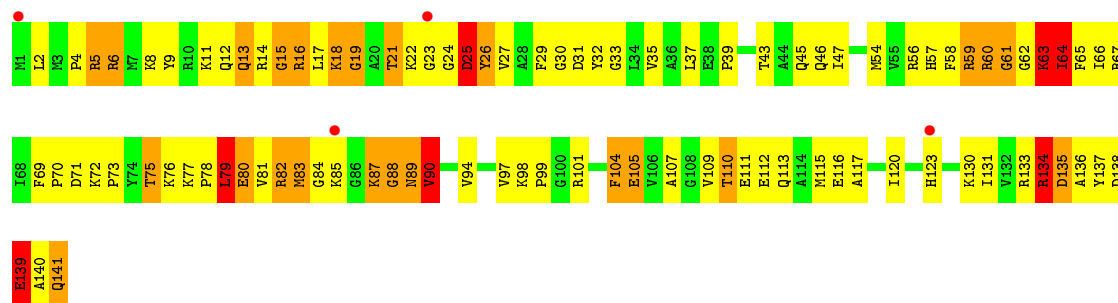




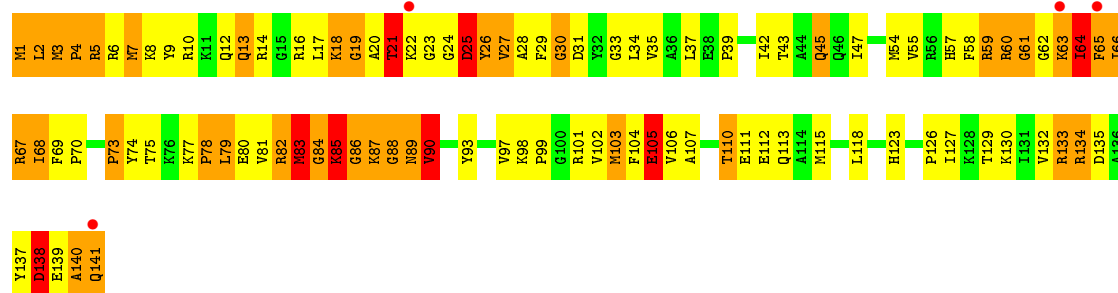
• Molecule 11: 50S ribosomal protein L15



• Molecule 12: 50S ribosomal protein L16

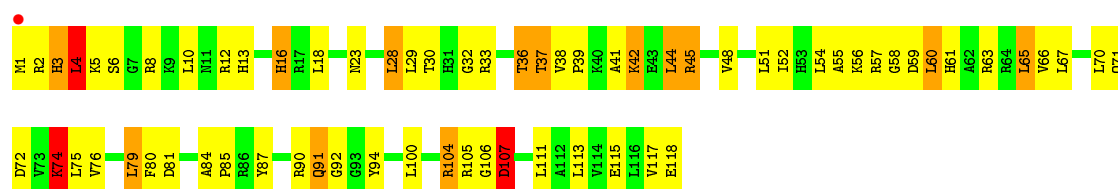


• Molecule 12: 50S ribosomal protein L16

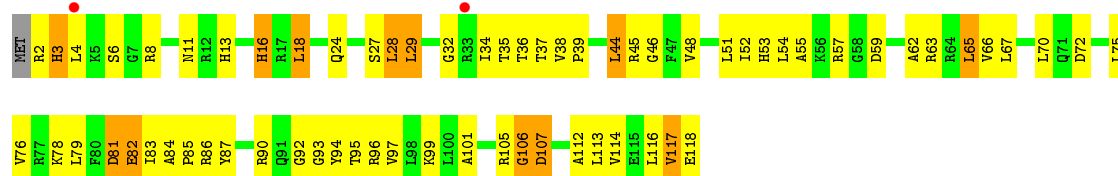
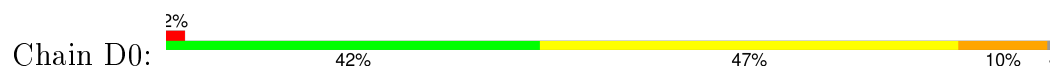


• Molecule 13: 50S ribosomal protein L17

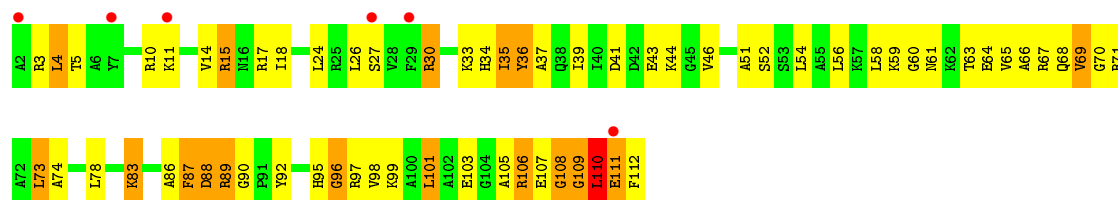
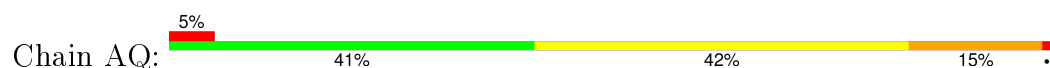




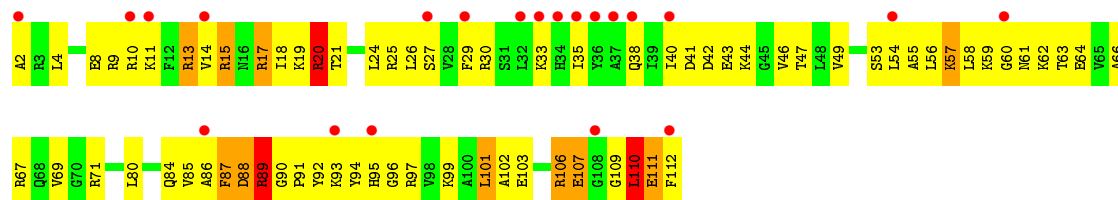
• Molecule 13: 50S ribosomal protein L17



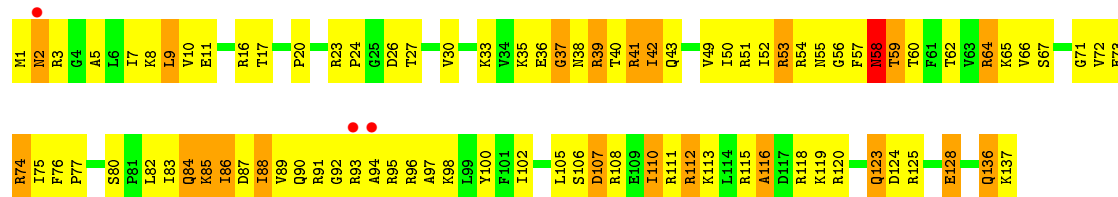
• Molecule 14: 50S ribosomal protein L18



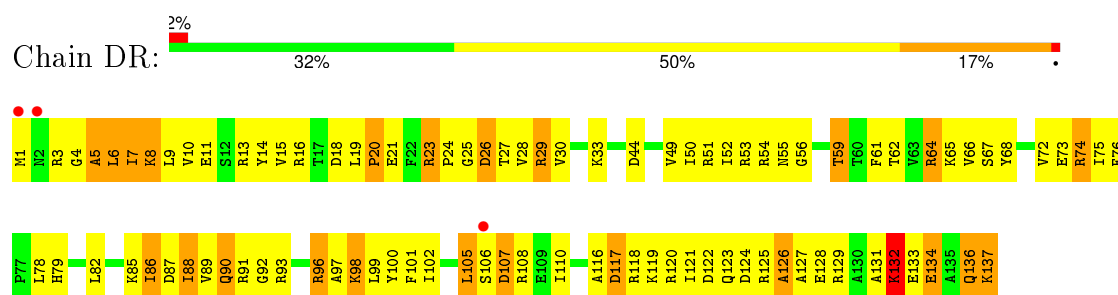
• Molecule 14: 50S ribosomal protein L18



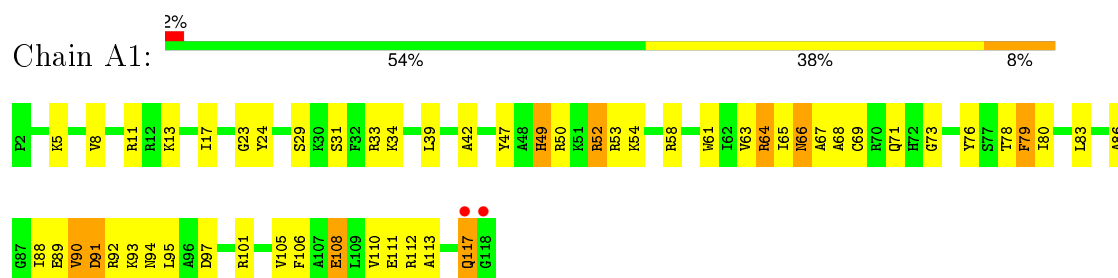
• Molecule 15: 50S ribosomal protein L19



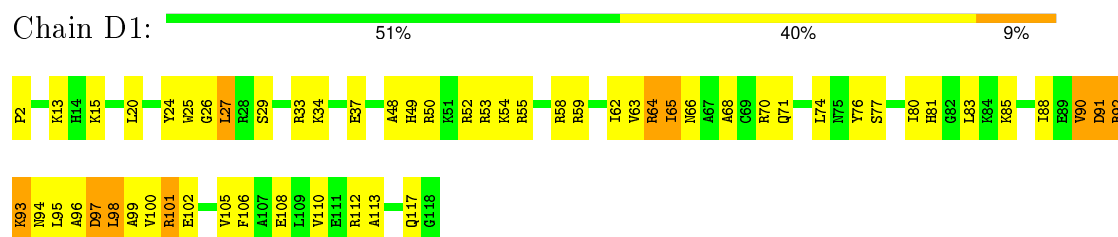
• Molecule 15: 50S ribosomal protein L19



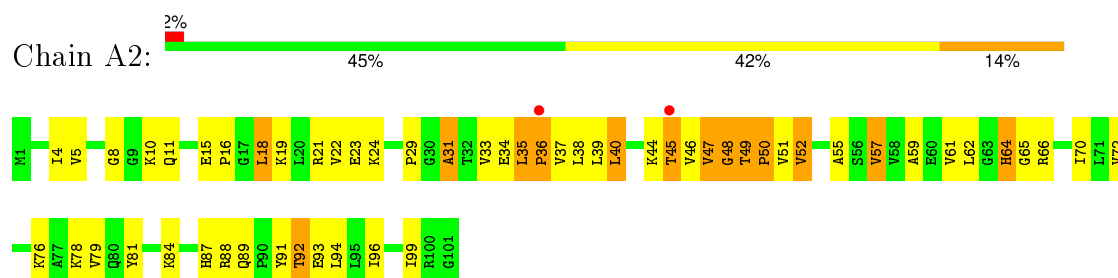
- Molecule 16: 50S ribosomal protein L20



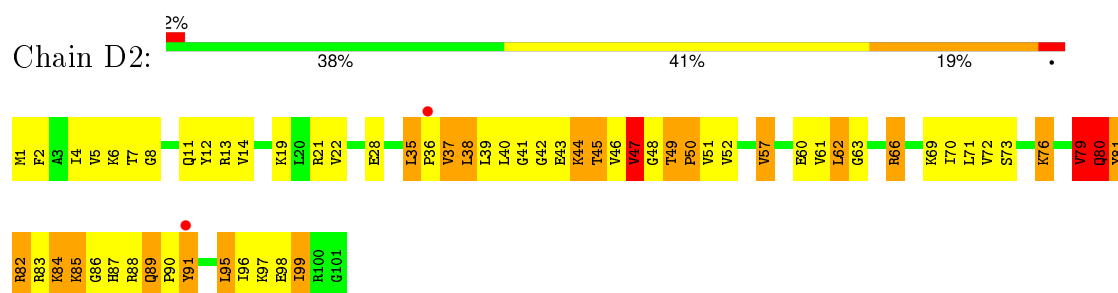
- Molecule 16: 50S ribosomal protein L20



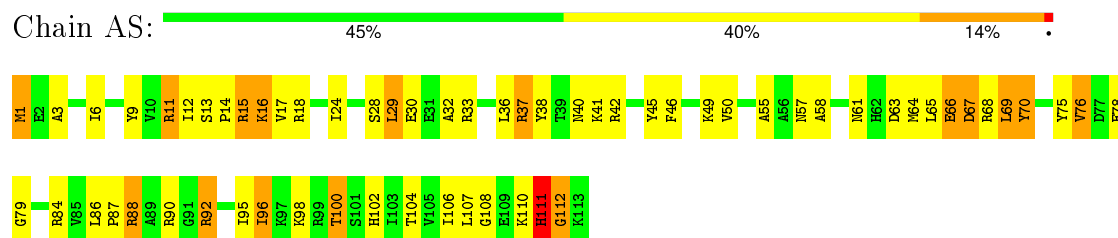
- Molecule 17: 50S ribosomal protein L21



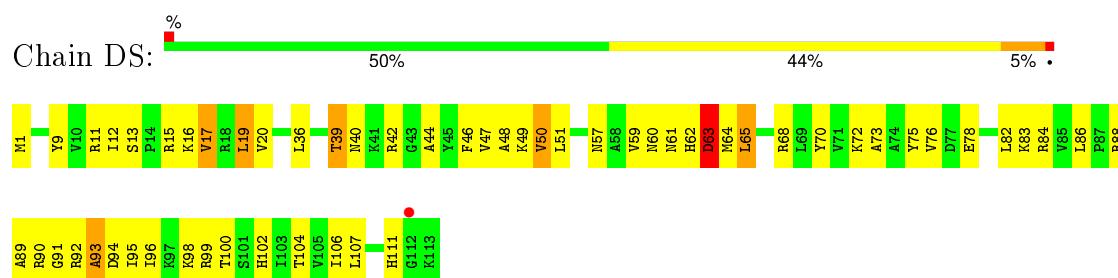
- Molecule 17: 50S ribosomal protein L21



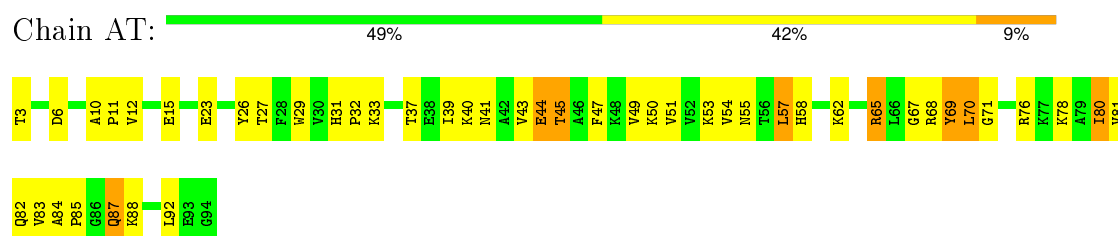
- Molecule 18: 50S ribosomal protein L22



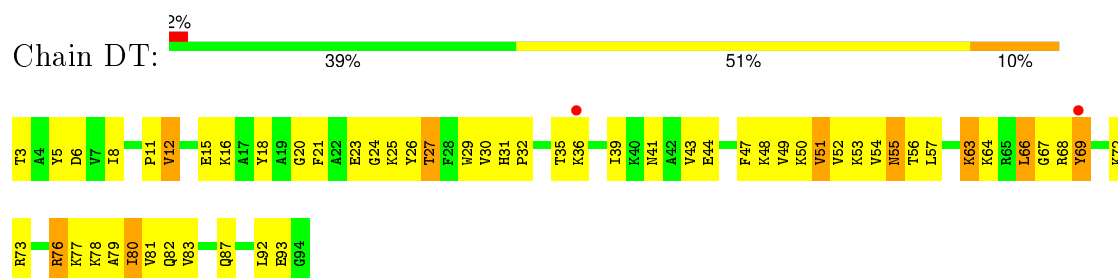
- Molecule 18: 50S ribosomal protein L22



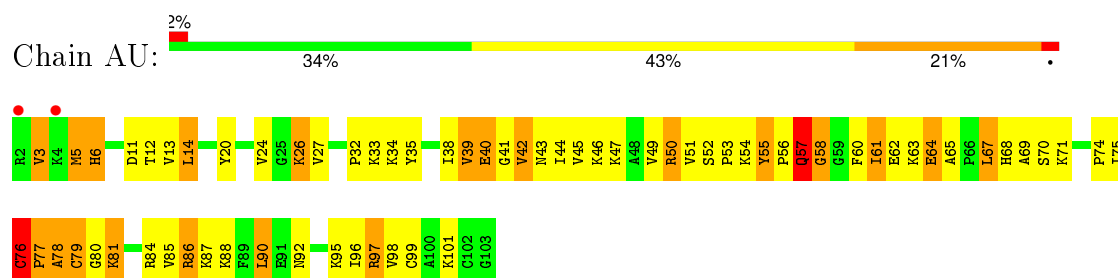
- Molecule 19: 50S ribosomal protein L23



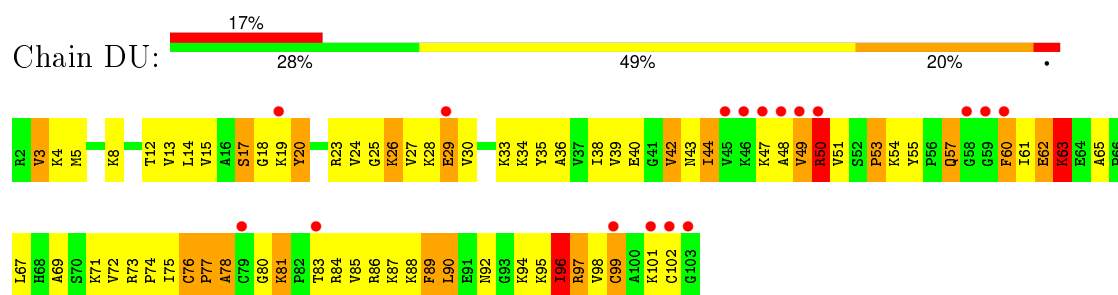
- Molecule 19: 50S ribosomal protein L23



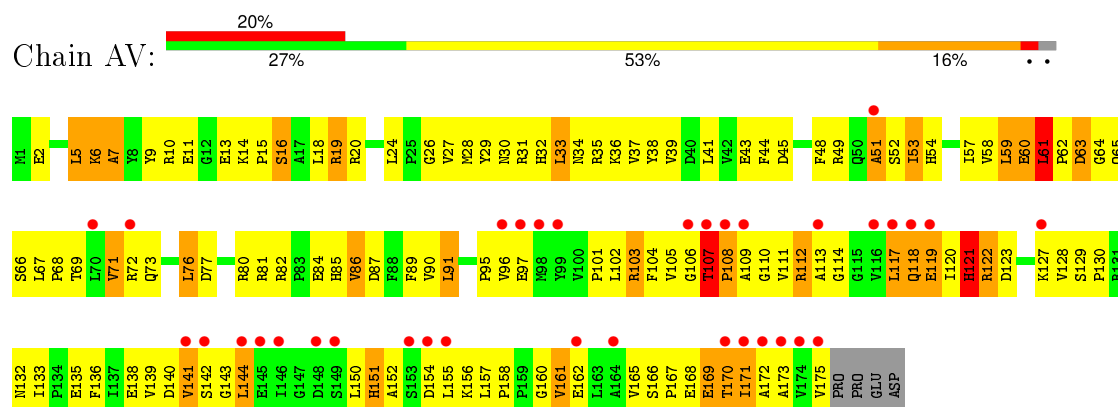
- Molecule 20: 50S ribosomal protein L24



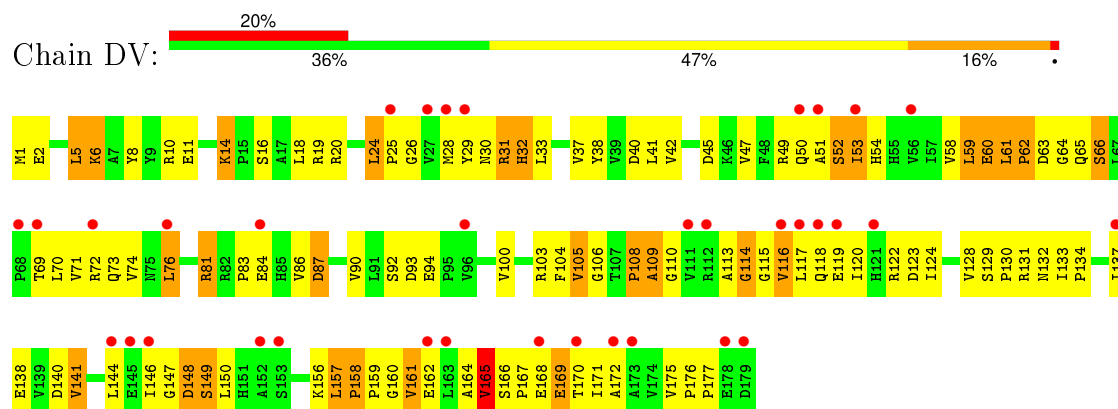
- Molecule 20: 50S ribosomal protein L24



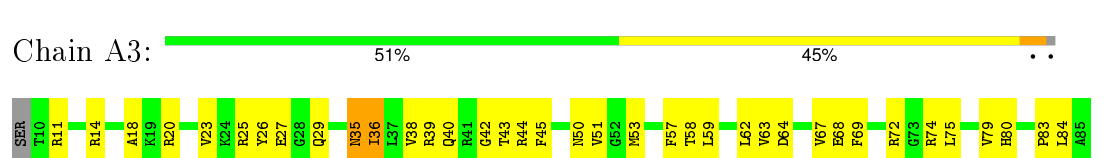
• Molecule 21: 50S ribosomal protein L25



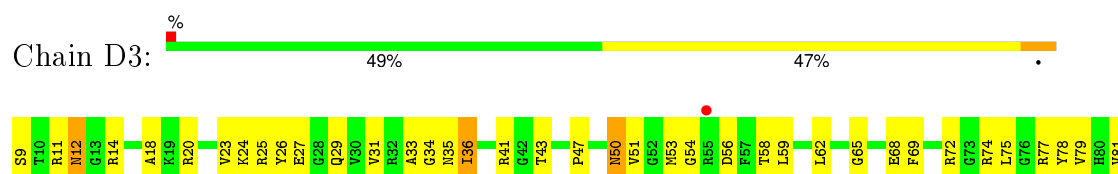
• Molecule 21: 50S ribosomal protein L25



• Molecule 22: 50S ribosomal protein L27

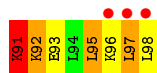


• Molecule 22: 50S ribosomal protein L27

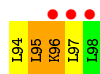




- Molecule 23: 50S ribosomal protein L28



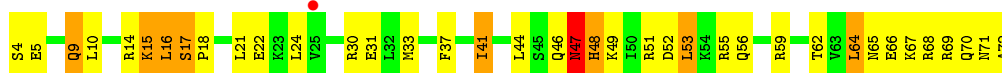
- Molecule 23: 50S ribosomal protein L28



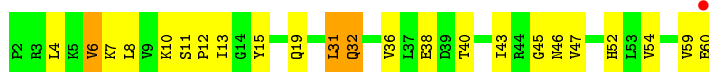
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29

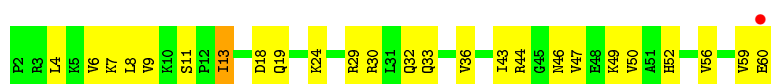


- Molecule 25: 50S ribosomal protein L30

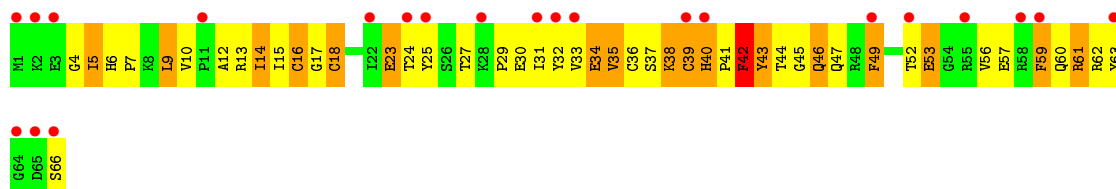


- Molecule 25: 50S ribosomal protein L30

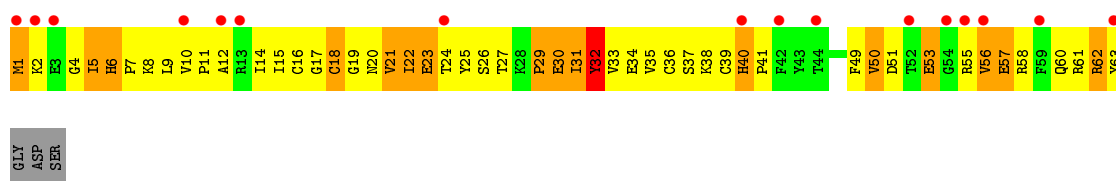
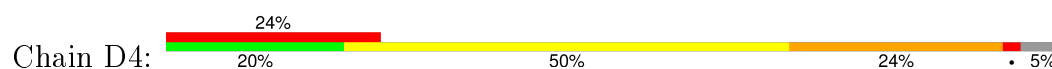




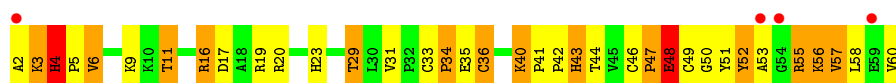
- Molecule 26: 50S ribosomal protein L31



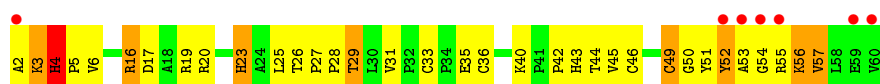
- Molecule 26: 50S ribosomal protein L31



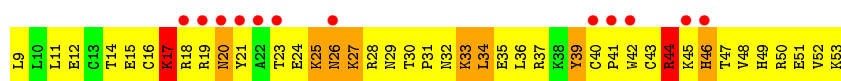
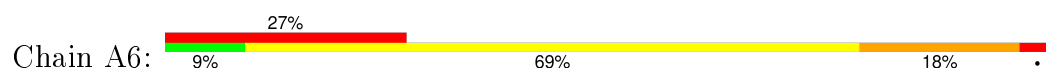
- Molecule 27: 50S ribosomal protein L32



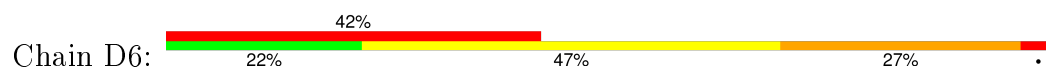
- Molecule 27: 50S ribosomal protein L32

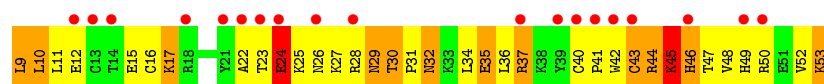


- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33





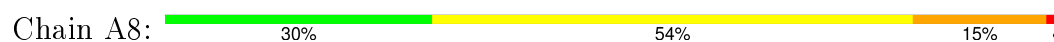
- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



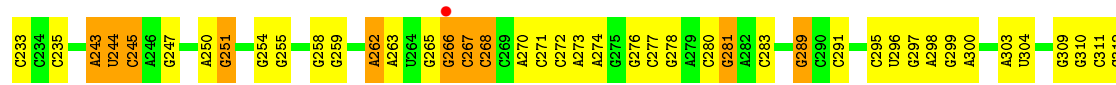
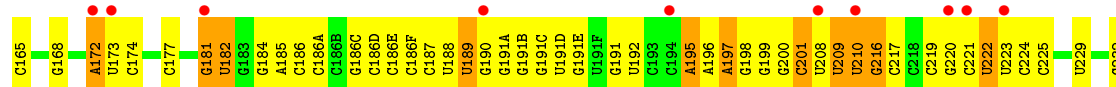
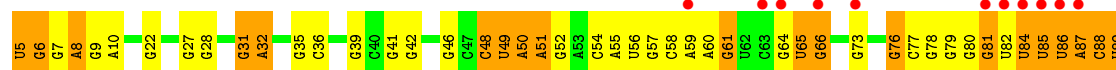
- Molecule 30: 50S ribosomal protein L35



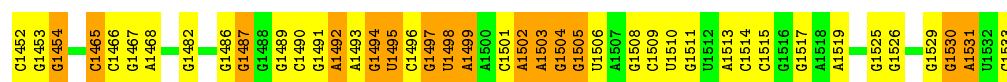
- Molecule 30: 50S ribosomal protein L35



