



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:16 PM GMT

PDB ID : 4V8D
Title : Structure analysis of ribosomal decoding (cognate tRNA-tyr complex).
Authors : Jenner, L.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2011-12-07
Resolution : 3.00 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

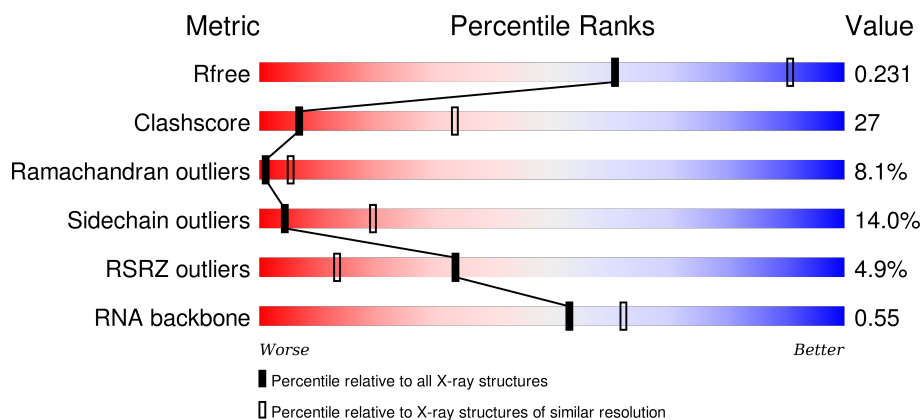
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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	1506	
1	CA	1506	
2	AE	256	
2	CE	256	


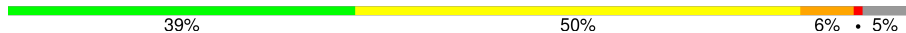



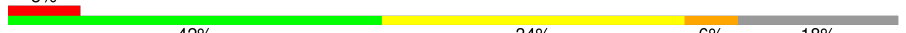
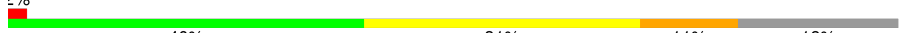




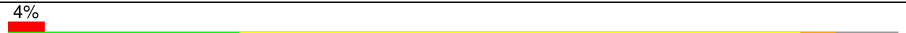








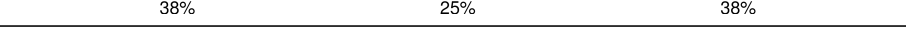




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AF	239	
3	CF	239	
4	AG	208	
4	CG	208	
5	AH	162	
5	CH	162	
6	AI	101	
6	CI	101	
7	AJ	156	
7	CJ	156	
8	AK	138	
8	CK	138	
9	AL	128	
9	CL	128	
10	AM	105	
10	CM	105	
11	AN	129	
11	CN	129	
12	AO	132	
12	CO	132	
13	AP	126	
13	CP	126	
14	AQ	61	
14	CQ	61	
15	AR	89	




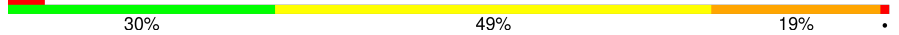

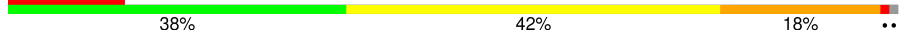
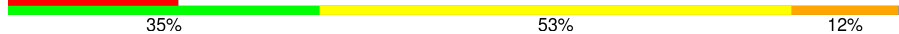
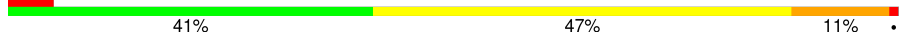
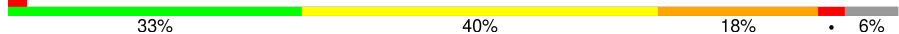
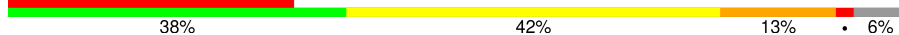
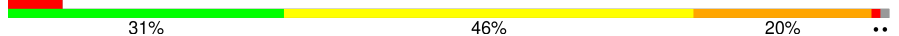
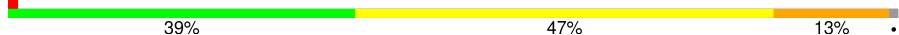
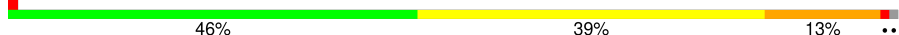
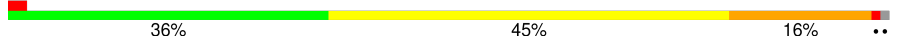



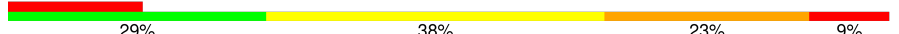

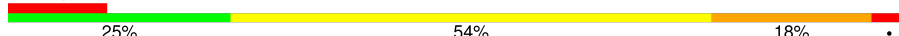





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CR	89	
16	AS	88	
16	CS	88	
17	AT	105	
17	CT	105	
18	AU	88	
18	CU	88	
19	AV	93	
19	CV	93	
20	AW	106	
20	CW	106	
21	AX	27	
21	CX	27	
22	AB	85	
22	AD	85	
22	CB	85	
22	CD	85	
23	AC	77	
23	CC	77	
24	A1	16	
24	C1	16	
25	BA	2912	
25	DA	2912	
26	BB	122	
26	DB	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	BD	276	
27	DD	276	
28	BE	206	
28	DE	206	
29	BF	210	
29	DF	210	
30	BG	182	
30	DG	182	
31	BH	180	
31	DH	180	
32	BK	148	
32	DK	148	
33	BM	140	
33	DM	140	
34	BN	122	
34	DN	122	
35	BO	150	
35	DO	150	
36	BP	141	
36	DP	141	
37	B0	118	
37	D0	118	
38	BQ	112	
38	DQ	112	
39	BR	146	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1601	-	-	-	X
55	MG	AA	1602	-	-	-	X
55	MG	AA	1605	-	-	-	X
55	MG	AA	1608	-	-	-	X
55	MG	AA	1610	-	-	-	X
55	MG	AA	1619	-	-	-	X
55	MG	AA	1620	-	-	-	X
55	MG	AA	1625	-	-	-	X
55	MG	AA	1628	-	-	-	X
55	MG	AA	1632	-	-	-	X
55	MG	AA	1636	-	-	-	X
55	MG	AA	1639	-	-	-	X
55	MG	AA	1646	-	-	-	X
55	MG	AA	1648	-	-	-	X
55	MG	AA	1652	-	-	-	X
55	MG	AA	1659	-	-	-	X
55	MG	AA	1662	-	-	-	X
55	MG	AA	1669	-	-	-	X
55	MG	AA	1681	-	-	-	X
55	MG	AA	1683	-	-	-	X
55	MG	AA	1698	-	-	-	X
55	MG	AA	1706	-	-	-	X
55	MG	AA	1709	-	-	-	X
55	MG	AA	1710	-	-	-	X
55	MG	AA	1739	-	-	-	X
55	MG	AA	1740	-	-	-	X
55	MG	AA	1788	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	AA	1790	-	-	-	X
55	MG	AA	1811	-	-	-	X
55	MG	AC	101	-	-	-	X
55	MG	AC	107	-	-	-	X
55	MG	AD	103	-	-	-	X
55	MG	AG	301	-	-	-	X
55	MG	B1	201	-	-	-	X
55	MG	B1	202	-	-	-	X
55	MG	BA	3001	-	-	-	X
55	MG	BA	3002	-	-	-	X
55	MG	BA	3004	-	-	-	X
55	MG	BA	3006	-	-	-	X
55	MG	BA	3010	-	-	-	X
55	MG	BA	3012	-	-	-	X
55	MG	BA	3014	-	-	-	X
55	MG	BA	3016	-	-	-	X
55	MG	BA	3018	-	-	-	X
55	MG	BA	3020	-	-	-	X
55	MG	BA	3021	-	-	-	X
55	MG	BA	3024	-	-	-	X
55	MG	BA	3026	-	-	-	X
55	MG	BA	3027	-	-	-	X
55	MG	BA	3039	-	-	-	X
55	MG	BA	3042	-	-	-	X
55	MG	BA	3044	-	-	-	X
55	MG	BA	3047	-	-	-	X
55	MG	BA	3048	-	-	-	X
55	MG	BA	3054	-	-	-	X
55	MG	BA	3055	-	-	-	X
55	MG	BA	3056	-	-	-	X
55	MG	BA	3057	-	-	-	X
55	MG	BA	3059	-	-	-	X
55	MG	BA	3070	-	-	-	X
55	MG	BA	3074	-	-	-	X
55	MG	BA	3076	-	-	-	X
55	MG	BA	3080	-	-	-	X
55	MG	BA	3083	-	-	-	X
55	MG	BA	3084	-	-	-	X
55	MG	BA	3086	-	-	-	X
55	MG	BA	3087	-	-	-	X
55	MG	BA	3088	-	-	-	X
55	MG	BA	3090	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3095	-	-	-	X
55	MG	BA	3101	-	-	-	X
55	MG	BA	3109	-	-	-	X
55	MG	BA	3110	-	-	-	X
55	MG	BA	3116	-	-	-	X
55	MG	BA	3117	-	-	-	X
55	MG	BA	3124	-	-	-	X
55	MG	BA	3127	-	-	-	X
55	MG	BA	3129	-	-	-	X
55	MG	BA	3130	-	-	-	X
55	MG	BA	3131	-	-	-	X
55	MG	BA	3134	-	-	-	X
55	MG	BA	3140	-	-	-	X
55	MG	BA	3144	-	-	-	X
55	MG	BA	3145	-	-	-	X
55	MG	BA	3147	-	-	-	X
55	MG	BA	3150	-	-	-	X
55	MG	BA	3157	-	-	-	X
55	MG	BA	3160	-	-	-	X
55	MG	BA	3161	-	-	-	X
55	MG	BA	3167	-	-	-	X
55	MG	BA	3169	-	-	-	X
55	MG	BA	3172	-	-	-	X
55	MG	BA	3174	-	-	-	X
55	MG	BA	3182	-	-	-	X
55	MG	BA	3184	-	-	-	X
55	MG	BA	3186	-	-	-	X
55	MG	BA	3202	-	-	-	X
55	MG	BA	3215	-	-	-	X
55	MG	BA	3223	-	-	-	X
55	MG	BA	3231	-	-	-	X
55	MG	BA	3232	-	-	-	X
55	MG	BA	3240	-	-	-	X
55	MG	BA	3241	-	-	-	X
55	MG	BA	3248	-	-	-	X
55	MG	BA	3262	-	-	-	X
55	MG	BA	3264	-	-	-	X
55	MG	BA	3272	-	-	-	X
55	MG	BA	3283	-	-	-	X
55	MG	BA	3286	-	-	-	X
55	MG	BA	3287	-	-	-	X
55	MG	BA	3290	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3299	-	-	-	X
55	MG	BA	3300	-	-	-	X
55	MG	BA	3313	-	-	-	X
55	MG	BA	3328	-	-	-	X
55	MG	BA	3330	-	-	-	X
55	MG	BA	3332	-	-	-	X
55	MG	BA	3334	-	-	-	X
55	MG	BA	3337	-	-	-	X
55	MG	BA	3346	-	-	-	X
55	MG	BA	3352	-	-	-	X
55	MG	BA	3356	-	-	-	X
55	MG	BA	3368	-	-	-	X
55	MG	BA	3389	-	-	-	X
55	MG	BA	3392	-	-	-	X
55	MG	BA	3407	-	-	-	X
55	MG	BA	3415	-	-	-	X
55	MG	BA	3435	-	-	-	X
55	MG	BA	3448	-	-	-	X
55	MG	BA	3454	-	-	-	X
55	MG	BA	3460	-	-	-	X
55	MG	BA	3469	-	-	-	X
55	MG	BA	3475	-	-	-	X
55	MG	BA	3486	-	-	-	X
55	MG	BA	3488	-	-	-	X
55	MG	BA	3490	-	-	-	X
55	MG	BA	3492	-	-	-	X
55	MG	BA	3493	-	-	-	X
55	MG	BA	3495	-	-	-	X
55	MG	BA	3496	-	-	-	X
55	MG	BA	3497	-	-	-	X
55	MG	BA	3498	-	-	-	X
55	MG	BA	3499	-	-	-	X
55	MG	BA	3505	-	-	-	X
55	MG	BA	3507	-	-	-	X
55	MG	BA	3518	-	-	-	X
55	MG	BA	3520	-	-	-	X
55	MG	BA	3521	-	-	-	X
55	MG	BA	3522	-	-	-	X
55	MG	BA	3524	-	-	-	X
55	MG	BA	3528	-	-	-	X
55	MG	BA	3534	-	-	-	X
55	MG	BA	3538	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	BA	3539	-	-	-	X
55	MG	BA	3540	-	-	-	X
55	MG	BA	3546	-	-	-	X
55	MG	BA	3549	-	-	-	X
55	MG	BA	3553	-	-	-	X
55	MG	BA	3555	-	-	-	X
55	MG	BB	202	-	-	-	X
55	MG	BB	210	-	-	-	X
55	MG	BB	215	-	-	-	X
55	MG	CA	1601	-	-	-	X
55	MG	CA	1602	-	-	-	X
55	MG	CA	1603	-	-	-	X
55	MG	CA	1613	-	-	-	X
55	MG	CA	1615	-	-	-	X
55	MG	CA	1616	-	-	-	X
55	MG	CA	1617	-	-	-	X
55	MG	CA	1631	-	-	-	X
55	MG	CA	1634	-	-	-	X
55	MG	CA	1638	-	-	-	X
55	MG	CA	1639	-	-	-	X
55	MG	CA	1645	-	-	-	X
55	MG	CA	1651	-	-	-	X
55	MG	CA	1656	-	-	-	X
55	MG	CA	1657	-	-	-	X
55	MG	CA	1676	-	-	-	X
55	MG	CA	1695	-	-	-	X
55	MG	CA	1720	-	-	-	X
55	MG	CA	1742	-	-	-	X
55	MG	CA	1744	-	-	-	X
55	MG	CA	1767	-	-	-	X
55	MG	CA	1776	-	-	-	X
55	MG	CA	1793	-	-	-	X
55	MG	CA	1806	-	-	-	X
55	MG	CA	1811	-	-	-	X
55	MG	CA	1813	-	-	-	X
55	MG	CA	1814	-	-	-	X
55	MG	CC	101	-	-	-	X
55	MG	CC	108	-	-	-	X
55	MG	CC	109	-	-	-	X
55	MG	DA	3002	-	-	-	X
55	MG	DA	3006	-	-	-	X
55	MG	DA	3008	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3009	-	-	-	X
55	MG	DA	3010	-	-	-	X
55	MG	DA	3015	-	-	-	X
55	MG	DA	3017	-	-	-	X
55	MG	DA	3018	-	-	-	X
55	MG	DA	3020	-	-	-	X
55	MG	DA	3028	-	-	-	X
55	MG	DA	3030	-	-	-	X
55	MG	DA	3043	-	-	-	X
55	MG	DA	3044	-	-	-	X
55	MG	DA	3045	-	-	-	X
55	MG	DA	3055	-	-	-	X
55	MG	DA	3056	-	-	-	X
55	MG	DA	3057	-	-	-	X
55	MG	DA	3058	-	-	-	X
55	MG	DA	3059	-	-	-	X
55	MG	DA	3061	-	-	-	X
55	MG	DA	3063	-	-	-	X
55	MG	DA	3068	-	-	-	X
55	MG	DA	3070	-	-	-	X
55	MG	DA	3071	-	-	-	X
55	MG	DA	3075	-	-	-	X
55	MG	DA	3084	-	-	-	X
55	MG	DA	3089	-	-	-	X
55	MG	DA	3094	-	-	-	X
55	MG	DA	3098	-	-	-	X
55	MG	DA	3106	-	-	-	X
55	MG	DA	3107	-	-	-	X
55	MG	DA	3115	-	-	-	X
55	MG	DA	3116	-	-	-	X
55	MG	DA	3119	-	-	-	X
55	MG	DA	3123	-	-	-	X
55	MG	DA	3124	-	-	-	X
55	MG	DA	3129	-	-	-	X
55	MG	DA	3131	-	-	-	X
55	MG	DA	3137	-	-	-	X
55	MG	DA	3144	-	-	-	X
55	MG	DA	3159	-	-	-	X
55	MG	DA	3162	-	-	-	X
55	MG	DA	3173	-	-	-	X
55	MG	DA	3174	-	-	-	X
55	MG	DA	3187	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3190	-	-	-	X
55	MG	DA	3196	-	-	-	X
55	MG	DA	3197	-	-	-	X
55	MG	DA	3200	-	-	-	X
55	MG	DA	3202	-	-	-	X
55	MG	DA	3207	-	-	-	X
55	MG	DA	3212	-	-	-	X
55	MG	DA	3220	-	-	-	X
55	MG	DA	3222	-	-	-	X
55	MG	DA	3233	-	-	-	X
55	MG	DA	3235	-	-	-	X
55	MG	DA	3236	-	-	-	X
55	MG	DA	3240	-	-	-	X
55	MG	DA	3241	-	-	-	X
55	MG	DA	3247	-	-	-	X
55	MG	DA	3250	-	-	-	X
55	MG	DA	3270	-	-	-	X
55	MG	DA	3282	-	-	-	X
55	MG	DA	3289	-	-	-	X
55	MG	DA	3307	-	-	-	X
55	MG	DA	3318	-	-	-	X
55	MG	DA	3321	-	-	-	X
55	MG	DA	3341	-	-	-	X
55	MG	DA	3362	-	-	-	X
55	MG	DA	3370	-	-	-	X
55	MG	DA	3383	-	-	-	X
55	MG	DA	3387	-	-	-	X
55	MG	DA	3390	-	-	-	X
55	MG	DA	3408	-	-	-	X
55	MG	DA	3428	-	-	-	X
55	MG	DA	3430	-	-	-	X
55	MG	DA	3432	-	-	-	X
55	MG	DA	3433	-	-	-	X
55	MG	DA	3435	-	-	-	X
55	MG	DA	3439	-	-	-	X
55	MG	DA	3450	-	-	-	X
55	MG	DA	3453	-	-	-	X
55	MG	DA	3456	-	-	-	X
55	MG	DA	3458	-	-	-	X
55	MG	DA	3463	-	-	-	X
55	MG	DA	3470	-	-	-	X
55	MG	DA	3471	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	DA	3474	-	-	-	X
55	MG	DB	208	-	-	-	X
55	MG	DB	212	-	-	-	X
55	MG	DB	213	-	-	-	X
55	MG	DD	301	-	-	-	X
55	MG	DE	301	-	-	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 299676 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1502	Total	C	N	O	P	0	0	0
			32284	14370	5982	10431	1501			
1	CA	1502	Total	C	N	O	P	0	0	0
			32287	14370	5982	10433	1502			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

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

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			
14	CQ	58	Total	C	N	O	S	0	0	0
			476	303	99	70	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			
19	CV	78	Total	C	N	O	S	0	0	0
			624	398	115	109	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 22 is a RNA chain called TRNA-TYR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
22	AB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
22	AD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
22	CB	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			
22	CD	85	Total	C	N	O	P	S	0	0	0
			1814	813	323	592	85	1			

- Molecule 23 is a RNA chain called TRNA-FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			
23	CC	77	Total	C	N	O	P	0	0	0
			1643	732	298	536	77			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	18	C	U	CONFLICT	GB AP012306.1
CC	18	C	U	CONFLICT	GB AP012306.1

- Molecule 24 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A1	16	Total	C	N	O	P	0	0	0
			346	156	69	105	16			
24	C1	16	Total	C	N	O	P	0	0	0
			346	156	69	105	16			

- Molecule 25 is a RNA chain called RNA (2912-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2912	Total	C	N	O	P	0	0	0
			62707	27911	11722	20163	2911			
25	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
BA	161	U	-	INSERTION	GB AP008226.1
BA	654A	A	G	CONFLICT	GB AP008226.1
BA	654E	C	G	CONFLICT	GB AP008226.1
BA	654P	G	C	CONFLICT	GB AP008226.1
BA	654T	A	C	CONFLICT	GB AP008226.1
BA	1058	U	G	CONFLICT	GB AP008226.1
BA	1080	A	C	CONFLICT	GB AP008226.1
DA	166	U	-	INSERTION	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 26 is a RNA chain called 5S RIBOSOMAL RNA.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	DE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
29	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			
31	DH	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

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

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BM	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

Continued on next page...

Continued from previous page...

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	B0	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
37	D0	117	Total	C	N	O	S	0	0	0
			960	599	202	159				

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
39	DR	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	B1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
40	D1	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	D2	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BT	92	Total	C	N	O	0	0	0
			725	471	131	123			
43	DT	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			
44	DU	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B3	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
46	D3	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			
48	DW	66	Total	C	N	O	S	0	0	0
			558	346	113	98	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	BX	59	Total	C	N	O	0	0	0
			469	298	90	81			

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	66	Total	C	N	O	S	0	0	0
			533	335	96	97	5			
50	D4	63	Total	C	N	O	S	0	0	0
			515	326	93	91	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			
52	D6	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			
53	D7	45	Total	C	N	O	S	0	0	0
			391	240	97	52	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			
54	D8	60	Total	C	N	O	S	0	0	0
			480	306	98	74	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	BA	568	Total 568	Mg 568	2	0
55	CA	219	Total 219	Mg 219	0	0
55	AB	4	Total 4	Mg 4	0	0
55	BE	3	Total 3	Mg 3	0	0
55	B1	2	Total 2	Mg 2	0	0
55	AN	1	Total 1	Mg 1	0	0
55	CR	1	Total 1	Mg 1	0	0
55	AS	1	Total 1	Mg 1	0	0
55	B5	1	Total 1	Mg 1	0	0
55	BB	18	Total 18	Mg 18	0	0
55	DO	1	Total 1	Mg 1	0	0
55	D8	1	Total 1	Mg 1	0	0
55	D3	1	Total 1	Mg 1	0	0
55	BF	3	Total 3	Mg 3	0	0
55	B2	1	Total 1	Mg 1	0	0
55	AA	220	Total 220	Mg 220	1	0
55	D7	1	Total 1	Mg 1	0	0
55	AR	1	Total 1	Mg 1	0	0
55	B6	1	Total 1	Mg 1	0	0
55	CG	2	Total 2	Mg 2	0	0
55	A1	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AD	3	Total 3	Mg 3	0	0
55	DD	3	Total 3	Mg 3	0	0
55	D0	1	Total 1	Mg 1	0	0
55	CC	9	Total 9	Mg 9	0	0
55	DE	1	Total 1	Mg 1	0	0
55	B3	3	Total 3	Mg 3	0	0
55	DA	488	Total 488	Mg 488	0	0
55	D5	2	Total 2	Mg 2	0	0
55	B7	1	Total 1	Mg 1	0	0
55	AG	2	Total 2	Mg 2	0	0
55	BO	2	Total 2	Mg 2	0	0
55	D1	1	Total 1	Mg 1	0	0
55	CB	4	Total 4	Mg 4	0	0
55	AC	8	Total 8	Mg 8	0	0
55	CD	1	Total 1	Mg 1	0	0
55	BD	1	Total 1	Mg 1	0	0
55	B0	1	Total 1	Mg 1	0	0
55	BW	1	Total 1	Mg 1	0	0
55	CK	1	Total 1	Mg 1	0	0
55	DB	20	Total 20	Mg 20	0	0

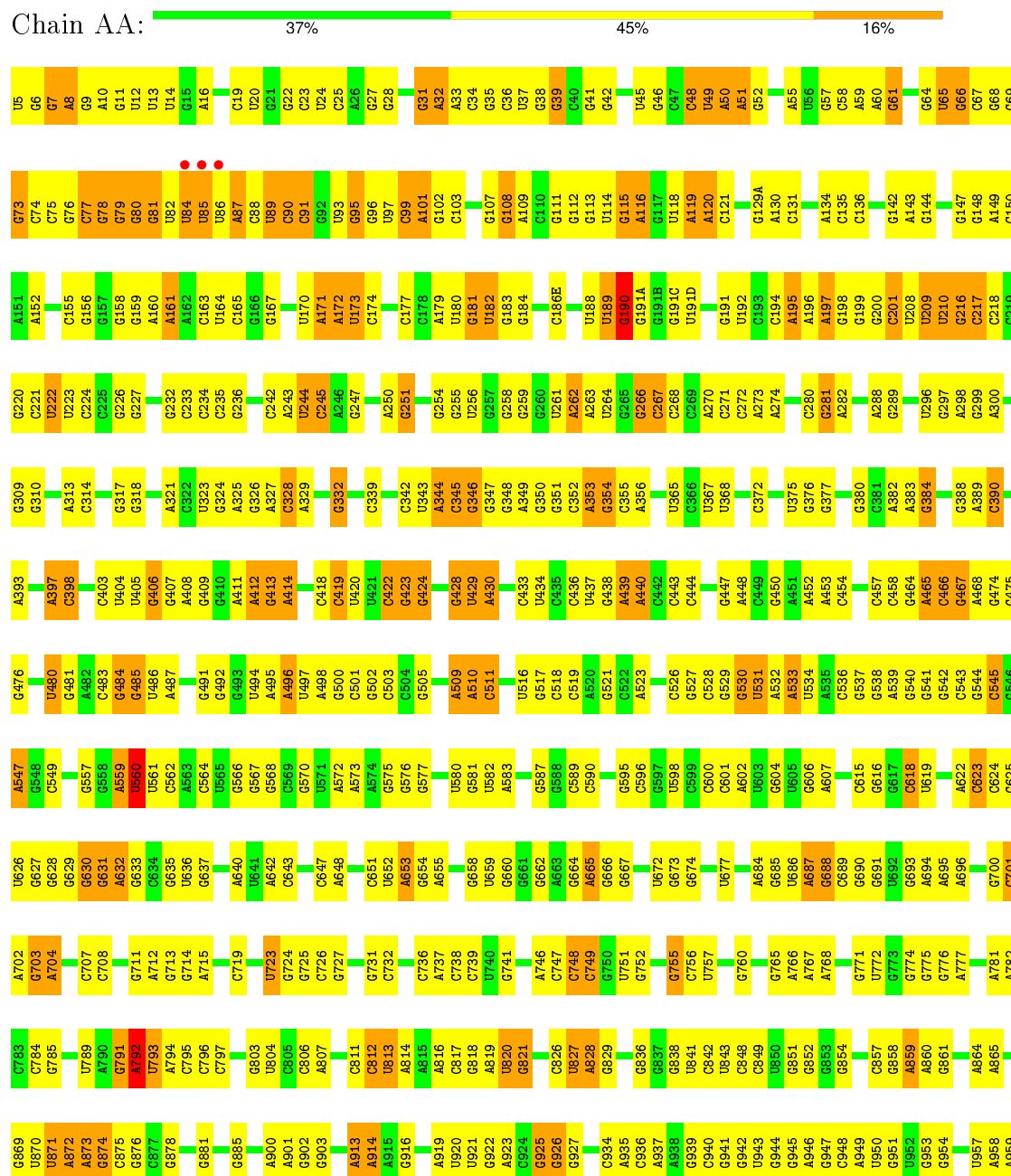
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

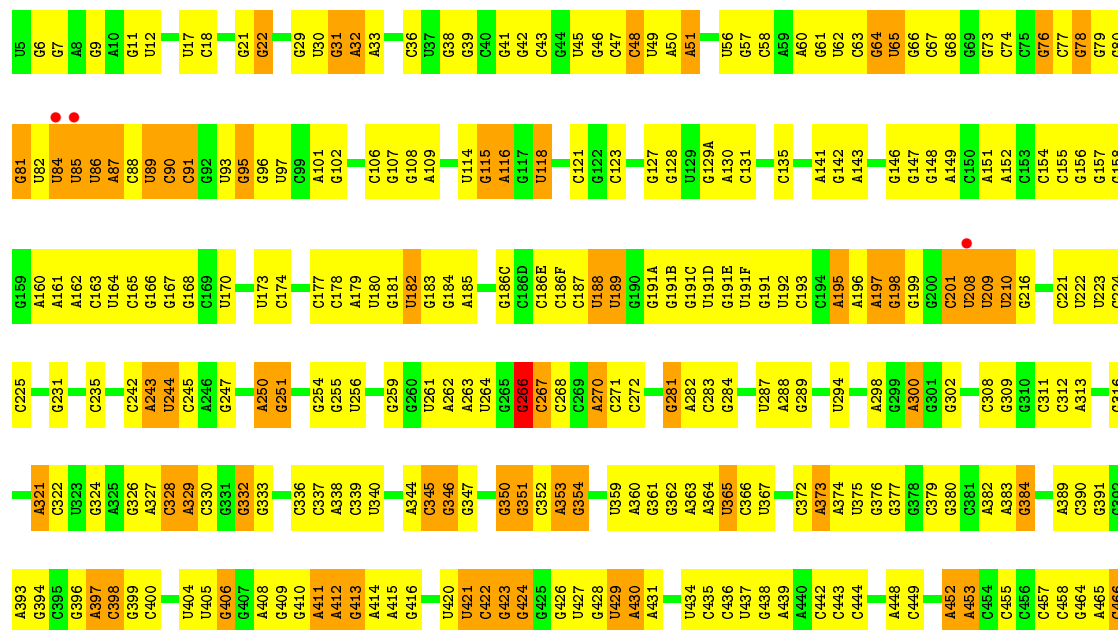
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AG	1	Total 1	Zn 1	0	0
56	AQ	1	Total 1	Zn 1	0	0
56	CQ	1	Total 1	Zn 1	0	0
56	CG	1	Total 1	Zn 1	0	0