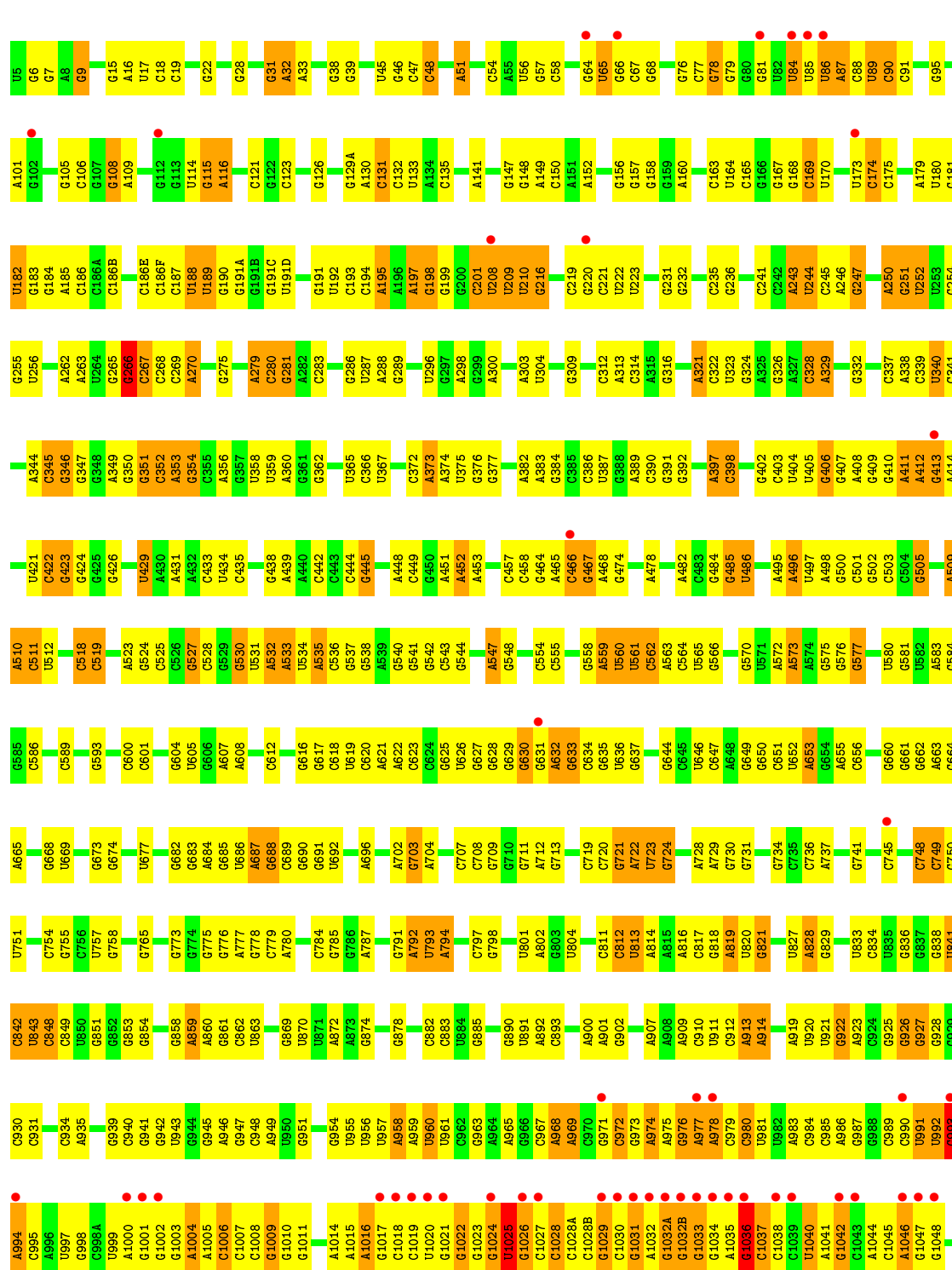
- Molecule 31: 16S ribosomal RNA

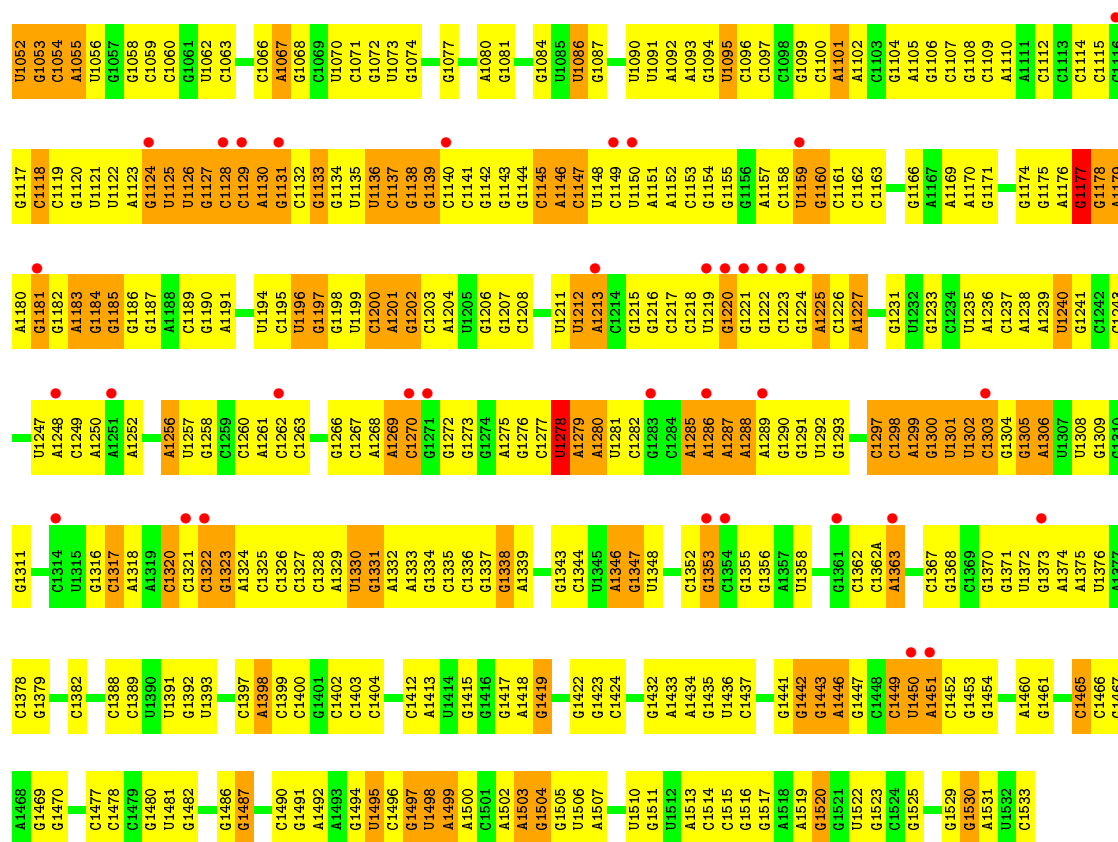


A1374	G1309	A1238	G1164	C1097	G1032A	G970	G881	A794	A712	G546	A478	C390	A313
A1375	G1310	A1239	G1165	C1098	G1032B	G971	G882	A802	G713	A547	C479	C397	G316
U1376	G1311	G1241	A1169	G1099	G1033	G972	G883	G803	G714	G548	G480	A398	
A1377	G1312	G1241	A1170	C1100	G1034	G973	G884	G804		C549	A482	G402	A321
G1378	G1313	A1250	G1171	A1101	G1035	A974	G885	C805	C719	G557	G483	G403	G322
U1380	U1314	A1251	G1172	A1102	G1036	A975	G886	G806	C720	G558	G484	C403	U323
U1381	U1315	A1251	G1173	C1103	G1037	G976	G887	C807	C721	A559	G485	U404	G324
	G1316	C1254	G1174	G1106	C1038	A977	A892	C811	A722	U560	U486	U405	G326
G1386	A1318	G1255	G1175	C1107	U1040	C979	A900	C812	U723	U561	G487	G406	
G1387	A1319	A1256	A1176	G1108	C980	C980	A901	A813	G724	G562	C488		
G1388	C1320	U1257	G1177	G1109	A1041	U981	G902	A815	G725	A563	G489	A411	
C1389	G1178	A1179	G1178	A1110	G1042	U982	G903	A816	A729	C564	G490	A412	G328
G1392	A1180	C1260	A1179	A1111	G1047	A983		C817	G730	U565	G491	G413	G330
U1391	G1181	C1260	A1180	C1112	G1048	C984	A913	A818	C731	G566	G492	A414	G332
G1392	G1182	C1263	G1182	G1117	U1049	C985	A914	A819	C732	G567	G493		
U1393	A1183	C1264	A1183	C1118	G1050	A986	A915	U820	A733	G568	U494	C419	G333
A1394	G1265	G1265			G1051	G987		G821	G734	C569	G495	U420	
	G1266				U1052	G988	A918	G822	C735	G570	A496	U421	G336
					G1053	C989	A919	G823	C736	U571	U497	C422	C337
C1397					C1054	C990	U920	C826	A737	A572	A498	G423	A338
A1398	U1194	A1269	U1194	A1122	U1055	U991	U921	C826	C738	A573	G500	G424	C339
C1399	C1195	C1270	C1195	A1123	U1056	U992	G922	U827		A574	C501		U340
G1400	U1196	G1197	G1197	G1124	G1057	G993	A923	A828	G741	G575	G502	G428	C341
G1401	G1197	G1273	G1198	U1125	G1058		C924		G742	G576	C503	U429	G342
C1402	G1198	G1274		G1127	C1059	G998	G925	C834	C745	G577	C504	A430	U343
G1403	U1199	G1275		C1128	C1060	C998A	G926	U835		C578	G505	A431	A344
C1404	C1200	A1276		G1129	G1061		G927	G836		G579		A432	C345
G1405	A1201	G1277		A1130	U1062	G1001	G928	G837	C748	U580	A509	U433	G346
	G1202	C1278		G1131	C1063	G1002		G838	C749	G581	A510	U434	G347
	C1203	A1204		C1132	G1064	G1003	G934	U841	G752	C596	C511	C435	G348
	U1204			G1133	U1065	A1004	A935	C842	G753	U512	U512	C436	
	G1206	U1205		G1134	C1066	A1005	G936	U843	A753	G597	C513	U437	G351
	G1207	C1282		U1135	A1067	C1006	A937	C848	C754	U598	C514	C438	C352
	C1208	G1283		U1136	G1068		A938	C849	G755		A439	C439	A353
	U1209	A1284		C1137	U1069	G1009	G939	U850	C756	C601	G517	A440	G354
	C1209	A1285		G1138	C1070	G1010	C940	G851	U757	A602	C518		
	A1286	A1286		C1139	C1071	G1011	G941	C852	G758			C443	U359
	U1281	U1281		G1140	U1072	G1012		G853		G606	A523	C444	
	C1282	C1282		U1141	G1073	G1013	G942	C857	G763	A607	A524	C445	U365
	G1283	G1283		C1142	U1074	A1014	A946	U858	C764	A608	G524	G446	U366
	C1284	A1284		G1143	G1075	A1015	G947	C859	A766	C526	C526	G447	U367
	G1290	A1289		C1144	C1076	C1016	C948	A859	A767	A611	G527	A448	U368
	G1291	G1291		U1145	G1077		A949	A860	A768	A614	C528	C449	
	U1292	U1292		C1146	U1078	G1019	U950				G529	G450	C372
	G1293	G1293		A1146	U1079	U1020	G951	A864	G771	C618	G530	A451	A373
	U1294	A1294		C1147	G1079	G1021	A952	A865	G772	U619	U531	A452	A374
	G1295	G1295		U1148	A1080	G1022	G953		U772	U619	A532	A453	U375
	C1296	C1296		C1149	G1081	G1023	G954	C868	G775	A621	A533		G376
	G1297	G1297		U1150	G1082	G1024	U955	C869	G776	A622		C454	G377
	U1298	U1298		A1151	U1083	U1025		U870	A777	C623	C836	G458	G380
	A1299	A1299		C1152	G1084	G1026	A958	U871		C624	G537	G464	G381
	G1300	G1300		G1153	U1085	C1027	A959	A872	G782	G625	G538	A465	A382
	U1301	U1301		A1157	U1086	C1028	U960	A873	A782	U626	A539	C466	A383
	A1225	C1226		U1158	G1088	G1028A	G874	C875	U789	U705	G540	G467	A384
	C1227	A1227		U1159	U1090	C1028B	A865		A790	G627	G541	A468	G385
	G1234	G1234		G1160	U1091	G1029	A965			G628	G542	G474	
	U1235	U1235		C1161	C1029B	G1029	G866			G629	C543	G475	
	A1236	A1236		U1094	U1094	C1030	C967	G878	A791	G630	G544	G476	G388
	G1237	G1237		C1096	C1096	A1032	A969	C880	U793	G631	C545	G477	G389

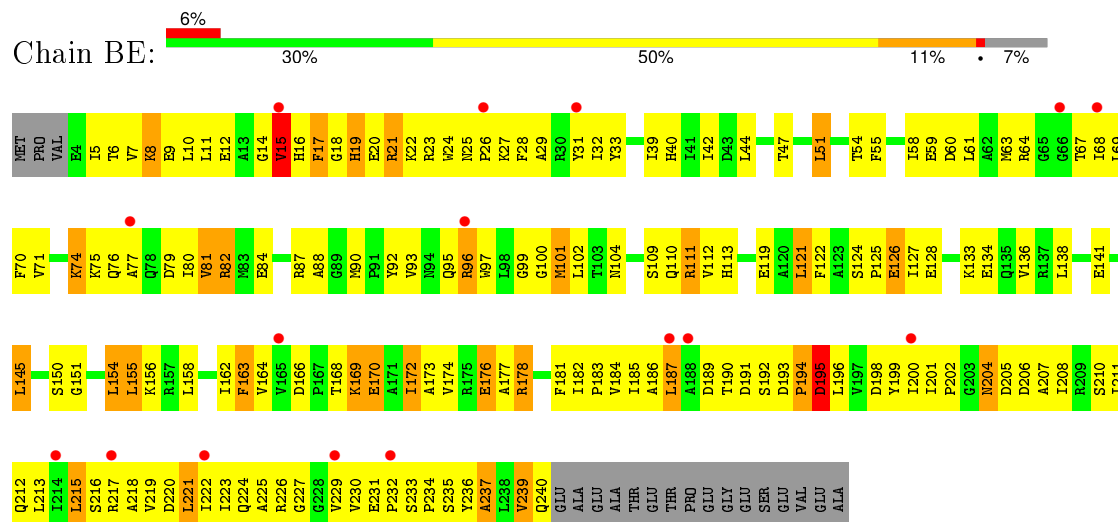


• Molecule 31: 16S ribosomal RNA

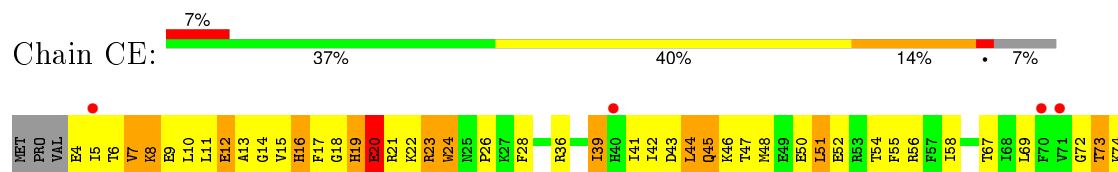


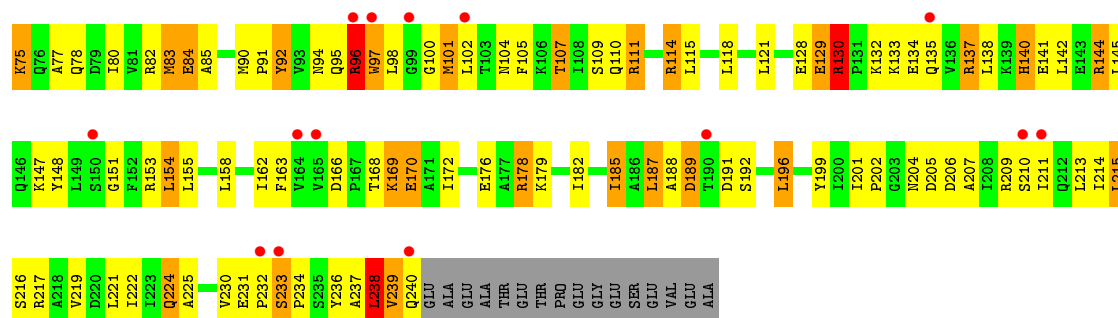


• Molecule 32: 30S RIBOSOMAL PROTEIN S2

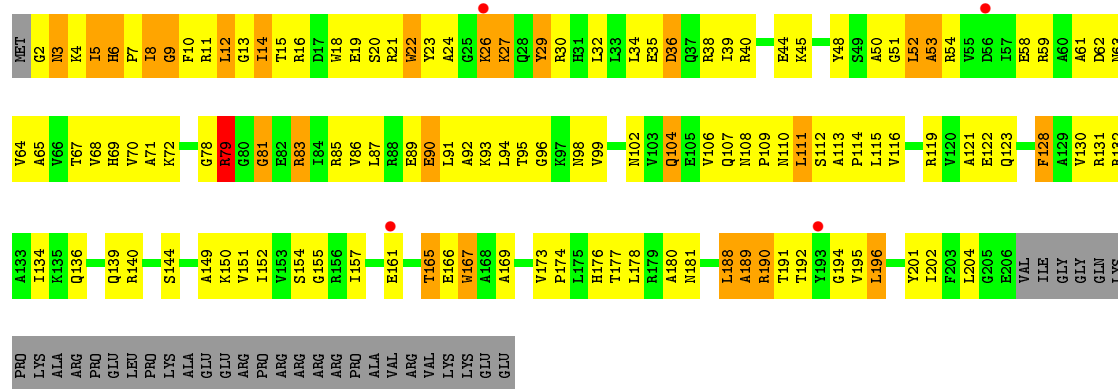


• Molecule 32: 30S RIBOSOMAL PROTEIN S2

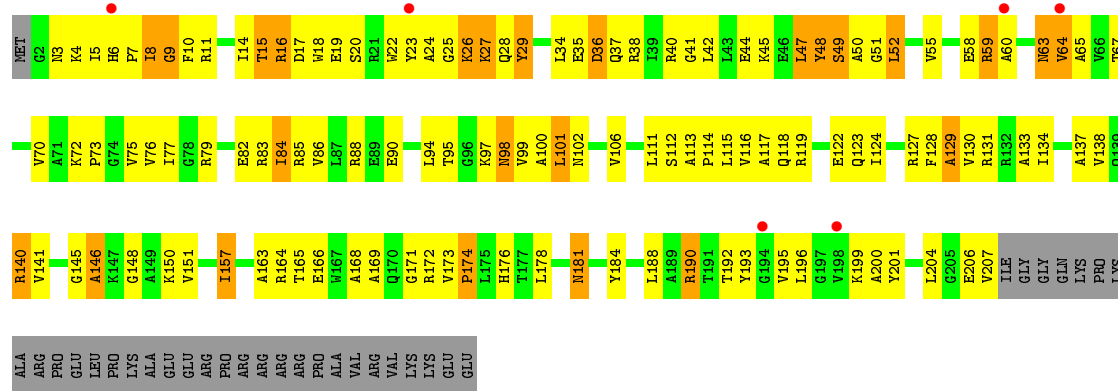




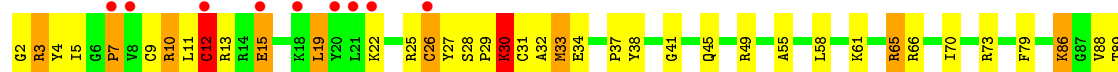
• Molecule 33: 30S RIBOSOMAL PROTEIN S3

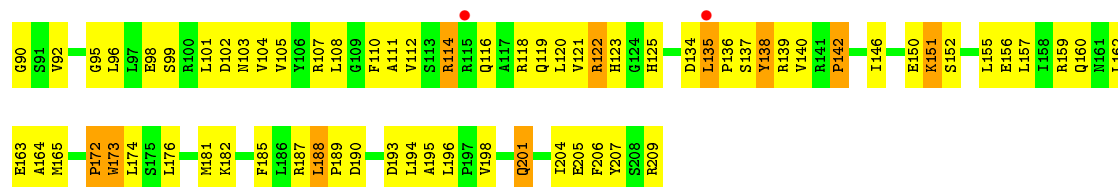


• Molecule 33: 30S RIBOSOMAL PROTEIN S3

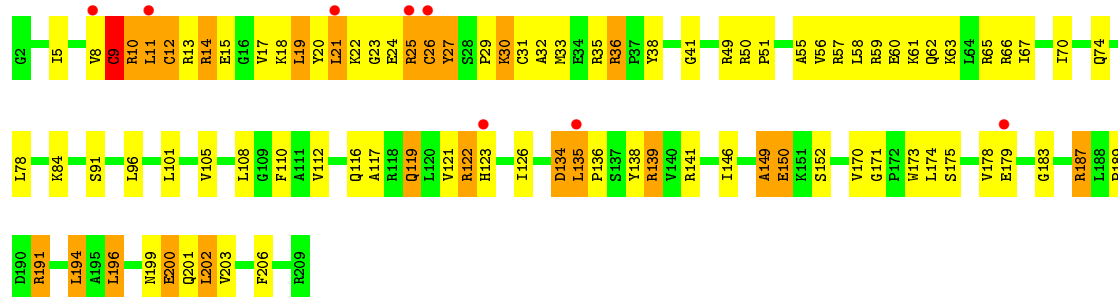


• Molecule 34: 30S RIBOSOMAL PROTEIN S4

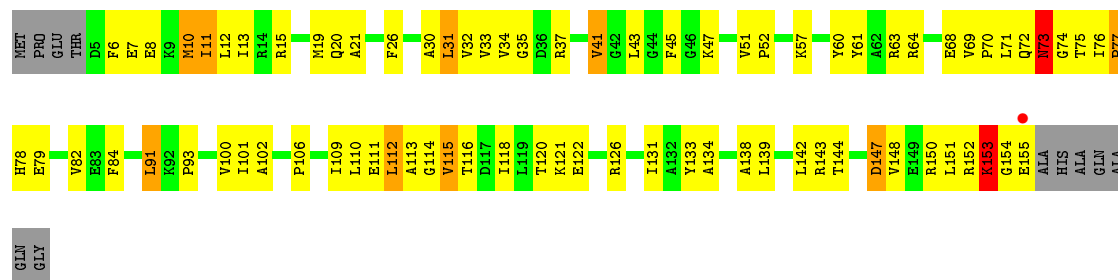




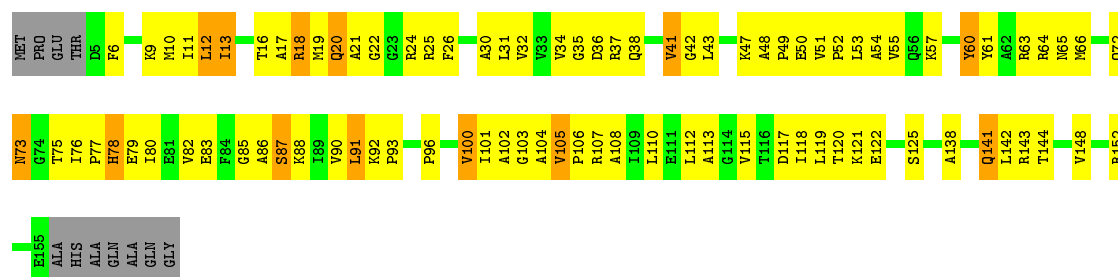
• Molecule 34: 30S RIBOSOMAL PROTEIN S4



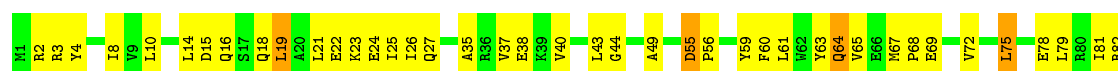
• Molecule 35: 30S RIBOSOMAL PROTEIN S5

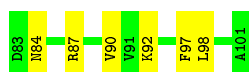


• Molecule 35: 30S RIBOSOMAL PROTEIN S5



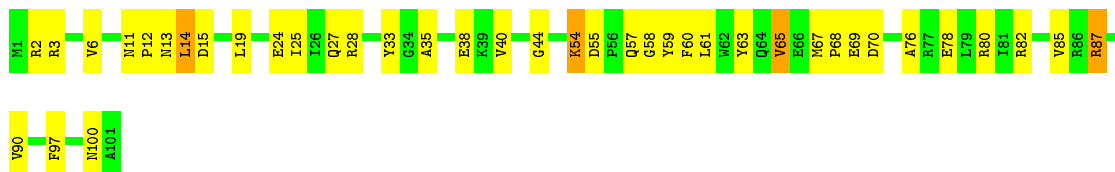
• Molecule 36: 30S RIBOSOMAL PROTEIN S6





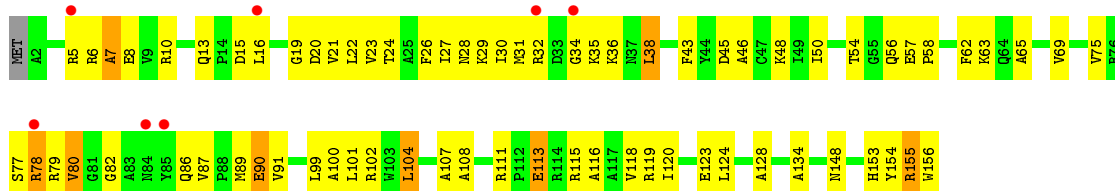
● Molecule 36: 30S RIBOSOMAL PROTEIN S6

Chain CI:



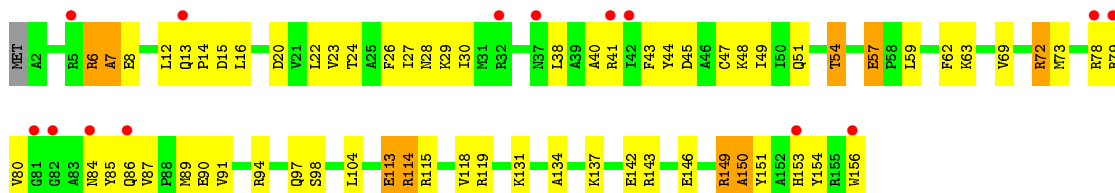
● Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain BJ:



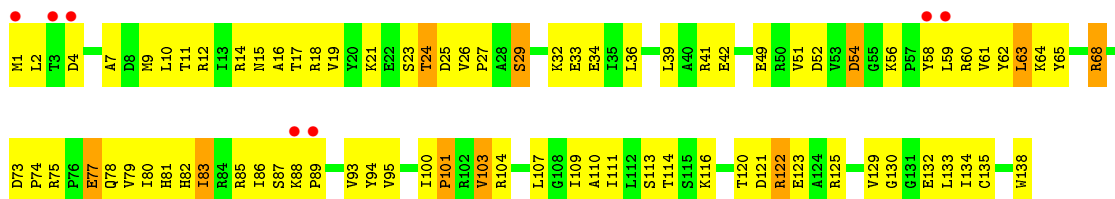
● Molecule 37: 30S RIBOSOMAL PROTEIN S7

Chain CJ:



● Molecule 38: 30S RIBOSOMAL PROTEIN S8

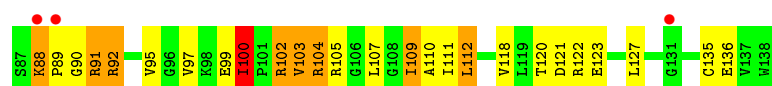
Chain BK:



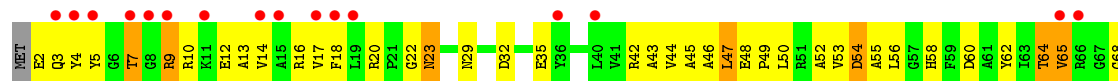
● Molecule 38: 30S RIBOSOMAL PROTEIN S8

Chain CK:





● Molecule 39: 30S RIBOSOMAL PROTEIN S9



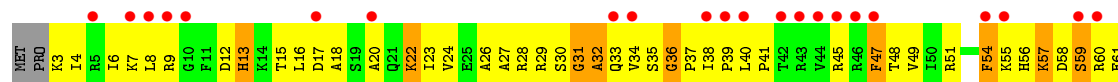
● Molecule 39: 30S RIBOSOMAL PROTEIN S9



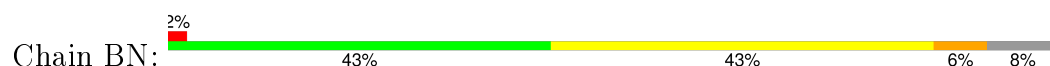
● Molecule 40: 30S RIBOSOMAL PROTEIN S10

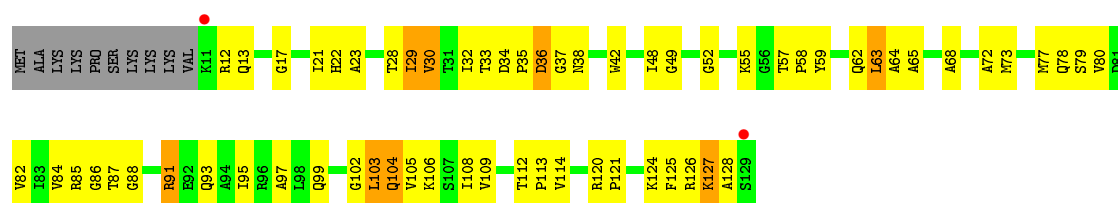


● Molecule 40: 30S RIBOSOMAL PROTEIN S10

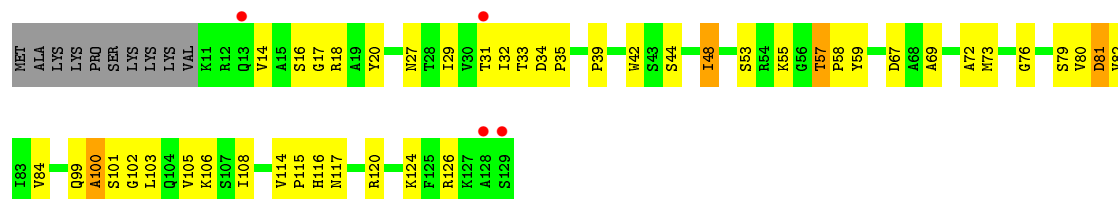


● Molecule 41: 30S RIBOSOMAL PROTEIN S11

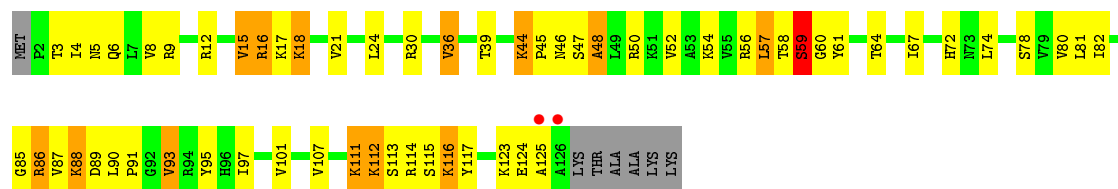




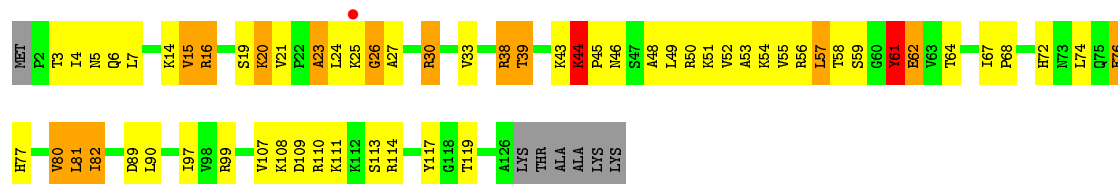
• Molecule 41: 30S RIBOSOMAL PROTEIN S11



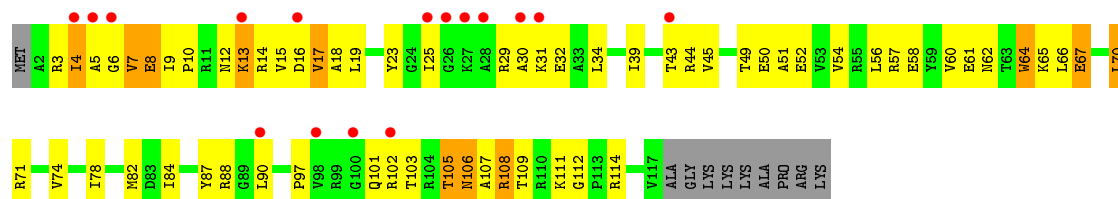
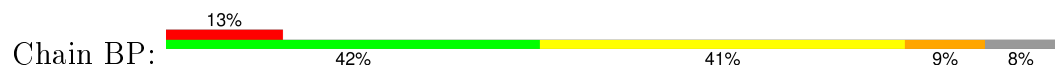
• Molecule 42: 30S RIBOSOMAL PROTEIN S12



• Molecule 42: 30S RIBOSOMAL PROTEIN S12



• Molecule 43: 30S RIBOSOMAL PROTEIN S13

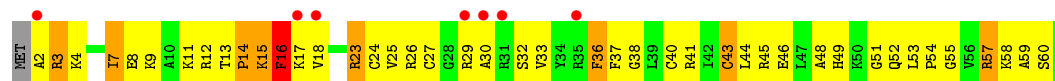
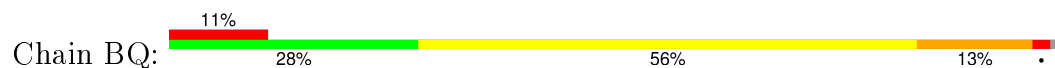


• Molecule 43: 30S RIBOSOMAL PROTEIN S13

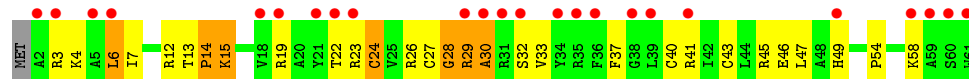
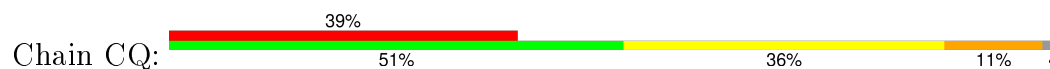




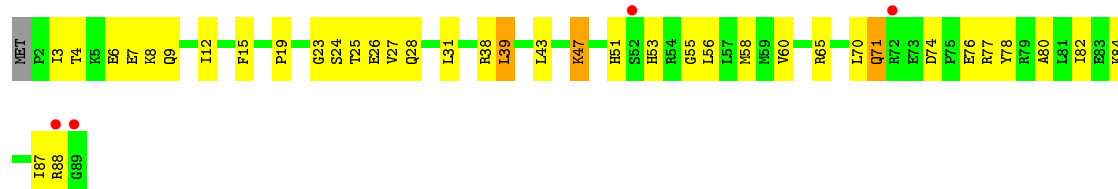
• Molecule 44: 30S RIBOSOMAL PROTEIN S14



• Molecule 44: 30S RIBOSOMAL PROTEIN S14



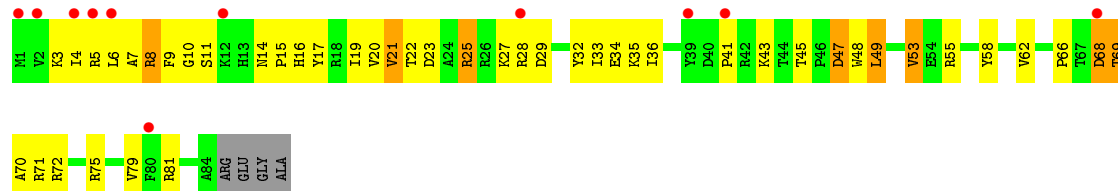
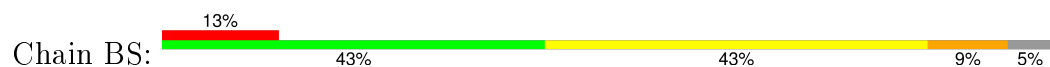
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



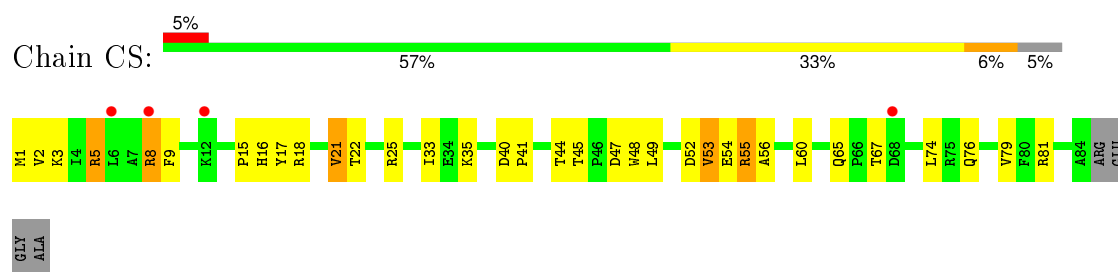
• Molecule 45: 30S RIBOSOMAL PROTEIN S15



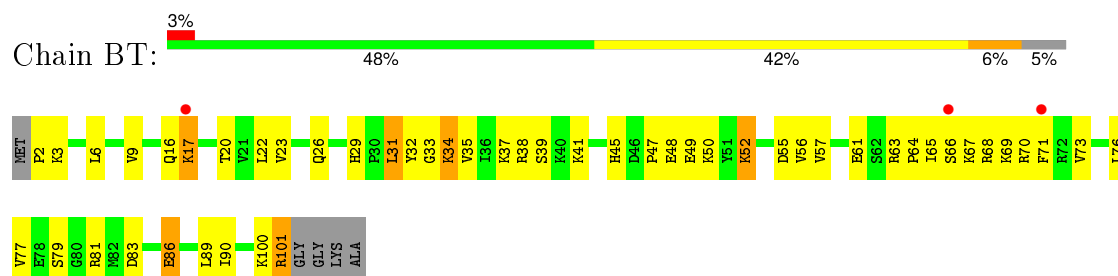
• Molecule 46: 30S RIBOSOMAL PROTEIN S16



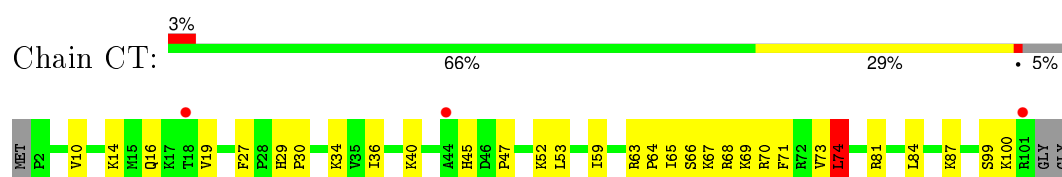
• Molecule 46: 30S RIBOSOMAL PROTEIN S16



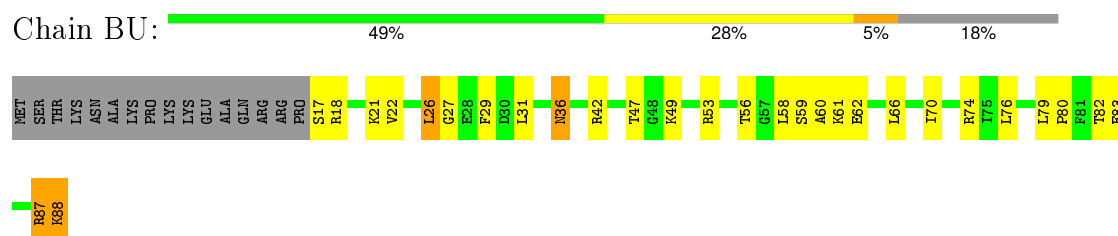
• Molecule 47: 30S RIBOSOMAL PROTEIN S17



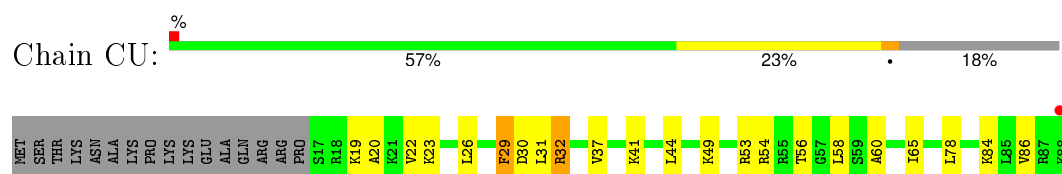
• Molecule 47: 30S RIBOSOMAL PROTEIN S17



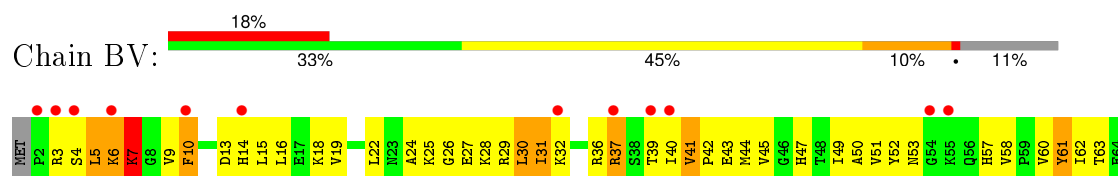
• Molecule 48: 30S RIBOSOMAL PROTEIN S18

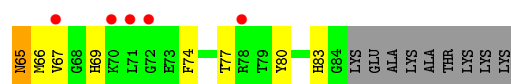


• Molecule 48: 30S RIBOSOMAL PROTEIN S18

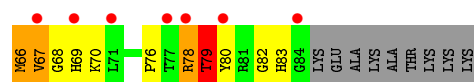
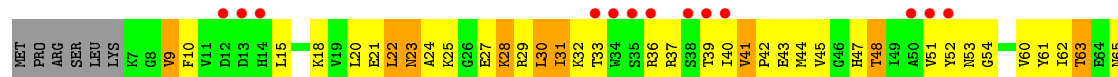


• Molecule 49: 30S RIBOSOMAL PROTEIN S19

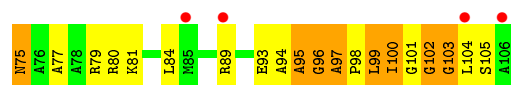




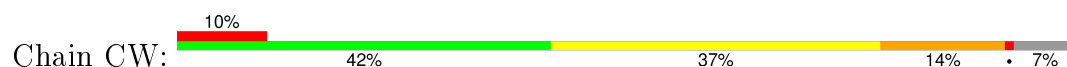
• Molecule 49: 30S RIBOSOMAL PROTEIN S19



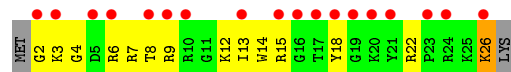
• Molecule 50: 30S RIBOSOMAL PROTEIN S20



• Molecule 50: 30S RIBOSOMAL PROTEIN S20



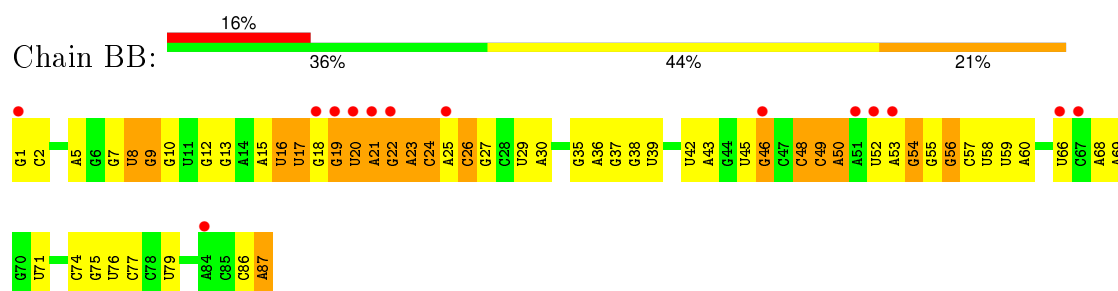
• Molecule 51: 30S RIBOSOMAL PROTEIN THX



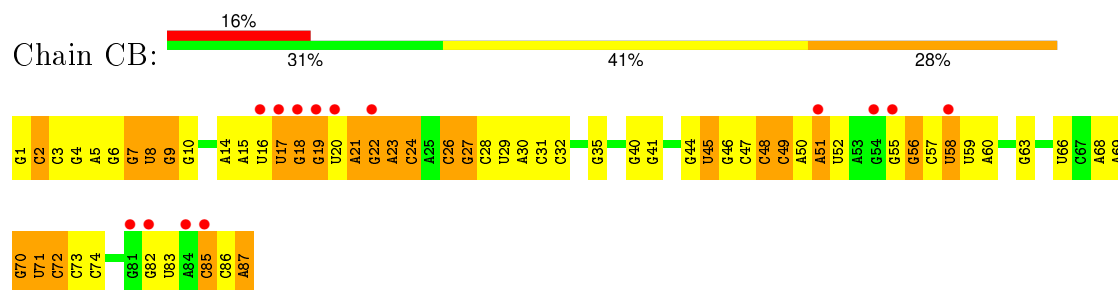
• Molecule 51: 30S RIBOSOMAL PROTEIN THX



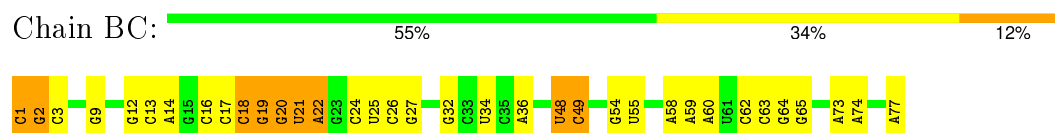
• Molecule 52: TRNA-LEU



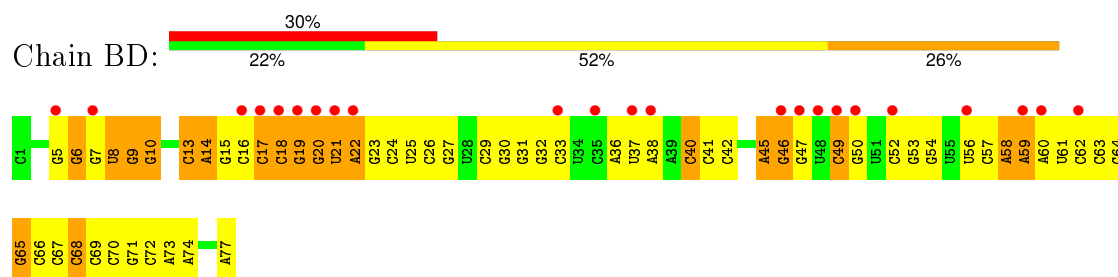
• Molecule 52: TRNA-LEU



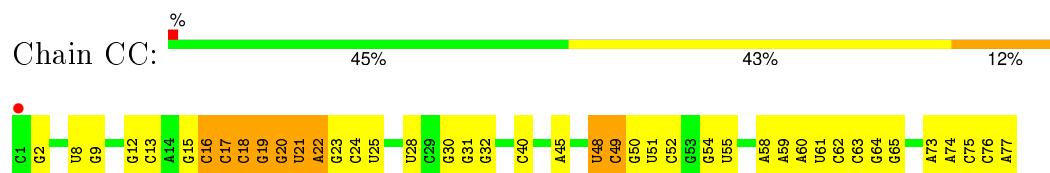
• Molecule 53: TRNA-FMET



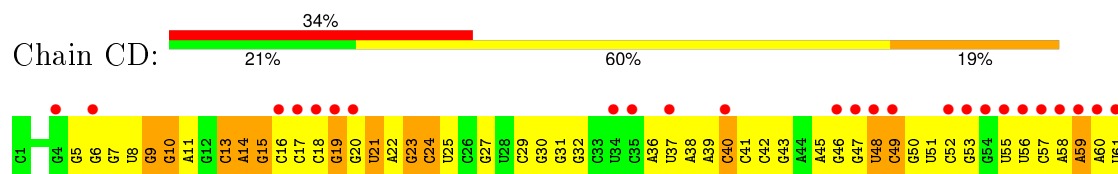
• Molecule 53: TRNA-FMET



• Molecule 53: TRNA-FMET



• Molecule 53: TRNA-FMET





● Molecule 54: MRNA



● Molecule 54: MRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.19Å 451.05Å 621.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.76 – 3.10 122.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (153.76-3.10) 91.7 (122.29-3.00)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_810)	Depositor
R, R_{free}	0.201 , 0.240 0.202 , 0.238	Depositor DCC
R_{free} test set	1675 reflections (0.17%)	DCC
Wilson B-factor (Å ²)	75.5	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 86.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1157389 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	299628	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/70233	0.74	48/109643 (0.0%)
1	DA	0.33	1/70122 (0.0%)	0.71	58/109469 (0.1%)
2	AB	0.31	0/2928	0.72	6/4568 (0.1%)
2	DB	0.27	0/2928	0.71	2/4568 (0.0%)
3	AD	0.31	0/2166	0.55	0/2919
3	DD	0.29	0/2165	0.52	0/2919
4	AE	0.27	0/1602	0.53	0/2160
4	DE	0.27	0/1601	0.54	0/2160
5	AF	0.31	1/1621 (0.1%)	0.50	0/2196
5	DF	0.25	0/1662	0.50	0/2249
6	AG	0.24	0/1499	0.42	0/2016
6	DG	0.22	0/1499	0.41	0/2016
7	AH	0.25	0/1333	0.50	0/1802
7	DH	0.21	0/1332	0.48	0/1802
8	AK	0.24	0/1152	0.49	0/1558
8	DK	0.23	0/1151	0.49	0/1558
9	AM	0.26	0/1132	0.47	0/1525
9	DM	0.23	0/1131	0.45	0/1525
10	AN	0.27	0/943	0.46	0/1269
10	DN	0.26	0/943	0.46	0/1269
11	AO	0.29	0/1162	0.57	0/1544
11	DO	0.26	0/1162	0.56	0/1544
12	AP	0.26	0/1143	0.41	0/1527
12	DP	0.58	1/1143 (0.1%)	0.40	0/1527
13	A0	0.26	0/982	0.50	0/1312
13	D0	0.25	0/974	0.45	0/1302
14	AQ	0.27	0/892	0.53	0/1187
14	DQ	0.23	0/892	0.46	0/1187
15	AR	0.28	0/1156	0.51	0/1542
15	DR	0.26	0/1155	0.45	0/1542
16	A1	0.29	0/982	0.48	0/1306
16	D1	0.24	0/982	0.43	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	A2	0.27	0/790	0.52	0/1057
17	D2	0.28	0/790	0.51	0/1057
18	AS	0.26	0/911	0.48	0/1220
18	DS	0.26	0/911	0.46	0/1220
19	AT	0.32	0/740	0.48	0/993
19	DT	0.31	0/739	0.46	0/993
20	AU	0.30	0/799	0.52	0/1064
20	DU	0.27	0/798	0.49	0/1064
21	AV	0.22	0/1427	0.48	0/1935
21	DV	0.21	0/1460	0.43	0/1982
22	A3	0.29	0/615	0.49	0/819
22	D3	0.26	0/621	0.43	0/827
23	AZ	0.28	0/770	0.52	0/1022
23	DZ	0.27	0/770	0.49	0/1022
24	AW	0.30	0/560	0.54	0/741
24	DW	0.25	0/583	0.48	0/771
25	AX	0.25	0/474	0.44	0/635
25	DX	0.22	0/474	0.42	0/635
26	A4	0.24	0/545	0.48	0/733
26	D4	0.24	0/527	0.48	0/709
27	A5	0.29	0/473	0.55	0/639
27	D5	0.27	0/473	0.57	0/639
28	A6	0.28	0/397	0.52	0/529
28	D6	0.25	0/396	0.51	0/529
29	A7	0.31	0/438	0.44	0/575
29	D7	0.26	0/438	0.43	0/575
30	A8	0.33	0/494	0.60	0/649
30	D8	0.34	0/494	0.68	0/649
31	BA	0.28	0/36234	0.65	19/56554 (0.0%)
31	CA	0.28	0/36237	0.65	15/56558 (0.0%)
32	BE	0.22	0/1959	0.42	0/2642
32	CE	0.22	0/1959	0.43	0/2642
33	BF	0.22	0/1629	0.41	0/2195
33	CF	0.21	0/1636	0.40	0/2205
34	BG	0.28	0/1733	0.45	0/2318
34	CG	0.26	0/1733	0.45	0/2318
35	BH	0.24	0/1171	0.44	0/1576
35	CH	0.24	0/1171	0.44	0/1576
36	BI	0.23	0/856	0.43	0/1154
36	CI	0.24	0/856	0.43	0/1154
37	BJ	0.22	0/1276	0.39	0/1709
37	CJ	0.22	0/1276	0.38	0/1709
38	BK	0.23	0/1136	0.44	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CK	0.22	0/1136	0.43	0/1527
39	BL	0.22	0/1029	0.42	0/1379
39	CL	0.22	0/1029	0.41	0/1379
40	BM	0.22	0/814	0.45	0/1095
40	CM	0.21	0/814	0.43	0/1095
41	BN	0.24	0/900	0.45	0/1213
41	CN	0.23	0/900	0.42	0/1213
42	BO	0.27	0/991	0.49	0/1327
42	CO	0.25	0/991	0.46	0/1327
43	BP	0.22	0/938	0.44	0/1258
43	CP	0.21	0/943	0.43	0/1265
44	BQ	0.26	0/501	0.49	0/664
44	CQ	0.23	0/501	0.43	0/664
45	BR	0.24	0/745	0.41	0/992
45	CR	0.23	0/745	0.40	0/992
46	BS	0.22	0/721	0.43	0/970
46	CS	0.24	0/721	0.43	0/970
47	BT	0.24	0/847	0.43	0/1131
47	CT	0.24	0/847	0.42	0/1131
48	BU	0.24	0/596	0.44	0/790
48	CU	0.24	0/596	0.43	0/790
49	BV	0.23	0/680	0.47	0/915
49	CV	0.22	0/638	0.44	0/860
50	BW	0.22	0/765	0.43	0/1007
50	CW	0.24	0/765	0.45	0/1007
51	BX	0.22	0/221	0.40	0/288
51	CX	0.21	0/221	0.41	0/288
52	BB	0.21	0/2080	0.51	0/3242
52	CB	0.20	0/2080	0.49	0/3242
53	BC	0.25	0/1835	0.56	0/2859
53	BD	0.16	0/1835	0.46	0/2859
53	CC	0.24	0/1835	0.57	0/2859
53	CD	0.16	0/1835	0.47	0/2859
54	B1	0.27	0/226	0.50	0/348
54	C1	0.37	0/226	0.73	1/348 (0.3%)
All	All	0.30	3/324084 (0.0%)	0.64	149/485290 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	AH	0	1
42	BO	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	DP	141	GLN	C-OXT	17.97	1.57	1.23
1	DA	1342	A	N7-C5	-5.40	1.36	1.39
5	AF	207	GLY	C-N	-5.12	1.23	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DA	933	A	C4-N9-C1'	10.03	144.35	126.30
1	DA	933	A	C6-C5-N7	-10.02	125.28	132.30
1	AA	673	C	C2-N3-C4	-9.52	115.14	119.90
1	DA	933	A	C8-N9-C1'	-9.44	110.72	127.70
31	BA	1025	U	C5-C4-O4	-9.10	120.44	125.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AH	153	LYS	Peptide
42	BO	44	LYS	Peptide

5.2 Too-close contacts [i](#)

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	62707	0	31614	1928	1
1	DA	62607	0	31565	1969	1
2	AB	2617	0	1328	93	0
2	DB	2617	0	1328	98	0
3	AD	2116	0	2195	197	0
3	DD	2115	0	2195	178	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AE	1569	0	1634	163	0
4	DE	1568	0	1634	175	0
5	AF	1586	0	1632	111	0
5	DF	1627	0	1680	126	0
6	AG	1474	0	1535	127	0
6	DG	1474	0	1535	99	0
7	AH	1308	0	1382	143	0
7	DH	1307	0	1382	102	1
8	AK	1137	0	1223	93	0
8	DK	1136	0	1223	92	0
9	AM	1105	0	1180	98	0
9	DM	1104	0	1180	84	0
10	AN	933	0	996	40	0
10	DN	933	0	996	38	0
11	AO	1145	0	1228	157	0
11	DO	1145	0	1228	169	0
12	AP	1122	0	1179	184	0
12	DP	1122	0	1179	204	0
13	A0	968	0	1033	63	0
13	D0	960	0	1021	69	0
14	AQ	882	0	943	85	0
14	DQ	882	0	943	73	0
15	AR	1142	0	1202	92	0
15	DR	1141	0	1202	96	0
16	A1	964	0	1022	76	0
16	D1	964	0	1022	88	0
17	A2	779	0	852	75	0
17	D2	779	0	852	117	0
18	AS	900	0	964	61	0
18	DS	900	0	964	41	0
19	AT	726	0	778	52	0
19	DT	725	0	778	56	0
20	AU	786	0	878	77	0
20	DU	785	0	878	97	0
21	AV	1397	0	1430	120	0
21	DV	1428	0	1454	100	0
22	A3	607	0	628	41	0
22	D3	613	0	633	45	0
23	AZ	763	0	848	40	0
23	DZ	763	0	848	50	0
24	AW	558	0	610	29	0
24	DW	581	0	629	49	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	AX	469	0	518	21	0
25	DX	469	0	518	22	0
26	A4	533	0	522	79	0
26	D4	515	0	510	83	0
27	A5	459	0	480	53	0
27	D5	459	0	480	43	0
28	A6	390	0	404	64	0
28	D6	389	0	404	50	0
29	A7	430	0	480	19	0
29	D7	430	0	480	28	0
30	A8	488	0	560	80	0
30	D8	488	0	560	86	0
31	BA	32369	0	16339	1082	1
31	CA	32372	0	16338	1075	2
32	BE	1924	0	1975	154	0
32	CE	1924	0	1975	162	0
33	BF	1605	0	1668	114	0
33	CF	1612	0	1677	115	0
34	BG	1703	0	1764	120	0
34	CG	1703	0	1763	94	1
35	BH	1155	0	1213	64	0
35	CH	1155	0	1213	75	0
36	BI	843	0	857	41	1
36	CI	843	0	857	38	0
37	BJ	1257	0	1296	65	0
37	CJ	1257	0	1296	62	0
38	BK	1116	0	1177	68	0
38	CK	1116	0	1177	50	0
39	BL	1010	0	1037	84	0
39	CL	1010	0	1037	96	0
40	BM	801	0	849	74	0
40	CM	801	0	849	70	0
41	BN	885	0	904	57	0
41	CN	885	0	904	34	0
42	BO	975	0	1062	52	0
42	CO	975	0	1062	67	0
43	BP	928	0	987	62	0
43	CP	933	0	992	71	0
44	BQ	492	0	529	46	0
44	CQ	492	0	530	38	0
45	BR	734	0	771	34	0
45	CR	734	0	771	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	BS	705	0	725	41	0
46	CS	705	0	725	32	0
47	BT	834	0	904	47	0
47	CT	834	0	904	31	0
48	BU	591	0	662	24	0
48	CU	591	0	662	18	0
49	BV	665	0	686	66	0
49	CV	624	0	636	65	0
50	BW	763	0	861	56	0
50	CW	763	0	861	47	0
51	BX	217	0	234	16	0
51	CX	217	0	234	20	0
52	BB	1861	0	938	50	0
52	CB	1861	0	938	62	0
53	BC	1643	0	837	48	0
53	BD	1643	0	837	65	0
53	CC	1643	0	837	50	0
53	CD	1643	0	837	79	0
54	B1	205	0	105	7	0
54	C1	205	0	105	5	0
55	A0	1	0	0	0	0
55	A1	1	0	0	0	0
55	A2	1	0	0	0	0
55	A3	1	0	0	0	0
55	A5	2	0	0	0	0
55	A6	1	0	0	0	0
55	A7	1	0	0	0	0
55	AA	630	0	0	0	0
55	AB	17	0	0	0	0
55	AD	2	0	0	0	0
55	AE	4	0	0	0	0
55	AF	3	0	0	0	0
55	AO	3	0	0	0	0
55	AU	1	0	0	0	0
55	B1	2	0	0	0	0
55	BA	244	0	0	0	0
55	BB	8	0	0	0	0
55	BC	9	0	0	0	0
55	BD	1	0	0	0	0
55	BG	1	0	0	0	0
55	BN	2	0	0	0	0
55	BQ	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CA	209	0	0	0	0
55	CB	5	0	0	0	0
55	CC	8	0	0	0	0
55	CG	3	0	0	0	0
55	CH	1	0	0	0	0
55	CS	1	0	0	0	0
55	D0	1	0	0	0	0
55	D1	2	0	0	0	0
55	D3	1	0	0	0	0
55	D5	1	0	0	0	0
55	DA	528	0	0	0	0
55	DB	14	0	0	0	0
55	DE	3	0	0	0	0
55	DP	1	0	0	0	0
55	DU	1	0	0	0	0
56	BG	1	0	0	0	0
56	BQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	299628	0	200976	12579	4

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 25.

The worst 5 of 12579 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)
6:AG:108:ASN:HA	26:A4:38:LYS:CG	1.41	1.51
6:AG:108:ASN:CA	26:A4:38:LYS:HG2	1.46	1.45
1:AA:1056:G:H21	1:AA:1103:A:N6	1.13	1.45
1:DA:226:G:H21	1:DA:228:A:N6	0.93	1.41
1:DA:226:G:N2	1:DA:228:A:H61	1.15	1.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:BA:85:U:O2'	7:DH:100:GLY:O[3_555]	1.87	0.33
1:AA:2137:C:OP1	31:CA:999:U:O2'[4_555]	1.89	0.31
36:BI:15:ASP:OD2	34:CG:27:TYR:OH[4_555]	2.05	0.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:CA:86:U:O2'	1:DA:276:A:OP2[3_545]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	270/272 (99%)	226 (84%)	31 (12%)	13 (5%)	3	17
3	DD	270/272 (99%)	231 (86%)	25 (9%)	14 (5%)	2	15
4	AE	203/205 (99%)	152 (75%)	33 (16%)	18 (9%)	1	5
4	DE	203/205 (99%)	128 (63%)	41 (20%)	34 (17%)	0	0
5	AF	201/208 (97%)	177 (88%)	13 (6%)	11 (6%)	2	13
5	DF	206/208 (99%)	162 (79%)	25 (12%)	19 (9%)	1	4
6	AG	179/181 (99%)	147 (82%)	21 (12%)	11 (6%)	2	11
6	DG	179/181 (99%)	141 (79%)	27 (15%)	11 (6%)	2	11
7	AH	168/170 (99%)	116 (69%)	22 (13%)	30 (18%)	0	0
7	DH	168/170 (99%)	108 (64%)	37 (22%)	23 (14%)	0	1
8	AK	144/146 (99%)	97 (67%)	27 (19%)	20 (14%)	0	1
8	DK	144/146 (99%)	106 (74%)	26 (18%)	12 (8%)	1	6
9	AM	136/138 (99%)	105 (77%)	18 (13%)	13 (10%)	1	4
9	DM	136/138 (99%)	108 (79%)	20 (15%)	8 (6%)	2	12
10	AN	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	11	43
10	DN	120/122 (98%)	108 (90%)	11 (9%)	1 (1%)	24	63
11	AO	148/150 (99%)	106 (72%)	25 (17%)	17 (12%)	0	2
11	DO	148/150 (99%)	92 (62%)	28 (19%)	28 (19%)	0	0
12	AP	139/141 (99%)	95 (68%)	25 (18%)	19 (14%)	0	1
12	DP	139/141 (99%)	91 (66%)	20 (14%)	28 (20%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	A0	116/118 (98%)	93 (80%)	15 (13%)	8 (7%)	1	8
13	D0	115/118 (98%)	93 (81%)	17 (15%)	5 (4%)	3	19
14	AQ	109/111 (98%)	77 (71%)	24 (22%)	8 (7%)	1	7
14	DQ	109/111 (98%)	78 (72%)	21 (19%)	10 (9%)	1	4
15	AR	135/137 (98%)	100 (74%)	25 (18%)	10 (7%)	1	7
15	DR	135/137 (98%)	103 (76%)	23 (17%)	9 (7%)	1	9
16	A1	115/117 (98%)	101 (88%)	7 (6%)	7 (6%)	2	11
16	D1	115/117 (98%)	93 (81%)	15 (13%)	7 (6%)	2	11
17	A2	99/101 (98%)	83 (84%)	9 (9%)	7 (7%)	1	8
17	D2	99/101 (98%)	73 (74%)	14 (14%)	12 (12%)	0	2
18	AS	111/113 (98%)	92 (83%)	14 (13%)	5 (4%)	3	17
18	DS	111/113 (98%)	99 (89%)	10 (9%)	2 (2%)	11	42
19	AT	90/92 (98%)	83 (92%)	6 (7%)	1 (1%)	17	55
19	DT	90/92 (98%)	75 (83%)	12 (13%)	3 (3%)	5	26
20	AU	100/102 (98%)	68 (68%)	19 (19%)	13 (13%)	0	1
20	DU	100/102 (98%)	61 (61%)	22 (22%)	17 (17%)	0	0
21	AV	173/179 (97%)	112 (65%)	36 (21%)	25 (14%)	0	1
21	DV	177/179 (99%)	120 (68%)	27 (15%)	30 (17%)	0	0
22	A3	74/77 (96%)	57 (77%)	15 (20%)	2 (3%)	6	31
22	D3	75/77 (97%)	62 (83%)	13 (17%)	0	100	100
23	AZ	95/97 (98%)	78 (82%)	10 (10%)	7 (7%)	1	7
23	DZ	95/97 (98%)	77 (81%)	7 (7%)	11 (12%)	0	2
24	AW	64/69 (93%)	56 (88%)	3 (5%)	5 (8%)	1	6
24	DW	67/69 (97%)	56 (84%)	5 (8%)	6 (9%)	1	5
25	AX	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
25	DX	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	11	42
26	A4	64/66 (97%)	38 (59%)	16 (25%)	10 (16%)	0	0
26	D4	61/66 (92%)	24 (39%)	25 (41%)	12 (20%)	0	0
27	A5	57/59 (97%)	40 (70%)	10 (18%)	7 (12%)	0	2
27	D5	57/59 (97%)	46 (81%)	7 (12%)	4 (7%)	1	8
28	A6	43/45 (96%)	25 (58%)	12 (28%)	6 (14%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	D6	43/45 (96%)	25 (58%)	12 (28%)	6 (14%)	0	1
29	A7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	9	37
29	D7	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
30	A8	59/61 (97%)	50 (85%)	5 (8%)	4 (7%)	1	8
30	D8	59/61 (97%)	39 (66%)	11 (19%)	9 (15%)	0	0
32	BE	235/256 (92%)	170 (72%)	47 (20%)	18 (8%)	1	6
32	CE	235/256 (92%)	188 (80%)	23 (10%)	24 (10%)	1	4
33	BF	203/239 (85%)	141 (70%)	46 (23%)	16 (8%)	1	6
33	CF	204/239 (85%)	152 (74%)	37 (18%)	15 (7%)	1	7
34	BG	206/208 (99%)	168 (82%)	27 (13%)	11 (5%)	2	14
34	CG	206/208 (99%)	171 (83%)	30 (15%)	5 (2%)	7	33
35	BH	149/162 (92%)	129 (87%)	14 (9%)	6 (4%)	4	21
35	CH	149/162 (92%)	134 (90%)	11 (7%)	4 (3%)	6	31
36	BI	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	9	38
36	CI	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	19	58
37	BJ	153/156 (98%)	137 (90%)	15 (10%)	1 (1%)	26	65
37	CJ	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	9	38
38	BK	136/138 (99%)	115 (85%)	14 (10%)	7 (5%)	2	15
38	CK	136/138 (99%)	122 (90%)	11 (8%)	3 (2%)	8	36
39	BL	125/128 (98%)	100 (80%)	22 (18%)	3 (2%)	7	33
39	CL	125/128 (98%)	102 (82%)	19 (15%)	4 (3%)	5	26
40	BM	97/105 (92%)	76 (78%)	19 (20%)	2 (2%)	9	37
40	CM	97/105 (92%)	75 (77%)	13 (13%)	9 (9%)	1	4
41	BN	117/129 (91%)	97 (83%)	15 (13%)	5 (4%)	3	19
41	CN	117/129 (91%)	100 (86%)	14 (12%)	3 (3%)	7	32
42	BO	123/132 (93%)	101 (82%)	13 (11%)	9 (7%)	1	7
42	CO	123/132 (93%)	96 (78%)	19 (15%)	8 (6%)	1	9
43	BP	114/126 (90%)	86 (75%)	20 (18%)	8 (7%)	1	8
43	CP	115/126 (91%)	83 (72%)	22 (19%)	10 (9%)	1	5
44	BQ	58/61 (95%)	42 (72%)	11 (19%)	5 (9%)	1	5
44	CQ	58/61 (95%)	41 (71%)	11 (19%)	6 (10%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BR	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	8	35
45	CR	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	16	52
46	BS	82/88 (93%)	65 (79%)	14 (17%)	3 (4%)	4	23
46	CS	82/88 (93%)	69 (84%)	13 (16%)	0	100	100
47	BT	98/105 (93%)	85 (87%)	11 (11%)	2 (2%)	9	38
47	CT	98/105 (93%)	92 (94%)	4 (4%)	2 (2%)	9	38
48	BU	70/88 (80%)	60 (86%)	8 (11%)	2 (3%)	6	29
48	CU	70/88 (80%)	63 (90%)	7 (10%)	0	100	100
49	BV	81/93 (87%)	63 (78%)	11 (14%)	7 (9%)	1	5
49	CV	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1	4
50	BW	97/106 (92%)	75 (77%)	12 (12%)	10 (10%)	1	4
50	CW	97/106 (92%)	73 (75%)	13 (13%)	11 (11%)	0	2
51	BX	23/27 (85%)	19 (83%)	3 (13%)	1 (4%)	3	19
51	CX	23/27 (85%)	19 (83%)	0	4 (17%)	0	0
All	All	11342/11844 (96%)	8910 (79%)	1590 (14%)	842 (7%)	1	7