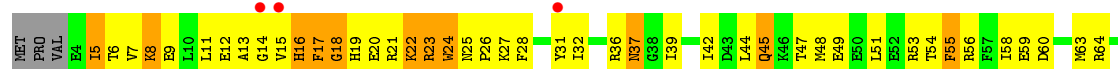
3 Residue-property plots

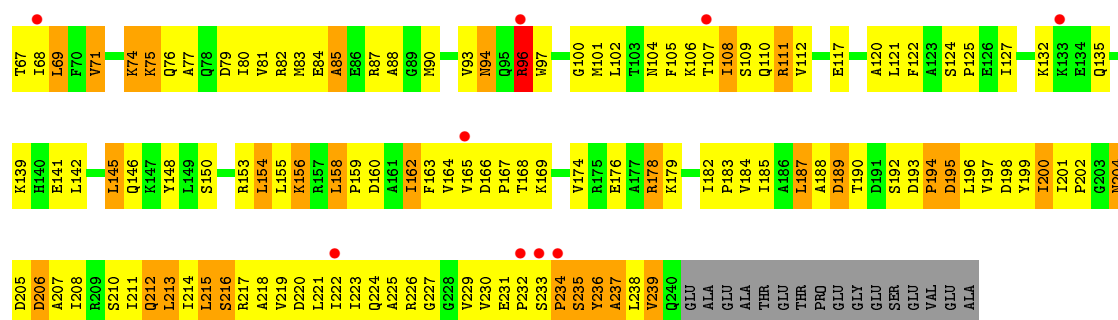
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S ribosomal RNA

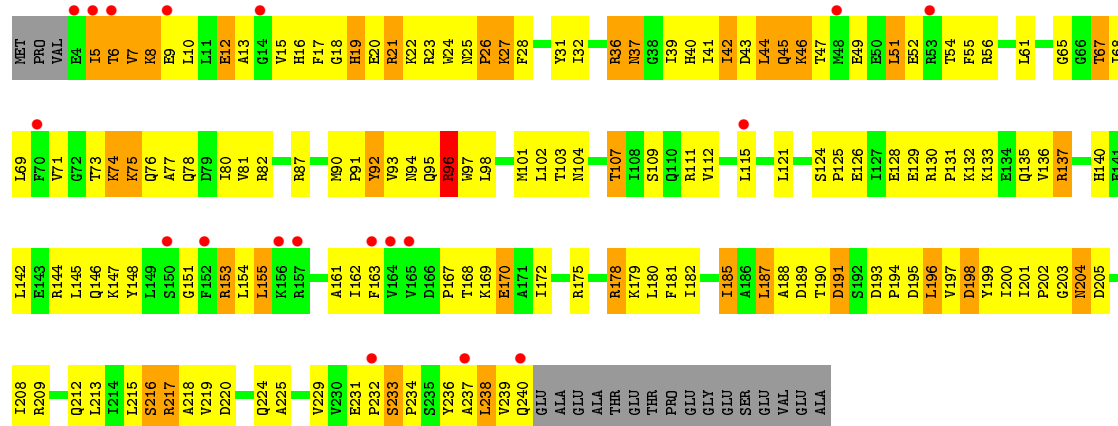




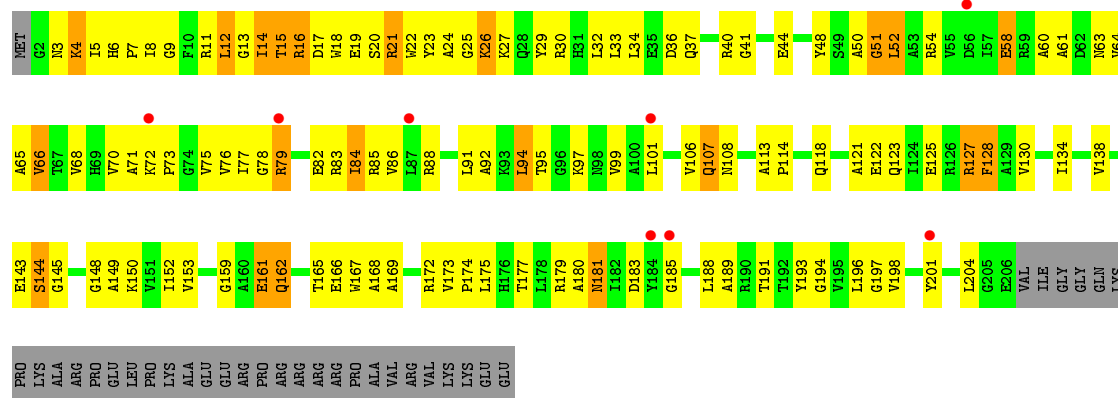




• Molecule 2: 30S RIBOSOMAL PROTEIN S2

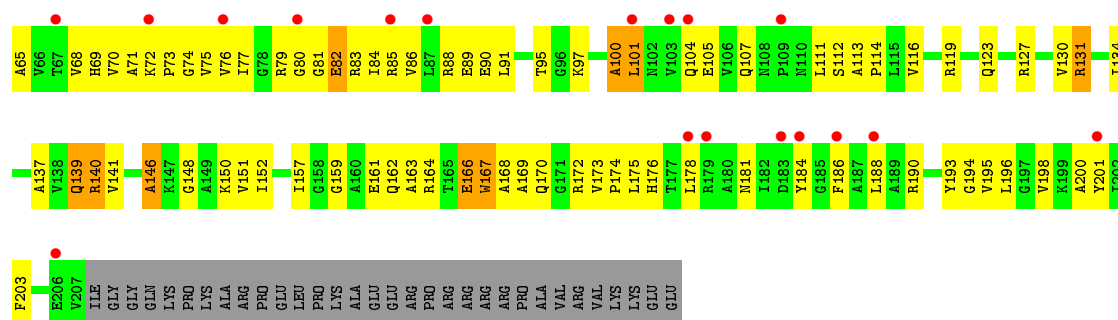


• Molecule 3: 30S RIBOSOMAL PROTEIN S3



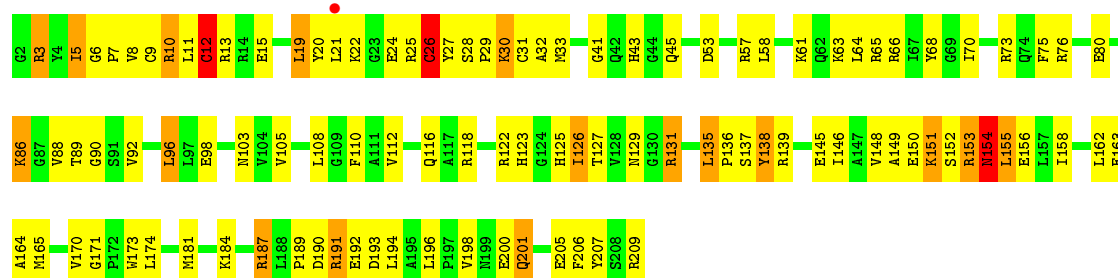
• Molecule 3: 30S RIBOSOMAL PROTEIN S3





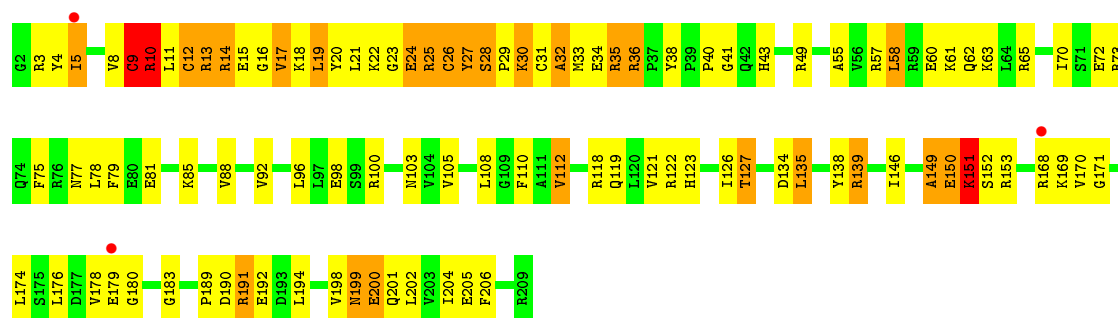
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AG: 50% 41% 8% .



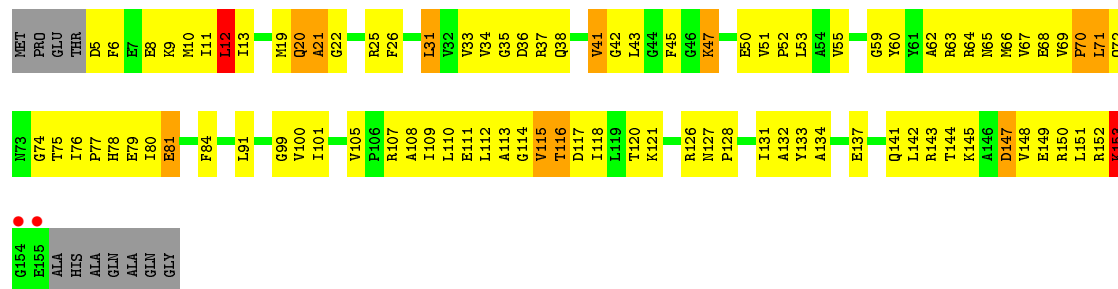
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CG: 50% 37% 12% .

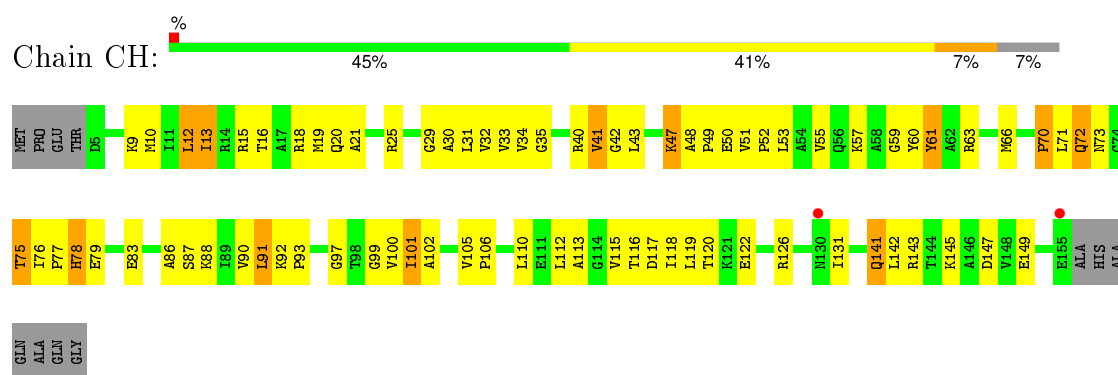


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

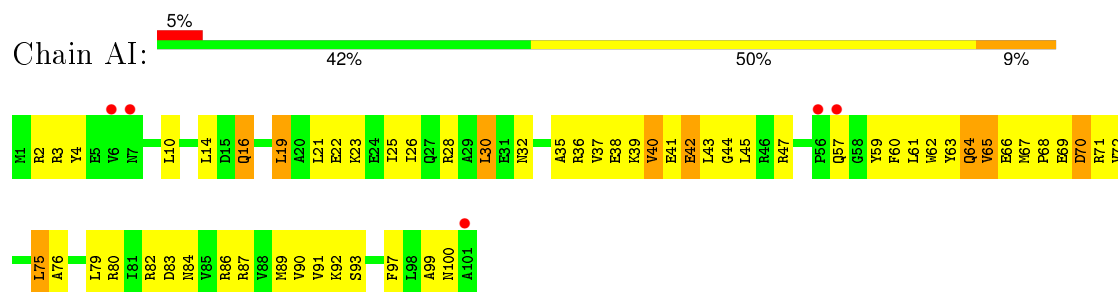
Chain AH: 36% 49% 7% 7% .