5 of 842 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	26	LYS
3	AD	28	GLU
3	AD	33	LEU
3	AD	122	ASP
3	AD	237	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	214/214 (100%)	182 (85%)	32 (15%)	3	15
3	DD	214/214 (100%)	179 (84%)	35 (16%)	3	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AE	165/165 (100%)	133 (81%)	32 (19%)	2	7
4	DE	165/165 (100%)	138 (84%)	27 (16%)	3	12
5	AF	161/165 (98%)	139 (86%)	22 (14%)	4	19
5	DF	165/165 (100%)	142 (86%)	23 (14%)	4	19
6	AG	155/155 (100%)	134 (86%)	21 (14%)	5	20
6	DG	155/155 (100%)	135 (87%)	20 (13%)	5	21
7	AH	142/142 (100%)	118 (83%)	24 (17%)	2	11
7	DH	142/142 (100%)	130 (92%)	12 (8%)	13	45
8	AK	122/122 (100%)	106 (87%)	16 (13%)	5	21
8	DK	122/122 (100%)	103 (84%)	19 (16%)	3	14
9	AM	117/117 (100%)	99 (85%)	18 (15%)	3	14
9	DM	117/117 (100%)	98 (84%)	19 (16%)	3	12
10	AN	100/100 (100%)	91 (91%)	9 (9%)	12	41
10	DN	100/100 (100%)	89 (89%)	11 (11%)	8	30
11	AO	116/116 (100%)	87 (75%)	29 (25%)	1	2
11	DO	116/116 (100%)	84 (72%)	32 (28%)	0	1
12	AP	111/111 (100%)	87 (78%)	24 (22%)	1	5
12	DP	111/111 (100%)	85 (77%)	26 (23%)	1	4
13	A0	101/101 (100%)	82 (81%)	19 (19%)	2	8
13	D0	100/101 (99%)	85 (85%)	15 (15%)	3	15
14	AQ	87/87 (100%)	68 (78%)	19 (22%)	1	5
14	DQ	87/87 (100%)	76 (87%)	11 (13%)	5	22
15	AR	120/120 (100%)	100 (83%)	20 (17%)	3	11
15	DR	120/120 (100%)	91 (76%)	29 (24%)	1	3
16	A1	93/93 (100%)	82 (88%)	11 (12%)	6	25
16	D1	93/93 (100%)	88 (95%)	5 (5%)	27	64
17	A2	82/82 (100%)	71 (87%)	11 (13%)	5	20
17	D2	82/82 (100%)	68 (83%)	14 (17%)	2	11
18	AS	92/92 (100%)	74 (80%)	18 (20%)	1	7
18	DS	92/92 (100%)	77 (84%)	15 (16%)	3	12
19	AT	74/74 (100%)	62 (84%)	12 (16%)	3	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	DT	74/74 (100%)	63 (85%)	11 (15%)	4	15
20	AU	85/85 (100%)	70 (82%)	15 (18%)	2	10
20	DU	85/85 (100%)	67 (79%)	18 (21%)	1	6
21	AV	154/158 (98%)	130 (84%)	24 (16%)	3	14
21	DV	158/158 (100%)	146 (92%)	12 (8%)	16	51
22	A3	61/62 (98%)	57 (93%)	4 (7%)	21	56
22	D3	62/62 (100%)	58 (94%)	4 (6%)	21	57
23	AZ	82/82 (100%)	72 (88%)	10 (12%)	6	24
23	DZ	82/82 (100%)	71 (87%)	11 (13%)	5	20
24	AW	62/64 (97%)	50 (81%)	12 (19%)	2	7
24	DW	64/64 (100%)	56 (88%)	8 (12%)	6	22
25	AX	51/51 (100%)	46 (90%)	5 (10%)	10	36
25	DX	51/51 (100%)	48 (94%)	3 (6%)	24	60
26	A4	59/59 (100%)	49 (83%)	10 (17%)	2	11
26	D4	57/59 (97%)	50 (88%)	7 (12%)	6	23
27	A5	51/51 (100%)	39 (76%)	12 (24%)	1	4
27	D5	51/51 (100%)	41 (80%)	10 (20%)	1	7
28	A6	44/44 (100%)	37 (84%)	7 (16%)	3	13
28	D6	44/44 (100%)	34 (77%)	10 (23%)	1	4
29	A7	42/42 (100%)	35 (83%)	7 (17%)	3	11
29	D7	42/42 (100%)	34 (81%)	8 (19%)	2	8
30	A8	51/51 (100%)	40 (78%)	11 (22%)	1	5
30	D8	51/51 (100%)	44 (86%)	7 (14%)	4	19
32	BE	205/220 (93%)	174 (85%)	31 (15%)	3	15
32	CE	205/220 (93%)	174 (85%)	31 (15%)	3	15
33	BF	159/188 (85%)	137 (86%)	22 (14%)	4	19
33	CF	160/188 (85%)	139 (87%)	21 (13%)	5	21
34	BG	180/180 (100%)	161 (89%)	19 (11%)	8	31
34	CG	180/180 (100%)	152 (84%)	28 (16%)	3	14
35	BH	116/123 (94%)	101 (87%)	15 (13%)	5	21
35	CH	116/123 (94%)	101 (87%)	15 (13%)	5	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	BI	90/90 (100%)	82 (91%)	8 (9%)	12	42
36	CI	90/90 (100%)	85 (94%)	5 (6%)	26	62
37	BJ	126/127 (99%)	113 (90%)	13 (10%)	9	32
37	CJ	126/127 (99%)	107 (85%)	19 (15%)	3	15
38	BK	119/119 (100%)	109 (92%)	10 (8%)	14	46
38	CK	119/119 (100%)	109 (92%)	10 (8%)	14	46
39	BL	98/99 (99%)	81 (83%)	17 (17%)	2	11
39	CL	98/99 (99%)	85 (87%)	13 (13%)	5	20
40	BM	89/92 (97%)	79 (89%)	10 (11%)	7	29
40	CM	89/92 (97%)	78 (88%)	11 (12%)	6	23
41	BN	90/99 (91%)	81 (90%)	9 (10%)	9	34
41	CN	90/99 (91%)	82 (91%)	8 (9%)	12	42
42	BO	104/109 (95%)	87 (84%)	17 (16%)	3	12
42	CO	104/109 (95%)	92 (88%)	12 (12%)	7	27
43	BP	94/101 (93%)	85 (90%)	9 (10%)	10	37
43	CP	94/101 (93%)	80 (85%)	14 (15%)	4	15
44	BQ	49/50 (98%)	40 (82%)	9 (18%)	2	9
44	CQ	49/50 (98%)	47 (96%)	2 (4%)	37	74
45	BR	79/80 (99%)	76 (96%)	3 (4%)	40	76
45	CR	79/80 (99%)	72 (91%)	7 (9%)	12	42
46	BS	72/74 (97%)	64 (89%)	8 (11%)	8	29
46	CS	72/74 (97%)	63 (88%)	9 (12%)	6	22
47	BT	95/97 (98%)	86 (90%)	9 (10%)	11	38
47	CT	95/97 (98%)	91 (96%)	4 (4%)	36	73
48	BU	63/77 (82%)	58 (92%)	5 (8%)	15	49
48	CU	63/77 (82%)	56 (89%)	7 (11%)	8	29
49	BV	72/80 (90%)	60 (83%)	12 (17%)	3	11
49	CV	67/80 (84%)	55 (82%)	12 (18%)	2	10
50	BW	76/82 (93%)	67 (88%)	9 (12%)	6	25
50	CW	76/82 (93%)	66 (87%)	10 (13%)	5	20
51	BX	20/22 (91%)	19 (95%)	1 (5%)	30	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	CX	20/22 (91%)	20 (100%)	0	100	100
All	All	9584/9828 (98%)	8234 (86%)	1350 (14%)	4	18

5 of 1350 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BO	17	LYS
34	CG	84	LYS
19	DT	63	LYS
43	BP	70	LEU
50	BW	73	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 259 such sidechains are listed below:

Mol	Chain	Res	Type
42	BO	46	ASN
34	CG	43	HIS
21	DV	65	GLN
43	BP	101	GLN
49	BV	56	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2911/2912 (99%)	555 (19%)	51 (1%)
1	DA	2905/2912 (99%)	601 (20%)	50 (1%)
2	AB	121/122 (99%)	24 (19%)	0
2	DB	121/122 (99%)	28 (23%)	0
31	BA	1506/1506 (100%)	291 (19%)	32 (2%)
31	CA	1505/1506 (99%)	315 (20%)	42 (2%)
52	BB	86/87 (98%)	26 (30%)	4 (4%)
52	CB	86/87 (98%)	30 (34%)	3 (3%)
53	BC	77/77 (100%)	12 (15%)	3 (3%)
53	BD	76/77 (98%)	25 (32%)	2 (2%)
53	CC	76/77 (98%)	14 (18%)	3 (3%)
53	CD	76/77 (98%)	16 (21%)	2 (2%)
54	B1	9/10 (90%)	2 (22%)	0
54	C1	9/10 (90%)	2 (22%)	0
All	All	9564/9582 (99%)	1941 (20%)	192 (2%)

5 of 1941 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	15	G
1	AA	23	G
1	AA	34	C
1	AA	35	G

5 of 192 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	BB	23	A
31	CA	560	U
1	DA	2210	G
53	BC	48	U
31	CA	209	U

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 1720 ligands modelled in this entry, 1720 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2912/2912 (100%)	0.62	128 (4%) 38 17	38, 71, 209, 243	0
1	DA	2907/2912 (99%)	0.66	159 (5%) 29 12	49, 82, 229, 246	0
2	AB	122/122 (100%)	0.40	0 100 100	73, 98, 119, 180	0
2	DB	122/122 (100%)	0.45	4 (3%) 50 26	87, 121, 145, 200	0
3	AD	272/272 (100%)	0.17	0 100 100	38, 61, 83, 107	0
3	DD	272/272 (100%)	0.17	1 (0%) 93 85	45, 69, 94, 125	0
4	AE	205/205 (100%)	0.21	4 (1%) 68 46	44, 82, 133, 147	0
4	DE	205/205 (100%)	0.43	9 (4%) 38 17	51, 90, 144, 167	0
5	AF	203/208 (97%)	0.09	0 100 100	40, 74, 116, 133	0
5	DF	208/208 (100%)	0.23	5 (2%) 62 39	54, 96, 161, 183	0
6	AG	181/181 (100%)	0.88	21 (11%) 6 2	91, 110, 140, 149	0
6	DG	181/181 (100%)	0.64	18 (9%) 9 3	112, 138, 161, 171	0
7	AH	170/170 (100%)	0.34	4 (2%) 62 39	80, 110, 129, 154	0
7	DH	170/170 (100%)	1.87	68 (40%) 0 0	150, 196, 217, 230	0
8	AK	146/146 (100%)	0.16	3 (2%) 67 44	75, 124, 142, 149	0
8	DK	146/146 (100%)	0.22	2 (1%) 78 60	76, 127, 150, 154	0
9	AM	138/138 (100%)	-0.01	0 100 100	63, 86, 124, 137	0
9	DM	138/138 (100%)	0.18	2 (1%) 78 60	74, 105, 136, 148	0
10	AN	122/122 (100%)	0.13	0 100 100	54, 74, 92, 103	0
10	DN	122/122 (100%)	0.09	0 100 100	62, 84, 106, 123	0
11	AO	150/150 (100%)	0.31	3 (2%) 68 46	45, 82, 112, 166	0
11	DO	150/150 (100%)	0.55	8 (5%) 30 13	50, 100, 140, 180	0
12	AP	141/141 (100%)	0.45	4 (2%) 56 32	58, 85, 110, 134	0
12	DP	141/141 (100%)	0.49	4 (2%) 56 32	58, 101, 131, 154	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	A0	118/118 (100%)	0.15	1 (0%) 87 75	55, 80, 102, 114	0
13	D0	117/118 (99%)	0.23	2 (1%) 73 52	58, 78, 100, 119	0
14	AQ	111/111 (100%)	0.44	6 (5%) 29 12	75, 96, 120, 136	0
14	DQ	111/111 (100%)	0.93	21 (18%) 2 1	80, 118, 143, 165	0
15	AR	137/137 (100%)	0.09	3 (2%) 65 42	69, 89, 140, 171	0
15	DR	137/137 (100%)	0.26	3 (2%) 65 42	70, 94, 158, 186	0
16	A1	117/117 (100%)	0.27	2 (1%) 73 52	46, 74, 108, 149	0
16	D1	117/117 (100%)	0.25	0 100 100	59, 95, 138, 157	0
17	A2	101/101 (100%)	-0.00	2 (1%) 68 46	47, 96, 125, 142	0
17	D2	101/101 (100%)	0.10	2 (1%) 68 46	57, 121, 140, 151	0
18	AS	113/113 (100%)	0.02	0 100 100	46, 70, 106, 155	0
18	DS	113/113 (100%)	0.10	1 (0%) 85 72	61, 74, 107, 155	0
19	AT	92/92 (100%)	0.05	0 100 100	54, 68, 98, 112	0
19	DT	92/92 (100%)	0.19	2 (2%) 65 42	64, 86, 112, 128	0
20	AU	102/102 (100%)	0.28	2 (1%) 68 46	70, 97, 148, 168	0
20	DU	102/102 (100%)	0.77	17 (16%) 2 1	85, 113, 163, 184	0
21	AV	175/179 (97%)	1.00	35 (20%) 1 0	87, 125, 190, 195	0
21	DV	179/179 (100%)	1.05	35 (19%) 1 0	112, 156, 209, 216	0
22	A3	76/77 (98%)	0.31	0 100 100	56, 75, 95, 135	0
22	D3	77/77 (100%)	0.38	1 (1%) 79 62	66, 88, 113, 152	0
23	AZ	97/97 (100%)	0.35	4 (4%) 41 19	50, 69, 126, 161	0
23	DZ	97/97 (100%)	0.39	4 (4%) 41 19	52, 78, 131, 156	0
24	AW	66/69 (95%)	-0.12	0 100 100	60, 77, 97, 134	0
24	DW	69/69 (100%)	0.28	1 (1%) 78 60	79, 105, 134, 172	0
25	AX	59/59 (100%)	0.16	1 (1%) 73 52	63, 80, 112, 127	0
25	DX	59/59 (100%)	0.22	1 (1%) 73 52	74, 100, 138, 162	0
26	A4	66/66 (100%)	1.67	22 (33%) 0 0	117, 153, 177, 184	0
26	D4	63/66 (95%)	1.23	16 (25%) 1 0	143, 184, 193, 201	0
27	A5	59/59 (100%)	0.39	4 (6%) 20 7	43, 85, 167, 172	0
27	D5	59/59 (100%)	0.57	7 (11%) 6 2	55, 83, 177, 186	0
28	A6	45/45 (100%)	1.39	12 (26%) 1 0	107, 136, 159, 163	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/45 (100%)	2.27	19 (42%) 0 0	121, 158, 176, 182	0
29	A7	49/49 (100%)	0.28	2 (4%) 41 19	38, 47, 95, 123	0
29	D7	49/49 (100%)	0.31	1 (2%) 68 46	49, 58, 115, 133	0
30	A8	61/61 (100%)	0.33	0 100 100	55, 68, 85, 108	0
30	D8	61/61 (100%)	0.64	2 (3%) 50 26	65, 81, 103, 120	0
31	BA	1506/1506 (100%)	0.68	71 (4%) 35 16	54, 103, 187, 244	0
31	CA	1506/1506 (100%)	0.72	85 (5%) 28 11	59, 109, 187, 245	0
32	BE	237/256 (92%)	0.40	16 (6%) 20 7	107, 142, 181, 191	0
32	CE	237/256 (92%)	0.55	18 (7%) 17 6	117, 158, 190, 208	0
33	BF	205/239 (85%)	0.07	4 (1%) 68 46	88, 118, 150, 162	0
33	CF	206/239 (86%)	0.28	6 (2%) 55 31	119, 143, 172, 183	0
34	BG	208/208 (100%)	0.45	11 (5%) 30 13	84, 110, 135, 149	0
34	CG	208/208 (100%)	0.29	8 (3%) 44 21	74, 101, 128, 142	0
35	BH	151/162 (93%)	0.20	1 (0%) 89 78	79, 101, 129, 159	0
35	CH	151/162 (93%)	0.27	0 100 100	90, 114, 139, 162	0
36	BI	101/101 (100%)	-0.09	0 100 100	77, 102, 122, 143	0
36	CI	101/101 (100%)	-0.17	0 100 100	73, 98, 121, 149	0
37	BJ	155/156 (99%)	0.24	7 (4%) 37 17	101, 122, 156, 167	0
37	CJ	155/156 (99%)	0.43	14 (9%) 12 4	105, 127, 158, 165	0
38	BK	138/138 (100%)	0.58	7 (5%) 32 13	84, 108, 123, 132	0
38	CK	138/138 (100%)	0.46	5 (3%) 46 23	93, 118, 131, 141	0
39	BL	127/128 (99%)	1.24	23 (18%) 2 1	91, 141, 160, 169	0
39	CL	127/128 (99%)	1.62	45 (35%) 0 0	107, 151, 168, 172	0
40	BM	99/105 (94%)	1.03	21 (21%) 1 0	87, 140, 171, 176	0
40	CM	99/105 (94%)	1.31	33 (33%) 0 0	113, 154, 173, 176	0
41	BN	119/129 (92%)	0.14	2 (1%) 73 52	63, 101, 133, 162	0
41	CN	119/129 (92%)	0.30	4 (3%) 49 24	77, 103, 141, 166	0
42	BO	125/132 (94%)	0.20	2 (1%) 74 55	61, 78, 116, 162	0
42	CO	125/132 (94%)	0.28	1 (0%) 87 75	70, 97, 130, 168	0
43	BP	116/126 (92%)	0.83	16 (13%) 4 2	87, 124, 144, 158	0
43	CP	117/126 (92%)	0.93	19 (16%) 3 1	105, 152, 166, 174	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	60/61 (98%)	0.89	7 (11%) 6 2	84, 107, 124, 134	0
44	CQ	60/61 (98%)	1.91	24 (40%) 0 0	120, 136, 153, 161	0
45	BR	88/89 (98%)	0.36	4 (4%) 37 17	73, 97, 120, 126	0
45	CR	88/89 (98%)	0.33	3 (3%) 49 24	75, 105, 129, 135	0
46	BS	84/88 (95%)	0.91	11 (13%) 5 2	98, 113, 141, 173	0
46	CS	84/88 (95%)	0.64	4 (4%) 34 15	79, 96, 122, 161	0
47	BT	100/105 (95%)	0.46	3 (3%) 54 29	85, 105, 123, 137	0
47	CT	100/105 (95%)	0.52	3 (3%) 54 29	81, 104, 126, 143	0
48	BU	72/88 (81%)	0.08	0 100 100	75, 102, 140, 169	0
48	CU	72/88 (81%)	0.11	1 (1%) 78 60	86, 109, 150, 165	0
49	BV	83/93 (89%)	1.01	17 (20%) 1 0	103, 129, 145, 156	0
49	CV	78/93 (83%)	1.41	20 (25%) 1 0	137, 160, 180, 183	0
50	BW	99/106 (93%)	0.85	10 (10%) 9 3	101, 123, 152, 162	0
50	CW	99/106 (93%)	0.77	11 (11%) 7 2	79, 110, 149, 164	0
51	BX	25/27 (92%)	2.67	18 (72%) 0 0	93, 114, 133, 155	0
51	CX	25/27 (92%)	3.33	18 (72%) 0 0	110, 134, 152, 170	0
52	BB	87/87 (100%)	0.98	14 (16%) 3 1	83, 164, 192, 209	0
52	CB	87/87 (100%)	1.00	14 (16%) 3 1	99, 167, 196, 209	0
53	BC	77/77 (100%)	0.36	0 100 100	66, 101, 139, 152	0
53	BD	77/77 (100%)	1.47	23 (29%) 1 0	75, 226, 239, 242	0
53	CC	77/77 (100%)	0.39	1 (1%) 79 62	77, 110, 148, 162	0
53	CD	77/77 (100%)	1.74	26 (33%) 0 0	78, 227, 239, 242	0
54	B1	10/10 (100%)	0.79	1 (10%) 9 3	73, 80, 132, 141	0
54	C1	10/10 (100%)	1.11	2 (20%) 1 0	81, 98, 145, 150	0
All	All	21111/21426 (98%)	0.56	1332 (6%) 23 9	38, 99, 184, 246	0

The worst 5 of 1332 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
16	A1	118	GLY	12.2
26	D4	63	TYR	10.8
41	CN	129	SER	10.6
28	A6	42	TRP	10.5
11	DO	64	LYS	9.7

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	AA	3591	1/1	0.89	1.30	104.66	80,80,80,80	0
55	MG	AA	3388	1/1	0.58	1.76	92.83	119,119,119,119	0
55	MG	DA	3324	1/1	0.79	1.34	79.60	89,89,89,89	0
55	MG	AA	3405	1/1	0.82	1.19	76.86	86,86,86,86	0
55	MG	AA	3307	1/1	0.95	1.05	66.62	75,75,75,75	0
55	MG	DA	3481	1/1	0.92	0.45	59.49	45,45,45,45	0
55	MG	AB	217	1/1	0.82	1.34	57.61	109,109,109,109	0
55	MG	DA	3337	1/1	0.86	0.90	56.34	75,75,75,75	0
55	MG	BA	1691	1/1	0.93	0.74	56.24	60,60,60,60	0
55	MG	AA	3138	1/1	0.97	0.74	48.99	41,41,41,41	0
55	MG	CA	1765	1/1	0.87	0.52	48.06	97,97,97,97	0
55	MG	AA	3321	1/1	0.84	0.76	47.40	68,68,68,68	0
55	MG	DA	3173	1/1	0.87	0.72	46.19	59,59,59,59	0
55	MG	DA	3499	1/1	0.83	0.91	46.09	78,78,78,78	0
55	MG	AA	3514	1/1	0.85	0.65	45.11	59,59,59,59	0
55	MG	AA	3154	1/1	0.97	0.63	44.87	55,55,55,55	0
55	MG	DA	3494	1/1	0.82	0.87	43.85	81,81,81,81	0
55	MG	DA	3140	1/1	0.95	0.76	42.94	49,49,49,49	0
55	MG	DA	3086	1/1	0.57	2.47	41.21	98,98,98,98	0
55	MG	DA	3303	1/1	0.97	0.86	41.06	61,61,61,61	0
55	MG	DA	3197	1/1	0.96	0.64	38.42	52,52,52,52	0
55	MG	BA	1835	1/1	0.77	0.68	37.52	82,82,82,82	0
55	MG	DA	3465	1/1	0.96	0.59	37.03	51,51,51,51	0
55	MG	DA	3471	1/1	0.82	0.73	35.91	89,89,89,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3104	1/1	0.97	0.60	35.14	38,38,38,38	0
55	MG	AA	3144	1/1	0.95	0.78	34.73	51,51,51,51	0
55	MG	AA	3567	1/1	0.96	0.56	34.34	38,38,38,38	0
55	MG	AA	3026	1/1	0.96	0.56	34.19	35,35,35,35	0
55	MG	CA	1704	1/1	-0.12	1.11	34.03	129,129,129,129	0
55	MG	AA	3592	1/1	0.93	0.72	33.22	69,69,69,69	0
55	MG	AA	3556	1/1	0.85	0.83	33.16	85,85,85,85	0
55	MG	DA	3203	1/1	0.98	0.78	32.42	52,52,52,52	0
55	MG	DA	3375	1/1	0.42	0.58	31.99	82,82,82,82	0
55	MG	AA	3160	1/1	0.99	0.60	31.61	31,31,31,31	0
55	MG	DA	3142	1/1	0.91	0.68	31.37	51,51,51,51	0
55	MG	AA	3276	1/1	0.67	0.60	30.71	59,59,59,59	0
55	MG	AA	3112	1/1	0.96	0.54	30.62	48,48,48,48	0
55	MG	DA	3514	1/1	0.98	0.55	30.60	49,49,49,49	0
55	MG	AA	3539	1/1	0.93	0.57	30.56	54,54,54,54	0
55	MG	AA	3605	1/1	0.99	0.49	30.18	45,45,45,45	0
55	MG	AA	3509	1/1	0.85	1.46	29.52	80,80,80,80	0
55	MG	BA	1700	1/1	0.76	1.21	29.15	97,97,97,97	0
55	MG	AA	3268	1/1	0.99	0.75	28.77	47,47,47,47	0
55	MG	AA	3092	1/1	0.92	0.56	28.68	59,59,59,59	0
55	MG	DA	3156	1/1	0.95	0.52	28.58	62,62,62,62	0
55	MG	DA	3130	1/1	0.93	0.54	28.49	64,64,64,64	0
55	MG	DA	3332	1/1	0.62	0.56	28.27	90,90,90,90	0
55	MG	AA	3213	1/1	0.98	0.55	27.44	50,50,50,50	0
55	MG	DA	3489	1/1	0.96	0.52	27.01	57,57,57,57	0
55	MG	BA	1822	1/1	0.67	0.92	26.92	107,107,107,107	0
55	MG	AA	3141	1/1	0.98	0.53	25.01	37,37,37,37	0
55	MG	BA	1794	1/1	0.79	1.59	24.29	94,94,94,94	0
55	MG	DA	3482	1/1	0.94	0.48	24.15	56,56,56,56	0
55	MG	DA	3233	1/1	0.67	0.96	23.45	84,84,84,84	0
55	MG	AA	3031	1/1	0.95	0.56	23.11	44,44,44,44	0
55	MG	AA	3412	1/1	0.75	0.85	22.86	88,88,88,88	0
55	MG	AA	3052	1/1	0.88	0.67	22.68	74,74,74,74	0
55	MG	AA	3549	1/1	0.97	0.63	22.64	41,41,41,41	0
55	MG	AA	3153	1/1	0.98	0.45	22.32	33,33,33,33	0
55	MG	DA	3153	1/1	0.96	0.53	22.22	54,54,54,54	0
55	MG	DE	303	1/1	0.96	0.59	22.11	52,52,52,52	0
55	MG	AA	3027	1/1	0.96	0.50	21.92	49,49,49,49	0
55	MG	DA	3427	1/1	0.77	0.48	21.67	78,78,78,78	0
55	MG	DA	3094	1/1	0.97	0.54	21.29	45,45,45,45	0
55	MG	DA	3139	1/1	0.97	0.54	21.24	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3174	1/1	0.81	0.50	21.18	49,49,49,49	0
55	MG	DA	3267	1/1	0.31	0.51	20.82	74,74,74,74	0
55	MG	AA	3176	1/1	0.95	0.56	20.65	38,38,38,38	0
55	MG	AA	3081	1/1	0.97	0.65	20.56	41,41,41,41	0
55	MG	DA	3387	1/1	0.95	0.55	20.26	45,45,45,45	0
55	MG	DA	3045	1/1	0.85	0.66	20.00	79,79,79,79	0
55	MG	AA	3537	1/1	0.98	0.50	19.66	39,39,39,39	0
55	MG	DA	3492	1/1	0.97	0.62	19.45	48,48,48,48	0
55	MG	DA	3486	1/1	0.91	0.66	19.23	46,46,46,46	0
55	MG	CA	1770	1/1	0.66	0.51	19.17	75,75,75,75	0
55	MG	DA	3463	1/1	0.95	0.68	19.04	44,44,44,44	0
55	MG	DA	3204	1/1	0.96	0.45	18.99	50,50,50,50	0
55	MG	CA	1676	1/1	0.95	0.40	18.89	55,55,55,55	0
55	MG	DA	3190	1/1	0.93	0.50	18.54	46,46,46,46	0
55	MG	AA	3162	1/1	0.91	0.60	18.21	45,45,45,45	0
55	MG	DA	3234	1/1	0.89	0.54	18.18	55,55,55,55	0
55	MG	AA	3004	1/1	0.97	0.43	17.76	37,37,37,37	0
55	MG	AA	3174	1/1	0.96	0.51	17.55	43,43,43,43	0
55	MG	CA	1671	1/1	0.98	0.62	17.41	51,51,51,51	0
55	MG	AA	3084	1/1	0.96	0.49	17.08	40,40,40,40	0
55	MG	BA	1610	1/1	0.92	0.46	17.06	53,53,53,53	0
55	MG	BA	1658	1/1	0.94	0.76	17.06	54,54,54,54	0
55	MG	AA	3124	1/1	0.96	0.65	17.00	56,56,56,56	0
55	MG	CA	1633	1/1	0.88	0.48	16.76	79,79,79,79	0
55	MG	AA	3125	1/1	0.97	0.47	16.70	49,49,49,49	0
55	MG	DA	3484	1/1	0.96	0.58	16.51	46,46,46,46	0
55	MG	AA	3135	1/1	0.79	0.35	16.43	66,66,66,66	0
55	MG	AA	3547	1/1	0.86	0.41	16.18	45,45,45,45	0
55	MG	AA	3018	1/1	0.98	0.57	16.17	38,38,38,38	0
55	MG	DA	3188	1/1	0.97	0.56	16.12	48,48,48,48	0
55	MG	AA	3122	1/1	0.84	0.71	15.92	87,87,87,87	0
55	MG	AA	3578	1/1	0.90	0.52	15.58	52,52,52,52	0
55	MG	DA	3088	1/1	0.97	0.58	15.15	49,49,49,49	0
55	MG	DA	3460	1/1	0.96	0.53	15.04	45,45,45,45	0
55	MG	AA	3265	1/1	0.95	0.59	14.96	42,42,42,42	0
55	MG	CA	1720	1/1	0.32	0.63	14.86	108,108,108,108	0
55	MG	DA	3469	1/1	0.89	0.38	14.81	64,64,64,64	0
55	MG	AA	3024	1/1	0.98	0.47	14.76	35,35,35,35	0
55	MG	AA	3080	1/1	0.91	0.48	14.75	52,52,52,52	0
55	MG	AA	3085	1/1	0.82	0.40	14.75	62,62,62,62	0
55	MG	DA	3141	1/1	0.95	0.58	14.61	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1750	1/1	0.78	0.56	14.59	91,91,91,91	0
55	MG	DA	3092	1/1	0.98	0.42	14.55	47,47,47,47	0
55	MG	AA	3604	1/1	0.84	0.65	14.38	84,84,84,84	0
55	MG	DA	3457	1/1	0.85	0.49	14.15	62,62,62,62	0
55	MG	DA	3221	1/1	0.96	0.58	14.09	66,66,66,66	0
55	MG	DA	3146	1/1	0.97	0.56	14.07	38,38,38,38	0
55	MG	AA	3500	1/1	0.78	0.50	13.99	32,32,32,32	0
55	MG	DA	3014	1/1	0.91	0.38	13.94	62,62,62,62	0
55	MG	DA	3339	1/1	0.75	0.57	13.92	77,77,77,77	0
55	MG	AA	3021	1/1	0.94	0.41	13.89	38,38,38,38	0
55	MG	AA	3051	1/1	0.92	0.46	13.82	51,51,51,51	0
55	MG	AA	3014	1/1	0.97	0.60	13.78	41,41,41,41	0
55	MG	DA	3143	1/1	0.91	0.58	13.35	69,69,69,69	0
55	MG	DA	3205	1/1	0.94	0.38	13.35	60,60,60,60	0
55	MG	DA	3189	1/1	0.95	0.46	13.29	43,43,43,43	0
55	MG	AA	3139	1/1	0.95	0.45	13.16	42,42,42,42	0
55	MG	CA	1646	1/1	0.92	0.46	12.98	56,56,56,56	0
55	MG	AA	3107	1/1	0.92	0.42	12.93	56,56,56,56	0
55	MG	AA	3221	1/1	0.95	0.44	12.90	51,51,51,51	0
55	MG	DA	3096	1/1	0.96	0.37	12.87	47,47,47,47	0
55	MG	CA	1754	1/1	0.77	0.43	12.86	84,84,84,84	0
55	MG	DA	3181	1/1	0.98	0.42	12.85	48,48,48,48	0
55	MG	AA	3001	1/1	0.96	0.61	12.63	49,49,49,49	0
55	MG	DA	3209	1/1	0.97	0.60	12.63	54,54,54,54	0
55	MG	DA	3145	1/1	0.97	0.57	12.51	54,54,54,54	0
55	MG	AA	3579	1/1	0.98	0.48	12.47	35,35,35,35	0
55	MG	AA	3569	1/1	0.95	0.58	12.27	40,40,40,40	0
55	MG	DA	3467	1/1	0.92	0.40	12.25	49,49,49,49	0
55	MG	CC	102	1/1	0.95	0.53	12.24	69,69,69,69	0
55	MG	BA	1823	1/1	0.73	0.56	12.19	93,93,93,93	0
55	MG	AA	3006	1/1	0.97	0.54	12.19	60,60,60,60	0
55	MG	AA	3248	1/1	0.93	0.46	12.07	53,53,53,53	0
55	MG	DA	3095	1/1	0.94	0.35	11.78	45,45,45,45	0
55	MG	AA	3540	1/1	0.97	0.34	11.71	44,44,44,44	0
55	MG	DA	3191	1/1	0.98	0.60	11.44	47,47,47,47	0
55	MG	DA	3292	1/1	0.92	0.70	11.41	56,56,56,56	0
55	MG	AA	3442	1/1	0.93	0.38	11.39	49,49,49,49	0
55	MG	DA	3198	1/1	0.97	0.53	11.30	68,68,68,68	0
55	MG	DA	3200	1/1	0.88	0.40	11.24	66,66,66,66	0
55	MG	DA	3155	1/1	0.90	0.54	11.13	49,49,49,49	0
55	MG	AA	3054	1/1	0.90	0.39	11.09	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	AA	3254	1/1	0.76	0.40	11.07	97,97,97,97	0
55	MG	AA	3205	1/1	0.95	0.37	10.93	43,43,43,43	0
55	MG	AA	3196	1/1	0.92	0.32	10.83	60,60,60,60	0
55	MG	DA	3291	1/1	0.88	0.50	10.72	70,70,70,70	0
55	MG	DA	3319	1/1	0.90	0.41	10.72	68,68,68,68	0
55	MG	AA	3012	1/1	0.96	0.46	10.71	45,45,45,45	0
55	MG	DA	3178	1/1	0.95	0.34	10.65	45,45,45,45	0
55	MG	AA	3628	1/1	0.76	0.36	10.46	89,89,89,89	0
55	MG	AA	3020	1/1	0.96	0.45	10.46	31,31,31,31	0
55	MG	AA	3227	1/1	0.94	0.40	10.44	66,66,66,66	0
55	MG	CA	1776	1/1	0.55	0.49	10.27	91,91,91,91	0
55	MG	DA	3148	1/1	0.95	0.45	10.04	42,42,42,42	0
55	MG	DA	3215	1/1	0.99	0.57	10.01	50,50,50,50	0
55	MG	AA	3057	1/1	0.93	0.29	9.98	52,52,52,52	0
55	MG	AA	3593	1/1	0.76	0.46	9.84	90,90,90,90	0
55	MG	DA	3236	1/1	0.91	0.56	9.56	57,57,57,57	0
55	MG	BA	1780	1/1	0.94	0.45	9.55	58,58,58,58	0
55	MG	CA	1647	1/1	0.94	0.41	9.51	65,65,65,65	0
55	MG	AA	3575	1/1	0.92	0.33	9.50	40,40,40,40	0
55	MG	DA	3272	1/1	0.86	0.30	9.32	117,117,117,117	0
55	MG	DA	3106	1/1	0.96	0.41	9.21	46,46,46,46	0
55	MG	AA	3483	1/1	0.87	0.41	8.67	70,70,70,70	0
55	MG	AA	3045	1/1	0.93	0.37	8.53	50,50,50,50	0
55	MG	DA	3464	1/1	0.96	0.39	8.52	55,55,55,55	0
55	MG	AA	3431	1/1	-0.40	1.25	8.45	197,197,197,197	0
55	MG	AA	3002	1/1	0.98	0.42	8.39	40,40,40,40	0
55	MG	AA	3626	1/1	0.90	0.38	8.26	63,63,63,63	0
55	MG	AA	3582	1/1	0.93	0.35	8.26	33,33,33,33	0
55	MG	BA	1661	1/1	0.81	0.34	8.22	49,49,49,49	0
55	MG	DA	3050	1/1	0.90	0.66	8.08	78,78,78,78	0
55	MG	BC	101	1/1	0.95	0.51	8.05	58,58,58,58	0
55	MG	D1	202	1/1	0.66	0.68	8.02	102,102,102,102	0
55	MG	BA	1601	1/1	0.96	0.36	8.01	65,65,65,65	0
55	MG	DA	3348	1/1	0.91	0.53	7.45	77,77,77,77	0
55	MG	AA	3010	1/1	0.96	0.33	7.24	52,52,52,52	0
55	MG	BA	1766	1/1	0.55	0.68	7.19	116,116,116,116	0
55	MG	DA	3258	1/1	0.92	0.56	7.10	56,56,56,56	0
55	MG	DA	3075	1/1	0.72	0.48	6.94	80,80,80,80	0
55	MG	AA	3345	1/1	0.71	0.37	6.94	78,78,78,78	0
55	MG	AA	3128	1/1	0.87	0.32	6.75	54,54,54,54	0
55	MG	AA	3123	1/1	0.98	0.40	6.74	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3132	1/1	0.82	0.29	6.67	89,89,89,89	0
55	MG	DA	3341	1/1	0.93	0.49	6.66	62,62,62,62	0
55	MG	AA	3311	1/1	0.90	0.36	6.64	58,58,58,58	0
55	MG	AA	3573	1/1	0.77	0.43	6.62	47,47,47,47	0
55	MG	CA	1755	1/1	0.80	0.45	6.55	94,94,94,94	0
55	MG	AA	3073	1/1	0.93	0.43	6.45	76,76,76,76	0
55	MG	DA	3058	1/1	0.74	0.33	6.42	75,75,75,75	0
55	MG	CA	1630	1/1	0.72	0.46	6.28	76,76,76,76	0
55	MG	AA	3308	1/1	0.84	0.32	6.20	58,58,58,58	0
55	MG	AA	3548	1/1	0.94	0.28	6.16	31,31,31,31	0
55	MG	DA	3035	1/1	0.87	0.90	6.00	102,102,102,102	0
55	MG	CA	1645	1/1	0.93	0.32	5.98	71,71,71,71	0
55	MG	AA	3306	1/1	0.86	0.38	5.93	63,63,63,63	0
55	MG	BA	1651	1/1	0.90	0.39	5.92	73,73,73,73	0
55	MG	BA	1645	1/1	0.98	0.43	5.88	52,52,52,52	0
55	MG	CA	1690	1/1	0.86	0.36	5.80	74,74,74,74	0
55	MG	AA	3263	1/1	0.93	0.30	5.77	56,56,56,56	0
55	MG	BA	1720	1/1	0.80	0.30	5.74	71,71,71,71	0
55	MG	CA	1801	1/1	0.90	0.52	5.68	71,71,71,71	0
55	MG	CA	1698	1/1	0.81	0.48	5.65	104,104,104,104	0
55	MG	AA	3397	1/1	0.98	0.39	5.52	40,40,40,40	0
55	MG	AA	3053	1/1	0.94	0.34	5.47	59,59,59,59	0
55	MG	DA	3516	1/1	0.90	0.33	5.36	60,60,60,60	0
55	MG	AA	3453	1/1	0.89	0.36	5.29	47,47,47,47	0
55	MG	DA	3114	1/1	0.85	0.45	5.28	70,70,70,70	0
55	MG	DA	3440	1/1	0.37	0.49	5.13	92,92,92,92	0
55	MG	A1	201	1/1	0.94	0.37	5.07	49,49,49,49	0
55	MG	CA	1617	1/1	0.96	0.31	5.06	91,91,91,91	0
55	MG	CA	1749	1/1	0.77	0.29	5.00	106,106,106,106	0
55	MG	D1	201	1/1	0.80	0.51	4.96	73,73,73,73	0
55	MG	CA	1668	1/1	0.92	0.32	4.95	75,75,75,75	0
55	MG	AA	3610	1/1	0.98	0.33	4.79	34,34,34,34	0
55	MG	AA	3178	1/1	0.96	0.39	4.75	49,49,49,49	0
55	MG	DA	3336	1/1	0.95	0.30	4.74	68,68,68,68	0
55	MG	DA	3509	1/1	0.96	0.48	4.58	65,65,65,65	0
55	MG	AA	3113	1/1	0.99	0.47	4.48	55,55,55,55	0
55	MG	AD	302	1/1	0.97	0.37	4.43	44,44,44,44	0
55	MG	DA	3512	1/1	0.95	0.33	4.42	70,70,70,70	0
55	MG	DA	3422	1/1	0.85	0.31	4.29	96,96,96,96	0
55	MG	AA	3034	1/1	0.95	0.32	4.28	61,61,61,61	0
55	MG	CA	1685	1/1	0.93	0.36	4.19	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
55	MG	BA	1606	1/1	0.95	0.39	3.98	88,88,88,88	0
55	MG	AA	3376	1/1	0.93	0.29	3.88	67,67,67,67	0
55	MG	DA	3160	1/1	0.98	0.28	3.86	65,65,65,65	0
55	MG	DA	3117	1/1	0.88	0.37	3.79	68,68,68,68	0
55	MG	AA	3546	1/1	0.96	0.32	3.74	33,33,33,33	0
55	MG	CA	1691	1/1	0.89	0.32	3.73	69,69,69,69	0
55	MG	A6	101	1/1	0.54	1.59	3.47	121,121,121,121	0
55	MG	DA	3194	1/1	0.96	0.34	3.45	59,59,59,59	0
55	MG	AA	3522	1/1	0.62	0.29	3.39	67,67,67,67	0
55	MG	CA	1758	1/1	0.76	0.29	3.37	64,64,64,64	0
55	MG	DA	3262	1/1	0.93	0.30	3.33	39,39,39,39	0
55	MG	DA	3382	1/1	0.45	0.26	3.31	84,84,84,84	0
55	MG	DA	3255	1/1	0.95	0.26	3.19	83,83,83,83	0
55	MG	AA	3529	1/1	0.86	0.27	3.19	78,78,78,78	0
55	MG	CA	1722	1/1	0.94	0.32	3.17	63,63,63,63	0
55	MG	AA	3261	1/1	0.86	0.29	3.14	30,30,30,30	0
55	MG	AB	215	1/1	0.84	0.29	3.09	92,92,92,92	0
55	MG	AA	3050	1/1	0.95	0.32	2.96	69,69,69,69	0
55	MG	AA	3232	1/1	0.96	0.24	2.88	47,47,47,47	0
55	MG	AA	3159	1/1	0.95	0.32	2.84	30,30,30,30	0
55	MG	AA	3313	1/1	0.89	0.34	2.79	62,62,62,62	0
55	MG	BA	1786	1/1	0.92	0.31	2.77	72,72,72,72	0
55	MG	CA	1606	1/1	0.77	0.29	2.65	96,96,96,96	0
55	MG	CA	1686	1/1	0.91	0.34	2.63	68,68,68,68	0
55	MG	BA	1682	1/1	0.90	0.41	2.61	98,98,98,98	0
55	MG	BA	1715	1/1	0.89	0.27	2.59	69,69,69,69	0
55	MG	AA	3016	1/1	0.98	0.29	2.51	53,53,53,53	0
55	MG	DA	3101	1/1	0.96	0.30	2.50	57,57,57,57	0
55	MG	DA	3206	1/1	0.89	0.24	2.43	65,65,65,65	0
55	MG	BA	1710	1/1	0.69	0.37	2.42	99,99,99,99	0
55	MG	DA	3517	1/1	0.91	0.29	2.40	62,62,62,62	0
55	MG	BA	1608	1/1	0.92	0.33	2.29	63,63,63,63	0
55	MG	AA	3246	1/1	0.93	0.33	2.23	73,73,73,73	0
55	MG	BA	1699	1/1	0.93	0.27	2.17	58,58,58,58	0
55	MG	BA	1679	1/1	0.80	0.30	2.14	86,86,86,86	0
55	MG	DA	3159	1/1	0.87	0.31	1.97	52,52,52,52	0
55	MG	AA	3040	1/1	0.96	0.35	1.91	67,67,67,67	0
55	MG	AA	3393	1/1	0.79	0.25	1.84	91,91,91,91	0
55	MG	AA	3083	1/1	0.89	0.28	1.79	47,47,47,47	0
55	MG	B1	101	1/1	0.96	0.25	1.70	64,64,64,64	0
55	MG	DA	3030	1/1	0.88	0.24	1.59	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3252	1/1	0.70	0.22	1.58	68,68,68,68	0
55	MG	DA	3129	1/1	0.95	0.27	1.49	55,55,55,55	0
55	MG	AA	3119	1/1	0.96	0.22	1.38	64,64,64,64	0
55	MG	AB	202	1/1	0.86	0.28	1.36	86,86,86,86	0
55	MG	AA	3168	1/1	0.92	0.29	1.29	64,64,64,64	0
55	MG	DB	206	1/1	-0.34	0.27	1.26	122,122,122,122	0
55	MG	BA	1751	1/1	0.52	0.32	1.25	122,122,122,122	0
55	MG	BA	1764	1/1	0.69	0.39	1.25	93,93,93,93	0
55	MG	AA	3341	1/1	0.94	0.22	1.21	63,63,63,63	0
55	MG	DA	3358	1/1	0.88	0.21	1.14	90,90,90,90	0
55	MG	BA	1632	1/1	0.89	0.27	1.09	72,72,72,72	0
55	MG	CA	1674	1/1	0.92	0.27	1.07	76,76,76,76	0
55	MG	CA	1742	1/1	0.46	0.34	0.96	93,93,93,93	0
55	MG	BA	1619	1/1	0.94	0.30	0.93	67,67,67,67	0
55	MG	AA	3518	1/1	0.80	0.23	0.88	71,71,71,71	0
55	MG	AA	3570	1/1	0.90	0.27	0.83	49,49,49,49	0
55	MG	BN	201	1/1	0.97	0.23	0.80	67,67,67,67	0
55	MG	AE	304	1/1	0.91	0.33	0.79	85,85,85,85	0
55	MG	CA	1669	1/1	0.84	0.24	0.78	67,67,67,67	0
55	MG	AA	3044	1/1	0.97	0.27	0.66	54,54,54,54	0
55	MG	DA	3128	1/1	0.97	0.27	0.65	66,66,66,66	0
55	MG	DA	3436	1/1	0.79	0.26	0.57	69,69,69,69	0
55	MG	BA	1701	1/1	0.84	0.25	0.45	73,73,73,73	0
55	MG	AE	301	1/1	0.93	0.27	0.44	52,52,52,52	0
55	MG	AA	3087	1/1	0.89	0.25	0.42	45,45,45,45	0
55	MG	AA	3304	1/1	0.83	0.34	0.41	59,59,59,59	0
55	MG	AA	3194	1/1	0.95	0.27	0.40	54,54,54,54	0
55	MG	DA	3280	1/1	0.93	0.20	0.36	80,80,80,80	0
55	MG	DA	3357	1/1	0.72	0.27	0.30	89,89,89,89	0
55	MG	AA	3457	1/1	0.81	0.24	0.29	73,73,73,73	0
55	MG	DA	3111	1/1	0.92	0.28	0.27	67,67,67,67	0
55	MG	BA	1713	1/1	0.84	0.22	0.27	107,107,107,107	0
55	MG	AA	3067	1/1	0.91	0.24	0.13	61,61,61,61	0
55	MG	DA	3135	1/1	0.83	0.23	0.01	64,64,64,64	0
55	MG	AA	3097	1/1	0.99	0.23	-0.15	65,65,65,65	0
55	MG	A0	201	1/1	0.96	0.25	-0.24	46,46,46,46	0
55	MG	DA	3213	1/1	0.84	0.19	-0.25	94,94,94,94	0
55	MG	BG	301	1/1	0.90	0.20	-0.32	110,110,110,110	0
55	MG	AA	3165	1/1	0.54	0.24	-0.33	71,71,71,71	0
55	MG	CA	1808	1/1	0.96	0.23	-0.33	73,73,73,73	0
55	MG	BA	1628	1/1	0.86	0.27	-0.37	86,86,86,86	0
55	MG	AA	3046	1/1	0.93	0.21	-0.43	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3071	1/1	0.87	0.15	-0.44	99,99,99,99	0
56	ZN	BG	302	1/1	0.95	0.34	-0.45	95,95,95,95	0
55	MG	AA	3137	1/1	0.94	0.24	-0.46	43,43,43,43	0
55	MG	D0	201	1/1	0.88	0.25	-0.46	78,78,78,78	0
55	MG	DE	302	1/1	0.93	0.21	-0.48	75,75,75,75	0
55	MG	DA	3359	1/1	0.81	0.22	-0.48	75,75,75,75	0
55	MG	BA	1678	1/1	0.80	0.26	-0.55	75,75,75,75	0
55	MG	DA	3296	1/1	0.93	0.20	-0.58	56,56,56,56	0
55	MG	AA	3255	1/1	0.92	0.21	-0.60	61,61,61,61	0
55	MG	BA	1602	1/1	0.88	0.22	-0.69	65,65,65,65	0
55	MG	DA	3246	1/1	0.95	0.22	-0.71	66,66,66,66	0
55	MG	CA	1719	1/1	0.68	0.18	-0.77	157,157,157,157	0
55	MG	BA	1605	1/1	0.82	0.20	-0.77	69,69,69,69	0
56	ZN	CQ	101	1/1	0.99	0.16	-0.86	113,113,113,113	0
55	MG	BA	1792	1/1	0.75	0.22	-0.94	94,94,94,94	0
55	MG	BA	1663	1/1	0.94	0.22	-0.94	47,47,47,47	0
56	ZN	CG	304	1/1	0.99	0.28	-0.99	112,112,112,112	0
55	MG	CA	1784	1/1	0.91	0.20	-1.02	102,102,102,102	0
55	MG	DA	3330	1/1	0.92	0.18	-1.09	74,74,74,74	0
55	MG	AA	3322	1/1	0.81	0.20	-1.12	83,83,83,83	0
55	MG	AA	3063	1/1	0.95	0.18	-1.22	64,64,64,64	0
55	MG	AA	3091	1/1	0.97	0.22	-1.30	69,69,69,69	0
55	MG	CA	1649	1/1	0.94	0.16	-1.35	70,70,70,70	0
56	ZN	BQ	103	1/1	0.98	0.10	-1.38	129,129,129,129	0
55	MG	BA	1636	1/1	0.88	0.16	-1.39	92,92,92,92	0
55	MG	CA	1622	1/1	0.85	0.19	-1.40	74,74,74,74	0
55	MG	AA	3349	1/1	0.89	0.18	-1.40	79,79,79,79	0
55	MG	AA	3216	1/1	0.89	0.21	-1.41	56,56,56,56	0
55	MG	CA	1650	1/1	0.98	0.21	-1.45	90,90,90,90	0
55	MG	AA	3510	1/1	0.89	0.17	-1.45	73,73,73,73	0
55	MG	BA	1761	1/1	0.85	0.15	-1.49	85,85,85,85	0
55	MG	AA	3093	1/1	0.77	0.20	-1.49	55,55,55,55	0
55	MG	CA	1639	1/1	0.94	0.21	-1.57	64,64,64,64	0
55	MG	CG	303	1/1	0.92	0.12	-1.61	100,100,100,100	0
55	MG	BA	1824	1/1	0.87	0.15	-1.61	97,97,97,97	0
55	MG	AA	3330	1/1	0.79	0.15	-1.61	61,61,61,61	0
55	MG	AA	3460	1/1	0.88	0.18	-1.64	89,89,89,89	0
55	MG	BA	1635	1/1	0.76	0.28	-1.67	87,87,87,87	0
55	MG	DA	3411	1/1	0.92	0.19	-1.71	77,77,77,77	0
55	MG	BA	1709	1/1	0.86	0.16	-1.75	101,101,101,101	0
55	MG	DA	3488	1/1	0.96	0.24	-1.77	45,45,45,45	0
55	MG	AA	3600	1/1	0.95	0.12	-1.79	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3370	1/1	0.90	0.14	-1.82	85,85,85,85	0
55	MG	CA	1625	1/1	0.75	0.12	-1.86	85,85,85,85	0
55	MG	CA	1783	1/1	0.90	0.14	-1.90	72,72,72,72	0
55	MG	AA	3612	1/1	0.98	0.20	-1.93	38,38,38,38	0
55	MG	BA	1789	1/1	0.91	0.19	-1.97	69,69,69,69	0
55	MG	AA	3266	1/1	0.97	0.18	-2.02	47,47,47,47	0
55	MG	CA	1623	1/1	0.82	0.15	-2.15	98,98,98,98	0
55	MG	AA	3042	1/1	0.88	0.13	-2.19	67,67,67,67	0
55	MG	CA	1658	1/1	0.94	0.18	-2.22	78,78,78,78	0
55	MG	AA	3185	1/1	0.91	0.21	-2.33	43,43,43,43	0
55	MG	DB	202	1/1	0.91	0.15	-2.35	101,101,101,101	0
55	MG	CA	1653	1/1	0.88	0.20	-2.50	73,73,73,73	0
55	MG	DA	3073	1/1	0.81	0.13	-2.59	69,69,69,69	0
55	MG	AF	301	1/1	0.93	0.12	-2.63	75,75,75,75	0
55	MG	BA	1759	1/1	0.94	0.16	-2.66	97,97,97,97	0
55	MG	AA	3334	1/1	0.95	0.10	-2.77	73,73,73,73	0
55	MG	DA	3080	1/1	0.92	0.08	-2.79	114,114,114,114	0
55	MG	AA	3037	1/1	0.95	0.14	-2.97	50,50,50,50	0
55	MG	AA	3421	1/1	0.87	0.19	-3.06	64,64,64,64	0
55	MG	AA	3446	1/1	0.82	0.20	-3.19	93,93,93,93	0
55	MG	CA	1610	1/1	0.91	0.17	-3.33	75,75,75,75	0
55	MG	DA	3441	1/1	0.93	0.10	-3.36	67,67,67,67	0
55	MG	DA	3116	1/1	0.82	0.15	-3.38	96,96,96,96	0
55	MG	AA	3426	1/1	0.95	0.10	-3.72	123,123,123,123	0
55	MG	DA	3122	1/1	0.76	0.14	-3.74	71,71,71,71	0
55	MG	DA	3407	1/1	0.88	0.12	-3.77	80,80,80,80	0
55	MG	CA	1654	1/1	0.91	0.15	-4.13	88,88,88,88	0
55	MG	BA	1644	1/1	0.90	0.16	-4.32	78,78,78,78	0
55	MG	DA	3147	1/1	0.95	0.18	-4.47	16,16,16,16	0
55	MG	AA	3177	1/1	0.90	0.16	-4.48	45,45,45,45	0
55	MG	AA	3383	1/1	0.83	0.09	-4.64	70,70,70,70	0
55	MG	DA	3289	1/1	0.84	0.17	-4.72	47,47,47,47	0
55	MG	CA	1678	1/1	0.89	0.13	-5.18	67,67,67,67	0
55	MG	DA	3070	1/1	0.90	0.15	-5.48	73,73,73,73	0
55	MG	AA	3585	1/1	0.97	0.09	-5.53	46,46,46,46	0
55	MG	DA	3044	1/1	0.99	0.13	-5.74	66,66,66,66	0
55	MG	DA	3251	1/1	0.88	0.15	-5.91	50,50,50,50	0
55	MG	DA	3405	1/1	0.84	0.10	-6.11	97,97,97,97	0
55	MG	BC	107	1/1	0.93	0.11	-7.62	88,88,88,88	0
55	MG	CA	1628	1/1	0.86	0.16	-10.14	86,86,86,86	0
55	MG	DA	3195	1/1	0.90	0.23	-	73,73,73,73	0
55	MG	BA	1829	1/1	0.85	0.34	-	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1803	1/1	0.89	0.19	-	87,87,87,87	0
55	MG	BA	1743	1/1	0.94	0.34	-	58,58,58,58	0
55	MG	AB	211	1/1	0.93	0.08	-	105,105,105,105	0
55	MG	BA	1828	1/1	0.92	0.45	-	85,85,85,85	0
55	MG	AA	3181	1/1	0.84	0.29	-	92,92,92,92	0
55	MG	DA	3309	1/1	0.84	0.38	-	69,69,69,69	0
55	MG	CA	1741	1/1	0.97	0.30	-	83,83,83,83	0
55	MG	DA	3185	1/1	0.94	0.36	-	64,64,64,64	0
55	MG	BQ	102	1/1	0.74	0.88	-	89,89,89,89	0
55	MG	CA	1781	1/1	0.90	0.32	-	92,92,92,92	0
55	MG	BA	1717	1/1	0.90	0.97	-	79,79,79,79	0