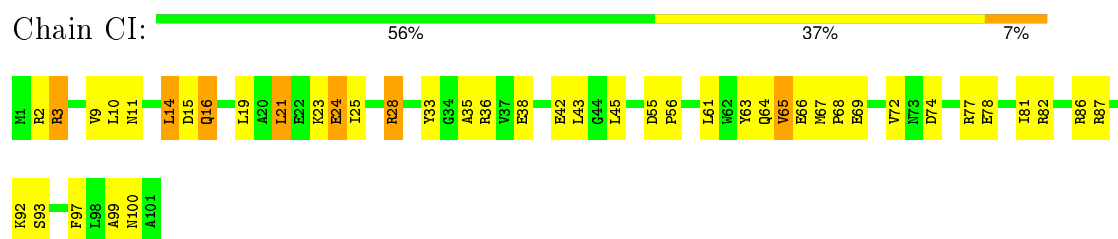
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



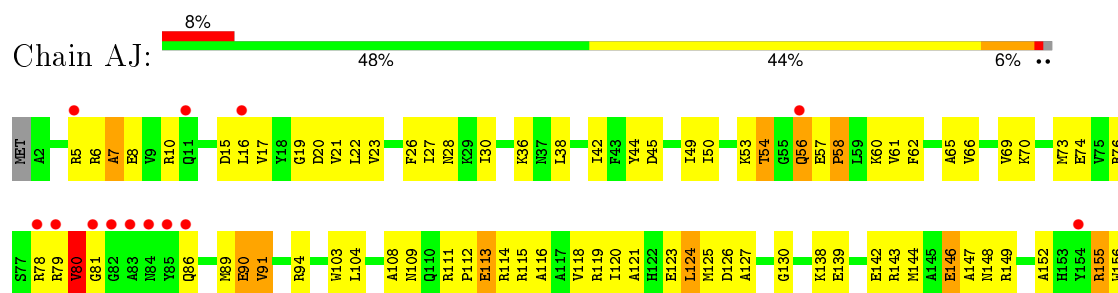
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



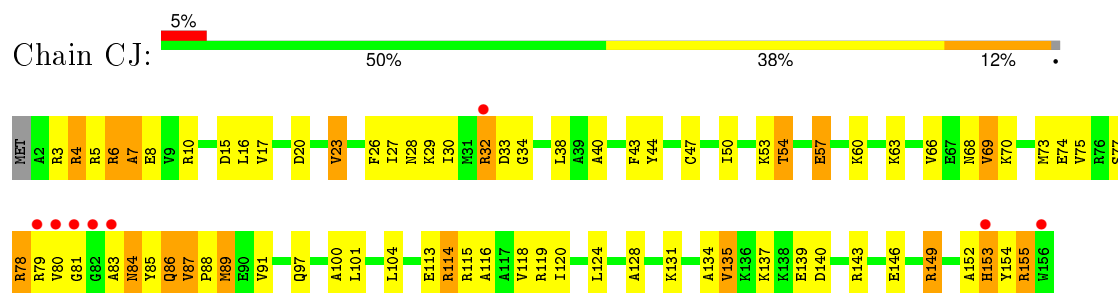
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

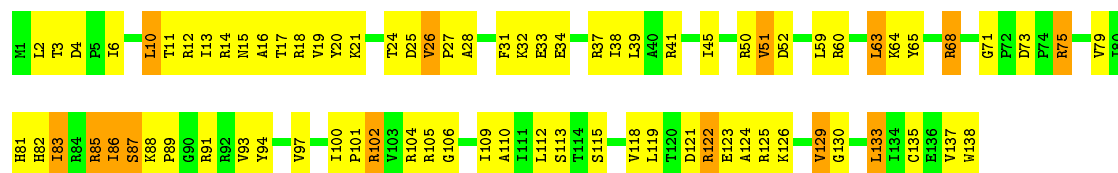


• Molecule 7: 30S RIBOSOMAL PROTEIN S7



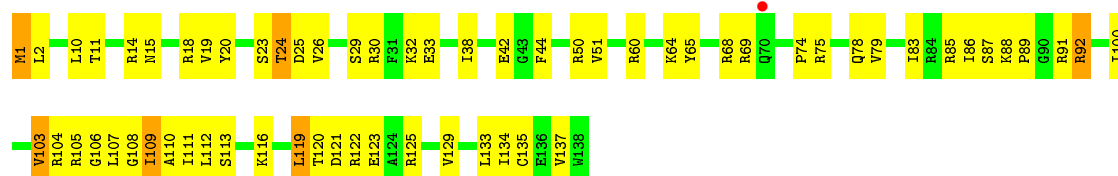
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AK: 



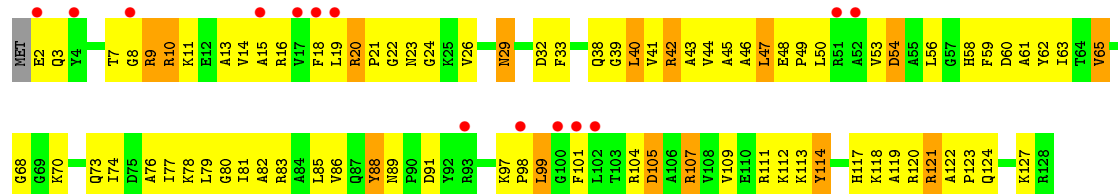
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CK: 



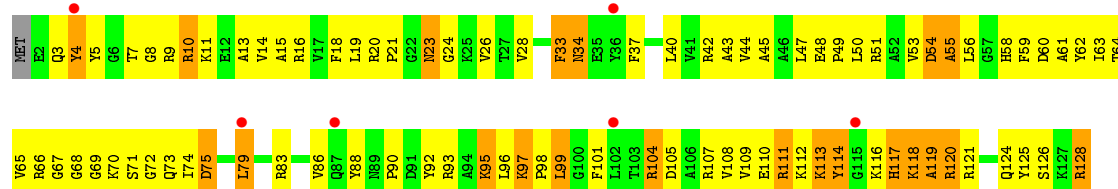
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AL: 



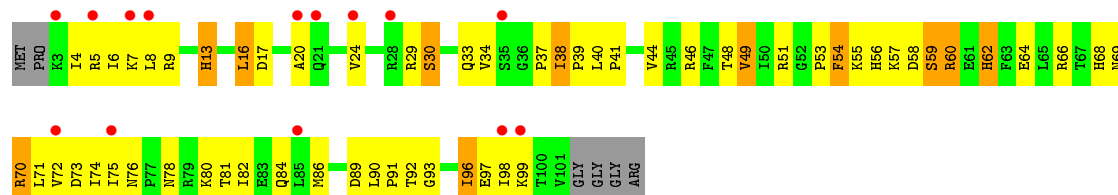
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CL: 

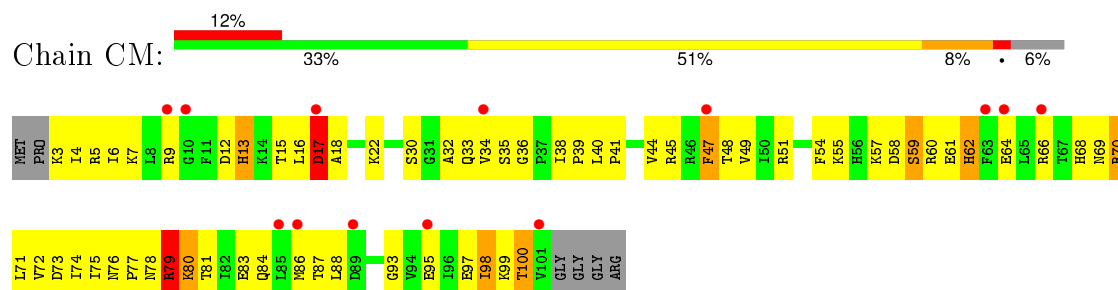


- Molecule 10: 30S RIBOSOMAL PROTEIN S10

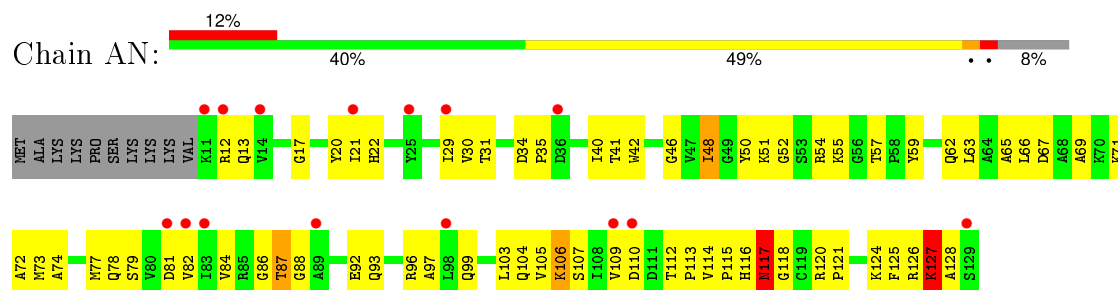
Chain AM: 



- Molecule 10: 30S RIBOSOMAL PROTEIN S10



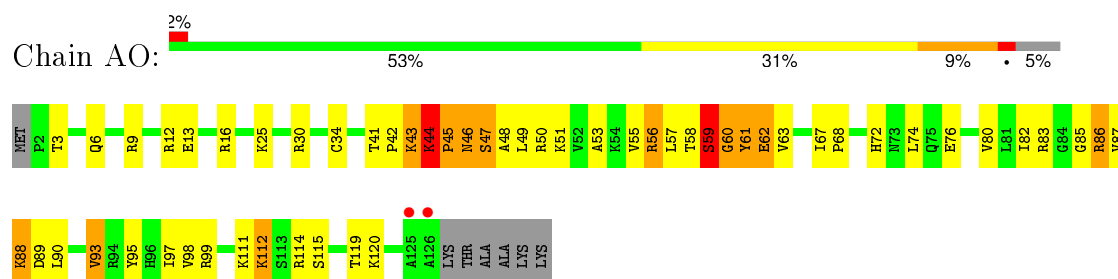
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



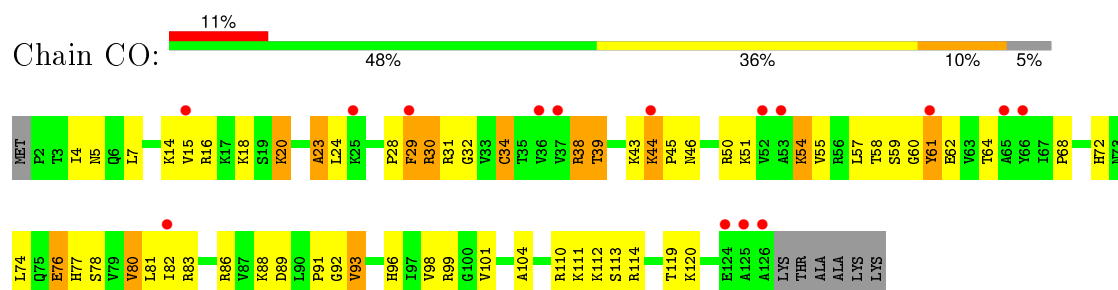
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



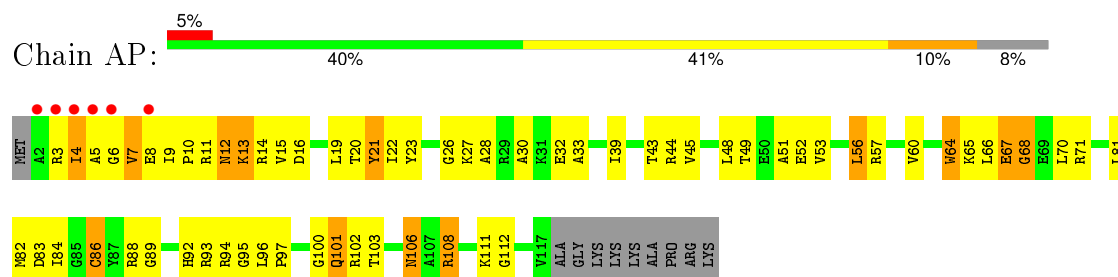
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



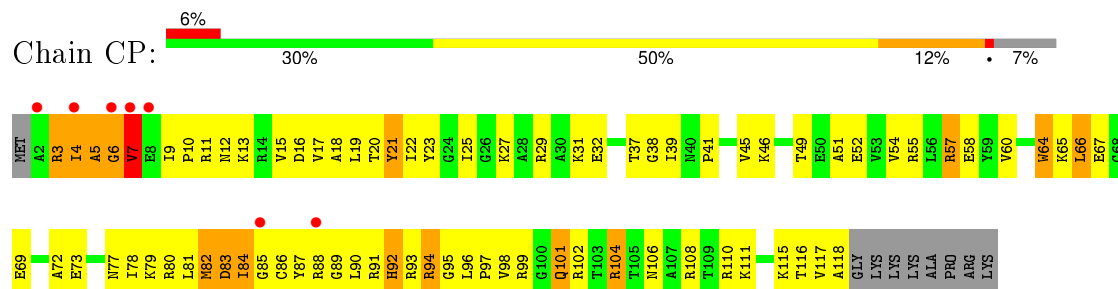
- Molecule 12: 30S RIBOSOMAL PROTEIN S12



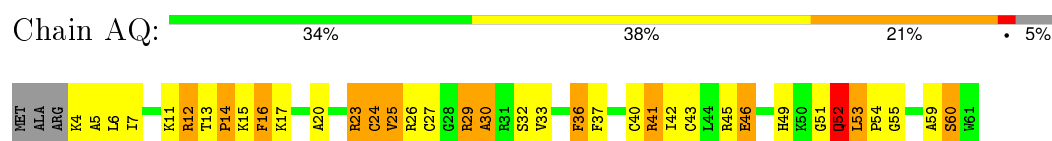
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



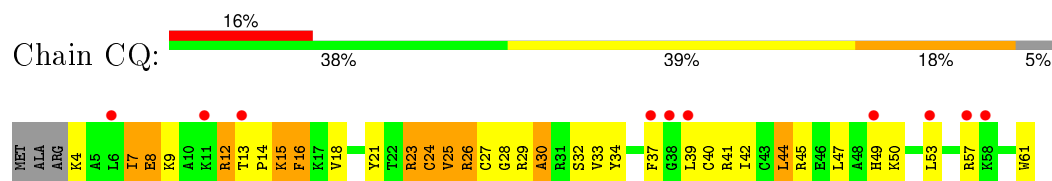
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



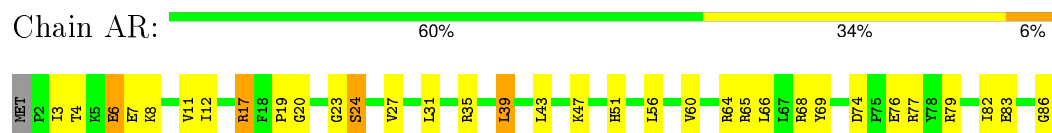
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



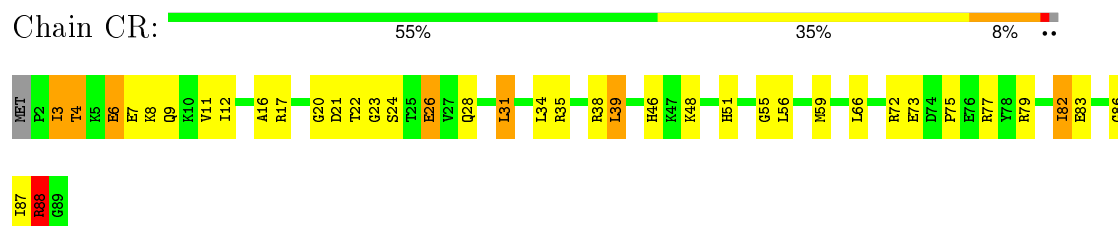
- Molecule 14: 30S RIBOSOMAL PROTEIN S14



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

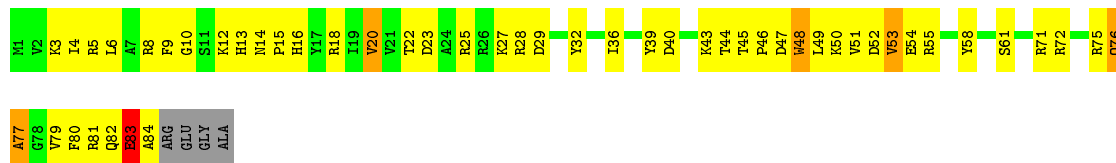


- Molecule 15: 30S RIBOSOMAL PROTEIN S15



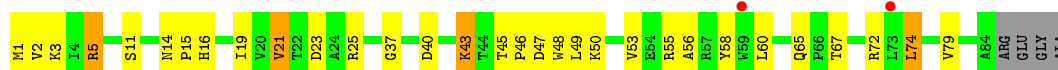
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AS: 



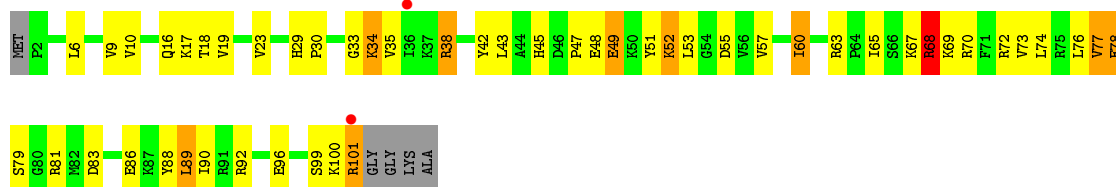
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CS: 



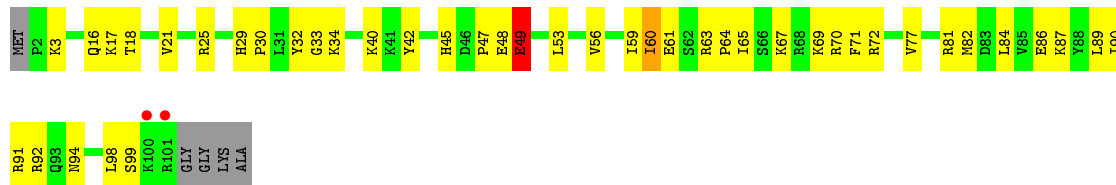
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AT: 



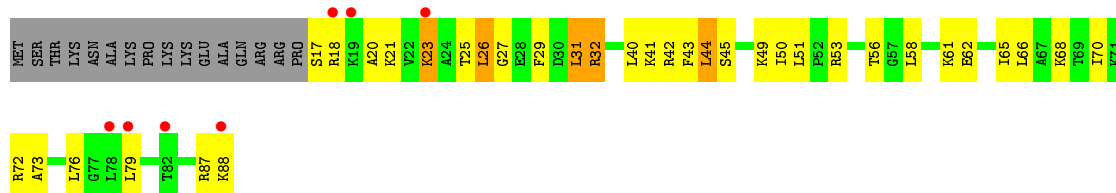
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CT: 



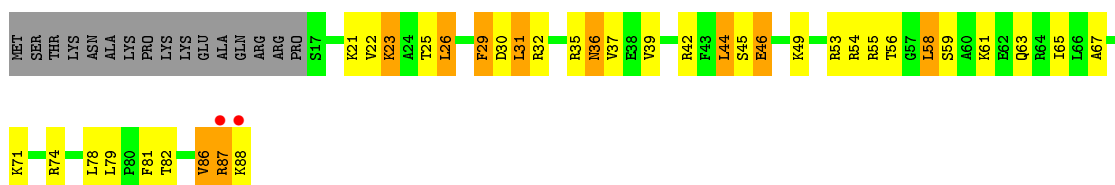
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AU: 

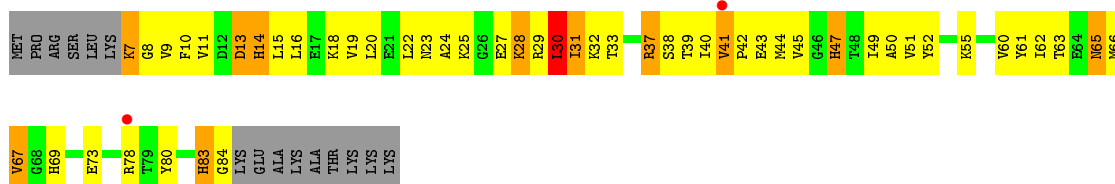


- Molecule 18: 30S RIBOSOMAL PROTEIN S18

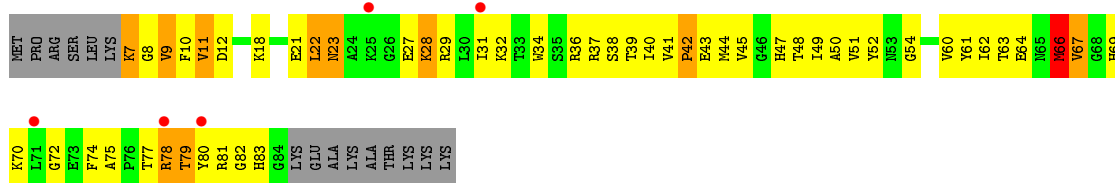
Chain CU: 



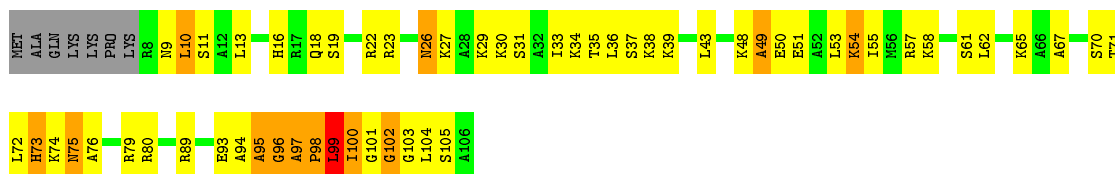
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



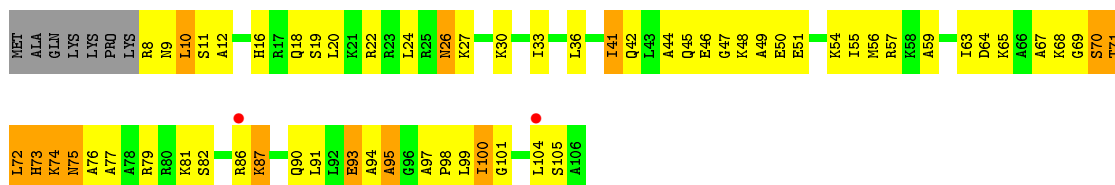
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

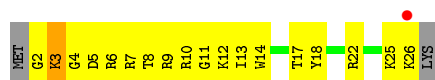


• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

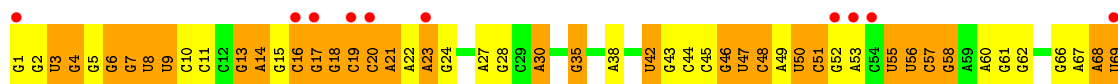
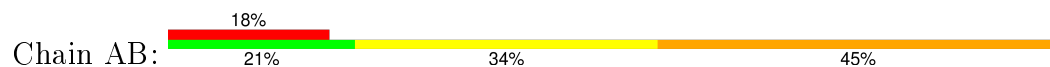




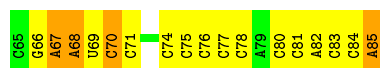
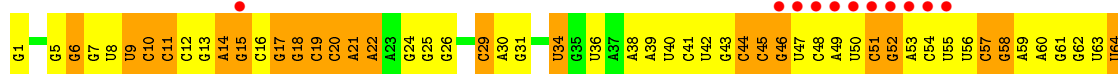
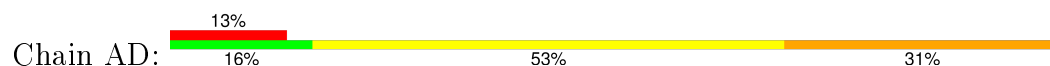
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



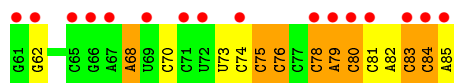
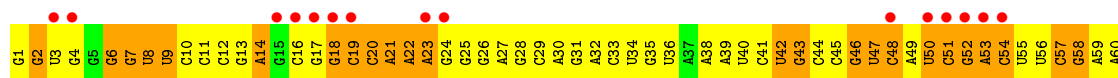
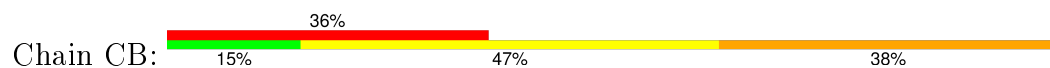
• Molecule 22: TRNA-TYR