55	MG	DA	3060	1/1	0.94	0.33	-	85,85,85,85	0
55	MG	BA	1696	1/1	0.83	0.24	-	90,90,90,90	0
55	MG	DA	3522	1/1	0.87	0.49	-	85,85,85,85	0
55	MG	DA	3473	1/1	0.60	0.25	-	103,103,103,103	0
55	MG	CA	1632	1/1	0.92	0.27	-	77,77,77,77	0
55	MG	BA	1706	1/1	0.98	0.74	-	55,55,55,55	0
55	MG	AA	3630	1/1	0.82	0.77	-	92,92,92,92	0
55	MG	DA	3334	1/1	0.52	0.60	-	95,95,95,95	0
55	MG	DA	3025	1/1	0.76	0.31	-	111,111,111,111	0
55	MG	DA	3404	1/1	0.71	1.21	-	91,91,91,91	0
55	MG	BA	1603	1/1	0.97	0.34	-	63,63,63,63	0
55	MG	CA	1737	1/1	0.90	0.28	-	109,109,109,109	0
55	MG	CA	1689	1/1	0.84	0.68	-	87,87,87,87	0
55	MG	AA	3161	1/1	0.95	0.61	-	41,41,41,41	0
55	MG	DB	211	1/1	0.87	0.26	-	104,104,104,104	0
55	MG	BQ	101	1/1	0.92	0.12	-	99,99,99,99	0
55	MG	CA	1733	1/1	0.96	0.34	-	66,66,66,66	0
55	MG	DA	3202	1/1	0.84	0.37	-	65,65,65,65	0
55	MG	AB	205	1/1	0.93	0.15	-	75,75,75,75	0
55	MG	CA	1710	1/1	0.88	0.11	-	105,105,105,105	0
55	MG	AA	3436	1/1	0.83	0.44	-	82,82,82,82	0
55	MG	DA	3298	1/1	0.47	0.41	-	95,95,95,95	0
55	MG	AA	3208	1/1	0.95	0.19	-	66,66,66,66	0
55	MG	CA	1791	1/1	0.91	0.71	-	70,70,70,70	0
55	MG	AA	3086	1/1	0.93	0.25	-	70,70,70,70	0
55	MG	AA	3062	1/1	0.63	0.41	-	73,73,73,73	0
55	MG	DA	3409	1/1	0.75	0.17	-	70,70,70,70	0
55	MG	AA	3056	1/1	0.91	0.22	-	64,64,64,64	0
55	MG	DA	3120	1/1	0.93	0.29	-	78,78,78,78	0
55	MG	AA	3136	1/1	0.98	0.21	-	40,40,40,40	0
55	MG	BA	1638	1/1	0.81	0.14	-	123,123,123,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3066	1/1	0.65	0.30	-	83,83,83,83	0
55	MG	AA	3350	1/1	0.91	0.67	-	59,59,59,59	0
55	MG	AA	3008	1/1	0.94	0.47	-	42,42,42,42	0
55	MG	DA	3390	1/1	0.57	0.19	-	81,81,81,81	0
55	MG	DA	3478	1/1	0.94	0.68	-	99,99,99,99	0
55	MG	CA	1709	1/1	0.93	0.37	-	81,81,81,81	0
55	MG	AA	3115	1/1	0.97	0.39	-	56,56,56,56	0
55	MG	AA	3625	1/1	0.92	0.74	-	70,70,70,70	0
55	MG	AA	3243	1/1	0.97	0.34	-	52,52,52,52	0
55	MG	DB	204	1/1	0.71	0.22	-	102,102,102,102	0
55	MG	CA	1611	1/1	0.70	0.71	-	76,76,76,76	0
55	MG	DA	3132	1/1	0.94	0.32	-	56,56,56,56	0
55	MG	AA	3367	1/1	0.61	0.39	-	101,101,101,101	0
55	MG	BB	108	1/1	0.91	0.21	-	106,106,106,106	0
55	MG	DA	3342	1/1	0.63	0.50	-	96,96,96,96	0
55	MG	CA	1641	1/1	0.84	0.49	-	101,101,101,101	0
55	MG	AA	3222	1/1	0.75	0.39	-	59,59,59,59	0
55	MG	DA	3192	1/1	0.94	0.40	-	51,51,51,51	0
55	MG	DA	3007	1/1	0.81	0.31	-	75,75,75,75	0
55	MG	AA	3292	1/1	0.92	0.44	-	80,80,80,80	0
55	MG	DA	3452	1/1	0.94	0.20	-	91,91,91,91	0
55	MG	BA	1736	1/1	0.75	1.14	-	89,89,89,89	0
55	MG	D5	101	1/1	0.95	0.50	-	50,50,50,50	0
55	MG	DA	3245	1/1	0.81	0.40	-	80,80,80,80	0
55	MG	BA	1729	1/1	0.82	0.15	-	85,85,85,85	0
55	MG	BA	1807	1/1	0.95	0.60	-	70,70,70,70	0
55	MG	AA	3309	1/1	0.80	0.34	-	64,64,64,64	0
55	MG	AA	3479	1/1	0.63	0.26	-	97,97,97,97	0
55	MG	DA	3047	1/1	0.76	0.39	-	84,84,84,84	0
55	MG	DA	3230	1/1	0.95	0.25	-	68,68,68,68	0
55	MG	CA	1736	1/1	0.66	1.27	-	90,90,90,90	0
55	MG	AA	3623	1/1	0.85	0.23	-	107,107,107,107	0
55	MG	AA	3448	1/1	0.91	0.19	-	85,85,85,85	0
55	MG	BA	1607	1/1	0.90	0.12	-	87,87,87,87	0
55	MG	CA	1747	1/1	0.76	0.34	-	114,114,114,114	0
55	MG	CB	101	1/1	0.78	0.76	-	102,102,102,102	0
55	MG	AA	3324	1/1	0.81	0.93	-	60,60,60,60	0
55	MG	AA	3584	1/1	0.89	0.24	-	94,94,94,94	0
55	MG	CA	1768	1/1	0.59	0.25	-	115,115,115,115	0
55	MG	AA	3432	1/1	0.97	0.65	-	41,41,41,41	0
55	MG	BA	1802	1/1	0.94	0.45	-	69,69,69,69	0
55	MG	DA	3294	1/1	0.86	0.25	-	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3278	1/1	0.85	1.04	-	81,81,81,81	0
55	MG	DA	3374	1/1	0.91	0.65	-	72,72,72,72	0
55	MG	AA	3226	1/1	0.93	0.91	-	85,85,85,85	0
55	MG	AA	3494	1/1	0.85	0.51	-	88,88,88,88	0
55	MG	DA	3355	1/1	0.86	0.43	-	93,93,93,93	0
55	MG	AA	3454	1/1	0.93	0.20	-	78,78,78,78	0
55	MG	DA	3458	1/1	0.67	0.88	-	88,88,88,88	0
55	MG	BA	1620	1/1	0.95	0.24	-	58,58,58,58	0
55	MG	BA	1760	1/1	0.93	0.52	-	67,67,67,67	0
55	MG	DA	3470	1/1	0.94	0.43	-	75,75,75,75	0
55	MG	CA	1794	1/1	0.92	0.44	-	72,72,72,72	0
55	MG	AA	3170	1/1	0.95	0.40	-	34,34,34,34	0
55	MG	CA	1712	1/1	0.75	0.36	-	86,86,86,86	0
55	MG	DA	3428	1/1	0.72	0.42	-	79,79,79,79	0
55	MG	AA	3422	1/1	0.95	0.84	-	73,73,73,73	0
55	MG	BA	1625	1/1	0.77	0.48	-	61,61,61,61	0
55	MG	AA	3260	1/1	0.95	0.26	-	70,70,70,70	0
55	MG	AA	3303	1/1	0.43	0.48	-	91,91,91,91	0
55	MG	AA	3244	1/1	0.86	0.27	-	69,69,69,69	0
55	MG	DA	3154	1/1	0.93	0.62	-	59,59,59,59	0
55	MG	DB	205	1/1	0.74	0.13	-	90,90,90,90	0
55	MG	CA	1748	1/1	0.41	0.44	-	91,91,91,91	0
55	MG	AA	3571	1/1	0.96	0.50	-	48,48,48,48	0
55	MG	BA	1779	1/1	0.42	0.77	-	105,105,105,105	0
55	MG	CC	105	1/1	0.76	0.46	-	74,74,74,74	0
55	MG	AA	3362	1/1	0.67	0.59	-	86,86,86,86	0
55	MG	DA	3220	1/1	0.91	0.51	-	67,67,67,67	0
55	MG	AA	3353	1/1	0.55	0.34	-	105,105,105,105	0
55	MG	DA	3067	1/1	0.95	0.22	-	75,75,75,75	0
55	MG	BA	1726	1/1	0.74	0.69	-	98,98,98,98	0
55	MG	AA	3402	1/1	0.90	0.41	-	94,94,94,94	0
55	MG	DA	3211	1/1	0.97	0.44	-	49,49,49,49	0
55	MG	AE	303	1/1	0.61	0.61	-	91,91,91,91	0
55	MG	AA	3076	1/1	0.85	0.07	-	109,109,109,109	0
55	MG	DA	3443	1/1	0.57	0.82	-	94,94,94,94	0
55	MG	DA	3033	1/1	0.95	0.09	-	94,94,94,94	0
55	MG	AA	3476	1/1	0.77	0.59	-	94,94,94,94	0
55	MG	AA	3435	1/1	0.65	0.29	-	137,137,137,137	0
55	MG	AA	3489	1/1	0.79	0.64	-	93,93,93,93	0
55	MG	BA	1801	1/1	0.94	0.11	-	93,93,93,93	0
55	MG	AA	3553	1/1	0.87	0.69	-	100,100,100,100	0
55	MG	AA	3225	1/1	0.93	0.29	-	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3385	1/1	0.94	0.19	-	75,75,75,75	0
55	MG	BA	1622	1/1	0.95	0.18	-	84,84,84,84	0
55	MG	BA	1650	1/1	0.92	0.42	-	78,78,78,78	0
55	MG	BA	1763	1/1	0.82	0.31	-	93,93,93,93	0
55	MG	AA	3534	1/1	0.86	0.49	-	100,100,100,100	0
55	MG	DA	3081	1/1	0.91	0.19	-	73,73,73,73	0
55	MG	AA	3621	1/1	0.91	0.21	-	100,100,100,100	0
55	MG	DA	3415	1/1	0.89	0.18	-	84,84,84,84	0
55	MG	CA	1615	1/1	0.44	0.41	-	92,92,92,92	0
55	MG	AD	301	1/1	0.73	1.41	-	100,100,100,100	0
55	MG	DA	3196	1/1	0.55	0.54	-	82,82,82,82	0
55	MG	AA	3179	1/1	0.86	0.54	-	70,70,70,70	0
55	MG	AA	3369	1/1	0.76	0.66	-	85,85,85,85	0
55	MG	BA	1769	1/1	0.54	0.35	-	86,86,86,86	0
55	MG	BA	1838	1/1	0.57	0.96	-	101,101,101,101	0
55	MG	BA	1675	1/1	0.74	0.48	-	89,89,89,89	0
55	MG	AA	3498	1/1	0.73	0.44	-	86,86,86,86	0
55	MG	CA	1766	1/1	0.82	0.24	-	75,75,75,75	0
55	MG	DA	3367	1/1	0.72	0.41	-	85,85,85,85	0
55	MG	AA	3368	1/1	0.94	0.46	-	83,83,83,83	0
55	MG	DA	3352	1/1	0.79	0.29	-	77,77,77,77	0
55	MG	BB	104	1/1	0.85	0.27	-	103,103,103,103	0
55	MG	BA	1690	1/1	0.58	0.25	-	109,109,109,109	0
55	MG	AA	3325	1/1	0.91	0.29	-	78,78,78,78	0
55	MG	DA	3408	1/1	0.86	0.30	-	61,61,61,61	0
55	MG	B1	102	1/1	0.90	0.50	-	69,69,69,69	0
55	MG	AA	3461	1/1	0.80	0.32	-	78,78,78,78	0
55	MG	AA	3011	1/1	0.98	0.51	-	38,38,38,38	0
55	MG	CA	1608	1/1	0.70	0.39	-	81,81,81,81	0
55	MG	AA	3068	1/1	0.96	0.43	-	49,49,49,49	0
55	MG	A5	102	1/1	0.81	0.41	-	75,75,75,75	0
55	MG	DA	3281	1/1	0.84	0.35	-	75,75,75,75	0
55	MG	AA	3245	1/1	0.73	0.33	-	81,81,81,81	0
55	MG	AB	201	1/1	0.85	0.18	-	91,91,91,91	0
55	MG	AA	3215	1/1	0.95	0.33	-	55,55,55,55	0
55	MG	AA	3543	1/1	0.96	0.61	-	61,61,61,61	0
55	MG	DA	3008	1/1	0.85	0.86	-	76,76,76,76	0
55	MG	DA	3071	1/1	0.92	0.25	-	74,74,74,74	0
55	MG	CA	1779	1/1	0.80	0.13	-	82,82,82,82	0
55	MG	BA	1744	1/1	0.88	0.35	-	93,93,93,93	0
55	MG	AA	3228	1/1	0.89	0.37	-	89,89,89,89	0
55	MG	DA	3461	1/1	0.92	0.40	-	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3049	1/1	0.86	0.98	-	72,72,72,72	0
55	MG	DA	3193	1/1	0.97	0.32	-	49,49,49,49	0
55	MG	AA	3312	1/1	0.66	0.38	-	88,88,88,88	0
55	MG	BA	1612	1/1	0.79	0.36	-	90,90,90,90	0
55	MG	AA	3588	1/1	0.88	0.67	-	63,63,63,63	0
55	MG	DB	209	1/1	0.92	0.62	-	103,103,103,103	0
55	MG	AA	3049	1/1	0.33	0.68	-	106,106,106,106	0
55	MG	BA	1659	1/1	0.94	0.87	-	70,70,70,70	0
55	MG	CA	1771	1/1	0.89	0.22	-	64,64,64,64	0
55	MG	DA	3518	1/1	0.93	0.52	-	63,63,63,63	0
55	MG	DA	3347	1/1	0.67	0.51	-	66,66,66,66	0
55	MG	DA	3386	1/1	0.76	0.27	-	88,88,88,88	0
55	MG	AA	3250	1/1	0.88	0.22	-	73,73,73,73	0
55	MG	AA	3408	1/1	0.95	0.72	-	70,70,70,70	0
55	MG	BA	1604	1/1	0.92	0.24	-	77,77,77,77	0
55	MG	A7	101	1/1	0.87	0.51	-	69,69,69,69	0
55	MG	CG	302	1/1	0.93	0.14	-	83,83,83,83	0
55	MG	BA	1799	1/1	0.94	0.29	-	85,85,85,85	0
55	MG	BA	1722	1/1	0.83	0.46	-	90,90,90,90	0
55	MG	CA	1681	1/1	0.87	0.36	-	71,71,71,71	0
55	MG	AA	3616	1/1	0.88	0.32	-	69,69,69,69	0
55	MG	BA	1641	1/1	0.98	0.59	-	62,62,62,62	0
55	MG	DA	3249	1/1	0.32	0.18	-	87,87,87,87	0
55	MG	AA	3166	1/1	0.97	0.30	-	63,63,63,63	0
55	MG	AA	3542	1/1	0.96	0.46	-	40,40,40,40	0
55	MG	AB	206	1/1	0.79	0.26	-	97,97,97,97	0
55	MG	AA	3318	1/1	0.28	0.97	-	120,120,120,120	0
55	MG	BA	1749	1/1	0.84	0.33	-	95,95,95,95	0
55	MG	BA	1667	1/1	0.94	0.29	-	78,78,78,78	0
55	MG	AA	3576	1/1	0.94	0.33	-	36,36,36,36	0
55	MG	AA	3477	1/1	0.72	0.23	-	65,65,65,65	0
55	MG	AA	3279	1/1	0.93	0.92	-	81,81,81,81	0
55	MG	AA	3438	1/1	0.62	0.26	-	77,77,77,77	0
55	MG	BA	1660	1/1	0.95	0.73	-	64,64,64,64	0
55	MG	BA	1703	1/1	0.61	0.68	-	118,118,118,118	0
55	MG	DA	3373	1/1	0.87	0.56	-	90,90,90,90	0
55	MG	DA	3279	1/1	0.88	0.31	-	66,66,66,66	0
55	MG	CA	1753	1/1	0.22	0.95	-	129,129,129,129	0
55	MG	CS	101	1/1	0.88	0.25	-	84,84,84,84	0
55	MG	DA	3385	1/1	0.78	0.53	-	90,90,90,90	0
55	MG	AA	3414	1/1	0.76	0.39	-	68,68,68,68	0
55	MG	AA	3288	1/1	0.90	0.85	-	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3326	1/1	0.90	0.53	-	63,63,63,63	0
55	MG	CA	1705	1/1	0.85	0.18	-	86,86,86,86	0
55	MG	DA	3011	1/1	0.83	0.51	-	68,68,68,68	0
55	MG	BA	1774	1/1	0.82	0.28	-	98,98,98,98	0
55	MG	DA	3519	1/1	0.79	0.36	-	114,114,114,114	0
55	MG	AA	3523	1/1	0.62	0.55	-	87,87,87,87	0
55	MG	DA	3167	1/1	0.84	0.27	-	72,72,72,72	0
55	MG	DA	3214	1/1	0.92	0.51	-	70,70,70,70	0
55	MG	AA	3622	1/1	0.90	0.20	-	71,71,71,71	0
55	MG	BA	1670	1/1	0.91	0.28	-	62,62,62,62	0
55	MG	BA	1754	1/1	0.42	0.35	-	80,80,80,80	0
55	MG	AA	3499	1/1	0.53	0.61	-	79,79,79,79	0
55	MG	CA	1735	1/1	0.83	0.13	-	86,86,86,86	0
55	MG	A5	101	1/1	0.90	0.61	-	49,49,49,49	0
55	MG	CA	1665	1/1	0.71	0.36	-	101,101,101,101	0
55	MG	AA	3258	1/1	0.81	0.15	-	80,80,80,80	0
55	MG	AA	3098	1/1	0.74	0.52	-	71,71,71,71	0
55	MG	DA	3006	1/1	0.90	0.43	-	78,78,78,78	0
55	MG	DA	3016	1/1	0.47	0.71	-	105,105,105,105	0
55	MG	BA	1740	1/1	0.91	0.12	-	72,72,72,72	0
55	MG	CA	1700	1/1	0.96	0.35	-	60,60,60,60	0
55	MG	AA	3274	1/1	0.79	0.23	-	77,77,77,77	0
55	MG	AA	3511	1/1	0.93	0.33	-	51,51,51,51	0
55	MG	AA	3513	1/1	0.73	0.54	-	73,73,73,73	0
55	MG	AA	3504	1/1	0.42	0.43	-	103,103,103,103	0
55	MG	BC	105	1/1	0.76	0.47	-	95,95,95,95	0
55	MG	DA	3013	1/1	0.95	0.56	-	55,55,55,55	0
55	MG	DA	3252	1/1	0.95	0.39	-	45,45,45,45	0
55	MG	BA	1816	1/1	0.89	0.34	-	87,87,87,87	0
55	MG	DA	3110	1/1	0.79	0.24	-	84,84,84,84	0
55	MG	DA	3466	1/1	0.94	0.63	-	78,78,78,78	0
55	MG	DA	3064	1/1	0.94	0.44	-	54,54,54,54	0
55	MG	AA	3409	1/1	0.68	0.91	-	98,98,98,98	0
55	MG	AA	3519	1/1	0.86	0.17	-	91,91,91,91	0
55	MG	BB	106	1/1	0.77	0.33	-	120,120,120,120	0
55	MG	AA	3411	1/1	0.89	0.17	-	84,84,84,84	0
55	MG	AA	3335	1/1	0.92	0.17	-	90,90,90,90	0
55	MG	AA	3398	1/1	0.86	0.17	-	91,91,91,91	0
55	MG	AA	3357	1/1	0.91	0.57	-	61,61,61,61	0
55	MG	AA	3580	1/1	0.96	0.80	-	44,44,44,44	0
55	MG	AA	3143	1/1	0.96	0.47	-	40,40,40,40	0
55	MG	DA	3523	1/1	0.77	0.72	-	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DB	208	1/1	0.38	0.55	-	114,114,114,114	0
55	MG	BA	1697	1/1	0.82	0.31	-	84,84,84,84	0
55	MG	CA	1761	1/1	0.61	0.45	-	96,96,96,96	0
55	MG	AA	3535	1/1	0.75	0.22	-	82,82,82,82	0
55	MG	DA	3430	1/1	0.75	0.69	-	102,102,102,102	0
55	MG	CA	1656	1/1	0.81	0.20	-	87,87,87,87	0
55	MG	DA	3349	1/1	0.98	0.18	-	83,83,83,83	0
55	MG	AA	3130	1/1	0.89	0.21	-	59,59,59,59	0
55	MG	AA	3473	1/1	0.82	0.35	-	70,70,70,70	0
55	MG	DA	3333	1/1	0.94	0.39	-	85,85,85,85	0
55	MG	BA	1812	1/1	0.82	0.31	-	76,76,76,76	0
55	MG	AA	3133	1/1	0.97	0.62	-	38,38,38,38	0
55	MG	DA	3308	1/1	0.79	0.11	-	95,95,95,95	0
55	MG	DA	3208	1/1	0.97	0.51	-	40,40,40,40	0
55	MG	DA	3210	1/1	0.98	0.37	-	51,51,51,51	0
55	MG	AA	3157	1/1	0.94	0.57	-	41,41,41,41	0
55	MG	DA	3018	1/1	0.76	0.59	-	85,85,85,85	0
55	MG	DA	3126	1/1	0.95	0.61	-	39,39,39,39	0
55	MG	AA	3568	1/1	0.93	0.56	-	29,29,29,29	0
55	MG	DA	3078	1/1	0.90	0.24	-	87,87,87,87	0
55	MG	AA	3134	1/1	0.81	0.53	-	59,59,59,59	0
55	MG	BA	1814	1/1	0.85	0.19	-	86,86,86,86	0
55	MG	AA	3417	1/1	0.73	0.36	-	78,78,78,78	0
55	MG	AA	3424	1/1	0.65	0.46	-	77,77,77,77	0
55	MG	AA	3281	1/1	0.91	0.28	-	67,67,67,67	0
55	MG	AA	3095	1/1	0.69	0.18	-	75,75,75,75	0
55	MG	AA	3452	1/1	0.74	0.16	-	95,95,95,95	0
55	MG	AA	3273	1/1	0.90	0.88	-	63,63,63,63	0
55	MG	DA	3057	1/1	0.73	0.59	-	81,81,81,81	0
55	MG	DA	3076	1/1	0.91	0.14	-	96,96,96,96	0
55	MG	DA	3163	1/1	0.86	0.44	-	97,97,97,97	0
55	MG	AA	3565	1/1	0.67	1.20	-	81,81,81,81	0
55	MG	BA	1803	1/1	0.84	0.22	-	81,81,81,81	0
55	MG	AA	3399	1/1	0.87	0.43	-	71,71,71,71	0
55	MG	CA	1718	1/1	0.80	0.12	-	78,78,78,78	0
55	MG	DA	3293	1/1	0.94	0.23	-	67,67,67,67	0
55	MG	CA	1675	1/1	0.93	0.57	-	65,65,65,65	0
55	MG	AA	3533	1/1	0.70	0.44	-	89,89,89,89	0
55	MG	DA	3314	1/1	0.92	0.40	-	78,78,78,78	0
55	MG	BA	1825	1/1	0.93	0.14	-	104,104,104,104	0
55	MG	BA	1773	1/1	0.75	0.58	-	79,79,79,79	0
55	MG	DA	3240	1/1	0.88	0.27	-	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	1800	1/1	0.64	0.31	-	101,101,101,101	0
55	MG	BA	1677	1/1	0.74	0.22	-	92,92,92,92	0
55	MG	CA	1721	1/1	0.87	0.37	-	94,94,94,94	0
55	MG	BA	1815	1/1	0.90	0.64	-	81,81,81,81	0
55	MG	CA	1767	1/1	0.57	0.42	-	94,94,94,94	0
55	MG	AA	3210	1/1	0.95	0.74	-	58,58,58,58	0
55	MG	AA	3441	1/1	0.89	0.21	-	76,76,76,76	0
55	MG	AA	3074	1/1	0.62	0.45	-	81,81,81,81	0
55	MG	BA	1796	1/1	0.66	0.24	-	78,78,78,78	0
55	MG	AA	3439	1/1	0.89	0.16	-	93,93,93,93	0
55	MG	BA	1770	1/1	0.78	0.17	-	106,106,106,106	0
55	MG	DA	3121	1/1	0.49	0.51	-	99,99,99,99	0
55	MG	DB	207	1/1	0.42	0.39	-	98,98,98,98	0
55	MG	AA	3538	1/1	0.98	0.42	-	37,37,37,37	0
55	MG	DA	3039	1/1	0.78	0.42	-	82,82,82,82	0
55	MG	AA	3033	1/1	0.97	0.33	-	46,46,46,46	0
55	MG	DA	3266	1/1	0.88	0.22	-	97,97,97,97	0
55	MG	DA	3479	1/1	0.80	1.44	-	87,87,87,87	0
55	MG	AA	3449	1/1	0.64	0.21	-	76,76,76,76	0
55	MG	AA	3480	1/1	0.90	0.23	-	77,77,77,77	0
55	MG	AA	3295	1/1	0.94	0.28	-	70,70,70,70	0
55	MG	BA	1817	1/1	0.89	0.55	-	92,92,92,92	0
55	MG	DA	3394	1/1	0.95	0.43	-	70,70,70,70	0
55	MG	AA	3140	1/1	0.88	0.52	-	53,53,53,53	0
55	MG	CC	103	1/1	0.94	1.08	-	72,72,72,72	0
55	MG	BA	1819	1/1	0.76	0.25	-	107,107,107,107	0
55	MG	DA	3361	1/1	0.88	0.55	-	102,102,102,102	0
55	MG	DA	3158	1/1	0.89	0.33	-	77,77,77,77	0
55	MG	AA	3420	1/1	0.87	0.18	-	107,107,107,107	0
55	MG	AA	3078	1/1	0.86	0.22	-	84,84,84,84	0
55	MG	AA	3541	1/1	0.66	0.88	-	94,94,94,94	0
55	MG	AA	3351	1/1	0.52	1.02	-	84,84,84,84	0
55	MG	DA	3315	1/1	0.80	0.32	-	82,82,82,82	0
55	MG	AA	3347	1/1	0.72	0.42	-	92,92,92,92	0
55	MG	AA	3035	1/1	0.98	0.28	-	46,46,46,46	0
55	MG	DA	3290	1/1	0.93	0.44	-	59,59,59,59	0
55	MG	AA	3180	1/1	0.98	0.41	-	56,56,56,56	0
55	MG	DA	3515	1/1	0.96	0.36	-	52,52,52,52	0
55	MG	DA	3125	1/1	0.85	0.26	-	86,86,86,86	0
55	MG	DA	3119	1/1	0.81	0.28	-	80,80,80,80	0
55	MG	AA	3415	1/1	0.80	0.30	-	86,86,86,86	0
55	MG	BA	1776	1/1	0.82	0.35	-	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3055	1/1	0.82	0.20	-	100,100,100,100	0
55	MG	DA	3395	1/1	0.82	0.70	-	80,80,80,80	0
55	MG	AA	3064	1/1	0.91	0.32	-	77,77,77,77	0
55	MG	AA	3102	1/1	0.66	0.28	-	108,108,108,108	0
55	MG	CA	1780	1/1	0.84	0.34	-	124,124,124,124	0
55	MG	DA	3476	1/1	0.93	0.65	-	76,76,76,76	0
55	MG	DA	3046	1/1	0.92	0.45	-	60,60,60,60	0
55	MG	BA	1738	1/1	0.86	0.31	-	73,73,73,73	0
55	MG	DA	3166	1/1	0.78	0.47	-	86,86,86,86	0
55	MG	CA	1805	1/1	0.80	0.18	-	81,81,81,81	0
55	MG	AA	3286	1/1	0.89	0.49	-	69,69,69,69	0
55	MG	BA	1723	1/1	0.89	0.35	-	95,95,95,95	0
55	MG	AA	3490	1/1	0.89	0.25	-	88,88,88,88	0
55	MG	DA	3112	1/1	0.89	0.11	-	70,70,70,70	0
55	MG	AA	3088	1/1	0.96	0.72	-	60,60,60,60	0
55	MG	AA	3105	1/1	0.97	0.27	-	64,64,64,64	0
55	MG	CA	1743	1/1	0.89	0.34	-	71,71,71,71	0
55	MG	DA	3510	1/1	0.73	0.79	-	67,67,67,67	0
55	MG	CA	1809	1/1	0.93	0.17	-	100,100,100,100	0
55	MG	CA	1760	1/1	0.87	0.27	-	103,103,103,103	0
55	MG	AA	3239	1/1	0.93	0.14	-	70,70,70,70	0
55	MG	BA	1806	1/1	0.93	0.28	-	75,75,75,75	0
55	MG	DA	3379	1/1	0.79	0.51	-	99,99,99,99	0
55	MG	DA	3502	1/1	0.71	0.33	-	96,96,96,96	0
55	MG	CA	1662	1/1	0.49	0.59	-	102,102,102,102	0
55	MG	AA	3277	1/1	0.56	0.67	-	98,98,98,98	0
55	MG	DA	3238	1/1	0.92	0.30	-	80,80,80,80	0
55	MG	DA	3475	1/1	0.83	1.12	-	81,81,81,81	0
55	MG	AA	3470	1/1	0.91	0.31	-	59,59,59,59	0
55	MG	AA	3007	1/1	0.98	0.28	-	33,33,33,33	0
55	MG	BA	1618	1/1	0.82	0.26	-	94,94,94,94	0
55	MG	DA	3237	1/1	0.83	0.94	-	84,84,84,84	0
55	MG	AA	3104	1/1	0.83	0.51	-	54,54,54,54	0
55	MG	BA	1694	1/1	0.61	0.30	-	99,99,99,99	0
55	MG	BB	105	1/1	0.59	0.37	-	115,115,115,115	0
55	MG	DA	3432	1/1	0.79	0.33	-	89,89,89,89	0
55	MG	CA	1798	1/1	0.90	0.12	-	96,96,96,96	0
55	MG	AA	3374	1/1	0.58	0.55	-	96,96,96,96	0
55	MG	AA	3348	1/1	0.75	0.35	-	92,92,92,92	0
55	MG	CA	1789	1/1	0.40	0.18	-	117,117,117,117	0
55	MG	AA	3271	1/1	0.93	0.48	-	68,68,68,68	0
55	MG	AA	3444	1/1	0.80	0.31	-	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3505	1/1	0.70	0.62	-	87,87,87,87	0
55	MG	DA	3235	1/1	0.95	0.34	-	53,53,53,53	0
55	MG	DA	3223	1/1	0.90	0.18	-	83,83,83,83	0
55	MG	AA	3594	1/1	0.58	0.26	-	97,97,97,97	0
55	MG	CA	1777	1/1	0.57	0.37	-	95,95,95,95	0
55	MG	DA	3273	1/1	0.79	0.74	-	108,108,108,108	0
55	MG	AA	3264	1/1	0.92	0.62	-	74,74,74,74	0
55	MG	BB	103	1/1	0.69	0.42	-	87,87,87,87	0
55	MG	DA	3241	1/1	0.86	0.21	-	85,85,85,85	0
55	MG	CC	106	1/1	0.78	0.62	-	115,115,115,115	0
55	MG	DA	3362	1/1	0.73	0.63	-	86,86,86,86	0
55	MG	DA	3364	1/1	0.65	0.40	-	85,85,85,85	0
55	MG	AA	3508	1/1	0.85	0.47	-	96,96,96,96	0
55	MG	DA	3401	1/1	0.85	0.40	-	75,75,75,75	0
55	MG	AA	3059	1/1	0.85	0.22	-	84,84,84,84	0
55	MG	BA	1681	1/1	0.56	0.23	-	79,79,79,79	0
55	MG	AA	3218	1/1	0.87	0.59	-	77,77,77,77	0
55	MG	DA	3328	1/1	0.68	0.39	-	83,83,83,83	0
55	MG	DA	3378	1/1	0.93	0.25	-	56,56,56,56	0
55	MG	AA	3491	1/1	0.71	0.14	-	93,93,93,93	0
55	MG	DA	3109	1/1	0.61	0.25	-	97,97,97,97	0
55	MG	AA	3333	1/1	0.67	0.20	-	80,80,80,80	0
55	MG	DA	3380	1/1	0.86	0.94	-	74,74,74,74	0
55	MG	DA	3311	1/1	0.67	0.26	-	80,80,80,80	0
55	MG	AA	3401	1/1	0.82	0.25	-	98,98,98,98	0
55	MG	DB	201	1/1	0.90	0.18	-	77,77,77,77	0
55	MG	BA	1753	1/1	0.92	0.18	-	91,91,91,91	0
55	MG	DA	3063	1/1	0.77	0.69	-	86,86,86,86	0
55	MG	AA	3410	1/1	0.93	0.26	-	99,99,99,99	0
55	MG	AA	3203	1/1	0.98	0.48	-	53,53,53,53	0
55	MG	CA	1731	1/1	0.89	0.61	-	85,85,85,85	0
55	MG	BA	1623	1/1	0.82	0.83	-	68,68,68,68	0
55	MG	CA	1659	1/1	0.89	0.15	-	111,111,111,111	0
55	MG	AA	3283	1/1	0.97	0.34	-	74,74,74,74	0
55	MG	AA	3406	1/1	0.61	0.14	-	99,99,99,99	0
55	MG	CA	1800	1/1	0.61	0.20	-	102,102,102,102	0
55	MG	DA	3318	1/1	0.95	0.66	-	93,93,93,93	0
55	MG	CA	1702	1/1	0.84	0.27	-	74,74,74,74	0
55	MG	AA	3572	1/1	0.96	0.49	-	40,40,40,40	0
55	MG	BA	1737	1/1	0.70	0.16	-	102,102,102,102	0
55	MG	DA	3376	1/1	0.74	0.22	-	88,88,88,88	0
55	MG	CA	1738	1/1	0.91	0.35	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	1833	1/1	0.82	0.30	-	88,88,88,88	0
55	MG	DA	3089	1/1	0.99	0.29	-	46,46,46,46	0
55	MG	AA	3075	1/1	0.83	0.33	-	71,71,71,71	0
55	MG	BA	1653	1/1	0.65	0.34	-	91,91,91,91	0
55	MG	AA	3305	1/1	0.95	0.41	-	62,62,62,62	0
55	MG	CA	1723	1/1	0.78	0.14	-	93,93,93,93	0
55	MG	BA	1672	1/1	0.56	0.47	-	104,104,104,104	0
55	MG	BA	1716	1/1	0.85	0.41	-	90,90,90,90	0
55	MG	AA	3101	1/1	0.58	0.16	-	69,69,69,69	0
55	MG	CA	1745	1/1	0.78	0.14	-	87,87,87,87	0
55	MG	AA	3524	1/1	0.82	0.28	-	72,72,72,72	0
55	MG	AA	3039	1/1	0.92	0.27	-	80,80,80,80	0
55	MG	CC	107	1/1	0.82	0.66	-	102,102,102,102	0
55	MG	DA	3431	1/1	0.76	0.16	-	93,93,93,93	0
55	MG	CA	1788	1/1	0.97	0.67	-	68,68,68,68	0
55	MG	DA	3222	1/1	0.93	0.51	-	57,57,57,57	0
55	MG	DA	3345	1/1	0.81	0.23	-	75,75,75,75	0
55	MG	BA	1609	1/1	0.67	0.49	-	84,84,84,84	0
55	MG	DA	3079	1/1	0.96	0.21	-	83,83,83,83	0
55	MG	DA	3504	1/1	0.92	0.17	-	119,119,119,119	0
55	MG	CA	1772	1/1	0.92	0.58	-	76,76,76,76	0
55	MG	CA	1703	1/1	0.91	0.13	-	88,88,88,88	0
55	MG	CA	1699	1/1	0.83	0.58	-	106,106,106,106	0
55	MG	DA	3438	1/1	0.89	0.55	-	102,102,102,102	0
55	MG	AA	3211	1/1	0.94	0.59	-	43,43,43,43	0
55	MG	AA	3464	1/1	0.68	0.61	-	83,83,83,83	0
55	MG	DA	3426	1/1	0.87	0.19	-	94,94,94,94	0
55	MG	AA	3280	1/1	0.91	0.46	-	65,65,65,65	0
55	MG	AA	3030	1/1	0.98	0.51	-	51,51,51,51	0
55	MG	DA	3439	1/1	0.86	0.65	-	92,92,92,92	0
55	MG	BA	1772	1/1	0.88	0.22	-	89,89,89,89	0
55	MG	BA	1739	1/1	0.66	0.20	-	79,79,79,79	0
55	MG	BA	1634	1/1	0.96	0.29	-	68,68,68,68	0
55	MG	BA	1704	1/1	0.94	0.45	-	87,87,87,87	0
55	MG	DA	3183	1/1	0.84	0.36	-	59,59,59,59	0
55	MG	AA	3425	1/1	0.93	0.36	-	70,70,70,70	0
55	MG	AA	3327	1/1	0.91	0.19	-	82,82,82,82	0
55	MG	DA	3265	1/1	0.96	0.25	-	63,63,63,63	0
55	MG	CA	1711	1/1	0.73	0.20	-	88,88,88,88	0
55	MG	AA	3564	1/1	0.99	0.57	-	54,54,54,54	0
55	MG	DA	3506	1/1	0.72	0.30	-	80,80,80,80	0
55	MG	AA	3120	1/1	0.82	0.39	-	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3609	1/1	0.97	0.36	-	39,39,39,39	0
55	MG	AA	3566	1/1	0.80	0.68	-	73,73,73,73	0
55	MG	DA	3450	1/1	0.93	0.19	-	86,86,86,86	0
55	MG	AA	3458	1/1	0.86	0.33	-	105,105,105,105	0
55	MG	AA	3372	1/1	0.94	0.19	-	77,77,77,77	0
55	MG	DA	3077	1/1	0.92	0.53	-	82,82,82,82	0
55	MG	DA	3175	1/1	0.96	0.53	-	70,70,70,70	0
55	MG	AA	3430	1/1	0.66	0.55	-	88,88,88,88	0
55	MG	AA	3437	1/1	0.67	0.16	-	105,105,105,105	0
55	MG	BA	1631	1/1	0.87	0.17	-	67,67,67,67	0
55	MG	DA	3320	1/1	0.94	0.23	-	73,73,73,73	0
55	MG	AA	3467	1/1	0.63	0.28	-	83,83,83,83	0
55	MG	DA	3270	1/1	0.56	0.55	-	73,73,73,73	0
55	MG	AA	3455	1/1	0.88	0.45	-	61,61,61,61	0
55	MG	DA	3414	1/1	0.86	0.32	-	74,74,74,74	0
55	MG	AA	3251	1/1	0.73	0.48	-	97,97,97,97	0
55	MG	AA	3036	1/1	0.93	0.41	-	34,34,34,34	0
55	MG	BA	1748	1/1	0.88	0.78	-	61,61,61,61	0
55	MG	DA	3098	1/1	0.90	0.35	-	41,41,41,41	0
55	MG	AA	3253	1/1	0.90	0.47	-	82,82,82,82	0
55	MG	DA	3219	1/1	0.71	0.61	-	79,79,79,79	0
55	MG	BC	102	1/1	0.61	0.32	-	100,100,100,100	0
55	MG	CA	1603	1/1	0.83	0.28	-	75,75,75,75	0
55	MG	BA	1630	1/1	0.80	0.83	-	105,105,105,105	0
55	MG	DA	3254	1/1	0.76	0.33	-	84,84,84,84	0
55	MG	AA	3029	1/1	0.98	0.30	-	50,50,50,50	0
55	MG	AA	3182	1/1	0.85	0.12	-	77,77,77,77	0
55	MG	BA	1820	1/1	0.93	0.35	-	97,97,97,97	0
55	MG	DA	3248	1/1	0.87	0.30	-	98,98,98,98	0
55	MG	CA	1620	1/1	0.77	0.70	-	70,70,70,70	0
55	MG	BA	1834	1/1	0.74	0.89	-	86,86,86,86	0
55	MG	DA	3444	1/1	0.80	0.16	-	82,82,82,82	0
55	MG	DA	3287	1/1	0.92	0.68	-	62,62,62,62	0
55	MG	DA	3042	1/1	0.61	0.54	-	84,84,84,84	0
55	MG	AA	3155	1/1	0.78	0.77	-	61,61,61,61	0
55	MG	DA	3425	1/1	0.73	0.50	-	88,88,88,88	0
55	MG	AA	3373	1/1	0.85	0.80	-	71,71,71,71	0
55	MG	BC	104	1/1	0.22	1.10	-	106,106,106,106	0
55	MG	DA	3468	1/1	0.94	0.47	-	53,53,53,53	0
55	MG	DA	3012	1/1	0.84	0.47	-	64,64,64,64	0
55	MG	BA	1837	1/1	0.81	0.66	-	88,88,88,88	0
55	MG	DA	3260	1/1	0.44	0.56	-	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1763	1/1	0.50	0.20	-	96,96,96,96	0
55	MG	AA	3597	1/1	0.90	0.53	-	67,67,67,67	0
55	MG	DA	3137	1/1	0.86	0.31	-	78,78,78,78	0
55	MG	DA	3253	1/1	0.92	0.32	-	83,83,83,83	0
55	MG	AA	3379	1/1	0.70	0.95	-	88,88,88,88	0
55	MG	BA	1730	1/1	0.75	0.26	-	97,97,97,97	0
55	MG	CA	1716	1/1	0.90	0.27	-	78,78,78,78	0
55	MG	BC	109	1/1	0.36	0.65	-	92,92,92,92	0
55	MG	DA	3286	1/1	0.94	0.89	-	86,86,86,86	0
55	MG	DA	3278	1/1	0.80	0.66	-	116,116,116,116	0
55	MG	AO	202	1/1	0.81	0.27	-	74,74,74,74	0
55	MG	BA	1680	1/1	0.92	0.32	-	71,71,71,71	0
55	MG	AA	3356	1/1	0.70	0.37	-	72,72,72,72	0
55	MG	CA	1785	1/1	0.90	0.23	-	81,81,81,81	0
55	MG	DA	3087	1/1	0.95	0.53	-	48,48,48,48	0
55	MG	AA	3236	1/1	0.87	0.26	-	93,93,93,93	0
55	MG	CA	1636	1/1	0.82	0.35	-	80,80,80,80	0
55	MG	BA	1687	1/1	0.73	0.26	-	74,74,74,74	0
55	MG	BA	1676	1/1	0.89	0.45	-	81,81,81,81	0
55	MG	BA	1614	1/1	0.90	0.28	-	93,93,93,93	0
55	MG	AA	3090	1/1	0.92	0.44	-	68,68,68,68	0
55	MG	DA	3034	1/1	0.94	0.28	-	72,72,72,72	0
55	MG	DA	3429	1/1	0.60	0.44	-	94,94,94,94	0
55	MG	CA	1799	1/1	0.68	0.58	-	95,95,95,95	0
55	MG	AA	3375	1/1	0.93	0.25	-	74,74,74,74	0
55	MG	AB	209	1/1	0.87	0.26	-	103,103,103,103	0
55	MG	BA	1731	1/1	0.92	0.42	-	67,67,67,67	0
55	MG	DA	3391	1/1	0.88	0.21	-	86,86,86,86	0
55	MG	CB	103	1/1	0.78	0.37	-	110,110,110,110	0
55	MG	AA	3163	1/1	0.93	0.51	-	48,48,48,48	0
55	MG	AA	3323	1/1	0.89	0.11	-	93,93,93,93	0
55	MG	DA	3124	1/1	0.10	1.32	-	111,111,111,111	0
55	MG	BA	1831	1/1	0.68	0.48	-	116,116,116,116	0
55	MG	AA	3371	1/1	0.80	0.52	-	69,69,69,69	0
55	MG	DA	3335	1/1	0.74	0.38	-	72,72,72,72	0
55	MG	BA	1642	1/1	0.92	0.43	-	69,69,69,69	0
55	MG	DA	3164	1/1	0.85	0.18	-	65,65,65,65	0
55	MG	DA	3323	1/1	0.49	0.65	-	85,85,85,85	0
55	MG	CA	1661	1/1	0.67	0.24	-	105,105,105,105	0
55	MG	DA	3074	1/1	0.71	0.35	-	89,89,89,89	0
55	MG	DA	3381	1/1	0.78	0.35	-	89,89,89,89	0
55	MG	DA	3199	1/1	0.97	0.36	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3419	1/1	0.66	0.62	-	90,90,90,90	0
55	MG	DA	3232	1/1	0.72	0.34	-	75,75,75,75	0
55	MG	AA	3079	1/1	0.49	0.56	-	100,100,100,100	0
55	MG	AA	3184	1/1	0.77	0.36	-	90,90,90,90	0
55	MG	AA	3015	1/1	0.97	0.50	-	30,30,30,30	0
55	MG	DA	3338	1/1	0.91	1.10	-	75,75,75,75	0
55	MG	AA	3058	1/1	0.85	0.09	-	85,85,85,85	0
55	MG	DA	3316	1/1	0.86	0.18	-	87,87,87,87	0
55	MG	DA	3149	1/1	0.94	0.69	-	60,60,60,60	0
55	MG	DA	3054	1/1	0.49	0.59	-	105,105,105,105	0
55	MG	DA	3423	1/1	0.72	0.35	-	102,102,102,102	0
55	MG	AA	3070	1/1	0.91	0.75	-	66,66,66,66	0
55	MG	AA	3223	1/1	0.40	0.64	-	72,72,72,72	0
55	MG	AA	3482	1/1	0.90	0.61	-	82,82,82,82	0
55	MG	CA	1601	1/1	0.76	0.39	-	95,95,95,95	0
55	MG	DA	3072	1/1	0.92	0.33	-	98,98,98,98	0
55	MG	AA	3354	1/1	0.94	0.57	-	79,79,79,79	0
55	MG	AA	3164	1/1	0.67	0.54	-	102,102,102,102	0
55	MG	AA	3217	1/1	0.96	0.37	-	58,58,58,58	0
55	MG	AA	3293	1/1	0.81	0.54	-	87,87,87,87	0
55	MG	DA	3297	1/1	0.85	0.34	-	70,70,70,70	0
55	MG	BA	1671	1/1	0.81	0.33	-	74,74,74,74	0
55	MG	BA	1624	1/1	0.76	0.42	-	92,92,92,92	0
55	MG	DA	3268	1/1	0.70	0.45	-	82,82,82,82	0
55	MG	DA	3363	1/1	0.91	0.38	-	73,73,73,73	0
55	MG	DA	3216	1/1	0.96	0.63	-	47,47,47,47	0
55	MG	AA	3521	1/1	0.79	0.31	-	87,87,87,87	0
55	MG	AA	3607	1/1	0.95	0.37	-	54,54,54,54	0
55	MG	BA	1784	1/1	0.53	0.19	-	106,106,106,106	0
55	MG	AA	3419	1/1	0.47	0.20	-	102,102,102,102	0
55	MG	DB	213	1/1	0.27	0.33	-	90,90,90,90	0
55	MG	AA	3109	1/1	0.94	0.31	-	33,33,33,33	0
55	MG	DA	3242	1/1	0.97	0.64	-	61,61,61,61	0
55	MG	DA	3313	1/1	0.79	0.48	-	75,75,75,75	0
55	MG	AA	3262	1/1	0.91	0.33	-	71,71,71,71	0
55	MG	DA	3299	1/1	0.77	0.30	-	92,92,92,92	0
55	MG	BA	1714	1/1	0.63	0.37	-	127,127,127,127	0
55	MG	AA	3206	1/1	0.89	0.45	-	53,53,53,53	0
55	MG	AA	3025	1/1	0.97	0.62	-	46,46,46,46	0
55	MG	CA	1797	1/1	0.72	0.27	-	94,94,94,94	0
55	MG	DA	3456	1/1	0.83	0.33	-	83,83,83,83	0
55	MG	DA	3317	1/1	0.82	0.38	-	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1717	1/1	0.74	0.67	-	106,106,106,106	0
55	MG	CA	1726	1/1	0.93	0.63	-	82,82,82,82	0
55	MG	AA	3147	1/1	0.91	0.59	-	77,77,77,77	0
55	MG	DA	3131	1/1	0.86	0.87	-	93,93,93,93	0
55	MG	DA	3004	1/1	0.82	0.26	-	91,91,91,91	0
55	MG	DA	3151	1/1	0.79	0.84	-	75,75,75,75	0
55	MG	AA	3528	1/1	0.81	0.20	-	88,88,88,88	0
55	MG	AB	203	1/1	0.77	0.23	-	70,70,70,70	0
55	MG	AA	3332	1/1	0.92	0.69	-	82,82,82,82	0
55	MG	AA	3574	1/1	0.96	0.49	-	29,29,29,29	0
55	MG	AA	3300	1/1	0.56	0.27	-	77,77,77,77	0
55	MG	DA	3493	1/1	0.95	0.67	-	46,46,46,46	0
55	MG	DA	3091	1/1	0.83	0.50	-	52,52,52,52	0
55	MG	DA	3310	1/1	0.79	0.69	-	80,80,80,80	0
55	MG	DA	3513	1/1	0.79	0.16	-	103,103,103,103	0
55	MG	DA	3052	1/1	0.88	0.21	-	84,84,84,84	0
55	MG	AA	3238	1/1	0.97	0.64	-	48,48,48,48	0
55	MG	AA	3219	1/1	0.98	0.28	-	60,60,60,60	0
55	MG	BC	103	1/1	0.75	0.47	-	65,65,65,65	0
55	MG	AA	3392	1/1	0.83	0.76	-	94,94,94,94	0
55	MG	AA	3193	1/1	0.57	0.35	-	94,94,94,94	0
55	MG	BA	1727	1/1	0.68	0.14	-	125,125,125,125	0
55	MG	BA	1685	1/1	0.70	0.87	-	82,82,82,82	0
55	MG	DA	3383	1/1	0.80	0.57	-	79,79,79,79	0
55	MG	AA	3188	1/1	0.82	0.42	-	72,72,72,72	0
55	MG	DA	3472	1/1	0.97	0.79	-	85,85,85,85	0
55	MG	AA	3624	1/1	0.97	0.20	-	80,80,80,80	0
55	MG	AA	3456	1/1	0.87	0.78	-	70,70,70,70	0
55	MG	DA	3403	1/1	0.69	0.15	-	78,78,78,78	0
55	MG	BA	1775	1/1	0.82	0.18	-	100,100,100,100	0
55	MG	BA	1771	1/1	0.89	0.23	-	100,100,100,100	0
55	MG	BA	1818	1/1	0.87	0.22	-	82,82,82,82	0
55	MG	AA	3224	1/1	0.81	0.33	-	77,77,77,77	0
55	MG	AA	3145	1/1	0.94	0.64	-	98,98,98,98	0
55	MG	DA	3269	1/1	0.69	0.53	-	86,86,86,86	0
55	MG	CA	1660	1/1	0.95	0.19	-	76,76,76,76	0
55	MG	DB	214	1/1	0.70	0.20	-	99,99,99,99	0
55	MG	AA	3043	1/1	0.93	0.26	-	83,83,83,83	0
55	MG	CA	1790	1/1	0.82	0.17	-	75,75,75,75	0
55	MG	CA	1752	1/1	0.87	0.24	-	70,70,70,70	0
55	MG	AA	3326	1/1	0.80	0.33	-	81,81,81,81	0
55	MG	AA	3297	1/1	0.85	0.47	-	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	1640	1/1	0.76	0.33	-	80,80,80,80	0
55	MG	AA	3175	1/1	0.80	0.61	-	70,70,70,70	0
55	MG	CA	1715	1/1	0.80	0.24	-	99,99,99,99	0
55	MG	CA	1634	1/1	0.93	0.90	-	90,90,90,90	0
55	MG	DB	203	1/1	0.90	0.22	-	71,71,71,71	0
55	MG	DA	3520	1/1	0.82	0.22	-	99,99,99,99	0
55	MG	DA	3420	1/1	0.77	0.81	-	73,73,73,73	0
55	MG	AA	3380	1/1	0.81	0.38	-	84,84,84,84	0
55	MG	DA	3369	1/1	0.96	0.59	-	61,61,61,61	0
55	MG	AA	3389	1/1	0.82	1.18	-	89,89,89,89	0
55	MG	BA	1643	1/1	0.77	0.34	-	80,80,80,80	0
55	MG	BA	1844	1/1	0.84	0.46	-	95,95,95,95	0
55	MG	AA	3544	1/1	0.85	0.86	-	67,67,67,67	0
55	MG	AA	3427	1/1	0.73	0.20	-	78,78,78,78	0
55	MG	BA	1686	1/1	0.96	0.26	-	94,94,94,94	0
55	MG	AA	3545	1/1	0.92	0.41	-	72,72,72,72	0
55	MG	DA	3218	1/1	0.87	0.73	-	75,75,75,75	0
55	MG	AA	3302	1/1	0.88	0.38	-	84,84,84,84	0
55	MG	AA	3259	1/1	0.78	0.31	-	91,91,91,91	0
55	MG	AA	3536	1/1	0.44	0.45	-	102,102,102,102	0
55	MG	BA	1718	1/1	0.45	0.37	-	104,104,104,104	0
55	MG	AA	3072	1/1	0.85	0.51	-	75,75,75,75	0
55	MG	DA	3028	1/1	0.86	0.39	-	71,71,71,71	0
55	MG	DA	3107	1/1	0.93	0.37	-	89,89,89,89	0
55	MG	DA	3068	1/1	0.90	0.17	-	100,100,100,100	0
55	MG	CA	1729	1/1	0.88	0.91	-	81,81,81,81	0
55	MG	DA	3447	1/1	0.81	0.53	-	86,86,86,86	0
55	MG	DA	3350	1/1	0.77	0.39	-	79,79,79,79	0
55	MG	AA	3298	1/1	0.92	0.52	-	80,80,80,80	0
55	MG	CA	1627	1/1	0.89	0.26	-	102,102,102,102	0
55	MG	AA	3017	1/1	0.97	0.41	-	59,59,59,59	0
55	MG	DA	3001	1/1	0.97	0.28	-	58,58,58,58	0
55	MG	CA	1786	1/1	0.62	0.17	-	97,97,97,97	0
55	MG	DA	3327	1/1	0.87	0.46	-	85,85,85,85	0
55	MG	DA	3019	1/1	0.73	0.72	-	66,66,66,66	0
55	MG	AA	3530	1/1	0.85	0.27	-	65,65,65,65	0
55	MG	CC	101	1/1	0.92	0.39	-	110,110,110,110	0
55	MG	CA	1684	1/1	0.74	0.61	-	77,77,77,77	0
55	MG	DA	3082	1/1	0.88	0.24	-	83,83,83,83	0
55	MG	AA	3433	1/1	0.84	0.46	-	77,77,77,77	0
55	MG	CA	1657	1/1	0.92	0.10	-	94,94,94,94	0
55	MG	AA	3618	1/1	0.88	0.43	-	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3131	1/1	0.84	0.69	-	88,88,88,88	0
55	MG	DA	3225	1/1	0.90	0.36	-	64,64,64,64	0
55	MG	DA	3023	1/1	0.82	0.11	-	107,107,107,107	0
55	MG	AA	3290	1/1	0.90	0.92	-	62,62,62,62	0
55	MG	BA	1656	1/1	0.76	0.23	-	78,78,78,78	0
55	MG	CA	1642	1/1	0.95	0.38	-	78,78,78,78	0
55	MG	BA	1732	1/1	0.79	0.30	-	94,94,94,94	0
55	MG	DA	3392	1/1	0.35	0.38	-	106,106,106,106	0
55	MG	AA	3082	1/1	0.97	0.51	-	39,39,39,39	0
55	MG	AA	3149	1/1	0.94	0.39	-	49,49,49,49	0
55	MG	DA	3201	1/1	0.74	0.41	-	75,75,75,75	0
55	MG	AA	3118	1/1	0.84	0.28	-	74,74,74,74	0
55	MG	AA	3038	1/1	0.86	0.15	-	70,70,70,70	0
55	MG	DA	3344	1/1	0.91	0.28	-	93,93,93,93	0
55	MG	CA	1744	1/1	0.91	0.21	-	70,70,70,70	0
55	MG	DA	3090	1/1	0.94	0.29	-	47,47,47,47	0
55	MG	AA	3100	1/1	0.89	0.13	-	79,79,79,79	0
55	MG	DA	3402	1/1	0.92	0.84	-	73,73,73,73	0
55	MG	AA	3559	1/1	0.64	0.68	-	93,93,93,93	0
55	MG	AA	3256	1/1	0.90	0.33	-	65,65,65,65	0
55	MG	DA	3144	1/1	0.89	0.94	-	68,68,68,68	0
55	MG	AA	3512	1/1	0.88	0.34	-	71,71,71,71	0
55	MG	AA	3492	1/1	0.76	0.39	-	84,84,84,84	0
55	MG	AA	3048	1/1	0.96	0.21	-	63,63,63,63	0
55	MG	BA	1719	1/1	0.73	0.28	-	91,91,91,91	0
55	MG	AA	3382	1/1	0.69	0.42	-	83,83,83,83	0
55	MG	DA	3032	1/1	0.93	0.54	-	73,73,73,73	0
55	MG	AA	3366	1/1	0.78	0.42	-	78,78,78,78	0
55	MG	DA	3040	1/1	0.95	0.42	-	92,92,92,92	0
55	MG	DA	3138	1/1	0.89	0.25	-	71,71,71,71	0
55	MG	AO	201	1/1	0.98	0.26	-	39,39,39,39	0
55	MG	AA	3617	1/1	0.82	0.63	-	92,92,92,92	0
55	MG	DA	3491	1/1	0.93	0.33	-	43,43,43,43	0
55	MG	BA	1788	1/1	0.30	0.15	-	108,108,108,108	0
55	MG	DA	3184	1/1	0.98	0.27	-	71,71,71,71	0
55	MG	CA	1644	1/1	0.95	0.17	-	59,59,59,59	0
55	MG	AA	3065	1/1	0.96	0.47	-	52,52,52,52	0
55	MG	CA	1643	1/1	0.70	0.17	-	97,97,97,97	0
55	MG	AA	3613	1/1	0.88	0.67	-	104,104,104,104	0
55	MG	CA	1619	1/1	0.94	0.74	-	62,62,62,62	0
55	MG	DA	3480	1/1	0.93	0.75	-	56,56,56,56	0
55	MG	AA	3563	1/1	0.76	0.80	-	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	1826	1/1	0.85	0.40	-	73,73,73,73	0
55	MG	BA	1702	1/1	0.73	0.21	-	98,98,98,98	0
55	MG	BA	1725	1/1	0.71	0.63	-	82,82,82,82	0
55	MG	BA	1795	1/1	0.88	0.55	-	66,66,66,66	0
55	MG	CA	1655	1/1	0.90	0.27	-	87,87,87,87	0
55	MG	AA	3558	1/1	0.48	0.58	-	110,110,110,110	0
55	MG	DA	3002	1/1	0.64	0.86	-	91,91,91,91	0
55	MG	CA	1618	1/1	0.76	0.21	-	89,89,89,89	0
55	MG	DA	3283	1/1	0.85	0.37	-	78,78,78,78	0
55	MG	AA	3595	1/1	0.83	0.57	-	90,90,90,90	0
55	MG	DA	3500	1/1	0.83	1.49	-	100,100,100,100	0
55	MG	AA	3586	1/1	0.89	0.30	-	80,80,80,80	0
55	MG	DA	3346	1/1	0.86	0.21	-	83,83,83,83	0
55	MG	CA	1775	1/1	0.80	0.38	-	66,66,66,66	0
55	MG	DA	3455	1/1	0.32	0.56	-	95,95,95,95	0
55	MG	AA	3377	1/1	0.95	0.51	-	85,85,85,85	0
55	MG	AF	303	1/1	0.67	0.54	-	77,77,77,77	0
55	MG	DA	3485	1/1	0.87	0.56	-	40,40,40,40	0
55	MG	DA	3413	1/1	0.81	0.47	-	96,96,96,96	0
55	MG	DA	3115	1/1	0.80	0.19	-	76,76,76,76	0
55	MG	AA	3342	1/1	0.90	0.24	-	65,65,65,65	0
55	MG	BA	1767	1/1	0.88	0.23	-	101,101,101,101	0
55	MG	AA	3172	1/1	0.74	0.63	-	102,102,102,102	0
55	MG	BA	1742	1/1	0.89	0.10	-	133,133,133,133	0
55	MG	CA	1778	1/1	0.93	0.32	-	69,69,69,69	0
55	MG	DA	3103	1/1	0.85	0.38	-	82,82,82,82	0
55	MG	DA	3083	1/1	0.59	0.39	-	108,108,108,108	0
55	MG	AA	3515	1/1	0.76	1.15	-	67,67,67,67	0
55	MG	BA	1791	1/1	0.89	0.47	-	89,89,89,89	0
55	MG	DA	3301	1/1	0.82	0.48	-	91,91,91,91	0
55	MG	DA	3417	1/1	0.92	0.18	-	83,83,83,83	0
55	MG	BA	1621	1/1	0.71	0.32	-	116,116,116,116	0
55	MG	DA	3396	1/1	0.85	0.26	-	89,89,89,89	0
55	MG	AA	3418	1/1	0.83	1.07	-	85,85,85,85	0
55	MG	DA	3229	1/1	0.58	0.48	-	109,109,109,109	0
55	MG	BA	1790	1/1	0.84	0.46	-	83,83,83,83	0
55	MG	DA	3271	1/1	0.89	0.37	-	76,76,76,76	0
55	MG	AA	3520	1/1	0.82	0.22	-	97,97,97,97	0
55	MG	DA	3371	1/1	0.71	0.36	-	82,82,82,82	0
55	MG	BA	1785	1/1	0.87	0.78	-	91,91,91,91	0
55	MG	AA	3199	1/1	0.84	0.40	-	66,66,66,66	0
55	MG	AA	3391	1/1	0.75	0.21	-	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1708	1/1	0.82	0.16	-	91,91,91,91	0
55	MG	DA	3243	1/1	0.94	0.28	-	83,83,83,83	0
55	MG	AA	3404	1/1	0.48	0.27	-	89,89,89,89	0
55	MG	DA	3496	1/1	0.78	0.48	-	85,85,85,85	0
55	MG	AA	3627	1/1	0.67	1.12	-	108,108,108,108	0
55	MG	AA	3611	1/1	0.96	0.36	-	54,54,54,54	0
55	MG	AA	3517	1/1	0.96	0.37	-	61,61,61,61	0
55	MG	CA	1664	1/1	0.72	0.22	-	97,97,97,97	0
55	MG	DA	3329	1/1	0.81	0.88	-	80,80,80,80	0
55	MG	DA	3418	1/1	0.76	0.43	-	81,81,81,81	0
55	MG	CA	1638	1/1	0.80	0.30	-	93,93,93,93	0
55	MG	DA	3250	1/1	0.93	0.30	-	54,54,54,54	0
55	MG	AA	3005	1/1	0.95	0.53	-	38,38,38,38	0
55	MG	AA	3495	1/1	0.90	0.48	-	98,98,98,98	0
55	MG	DA	3487	1/1	0.90	0.60	-	59,59,59,59	0
55	MG	DA	3446	1/1	0.46	0.31	-	98,98,98,98	0
55	MG	CA	1605	1/1	0.91	0.27	-	72,72,72,72	0
55	MG	AA	3363	1/1	0.75	0.41	-	80,80,80,80	0
55	MG	CA	1604	1/1	0.92	0.14	-	78,78,78,78	0
55	MG	AB	216	1/1	0.77	0.17	-	112,112,112,112	0
55	MG	AA	3602	1/1	0.72	0.24	-	70,70,70,70	0
55	MG	BA	1689	1/1	0.83	0.12	-	110,110,110,110	0
55	MG	AB	207	1/1	0.92	0.14	-	97,97,97,97	0
55	MG	CA	1602	1/1	0.81	0.19	-	81,81,81,81	0
55	MG	CA	1713	1/1	0.75	0.40	-	109,109,109,109	0
55	MG	AO	203	1/1	0.96	0.55	-	63,63,63,63	0
55	MG	DA	3168	1/1	0.94	0.47	-	49,49,49,49	0
55	MG	AA	3381	1/1	0.66	0.35	-	88,88,88,88	0
55	MG	DA	3424	1/1	0.97	0.43	-	79,79,79,79	0
55	MG	CA	1707	1/1	0.80	0.47	-	88,88,88,88	0
55	MG	CA	1682	1/1	0.91	0.36	-	97,97,97,97	0
55	MG	BA	1797	1/1	0.82	0.32	-	89,89,89,89	0
55	MG	AA	3111	1/1	0.96	0.62	-	43,43,43,43	0
55	MG	CA	1782	1/1	0.87	0.33	-	104,104,104,104	0
55	MG	AA	3317	1/1	0.69	0.62	-	95,95,95,95	0
55	MG	AB	204	1/1	0.48	0.20	-	94,94,94,94	0
55	MG	DA	3435	1/1	0.80	0.58	-	104,104,104,104	0
55	MG	BA	1611	1/1	0.74	0.38	-	97,97,97,97	0
55	MG	BA	1657	1/1	0.97	0.44	-	44,44,44,44	0
55	MG	AA	3413	1/1	0.95	0.32	-	82,82,82,82	0
55	MG	AA	3434	1/1	0.78	0.43	-	65,65,65,65	0
55	MG	CA	1734	1/1	0.79	0.28	-	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3020	1/1	0.97	0.59	-	51,51,51,51	0
55	MG	AA	3249	1/1	0.77	0.24	-	92,92,92,92	0
55	MG	AA	3121	1/1	0.42	0.59	-	93,93,93,93	0
55	MG	DA	3503	1/1	0.96	0.36	-	52,52,52,52	0
55	MG	AA	3234	1/1	0.78	0.61	-	83,83,83,83	0
55	MG	AA	3103	1/1	0.89	0.45	-	75,75,75,75	0
55	MG	DA	3305	1/1	0.89	0.45	-	83,83,83,83	0
55	MG	AA	3503	1/1	0.91	0.18	-	72,72,72,72	0
55	MG	AA	3150	1/1	0.96	0.63	-	58,58,58,58	0
55	MG	CA	1670	1/1	0.94	0.47	-	54,54,54,54	0
55	MG	DA	3285	1/1	0.40	0.40	-	109,109,109,109	0
55	MG	DA	3177	1/1	0.97	0.51	-	51,51,51,51	0
55	MG	AA	3127	1/1	0.99	0.30	-	47,47,47,47	0
55	MG	DA	3176	1/1	0.92	0.73	-	78,78,78,78	0
55	MG	AA	3126	1/1	0.87	0.23	-	63,63,63,63	0
55	MG	DA	3263	1/1	0.55	0.39	-	88,88,88,88	0
55	MG	BC	108	1/1	0.89	0.72	-	101,101,101,101	0
55	MG	BA	1768	1/1	0.84	0.49	-	86,86,86,86	0
55	MG	DA	3521	1/1	0.77	0.57	-	89,89,89,89	0
55	MG	DA	3123	1/1	0.89	0.14	-	73,73,73,73	0
55	MG	AA	3465	1/1	0.75	0.30	-	88,88,88,88	0
55	MG	AA	3214	1/1	0.90	0.47	-	66,66,66,66	0
55	MG	CC	108	1/1	0.78	0.71	-	110,110,110,110	0
55	MG	DA	3043	1/1	0.94	0.23	-	81,81,81,81	0
55	MG	AA	3590	1/1	0.94	0.60	-	56,56,56,56	0
55	MG	BA	1781	1/1	0.97	0.43	-	57,57,57,57	0
55	MG	AA	3315	1/1	0.93	0.67	-	68,68,68,68	0
55	MG	AA	3106	1/1	0.79	0.70	-	65,65,65,65	0
55	MG	BB	101	1/1	0.94	0.24	-	88,88,88,88	0
55	MG	BC	106	1/1	0.82	0.23	-	80,80,80,80	0
55	MG	AA	3598	1/1	0.83	0.34	-	84,84,84,84	0
55	MG	AF	302	1/1	0.65	0.78	-	80,80,80,80	0
55	MG	BA	1842	1/1	0.90	0.36	-	88,88,88,88	0
55	MG	BA	1733	1/1	0.88	0.28	-	88,88,88,88	0
55	MG	AA	3269	1/1	0.85	0.32	-	72,72,72,72	0
55	MG	DA	3053	1/1	0.73	0.64	-	86,86,86,86	0
55	MG	AA	3496	1/1	0.82	0.37	-	91,91,91,91	0
55	MG	BA	1836	1/1	0.89	0.55	-	73,73,73,73	0
55	MG	AA	3469	1/1	0.90	0.46	-	76,76,76,76	0
55	MG	DA	3099	1/1	0.98	0.35	-	51,51,51,51	0
55	MG	AA	3233	1/1	0.83	0.25	-	74,74,74,74	0
55	MG	AA	3116	1/1	0.95	0.39	-	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3151	1/1	0.93	0.57	-	61,61,61,61	0
55	MG	CA	1697	1/1	0.94	0.29	-	56,56,56,56	0
55	MG	CA	1701	1/1	0.88	0.30	-	77,77,77,77	0
55	MG	DE	301	1/1	0.97	0.45	-	43,43,43,43	0
55	MG	AA	3328	1/1	0.84	0.47	-	71,71,71,71	0
55	MG	DA	3421	1/1	0.77	0.32	-	76,76,76,76	0
55	MG	BA	1745	1/1	0.73	0.48	-	90,90,90,90	0
55	MG	DA	3021	1/1	0.91	0.68	-	61,61,61,61	0
55	MG	DA	3437	1/1	0.72	0.74	-	140,140,140,140	0
55	MG	DA	3027	1/1	0.85	0.40	-	93,93,93,93	0
55	MG	DA	3498	1/1	0.59	1.56	-	90,90,90,90	0
55	MG	CA	1714	1/1	0.08	1.37	-	115,115,115,115	0
55	MG	DA	3062	1/1	0.80	0.33	-	85,85,85,85	0
55	MG	CA	1637	1/1	0.67	0.55	-	97,97,97,97	0
55	MG	BA	1809	1/1	0.77	1.35	-	88,88,88,88	0
55	MG	AA	3484	1/1	0.77	0.38	-	86,86,86,86	0
55	MG	AA	3108	1/1	0.80	0.72	-	79,79,79,79	0
55	MG	CA	1725	1/1	0.72	0.20	-	75,75,75,75	0
55	MG	DA	3048	1/1	0.88	0.58	-	84,84,84,84	0
55	MG	DA	3412	1/1	0.73	0.43	-	97,97,97,97	0
55	MG	DA	3239	1/1	0.85	0.57	-	75,75,75,75	0
55	MG	DA	3182	1/1	0.95	0.64	-	72,72,72,72	0
55	MG	AA	3423	1/1	0.80	0.26	-	69,69,69,69	0
55	MG	AA	3329	1/1	0.79	0.25	-	77,77,77,77	0
55	MG	DA	3365	1/1	0.75	0.57	-	89,89,89,89	0
55	MG	CA	1759	1/1	0.53	0.22	-	100,100,100,100	0
55	MG	AA	3270	1/1	0.70	0.33	-	96,96,96,96	0
55	MG	CA	1762	1/1	0.43	0.47	-	105,105,105,105	0
55	MG	AA	3019	1/1	0.99	0.38	-	35,35,35,35	0
55	MG	AA	3200	1/1	0.82	0.33	-	80,80,80,80	0
55	MG	DA	3217	1/1	0.92	0.61	-	51,51,51,51	0
55	MG	AA	3282	1/1	0.96	0.27	-	87,87,87,87	0
55	MG	AA	3198	1/1	0.95	0.70	-	57,57,57,57	0
55	MG	CA	1680	1/1	0.82	0.55	-	68,68,68,68	0
55	MG	AA	3551	1/1	0.78	0.60	-	73,73,73,73	0
55	MG	AA	3096	1/1	0.87	0.25	-	75,75,75,75	0
55	MG	AA	3257	1/1	0.80	0.29	-	84,84,84,84	0
55	MG	AA	3599	1/1	0.82	1.00	-	84,84,84,84	0
55	MG	DA	3169	1/1	0.95	0.77	-	68,68,68,68	0
55	MG	DA	3307	1/1	0.65	0.51	-	77,77,77,77	0
55	MG	DA	3108	1/1	0.90	0.33	-	69,69,69,69	0
55	MG	CH	201	1/1	0.74	0.17	-	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3009	1/1	0.95	0.29	-	48,48,48,48	0
55	MG	AA	3387	1/1	0.81	0.46	-	102,102,102,102	0
55	MG	DA	3051	1/1	0.94	0.40	-	81,81,81,81	0
55	MG	AA	3488	1/1	0.71	0.48	-	94,94,94,94	0
55	MG	AA	3501	1/1	0.80	0.39	-	73,73,73,73	0
55	MG	DA	3366	1/1	0.56	0.50	-	97,97,97,97	0