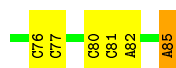
• Molecule 22: TRNA-TYR



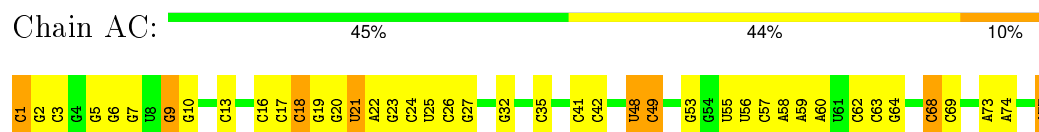
• Molecule 22: TRNA-TYR



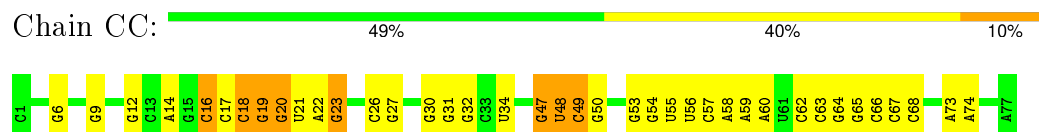
• Molecule 22: TRNA-TYR



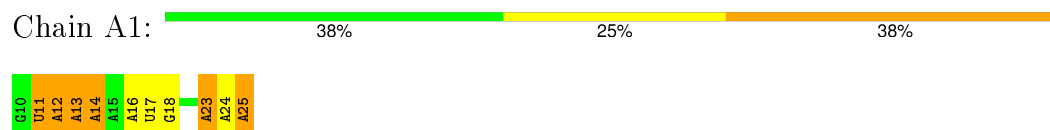
• Molecule 23: TRNA-FMET



- Molecule 23: TRNA-FMET



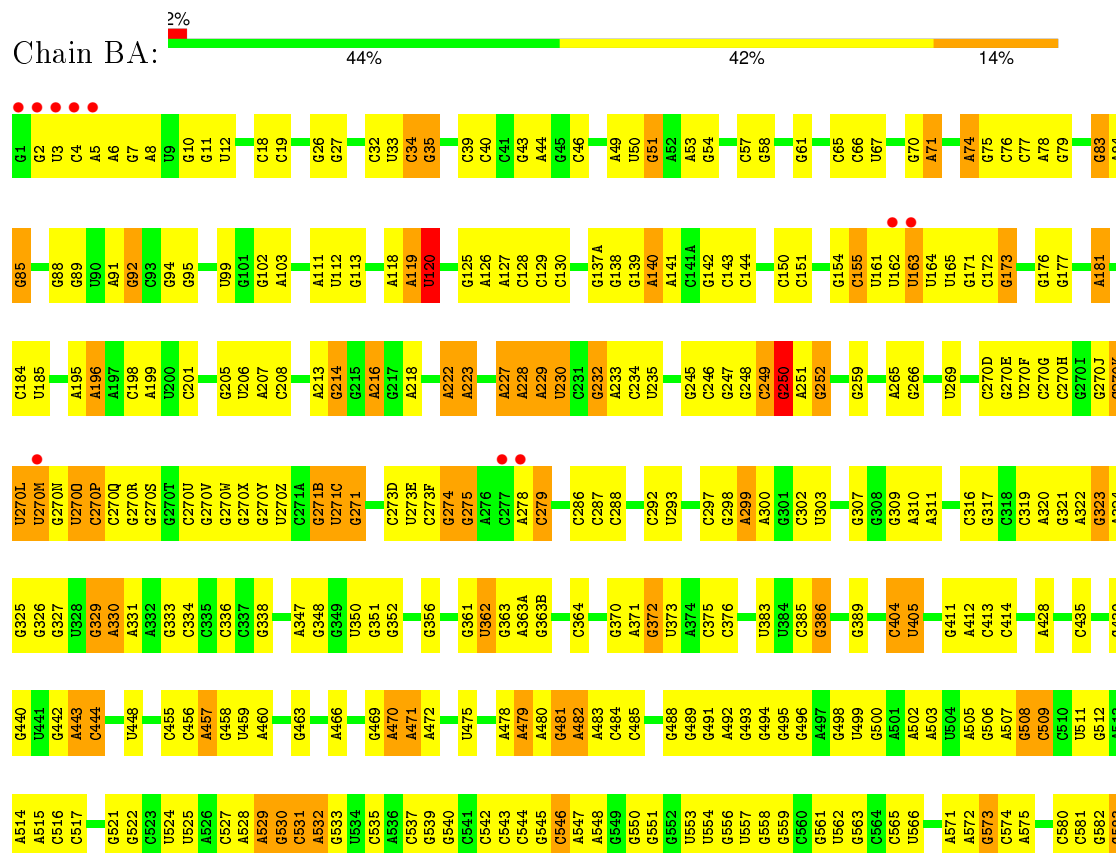
- Molecule 24: MRNA



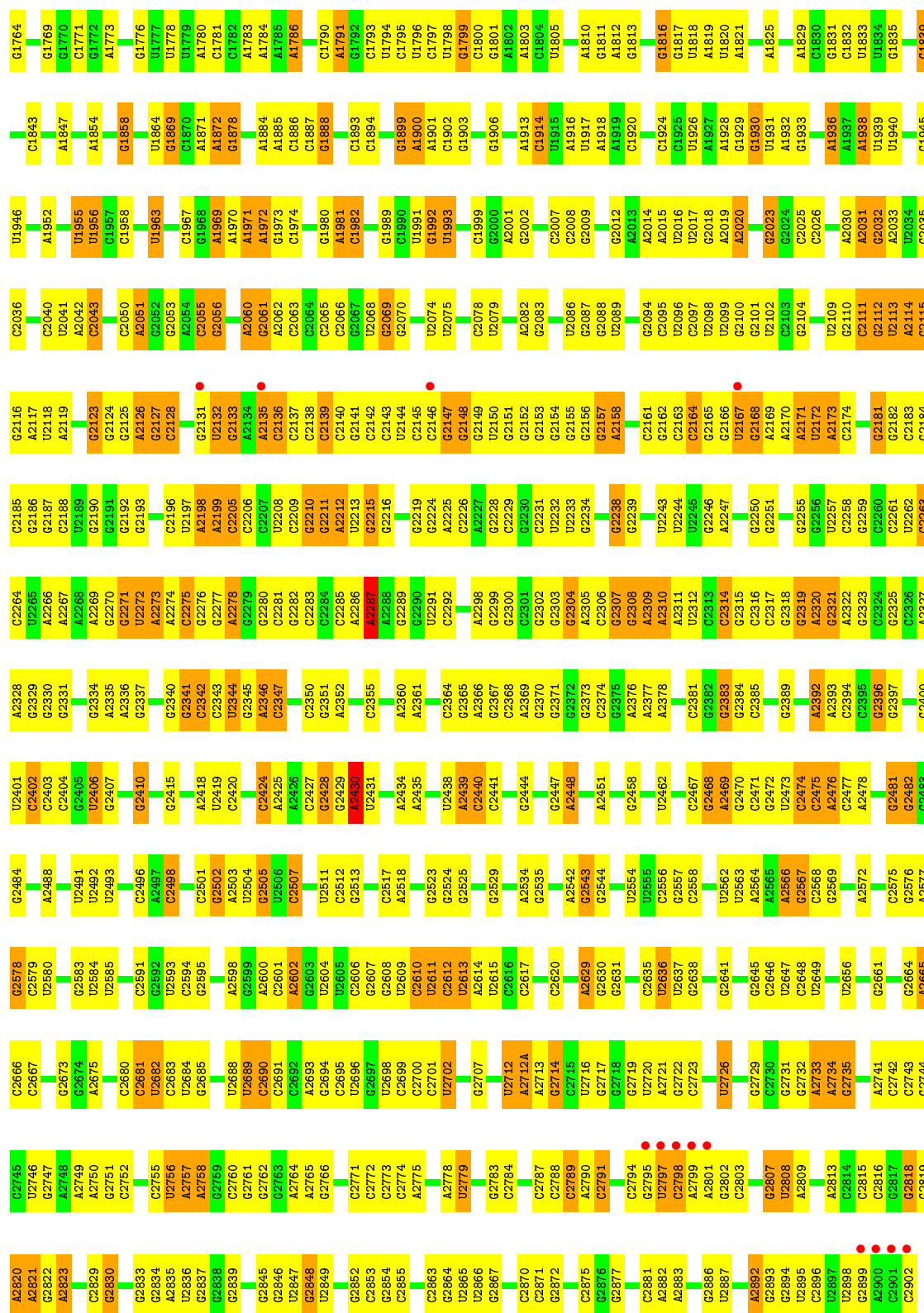
- Molecule 24: MRNA



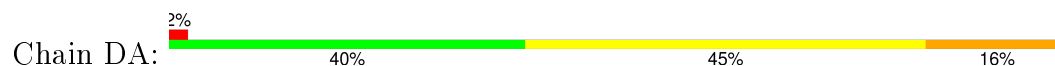
- Molecule 25: RNA (2912-MER)



C1657	A1566	A1494	C1411	G1330	G1250	G1173	U1097	A1029	G956	A878	C797	C721	A654A	A586
C1658	A1567	A1495	A1412	A1331	C1261	A1174	C1100	U1033	G957	G879	A802	A722	C654B	C587
C1661	A1568	A1496	G1413	G1332	G1262	U1175	U1101	G1034	A957	G880	A802	G723	G654C	U588
C1662	A1569	A1497	G1416	A1263	A1263	G1176	C1101	G1034	U958	G881	A802	U724	G654D	C589
C1667	A1570	C1498	G1417	U1340	G1256	A1177	C1102	G1042	A959	G882	C806	G725	G654E	C590
A1668	A1571	C1499	G1418	U1341	G1256	C1179	C1103	C1043	A960	G883	C806	G726	G654F	C591
A1669	A1575	G1500	G1419	G1348	C1261	C1180	C1104	C1043	C961	C884	U807	C730	G654G	C592
G1674	U1576	C1505	A1420	A1349	A1262	G1186	U1105	G1044	G966	C885	U811	C733	G654H	G593
C1675	C1577	A1506	G1421	U1263	A1262	C1185	G1106	A1045	G967	C886	U811	G733	G654I	G598
A1676	A1578	A1507	G1422	G1264	G1264	U1175	G1107	A1046	C968	A887	C812	G733	G654J	G602
A1677	A1579	A1508	A1427	A1352	G1265	G1186	U1108	G1047	G968	C888	U812	G733	G654K	A603
G1678	A1580	C1509	C1428	A1354	G1266	U1187	C1109	A1048	U969	C889	C814	G733	G654L	A603
G1679	G1581	A1510	G1429	G1355	G1266	U1188	G1110	A1049	C970	A890	C817	U740	G654M	G604
G1680	G1582	A1511	C1430	G1356	A1269	A1189	A1111	A1050	C971	G892	C817	G743	G654N	C805
A1681	C1583	G1512	U1431	U1357	C1270	G1191	G1112	C1051	G972	C893	A819	G743	G654O	G605
A1682	A1584	C1513	G1432	G1358	G1271	G1191	U1113	C1052	A973	C894	A819	G743	G654P	C805
C1686	A1587	U1514	A1434	A1359	G1272	G1195	C1121	A1054	G974	C897	A821	G743	G654Q	U606
C1687	A1588	C1515	G1442	A1360	U1273	U1198	G1122	G1055	G975	C898	A821	G743	G654R	U607
C1688	C1516	U1516	G1443	C1363	A1278	U1198	G1122	G1056	G978	C899	U826	G743	G654S	G612
C1689	U1517	G1517	G1444	G1364	G1279	C1201	G1125	G1057	U978	C899	U827	G743	G654T	U613
A1690	G1518	C1518	A1444	A1365	G1279	G1202	A1126	U1058	A983	A900	U828	G743	G654U	U614
A1691	G1519	G1519	A1444A	A1365	G1279	C1202	A1127	G1059	A983	A901	U829	G743	G654V	G615
G1692	U1520	G1520	C1445	A1368	A1284	G1203	A1128	U1060	C986	C902	G830	G752	G654W	A616
C1693	G1521	G1521	G1446	G1369	A1285	A1204	A1129	U1061	C987	C903	G831	G753	G654X	A617
C1694	G1522	G1522	G1447	G1370	A1286	U1205	U1130	G1062	G988	C904	G832	G754	G654Y	G618
C1695	C1525	G1525	G1448	C1371	A1287	G1206	G1131	G1063	G989	U905	U833	G755	G654Z	C618A
C1696	U1526	G1526	A1449	U1372	U1288	C1207	G1136	C1064	G990	G906	C834	G756	G654A	G619
A1698	G1527	C1527	G1450	A1373	C1289	G1208	G1137	U1066	A991	U907	U839	G760	G654B	G620
C1702	G1528	A1528	C1451	G1374	C1291	U1210	G1138	A1067	C992	C908	U839	G760	G654C	A621
C1703	A1533	A1533	C1458	A1379	U1292	U1211	G1138	G1068	C993	A910	U839	G760	G654D	G622
G1704	G1534	G1534	A1459	C1380	C1293	G1212	G1139	U1069	C994	A911	U839	G760	G654E	G625
G1705	U1535	G1535	A1460	G1381	C1298	A1213	G1140	A1069	C995	A912	U839	G760	G654F	U626
U1706	A1536	G1536	G1461	G1382	G1299	G1214	U1141	G1071	A996	C912	U839	G760	G654G	G627
U1709	C1537	C1537	C1464	C1383	U1300	G1215	U1142	C1072	G1003	C914	U839	G760	G654H	G628
C1710	G1538	G1538	G1465	A1384	A1301	C1218	A1143	G1074	C1004	G915	U839	G760	G654I	G629
C1711	G1539	G1539	G1466	G1385	A1302	G1219	G1144	C1075	C1005	A917	U839	G760	G654J	A631
U1727	G1540	G1540	C1467	C1386	G1303	A1220	C1145	C1076	C1006	A918	U839	G760	G654K	A632
A1728	U1541	U1541	G1468	C1387	G1309	C1222	C1146	A1077	U1009	G919	U839	G760	G654L	A633
U1729	A1542	A1542	A1469	G1388	G1310	G1228	C1147	C1078	A1010	C925	U839	G760	G654M	C634
U1730	A1543	G1543	G1470	G1389	G1311	G1228	A1148	G1079	G1011	G890	U839	G760	G654N	C635
G1731	C1544	C1544	A1471	U1394	U1312	G1228	G1151	A1080	G1012	C691	U839	G760	G654O	G636
G1732	A1545	A1545	A1472	U1395	U1313	G1228	C1152	U1081	U988	C692	U839	G760	G654P	A637
G1733	A1546	A1546A	G1473	U1396	C1314	G1230	C1153	U1082	C693	A638	U839	G760	G654Q	G638
G1734	C1547	C1547	C1474	U1397	C1315	G1231	C1153	U1083	U1014	U694	U839	G760	G654R	U639
G1735	A1641	C1547	G1475	U1316	G1316	G1235	A1156	A1084	G1015	G938	U839	G760	G654S	C640
C1741	G1642	C1548	C1476	A1317	A1317	G1236	G1157	A1085	G1016	A861	U839	G760	G654T	G641
C1742	C1549	C1549	A1477	G1318	G1318	G1237	G1158	A1086	U1019	A862	U839	G760	G654U	G642
G1743	C1550	C1550	G1478	G1319	G1319	G1238	C1158	G1087	A1020	A863	U839	G760	G654V	A643
G1744	C1551	C1551	G1479	C1320	C1320	G1239	C1158	A1088	A1021	C694	U839	G760	G654W	A644
C1754	G1552	G1552	C1483	U1404	U1240	G1240	G1162	G1089	G1022	A866	U839	G760	G654X	C645
A1755	A1651	A1651	G1483	U1405	U1323	A1241	G1163	U1090	G1023	C867	U839	G760	G654Y	A646
G1756	A1652	C1557	U1406	G1324	G1324	A1242	G1164	G1091	G1024	G946	U839	G760	G654Z	G647
C1762	A1653	A1653	C1407	U1407	G1327	G1243	U1165	C1092	G1025	G850	U839	G760	G654A	C650
A1762	A1654	A1654	G1487	C1408	C1327	G1244	C1166	G1093	A1027	C951	U839	G760	G654B	A653
G1763	C1656	G1560	C1493	G1410	U1329	G1249	G1171	A1096	A1028	A953	U839	G760	G654C	A654

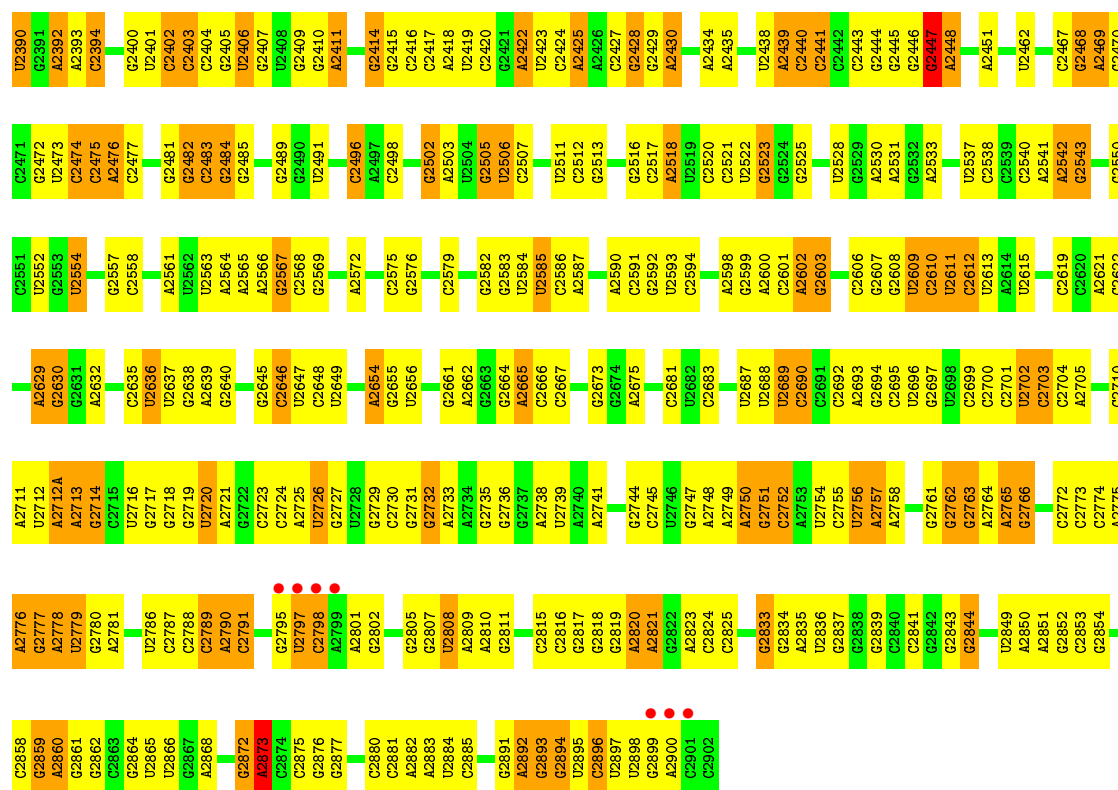


• Molecule 25: RNA (2912-MER)