55	MG	BA	1616	1/1	0.86	0.19	-	92,92,92,92	0
55	MG	DA	3302	1/1	0.79	0.66	-	91,91,91,91	0
55	MG	CA	1796	1/1	0.81	0.31	-	81,81,81,81	0
55	MG	AA	3451	1/1	0.90	0.40	-	85,85,85,85	0
55	MG	BA	1734	1/1	0.50	0.69	-	96,96,96,96	0
55	MG	DA	3312	1/1	0.90	0.19	-	101,101,101,101	0
55	MG	AA	3525	1/1	0.95	0.33	-	67,67,67,67	0
55	MG	AA	3275	1/1	0.95	0.45	-	65,65,65,65	0
55	MG	AB	214	1/1	0.85	0.21	-	88,88,88,88	0
55	MG	DA	3353	1/1	0.90	0.66	-	70,70,70,70	0
55	MG	CA	1696	1/1	0.81	0.15	-	79,79,79,79	0
55	MG	BA	1627	1/1	0.97	0.27	-	62,62,62,62	0
55	MG	BA	1755	1/1	0.93	1.03	-	106,106,106,106	0
55	MG	AA	3061	1/1	0.94	0.25	-	75,75,75,75	0
55	MG	CB	104	1/1	0.45	0.29	-	114,114,114,114	0
55	MG	AA	3365	1/1	0.92	0.23	-	83,83,83,83	0
55	MG	AA	3285	1/1	0.77	0.32	-	77,77,77,77	0
55	MG	AA	3361	1/1	0.85	0.41	-	88,88,88,88	0
55	MG	DA	3372	1/1	0.45	0.41	-	108,108,108,108	0
55	MG	AA	3195	1/1	0.82	0.18	-	62,62,62,62	0
55	MG	DA	3085	1/1	0.85	0.31	-	89,89,89,89	0
55	MG	AA	3336	1/1	0.88	0.52	-	48,48,48,48	0
55	MG	DA	3322	1/1	0.89	0.78	-	83,83,83,83	0
55	MG	AA	3189	1/1	0.88	0.39	-	57,57,57,57	0
55	MG	DA	3416	1/1	0.98	0.28	-	75,75,75,75	0
55	MG	BA	1750	1/1	0.92	0.51	-	79,79,79,79	0
55	MG	AA	3355	1/1	0.90	0.58	-	87,87,87,87	0
55	MG	BA	1668	1/1	0.84	0.51	-	73,73,73,73	0
55	MG	BA	1629	1/1	0.89	0.49	-	100,100,100,100	0
55	MG	BA	1615	1/1	0.71	0.31	-	104,104,104,104	0
55	MG	AA	3403	1/1	0.82	0.20	-	74,74,74,74	0
55	MG	DA	3093	1/1	0.99	0.36	-	51,51,51,51	0
55	MG	AA	3099	1/1	0.93	0.37	-	64,64,64,64	0
55	MG	DA	3024	1/1	0.73	1.27	-	100,100,100,100	0
55	MG	BA	1698	1/1	0.88	0.68	-	73,73,73,73	0
55	MG	BA	1613	1/1	0.62	1.36	-	96,96,96,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3475	1/1	0.87	0.31	-	67,67,67,67	0
55	MG	AA	3060	1/1	0.94	0.23	-	57,57,57,57	0
55	MG	BA	1665	1/1	0.94	0.68	-	66,66,66,66	0
55	MG	AA	3428	1/1	0.69	0.35	-	106,106,106,106	0
55	MG	AU	201	1/1	0.93	0.28	-	74,74,74,74	0
55	MG	AA	3301	1/1	0.70	0.88	-	113,113,113,113	0
55	MG	DA	3161	1/1	0.93	0.42	-	73,73,73,73	0
55	MG	BA	1840	1/1	0.81	0.43	-	80,80,80,80	0
55	MG	AA	3343	1/1	0.77	0.29	-	94,94,94,94	0
55	MG	BA	1708	1/1	0.71	0.21	-	78,78,78,78	0
55	MG	DA	3037	1/1	0.66	0.21	-	84,84,84,84	0
55	MG	CA	1706	1/1	0.95	0.34	-	77,77,77,77	0
55	MG	BA	1674	1/1	0.43	0.19	-	113,113,113,113	0
55	MG	CA	1640	1/1	0.58	0.36	-	78,78,78,78	0
55	MG	AA	3552	1/1	0.90	0.81	-	75,75,75,75	0
55	MG	DA	3511	1/1	0.94	0.43	-	65,65,65,65	0
55	MG	AB	213	1/1	0.92	0.21	-	54,54,54,54	0
55	MG	CA	1673	1/1	0.94	0.72	-	65,65,65,65	0
55	MG	AA	3207	1/1	0.95	0.54	-	44,44,44,44	0
55	MG	AA	3235	1/1	0.71	0.44	-	86,86,86,86	0
55	MG	DA	3226	1/1	0.90	0.41	-	57,57,57,57	0
55	MG	DA	3434	1/1	0.84	0.47	-	75,75,75,75	0
55	MG	DA	3284	1/1	0.60	0.88	-	81,81,81,81	0
55	MG	DA	3105	1/1	0.89	0.32	-	72,72,72,72	0
55	MG	DA	3022	1/1	0.85	0.80	-	66,66,66,66	0
55	MG	DA	3227	1/1	0.74	0.29	-	81,81,81,81	0
55	MG	BA	1783	1/1	0.72	0.95	-	91,91,91,91	0
55	MG	BA	1752	1/1	0.68	0.48	-	116,116,116,116	0
55	MG	AA	3358	1/1	0.91	0.51	-	79,79,79,79	0
55	MG	AA	3478	1/1	0.89	0.13	-	93,93,93,93	0
55	MG	AA	3396	1/1	0.88	0.31	-	58,58,58,58	0
55	MG	DA	3069	1/1	0.76	0.40	-	82,82,82,82	0
55	MG	CA	1751	1/1	0.70	0.93	-	102,102,102,102	0
55	MG	AA	3310	1/1	0.92	0.39	-	74,74,74,74	0
55	MG	AA	3466	1/1	0.78	0.60	-	106,106,106,106	0
55	MG	AA	3220	1/1	0.93	0.28	-	44,44,44,44	0
55	MG	DA	3097	1/1	0.94	0.33	-	42,42,42,42	0
55	MG	AA	3114	1/1	0.94	0.47	-	41,41,41,41	0
55	MG	AA	3047	1/1	0.84	0.29	-	87,87,87,87	0
55	MG	AA	3339	1/1	0.72	0.24	-	95,95,95,95	0
55	MG	AA	3289	1/1	0.98	0.36	-	62,62,62,62	0
55	MG	BB	107	1/1	0.84	0.23	-	97,97,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3183	1/1	0.77	0.30	-	79,79,79,79	0
55	MG	AA	3287	1/1	0.95	0.12	-	88,88,88,88	0
55	MG	BA	1647	1/1	0.58	0.27	-	93,93,93,93	0
55	MG	D3	101	1/1	0.84	0.37	-	68,68,68,68	0
55	MG	DA	3065	1/1	0.72	0.57	-	95,95,95,95	0
55	MG	DA	3282	1/1	0.80	0.58	-	55,55,55,55	0
55	MG	AA	3596	1/1	0.64	0.18	-	87,87,87,87	0
55	MG	AA	3209	1/1	0.66	0.77	-	71,71,71,71	0
55	MG	BA	1655	1/1	0.86	0.17	-	89,89,89,89	0
55	MG	AA	3187	1/1	0.94	0.63	-	65,65,65,65	0
55	MG	AA	3242	1/1	0.98	0.38	-	58,58,58,58	0
55	MG	BA	1798	1/1	0.80	0.31	-	89,89,89,89	0
55	MG	DA	3162	1/1	0.97	0.24	-	70,70,70,70	0
55	MG	AA	3316	1/1	0.80	0.71	-	87,87,87,87	0
55	MG	BA	1813	1/1	0.70	0.36	-	80,80,80,80	0
55	MG	AA	3583	1/1	0.80	0.60	-	44,44,44,44	0
55	MG	DA	3228	1/1	0.96	0.42	-	71,71,71,71	0
55	MG	DA	3005	1/1	0.84	0.45	-	83,83,83,83	0
55	MG	AA	3319	1/1	0.92	0.22	-	61,61,61,61	0
55	MG	BA	1688	1/1	0.87	0.26	-	76,76,76,76	0
55	MG	AA	3589	1/1	0.92	0.21	-	72,72,72,72	0
55	MG	AA	3360	1/1	0.69	0.41	-	89,89,89,89	0
55	MG	AA	3378	1/1	0.75	0.92	-	86,86,86,86	0
55	MG	AA	3606	1/1	0.59	0.25	-	77,77,77,77	0
55	MG	CA	1624	1/1	0.78	0.21	-	83,83,83,83	0
55	MG	BA	1711	1/1	0.74	0.43	-	86,86,86,86	0
55	MG	AA	3527	1/1	0.93	0.11	-	77,77,77,77	0
55	MG	DA	3508	1/1	0.75	0.72	-	77,77,77,77	0
55	MG	CA	1652	1/1	0.93	0.30	-	70,70,70,70	0
55	MG	AA	3240	1/1	0.83	0.41	-	76,76,76,76	0
55	MG	BA	1712	1/1	0.24	0.46	-	125,125,125,125	0
55	MG	DB	212	1/1	0.87	0.41	-	94,94,94,94	0
55	MG	AA	3562	1/1	0.84	0.33	-	96,96,96,96	0
55	MG	BD	101	1/1	0.63	0.51	-	108,108,108,108	0
55	MG	BA	1654	1/1	0.94	0.21	-	74,74,74,74	0
55	MG	AA	3337	1/1	0.91	0.86	-	88,88,88,88	0
55	MG	BA	1617	1/1	0.81	0.54	-	64,64,64,64	0
55	MG	CB	105	1/1	0.89	0.28	-	80,80,80,80	0
55	MG	DA	3009	1/1	0.92	0.31	-	88,88,88,88	0
55	MG	BA	1741	1/1	0.61	0.37	-	124,124,124,124	0
55	MG	AA	3370	1/1	0.62	0.17	-	103,103,103,103	0
55	MG	DA	3059	1/1	0.52	0.61	-	104,104,104,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3202	1/1	0.88	0.42	-	55,55,55,55	0
55	MG	BA	1684	1/1	0.89	0.89	-	100,100,100,100	0
55	MG	DA	3127	1/1	0.99	0.72	-	44,44,44,44	0
55	MG	DA	3256	1/1	0.88	0.44	-	82,82,82,82	0
55	MG	DA	3010	1/1	0.53	0.41	-	121,121,121,121	0
55	MG	AA	3386	1/1	0.84	0.31	-	74,74,74,74	0
55	MG	AA	3346	1/1	0.40	0.85	-	98,98,98,98	0
55	MG	CA	1609	1/1	0.91	0.21	-	108,108,108,108	0
55	MG	DA	3038	1/1	0.76	0.22	-	102,102,102,102	0
55	MG	DA	3247	1/1	0.94	0.42	-	71,71,71,71	0
55	MG	CA	1732	1/1	0.82	0.14	-	93,93,93,93	0
55	MG	CA	1807	1/1	0.80	0.98	-	121,121,121,121	0
55	MG	DA	3231	1/1	0.99	0.30	-	55,55,55,55	0
55	MG	AA	3192	1/1	0.71	0.27	-	90,90,90,90	0
55	MG	AA	3474	1/1	0.83	0.20	-	93,93,93,93	0
55	MG	BA	1757	1/1	0.77	0.40	-	88,88,88,88	0
55	MG	DA	3055	1/1	0.87	0.80	-	80,80,80,80	0
55	MG	DA	3340	1/1	0.49	0.31	-	107,107,107,107	0
55	MG	BA	1793	1/1	0.90	0.22	-	82,82,82,82	0
55	MG	DA	3442	1/1	0.88	0.25	-	96,96,96,96	0
55	MG	DA	3528	1/1	0.71	0.37	-	87,87,87,87	0
55	MG	DA	3445	1/1	0.89	0.26	-	72,72,72,72	0
55	MG	DA	3483	1/1	0.97	0.81	-	45,45,45,45	0
55	MG	CA	1730	1/1	0.74	0.16	-	118,118,118,118	0
55	MG	AA	3229	1/1	0.94	0.13	-	18,18,18,18	0
55	MG	AA	3110	1/1	0.98	0.24	-	39,39,39,39	0
55	MG	BA	1762	1/1	0.82	0.62	-	85,85,85,85	0
55	MG	AA	3429	1/1	0.86	0.25	-	85,85,85,85	0
55	MG	BA	1724	1/1	0.61	0.49	-	100,100,100,100	0
55	MG	DA	3036	1/1	0.71	0.32	-	87,87,87,87	0
55	MG	AA	3463	1/1	0.26	0.77	-	108,108,108,108	0
55	MG	DA	3264	1/1	0.73	0.20	-	76,76,76,76	0
55	MG	BA	1633	1/1	0.85	0.28	-	75,75,75,75	0
55	MG	AA	3320	1/1	0.86	0.40	-	70,70,70,70	0
55	MG	CG	301	1/1	0.88	0.40	-	86,86,86,86	0
55	MG	DA	3451	1/1	0.86	0.66	-	65,65,65,65	0
55	MG	BA	1692	1/1	0.84	0.48	-	132,132,132,132	0
55	MG	CA	1679	1/1	0.65	0.39	-	84,84,84,84	0
55	MG	BA	1695	1/1	0.85	0.14	-	101,101,101,101	0
55	MG	AA	3601	1/1	0.82	0.38	-	79,79,79,79	0
55	MG	A2	201	1/1	0.91	0.38	-	81,81,81,81	0
55	MG	BA	1649	1/1	0.88	0.26	-	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3191	1/1	0.97	0.35	-	61,61,61,61	0
55	MG	DA	3187	1/1	0.98	0.54	-	40,40,40,40	0
55	MG	DA	3507	1/1	0.89	0.33	-	88,88,88,88	0
55	MG	AA	3608	1/1	0.82	0.52	-	69,69,69,69	0
55	MG	AA	3169	1/1	0.86	0.23	-	74,74,74,74	0
55	MG	CB	102	1/1	0.91	0.52	-	94,94,94,94	0
55	MG	AA	3554	1/1	0.81	0.47	-	86,86,86,86	0
55	MG	DA	3356	1/1	0.87	0.40	-	80,80,80,80	0
55	MG	AB	210	1/1	0.89	0.31	-	71,71,71,71	0
55	MG	AA	3129	1/1	0.91	0.25	-	75,75,75,75	0
55	MG	BA	1669	1/1	0.94	0.35	-	76,76,76,76	0
55	MG	AA	3089	1/1	0.97	0.41	-	44,44,44,44	0
55	MG	DA	3449	1/1	0.84	0.53	-	96,96,96,96	0
55	MG	AA	3272	1/1	0.85	0.10	-	86,86,86,86	0
55	MG	DA	3300	1/1	0.82	0.43	-	71,71,71,71	0
55	MG	BA	1646	1/1	0.81	0.28	-	70,70,70,70	0
55	MG	AA	3497	1/1	0.49	0.27	-	105,105,105,105	0
55	MG	CA	1693	1/1	0.97	0.62	-	73,73,73,73	0
55	MG	DA	3179	1/1	0.94	0.55	-	56,56,56,56	0
55	MG	BA	1662	1/1	0.76	0.79	-	80,80,80,80	0
55	MG	BA	1804	1/1	0.76	0.54	-	80,80,80,80	0
55	MG	DA	3003	1/1	0.91	0.58	-	70,70,70,70	0
55	MG	AA	3550	1/1	0.94	0.69	-	52,52,52,52	0
55	MG	DU	201	1/1	0.80	0.23	-	72,72,72,72	0
55	MG	DA	3525	1/1	0.89	0.33	-	88,88,88,88	0
55	MG	AA	3462	1/1	0.84	0.42	-	69,69,69,69	0
55	MG	DA	3321	1/1	0.93	0.25	-	81,81,81,81	0
55	MG	AA	3028	1/1	0.91	0.40	-	51,51,51,51	0
55	MG	AA	3190	1/1	0.85	0.20	-	83,83,83,83	0
55	MG	AA	3146	1/1	0.93	0.44	-	62,62,62,62	0
55	MG	DA	3399	1/1	0.86	0.24	-	97,97,97,97	0
55	MG	AA	3557	1/1	0.71	0.62	-	68,68,68,68	0
55	MG	DA	3133	1/1	0.80	0.30	-	77,77,77,77	0
55	MG	AA	3344	1/1	0.91	0.64	-	71,71,71,71	0
55	MG	DA	3061	1/1	0.97	0.43	-	67,67,67,67	0
55	MG	AA	3516	1/1	0.83	0.54	-	57,57,57,57	0
55	MG	CA	1769	1/1	0.49	0.21	-	109,109,109,109	0
55	MG	AA	3212	1/1	0.97	0.60	-	56,56,56,56	0
55	MG	CA	1802	1/1	0.91	0.11	-	107,107,107,107	0
55	MG	DA	3398	1/1	0.51	0.23	-	107,107,107,107	0
55	MG	DA	3261	1/1	0.59	0.37	-	89,89,89,89	0
55	MG	CA	1757	1/1	0.88	0.15	-	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	3247	1/1	0.80	0.55	-	76,76,76,76	0
55	MG	AB	212	1/1	0.86	0.33	-	76,76,76,76	0
55	MG	BA	1782	1/1	0.83	0.27	-	88,88,88,88	0
55	MG	AA	3450	1/1	0.81	0.38	-	84,84,84,84	0
55	MG	CA	1683	1/1	0.83	0.50	-	84,84,84,84	0
55	MG	DA	3157	1/1	0.98	0.49	-	51,51,51,51	0
55	MG	AA	3013	1/1	0.95	0.39	-	49,49,49,49	0
55	MG	DA	3524	1/1	0.67	1.38	-	99,99,99,99	0
55	MG	BA	1664	1/1	0.91	0.33	-	52,52,52,52	0
55	MG	AA	3487	1/1	0.90	0.50	-	78,78,78,78	0
55	MG	DA	3448	1/1	0.84	0.43	-	75,75,75,75	0
55	MG	BA	1827	1/1	0.71	0.41	-	85,85,85,85	0
55	MG	DA	3102	1/1	0.89	0.27	-	72,72,72,72	0
55	MG	AA	3493	1/1	0.85	0.45	-	89,89,89,89	0
55	MG	BA	1666	1/1	0.82	0.56	-	74,74,74,74	0
55	MG	AA	3481	1/1	0.82	0.74	-	66,66,66,66	0
55	MG	CA	1792	1/1	0.91	0.24	-	91,91,91,91	0
55	MG	CA	1694	1/1	0.93	0.25	-	94,94,94,94	0
55	MG	AA	3440	1/1	0.92	0.35	-	83,83,83,83	0
55	MG	DA	3306	1/1	0.72	0.94	-	73,73,73,73	0
55	MG	DA	3118	1/1	0.92	0.16	-	72,72,72,72	0
55	MG	AA	3173	1/1	0.77	0.60	-	70,70,70,70	0
55	MG	CA	1621	1/1	0.83	0.53	-	84,84,84,84	0
55	MG	AA	3204	1/1	0.96	0.32	-	56,56,56,56	0
55	MG	DA	3275	1/1	0.85	0.35	-	81,81,81,81	0
55	MG	AB	208	1/1	0.71	0.33	-	87,87,87,87	0
55	MG	CA	1626	1/1	0.27	0.28	-	103,103,103,103	0
55	MG	BA	1735	1/1	0.83	0.21	-	80,80,80,80	0
55	MG	DA	3454	1/1	0.94	0.18	-	108,108,108,108	0
55	MG	DA	3389	1/1	0.54	0.77	-	85,85,85,85	0
55	MG	DA	3304	1/1	0.51	0.33	-	106,106,106,106	0
55	MG	AA	3142	1/1	0.94	0.23	-	61,61,61,61	0
55	MG	DA	3495	1/1	0.84	0.78	-	65,65,65,65	0
55	MG	AA	3230	1/1	0.32	0.19	-	112,112,112,112	0
55	MG	DA	3393	1/1	0.92	0.19	-	93,93,93,93	0
55	MG	AA	3241	1/1	0.59	0.32	-	101,101,101,101	0
55	MG	AA	3022	1/1	0.98	0.33	-	43,43,43,43	0
55	MG	CA	1666	1/1	0.90	0.16	-	76,76,76,76	0
55	MG	AA	3331	1/1	0.83	0.40	-	79,79,79,79	0
55	MG	DA	3171	1/1	0.90	0.39	-	81,81,81,81	0
55	MG	AA	3069	1/1	0.95	0.18	-	64,64,64,64	0
55	MG	AA	3231	1/1	0.36	0.51	-	120,120,120,120	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BB	102	1/1	0.88	0.29	-	86,86,86,86	0
55	MG	CA	1635	1/1	0.88	0.27	-	87,87,87,87	0
55	MG	AA	3620	1/1	0.88	0.28	-	99,99,99,99	0
55	MG	AA	3472	1/1	0.71	0.20	-	81,81,81,81	0
55	MG	AA	3158	1/1	0.94	0.73	-	66,66,66,66	0
55	MG	CA	1739	1/1	0.92	0.53	-	69,69,69,69	0
55	MG	DA	3259	1/1	0.97	0.81	-	56,56,56,56	0
55	MG	AA	3560	1/1	0.88	0.65	-	84,84,84,84	0
55	MG	AA	3077	1/1	0.73	0.51	-	94,94,94,94	0
55	MG	AE	302	1/1	0.98	0.47	-	38,38,38,38	0
55	MG	CA	1688	1/1	0.93	0.42	-	75,75,75,75	0
55	MG	AA	3340	1/1	0.94	0.44	-	61,61,61,61	0
55	MG	CA	1728	1/1	0.95	0.47	-	58,58,58,58	0
55	MG	DB	210	1/1	0.87	0.20	-	76,76,76,76	0
55	MG	AA	3471	1/1	0.94	0.26	-	69,69,69,69	0
55	MG	CA	1804	1/1	0.83	0.18	-	81,81,81,81	0
55	MG	DA	3172	1/1	0.67	0.41	-	59,59,59,59	0
55	MG	AA	3267	1/1	0.88	0.22	-	80,80,80,80	0
55	MG	BA	1830	1/1	0.87	0.22	-	96,96,96,96	0
55	MG	BA	1637	1/1	0.92	0.42	-	93,93,93,93	0
55	MG	DA	3015	1/1	0.93	0.23	-	83,83,83,83	0
55	MG	DA	3497	1/1	0.79	0.17	-	62,62,62,62	0
55	MG	DA	3406	1/1	0.80	0.96	-	72,72,72,72	0
55	MG	BA	1693	1/1	0.79	0.23	-	80,80,80,80	0
55	MG	DA	3152	1/1	0.97	0.25	-	44,44,44,44	0
55	MG	DA	3351	1/1	0.86	0.35	-	70,70,70,70	0
55	MG	BA	1777	1/1	0.96	0.09	-	88,88,88,88	0
55	MG	DA	3084	1/1	0.91	0.44	-	87,87,87,87	0
55	MG	AA	3152	1/1	0.96	0.51	-	53,53,53,53	0
55	MG	DA	3325	1/1	0.82	0.32	-	70,70,70,70	0
55	MG	DA	3056	1/1	0.81	0.78	-	100,100,100,100	0
55	MG	DA	3170	1/1	0.91	0.85	-	66,66,66,66	0
55	MG	AA	3023	1/1	0.96	0.51	-	52,52,52,52	0
55	MG	BA	1707	1/1	0.64	0.40	-	94,94,94,94	0
55	MG	DA	3212	1/1	0.86	0.47	-	70,70,70,70	0
55	MG	CA	1651	1/1	0.92	0.13	-	79,79,79,79	0
55	MG	AA	3486	1/1	0.78	0.28	-	96,96,96,96	0
55	MG	CA	1787	1/1	0.82	0.47	-	84,84,84,84	0
55	MG	AA	3390	1/1	0.83	0.43	-	73,73,73,73	0
55	MG	BA	1810	1/1	0.65	0.24	-	110,110,110,110	0
55	MG	BA	1705	1/1	0.94	0.33	-	70,70,70,70	0
55	MG	CA	1756	1/1	0.84	0.62	-	93,93,93,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	BA	1787	1/1	0.77	0.23	-	107,107,107,107	0
55	MG	BA	1843	1/1	0.37	0.67	-	87,87,87,87	0
55	MG	DA	3377	1/1	0.82	0.97	-	92,92,92,92	0
55	MG	AA	3561	1/1	0.79	0.18	-	88,88,88,88	0
55	MG	AA	3171	1/1	0.85	0.50	-	81,81,81,81	0
55	MG	DA	3186	1/1	0.97	0.42	-	56,56,56,56	0
55	MG	BA	1811	1/1	0.92	0.20	-	86,86,86,86	0
55	MG	CA	1740	1/1	0.87	0.42	-	75,75,75,75	0
55	MG	DA	3244	1/1	0.38	0.95	-	106,106,106,106	0
55	MG	AA	3384	1/1	0.93	0.55	-	79,79,79,79	0
55	MG	DA	3360	1/1	0.35	0.31	-	96,96,96,96	0
55	MG	AA	3447	1/1	0.81	0.24	-	51,51,51,51	0
55	MG	DA	3134	1/1	0.95	0.51	-	56,56,56,56	0
55	MG	DA	3433	1/1	0.46	0.39	-	110,110,110,110	0
55	MG	AA	3603	1/1	0.82	0.40	-	65,65,65,65	0
55	MG	AA	3117	1/1	0.98	0.30	-	62,62,62,62	0
55	MG	AA	3291	1/1	0.79	0.74	-	70,70,70,70	0
55	MG	AA	3459	1/1	0.29	0.88	-	110,110,110,110	0
55	MG	AA	3167	1/1	0.94	0.36	-	51,51,51,51	0
55	MG	AA	3066	1/1	0.67	0.89	-	103,103,103,103	0
55	MG	CA	1613	1/1	0.70	0.18	-	84,84,84,84	0
55	MG	DA	3453	1/1	0.72	0.60	-	94,94,94,94	0
55	MG	AA	3359	1/1	0.89	0.50	-	60,60,60,60	0
55	MG	DA	3400	1/1	0.57	0.66	-	82,82,82,82	0
55	MG	BA	1805	1/1	0.91	0.59	-	62,62,62,62	0
55	MG	BA	1648	1/1	0.78	0.22	-	77,77,77,77	0
55	MG	DA	3462	1/1	0.94	0.74	-	67,67,67,67	0
55	MG	BA	1683	1/1	0.76	0.41	-	112,112,112,112	0
55	MG	AA	3526	1/1	0.69	0.37	-	57,57,57,57	0
55	MG	DA	3354	1/1	0.64	0.19	-	92,92,92,92	0
55	MG	DA	3490	1/1	0.96	0.45	-	49,49,49,49	0
55	MG	DA	3288	1/1	0.75	0.90	-	82,82,82,82	0
55	MG	DA	3459	1/1	0.98	0.58	-	49,49,49,49	0
55	MG	AA	3296	1/1	0.88	0.16	-	75,75,75,75	0
55	MG	DA	3150	1/1	0.95	1.01	-	76,76,76,76	0
55	MG	DA	3026	1/1	0.79	0.59	-	82,82,82,82	0
55	MG	DA	3165	1/1	0.92	0.32	-	73,73,73,73	0
55	MG	DA	3276	1/1	0.89	0.18	-	86,86,86,86	0
55	MG	AA	3294	1/1	0.48	0.49	-	99,99,99,99	0
55	MG	AA	3003	1/1	0.97	0.48	-	43,43,43,43	0
55	MG	AA	3186	1/1	0.86	0.44	-	77,77,77,77	0
55	MG	AA	3338	1/1	0.91	0.30	-	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1695	1/1	0.81	0.33	-	77,77,77,77	0
55	MG	AA	3531	1/1	0.93	0.61	-	53,53,53,53	0
55	MG	BA	1626	1/1	0.88	0.77	-	76,76,76,76	0
55	MG	DA	3277	1/1	0.45	0.38	-	77,77,77,77	0
55	MG	AA	3507	1/1	0.90	0.29	-	62,62,62,62	0
55	MG	DA	3397	1/1	-0.06	0.90	-	150,150,150,150	0
55	MG	DA	3207	1/1	0.90	0.39	-	61,61,61,61	0
55	MG	AA	3314	1/1	0.48	0.43	-	82,82,82,82	0
55	MG	AA	3445	1/1	0.95	0.51	-	69,69,69,69	0
55	MG	BA	1639	1/1	0.83	0.24	-	94,94,94,94	0
55	MG	AA	3237	1/1	0.86	0.31	-	81,81,81,81	0
55	MG	DA	3257	1/1	0.85	0.17	-	75,75,75,75	0
55	MG	CA	1687	1/1	0.68	0.35	-	99,99,99,99	0
55	MG	AA	3416	1/1	0.88	0.30	-	70,70,70,70	0
55	MG	DA	3113	1/1	0.96	0.35	-	44,44,44,44	0
55	MG	AA	3407	1/1	0.78	0.33	-	84,84,84,84	0
55	MG	BA	1808	1/1	0.86	0.43	-	69,69,69,69	0
55	MG	CA	1773	1/1	0.56	0.57	-	115,115,115,115	0
55	MG	BA	1821	1/1	0.88	0.23	-	78,78,78,78	0
55	MG	DA	3368	1/1	0.85	0.58	-	87,87,87,87	0
55	MG	AA	3032	1/1	0.92	0.39	-	60,60,60,60	0
55	MG	DA	3527	1/1	0.81	0.42	-	96,96,96,96	0
55	MG	CA	1795	1/1	0.52	0.23	-	110,110,110,110	0
55	MG	BA	1728	1/1	0.73	1.08	-	90,90,90,90	0
55	MG	AA	3485	1/1	0.74	0.51	-	96,96,96,96	0
55	MG	AA	3400	1/1	0.87	1.04	-	86,86,86,86	0
55	MG	CC	104	1/1	0.78	0.51	-	90,90,90,90	0
55	MG	DA	3274	1/1	0.89	0.48	-	80,80,80,80	0
55	MG	DA	3136	1/1	0.79	0.26	-	97,97,97,97	0
55	MG	CA	1746	1/1	0.94	0.63	-	59,59,59,59	0
55	MG	BA	1841	1/1	0.23	0.74	-	105,105,105,105	0
55	MG	AA	3395	1/1	0.96	0.17	-	57,57,57,57	0
55	MG	AA	3532	1/1	0.90	0.61	-	89,89,89,89	0
55	MG	AA	3502	1/1	0.83	0.48	-	81,81,81,81	0
55	MG	DA	3384	1/1	0.91	0.62	-	64,64,64,64	0
55	MG	DA	3224	1/1	0.93	0.35	-	59,59,59,59	0
55	MG	CA	1774	1/1	0.87	0.28	-	72,72,72,72	0
55	MG	BA	1758	1/1	0.58	0.22	-	110,110,110,110	0
55	MG	AA	3352	1/1	0.77	0.59	-	91,91,91,91	0
55	MG	CA	1607	1/1	0.92	0.39	-	77,77,77,77	0
55	MG	AA	3094	1/1	0.96	0.30	-	81,81,81,81	0
55	MG	DA	3041	1/1	0.85	0.64	-	91,91,91,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3474	1/1	0.53	0.67	-	103,103,103,103	0
55	MG	AA	3619	1/1	0.69	0.60	-	94,94,94,94	0
55	MG	CA	1672	1/1	0.86	0.64	-	76,76,76,76	0
55	MG	AA	3197	1/1	0.92	0.62	-	63,63,63,63	0
55	MG	DA	3029	1/1	0.83	0.33	-	92,92,92,92	0
55	MG	DA	3017	1/1	0.80	0.66	-	88,88,88,88	0
55	MG	DA	3180	1/1	0.98	0.51	-	50,50,50,50	0
55	MG	AA	3156	1/1	0.83	0.31	-	87,87,87,87	0
55	MG	CA	1692	1/1	0.90	0.26	-	75,75,75,75	0
55	MG	CA	1614	1/1	0.54	0.46	-	95,95,95,95	0
55	MG	DA	3410	1/1	0.69	0.53	-	99,99,99,99	0
55	MG	A3	101	1/1	0.79	0.45	-	80,80,80,80	0
55	MG	AA	3555	1/1	0.72	0.51	-	68,68,68,68	0
55	MG	DA	3100	1/1	0.96	0.25	-	62,62,62,62	0
55	MG	CA	1677	1/1	0.88	0.26	-	68,68,68,68	0
55	MG	AA	3629	1/1	0.37	0.50	-	107,107,107,107	0
55	MG	DA	3331	1/1	0.72	0.23	-	76,76,76,76	0
55	MG	AA	3201	1/1	0.98	0.42	-	42,42,42,42	0
55	MG	CA	1727	1/1	0.83	0.16	-	84,84,84,84	0
55	MG	CA	1764	1/1	0.93	0.49	-	67,67,67,67	0
55	MG	CA	1667	1/1	0.08	0.34	-	144,144,144,144	0
55	MG	DA	3343	1/1	0.56	0.88	-	145,145,145,145	0
55	MG	BA	1832	1/1	0.74	0.35	-	100,100,100,100	0
55	MG	CA	1612	1/1	0.66	0.41	-	91,91,91,91	0
55	MG	BA	1673	1/1	0.89	0.24	-	80,80,80,80	0
55	MG	CA	1616	1/1	0.71	0.12	-	90,90,90,90	0
55	MG	AA	3506	1/1	0.42	0.56	-	73,73,73,73	0
55	MG	BA	1839	1/1	0.89	0.22	-	61,61,61,61	0
55	MG	AA	3505	1/1	0.74	0.27	-	103,103,103,103	0
55	MG	DA	3477	1/1	0.48	0.74	-	125,125,125,125	0
55	MG	AA	3614	1/1	0.97	0.51	-	91,91,91,91	0
55	MG	AA	3587	1/1	0.93	0.19	-	28,28,28,28	0
55	MG	AA	3299	1/1	0.84	0.20	-	94,94,94,94	0
55	MG	BA	1747	1/1	0.84	0.19	-	97,97,97,97	0
55	MG	BA	1652	1/1	0.89	0.25	-	86,86,86,86	0
55	MG	CA	1631	1/1	0.65	0.21	-	95,95,95,95	0
55	MG	AA	3581	1/1	0.74	0.71	-	67,67,67,67	0
55	MG	DA	3031	1/1	0.94	0.36	-	69,69,69,69	0
55	MG	DA	3526	1/1	0.95	0.28	-	92,92,92,92	0
55	MG	BA	1756	1/1	0.86	0.78	-	96,96,96,96	0
55	MG	BA	1721	1/1	0.61	0.40	-	109,109,109,109	0
55	MG	DA	3295	1/1	0.93	0.57	-	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1648	1/1	0.96	0.28	-	65,65,65,65	0
55	MG	CA	1793	1/1	0.94	0.45	-	78,78,78,78	0
55	MG	AA	3615	1/1	0.86	0.35	-	84,84,84,84	0
55	MG	AA	3443	1/1	0.32	0.23	-	95,95,95,95	0
55	MG	CA	1663	1/1	0.86	0.27	-	72,72,72,72	0
55	MG	BA	1778	1/1	0.76	0.23	-	93,93,93,93	0
55	MG	AA	3041	1/1	0.95	0.23	-	62,62,62,62	0
55	MG	AA	3468	1/1	0.91	0.44	-	92,92,92,92	0
55	MG	AA	3394	1/1	0.95	0.15	-	85,85,85,85	0
55	MG	CA	1806	1/1	0.88	0.23	-	115,115,115,115	0
55	MG	AA	3148	1/1	0.54	0.46	-	70,70,70,70	0
55	MG	BN	202	1/1	0.56	0.68	-	104,104,104,104	0
55	MG	CA	1724	1/1	0.90	0.65	-	88,88,88,88	0
55	MG	BA	1746	1/1	0.71	0.42	-	95,95,95,95	0
55	MG	BA	1765	1/1	0.64	0.20	-	99,99,99,99	0
55	MG	AA	3577	1/1	0.95	0.44	-	42,42,42,42	0
55	MG	DA	3388	1/1	0.89	0.53	-	85,85,85,85	0
55	MG	AA	3284	1/1	0.83	0.47	-	80,80,80,80	0
55	MG	DP	201	1/1	0.95	0.35	-	63,63,63,63	0
55	MG	CA	1629	1/1	0.87	0.23	-	82,82,82,82	0
55	MG	AA	3364	1/1	0.56	0.52	-	89,89,89,89	0
55	MG	DA	3501	1/1	0.89	0.36	-	77,77,77,77	0

6.5 Other polymers

There are no such residues in this entry.