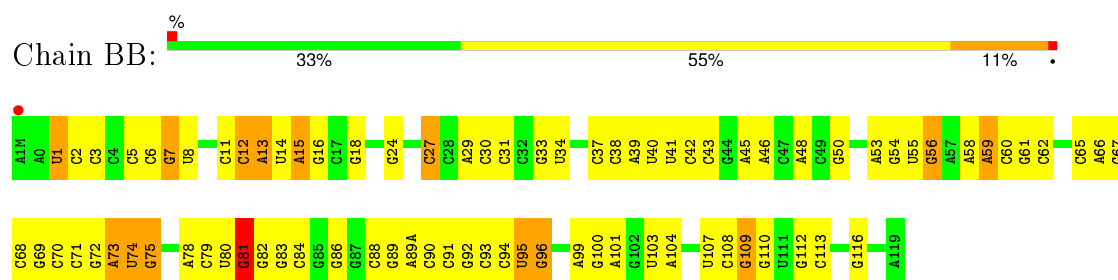


A1085	U1019	C951	C884	C817	A746	G666	G619	C537	U459	U358	A282	A241	C153	U72	G1
A1086	A1020	G962	C885	G818	U747	G667	G620	C543	G463	G361	A283	A242	G154	A73	G2
G1087	A1021	A953	C886	A819	G748	G668	G622	C543	U464	G362	C285	U243	C155	A74	U3
A1088	G1022	G954	A887	A820		G669		A547	A465	A363	C286	G247	U	G75	C4
U1089	G1023	C955	C888	A821	A751	A670	U626	A547	A466	A363A	C287	G248	U	A78	A5
U1090	G1024	C956	C889	A824	A752	C753	A627	A548	A467	A363B	C288	C248	U	G79	A6
G1091	G1025	A957	A890	C825	C754	C671	G628	C549	G468	G363C	C289	C249	U	U9	A7
C1092	U1026	U958	G992	C826	C755	C672		G550	G469	G363D	C291	G250	G171	G83	A8
G1093	A1027	A959	C893	U826	C756	A674	A631	G556	A470	A363E	C291	G251	C172	A84	A9
U1094	A1028	A960	C894	U827	C757	A675	A632	U557		A363F	C291	G252	G173	G85	G10
A1095	A1029	C961	U895	U828	U757	A676	A633	G558	A478	C364	C297	G256	C174		A13
U1096	G1030	G962	A896	A829	C758	A677	A634	G559	A479		C297	A256	G175	U90	
U1097			C897	G830		A677	C835	G560	A480	G370	C298		G176	A91	G16
A1098	U1035	U969	C898	G831	A761		C836	G561	A481	A371	G301	G259	G177	G92	G17
G1099	G1036	C970	A899	G832	U762	G681	G636	G562	G481	G372	G302	G260	G178	C93	C18
C1100	G1037	C971	A900	U833	G763	G682	A637	U562	A482	U373	G303	A265	G179	C94	C19
U1101	G1038	G972	A901	C834	A764	G683	G638	G563	A483		U303	A266	C182	G95	C20
	A1039	A973	C902	A835		G684	U639	A571		G386	G304	G266	C183	A21	C22
C1104	C1040	C903	C903	C836	G768	A685	C640	A572	G491				C184		
U1105	C1041	C904	C904	C837		G686	C641	A573	A492	G389	G307	A270	U185	U99	
	G1042	U905	U905	G838	U773		G642	G573	G493	G390	G308	A270A	C198	G101	G26
C1109	C1043	G906	G906	U839	A774	G690	A643	C574	G494	G391	G309	A270B	U193	G102	G27
G1110	G1044	G977	A907	C844	G775		A644	A575	G495		A310	U270F	G194	A103	G30
A1111	U1045	G978	C908	C845	G776	A699	C645	U576		A394	A311	C270G	A196	C105	C31
G1112	A1046	G979	A909	C846		G700	A646	G577	U499	U395	G312	C270H	A197	C106	C32
U1113	G1047	A980	A910	U847	U779	G701	G647		G500	G396		C270I	C198	C107	U33
	A1048	C981	A911	G848	G780	U702		C580	A501		G315	C270J	A199	U108	G35
C1116	C1049	C982	C912	A849	A781	U703	C650	C581	A502	G411	G316	C270K	U200	A111	
G1117	G1050	A983	U913	C850	A782	G704	G651	G582	A503	C414		C270L	C201	U112	
U1119	A1051	G984	C914	U851	A783	A705	C652	G583	U504	A405		C270M		C116	
C1120	C985	G915	G915	G854	A784	A706	A653		A505	G411	G320	U270N		G117	C41
G1121	G916	C986	G916	G855	G785	G707	A654	U588	G506		G321	C270O	A119	A44	
C1122	A1056	A988	A918	C856	G786	U708	C654A	C589	A507	C415	A322	C270P	A126	G48	
	A1057	G989	G919	C857	U787	U709	C654B	G592	G508	A415	G323	C270Q	G125	A49	
G1125	U1058	A990	G920	U858	A789	G710	G654C	G593	U509	U427	G325	C270R	A127	U50	
A1126	G1059	C991	G921	G859	C790	G715	C654D		G511	A428	G327	C270S	A213	G51	
A1127	U1060	C992		U860	C791	A716	C654E	G596	G512		U328	G270T	G215	C46	
A1128	U1061	G993	C924	A861	G792	G717	C654F	U597	A513	G439	C335	U271B	A221	G55	
U1129	G1062	C994	C925	G862	A793		C654G	G598	A514	G440	C336	U271C	A222	G56	
G1130	C1063	C995	A926	A863	A794	C720	C654H	G599	A515	U441	C337	G271	G224	A56	
U1131	C1064	A996	G928	G864	C795	C721	C654I		G516	G442	G338	G272	G225	C57	
A1132	U1065	G997	G929	C865	C796	A722	C654J	G602	G517	A443	U339	G273	G226	G58	
U1133	U1066	C998	U930	A866	C797	G723	C654K	G603		C444	A340	C273D	A227	U59	
C1135	A1067	U999	G931	C867	C797	U724	C654L	G604	G521	C445	G341	U273E	A228	G60	
U1136	G1068	A1000	G932	U868	U725	G732	C654M		G522	U449	C342	C273F	A229	G64	
G1137	A1069	A1001	A933	G869	G726	G733	C654N	U607	C523	U441	C343	G274	G230	A64	
U1138	A1070	G1002	G934	A870	U803	A734	G654O	A608	U524	G442	G344	G275	U230	C65	
G1139	G1071			U871	A804	G729	C654P	A609	U525	A443	U339	G276	G233	C66	
C1140	C1072	C1005	G938		G805	C730	C654Q	G609A	A526	C444	A340	C273D	A227	U67	
U1141	A1073	C1006		G874	C806	G731	G654R	G610	G527	C445	G341	U273E	A228	G68	
U1142	G1074	C1007	A941	G875	U807	G732	A654T	G611	A528	U449	C344	C273F	A229	G69	
A1142A	C1075	G1011	G942	U877	U810	G733	A654U	G612	A529	U449	G344	G275	U230	G70	
A1143	C1076	U1012	U943	U878	U811	A734	A655	U613	G530	A449	G344	G276	G233	C150	
G1144	A1077	U1013	G944	A878	U812	G738	G656	U614	C531	A454	G352	C277	G235	G143	
C1145	U1078	A945	A945	G879	C812	G739	U857	U615	A532	A454	G352	A278	G235	U67	
G1146	C1079	U1014	G946	G880	U813	G739	G656	A616	G533	C455	G355	A279	G239	G68	
A1147	A1080	G1015	G947	G881	C814	G744	U857	G617	U534	A456	G356	C280	U239	G70	
A1148	U1081	G1016	G948	G882	C815	G744	C859	G618	C535	A457	G356	C280	G240	A71	

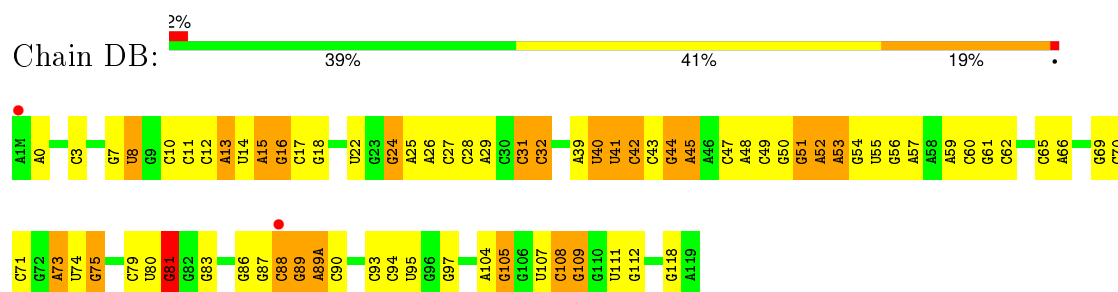
G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	G2388	G2389																																																																																																																																																																																																																																																																																																																																																																																																																																																								
G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	G2197	G2198	G2199	G2200	G2201	G2202	G2203	G2204	G2205	G2206	G2207	G2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	G2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	G2241	G2242	G2243	G2244	G2245	G2246	G2247	G2248	G2249	G2250	G2251	G2252	G2253																																																																																																																																																																																																																																																																																																																																																																																																																													
G2101	G2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	G2197	G2198	G2199	G2200	G2201	G2202	G2203	G2204	G2205	G2206	G2207	G2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	G2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	G2241	G2242	G2243	G2244	G2245	G2246	G2247	G2248	G2249	G2250	G2251	G2252	G2253																																																																																																																																																																																																																																																																																																																																																																
U2016	U2017	U2018	U2019	U2020	U2021	U2022	U2023	U2024	U2025	U2026	U2027	U2028	U2029	U2030	U2031	U2032	U2033	U2034	U2035	U2036	U2037	U2038	U2039	U2040	U2041	U2042	U2043	U2044	U2045	U2046	U2047	U2048	U2049	U2050	U2051	U2052	U2053	U2054	U2055	U2056	U2057	U2058	U2059	U2060	U2061	U2062	U2063	U2064	U2065	U2066	U2067	U2068	U2069	U2070	U2071	U2072	U2073	U2074	U2075	U2076	U2077	U2078	U2079	U2080	U2081	U2082	U2083	U2084	U2085	U2086	U2087	U2088	U2089	U2090	U2091	U2092	U2093	U2094	U2095	U2096	U2097	U2098	U2099	U2100	U2101	U2102	U2103	U2104	U2105	U2106	U2107	U2108	U2109	U2110	U2111	U2112	U2113	U2114	U2115	U2116	U2117	U2118	U2119	U2120	U2121	U2122	U2123	U2124	U2125	U2126	U2127	U2128	U2129	U2130	U2131	U2132	U2133	U2134	U2135	U2136	U2137	U2138	U2139	U2140	U2141	U2142	U2143	U2144	U2145	U2146	U2147	U2148	U2149	U2150	U2151	U2152	U2153	U2154	U2155	U2156	U2157	U2158	U2159	U2160	U2161	U2162	U2163	U2164	U2165	U2166	U2167	U2168	U2169	U2170	U2171	U2172	U2173	U2174	U2175	U2176	U2177	U2178	U2179	U2180	U2181	U2182	U2183	U2184	U2185	U2186	U2187	U2188	U2189	U2190	U2191	U2192	U2193	U2194	U2195	U2196	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2204	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230	U2231	U2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240	U2241	U2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2251	U2252	U2253																																																																																																																																																																																																																																																																											
C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283	C2284	C2285	C2286	C2287	C2288	C2289	C2290	C2291	C2292	C2293	C2294	C2295	C2296	C2297	C2298	C2299	C2300	C2301	C2302	C2303	C2304	C2305	C2306	C2307	C2308	C2309	C2310	C2311	C2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	C2320	C2321	C2322	C2323	C2324	C2325	C2326	C2327	C2328	C2329	C2330	C2331	C2332	C2333	C2334	C2335	C2336	C2337	C2338	C2339	C2340	C2341	C2342	C2343	C2344	C2345	C2346	C2347	C2348	C2349	C2350	C2351	C2352	C2353	C2354	C2355	C2356	C2357	C2358	C2359	C2360	C2361	C2362	C2363	C2364	C2365	C2366	C2367	C2368	C2369	C2370	C2371	C2372	C2373	C2374	C2375	C2376	C2377	C2378	C2379	C2380	C2381	C2382	C2383	C2384	C2385	C2386	C2387	C2388	C2389																																																																																																																																																																																																																																																																																																																																																																																	
G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	G1500	G1501	G1502	G1503	G1504	G1505	G1506	G1507	G1508	G1509	G1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520	G1521	G1522	G1523	G1524	G1525	G1526	G1527	G1528	G1529	G1530	G1531	G1532	G1533	G1534	G1535	G1536	G1537	G1538	G1539	G1540	G1541	G1542	G1543	G1544	G1545	G1546	G1547	G1548	G1549	G1550	G1551	G1552	G1553	G1554	G1555	G1556	G1557	G1558	G1559	G1560	G1561	G1562	G1563	G1564	G1565	G1566	G1567	G1568	G1569	G1570	G1571	G1572	G1573	G1574	G1575	G1576	G1577	G1578	G1579	G1580	G1581	G1582	G1583	G1584	G1585	G1586	G1587	G1588	G1589	G1590	G1591	G1592	G1593	G1594	G1595	G1596	G1597	G1598	G1599	G1600	G1601	G1602	G1603	G1604	G1605	G1606	G1607	G1608	G1609	G1610	G1611	G1612	G1613	G1614	G1615	G1616	G1617	G1618	G1619	G1620	G1621	G1622	G1623	G1624	G1625	G1626	G1627	G1628	G1629	G1630	G1631	G1632	G1633	G1634	G1635	G1636	G1637	G1638	G1639	G1640	G1641	G1642	G1643	G1644	G1645	G1646	G1647	G1648	G1649	G1650	G1651	G1652	G1653	G1654	G1655	G1656	G1657	G1658	G1659	G1660	G1661	G1662	G1663	G1664	G1665	G1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	G1677	G1678	G1679	G1680	G1681	G1682	G1683	G1684	G1685	G1686	G1687	G1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1712	G1713	G1714	G1715	G1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1733	G1734	G1735	G1736	G1737	G1738	G1739	G1740	G1741	G1742	G1743	G1744	G1745	G1746	G1747	G1748	G1749	G1750	G1751	G1752	G1753	G1754	G1755	G1756	G1757	G1758	G1759	G1760	G1761	G1762	G1763	G1764	G1765	G1766	G1767	G1768	G1769	G1770	G1771	G1772	G1773	G1774	G1775	G1776	G1777	G1778	G1779	G1780	G1781	G1782	G1783	G1784	G1785	G1786	G1787	G1788	G1789	G1790	G1791	G1792	G1793	G1794	G1795	G1796	G1797	G1798	G1799	G1800	G1801	G1802	G1803	G1804	G1805	G1806	G1807	G1808	G1809	G1810	G1811	G1812	G1813	G1814	G1815	G1816	G1817	G1818	G1819	G1820	G1821	G1822	G1823	G1824	G1825	G1826	G1827	G1828	G1829	G1830	G1831	G1832	G1833	G1834	G1835	G1836	G1837	G1838	G1839	G1840	G1841	G1842	G1843	G1844	G1845	G1846	G1847	G1848	G1849	G1850	G1851	G1852	G1853	G1854	G1855	G1856	G1857	G1858	G1859	G1860	G1861	G1862	G1863	G1864	G1865	G1866	G1867	G1868	G1869	G1870	G1871	G1872	G1873	G1874	G1875	G1876	G1877	G1878	G1879	G1880	G1881	G1882	G1883	G1884	G1885	G1886	G1887	G1888	G1889	G1890	G1891	G1892



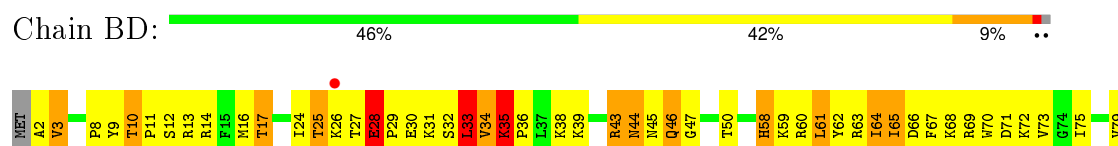
• Molecule 26: 5S RIBOSOMAL RNA

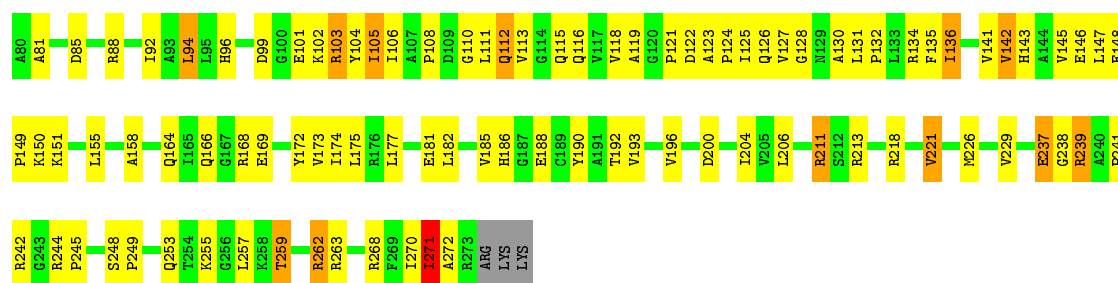


• Molecule 26: 5S RIBOSOMAL RNA



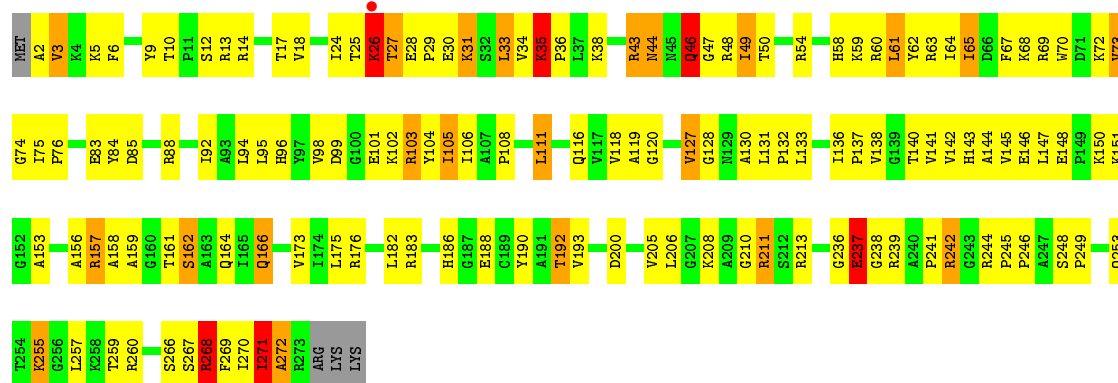
• Molecule 27: 50S ribosomal protein L2





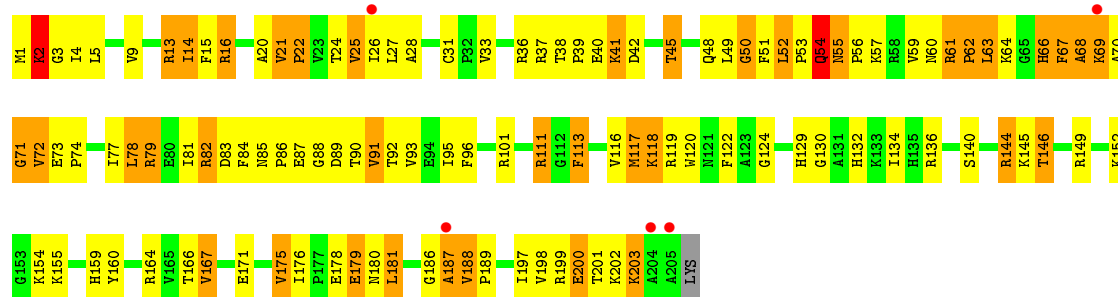
• Molecule 27: 50S ribosomal protein L2

Chain DD: 48% 41% 8% ..



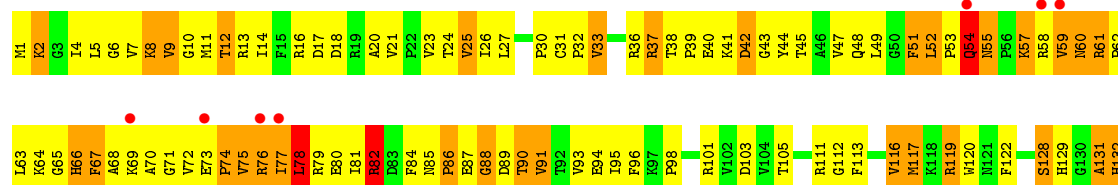
• Molecule 28: 50S ribosomal protein L3

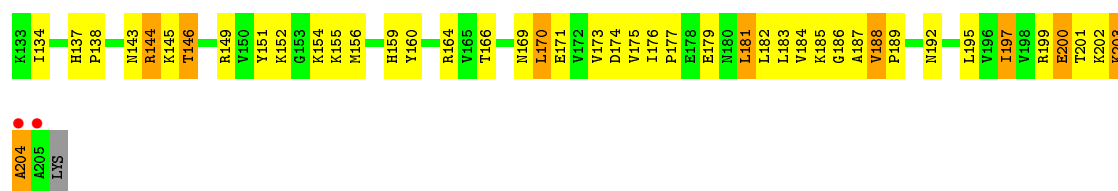
Chain BE: 2% 43% 37% 18% .



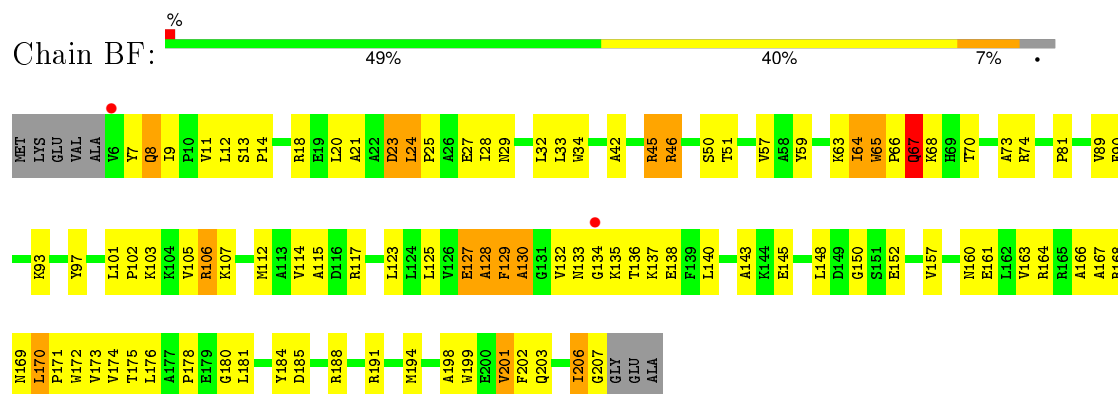
• Molecule 28: 50S ribosomal protein L3

Chain DE: 4% 30% 49% 19% .

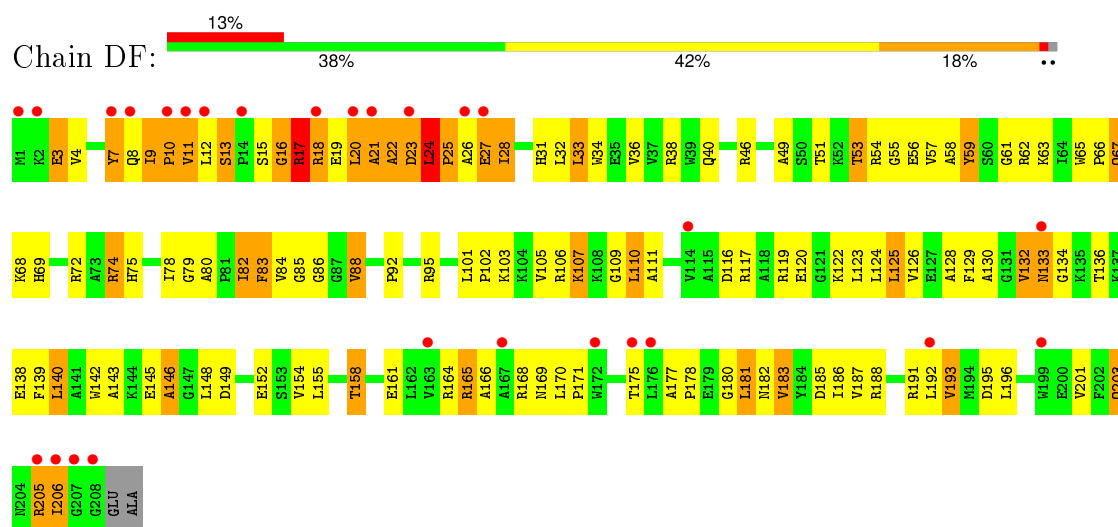




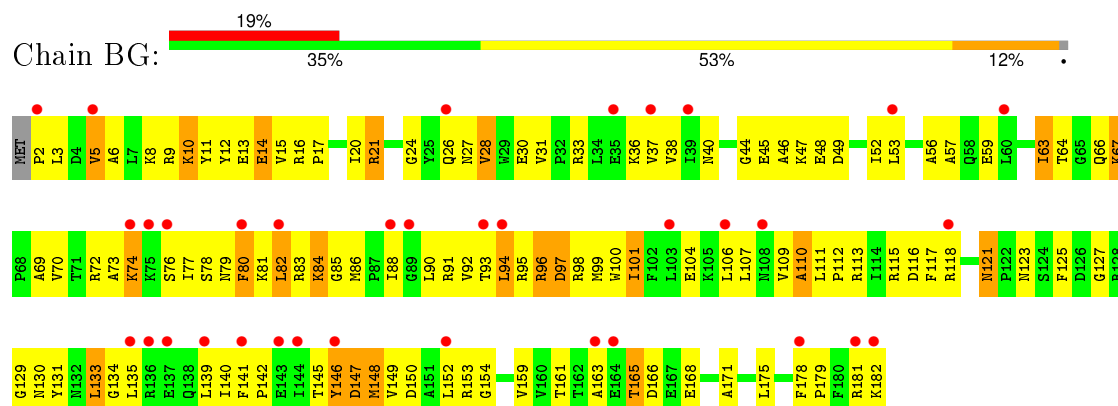
• Molecule 29: 50S ribosomal protein L4



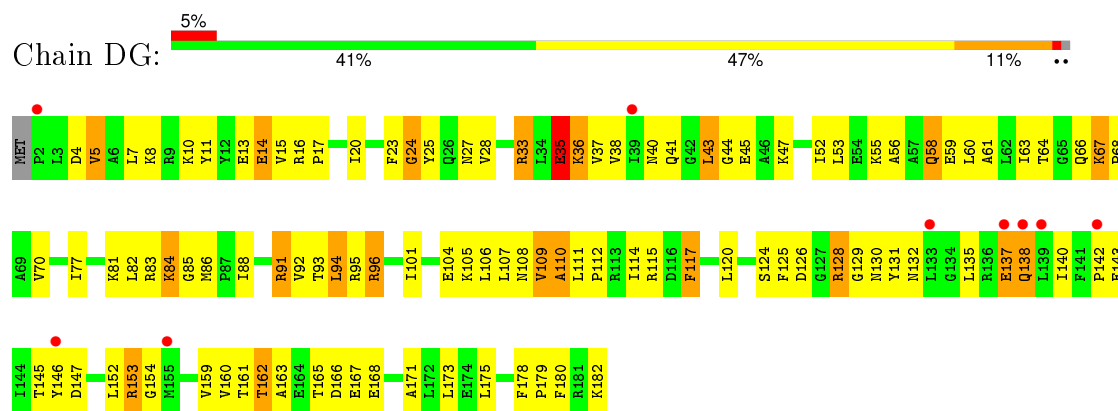
• Molecule 29: 50S ribosomal protein L4



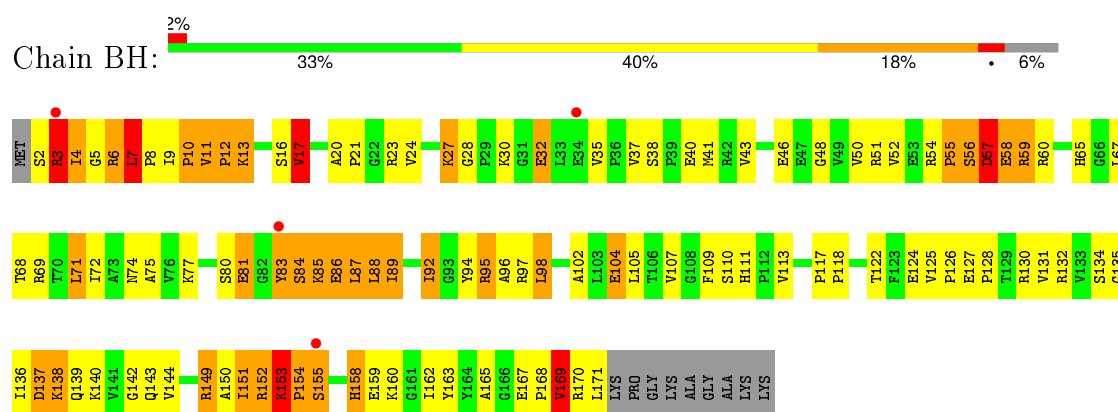
• Molecule 30: 50S ribosomal protein L5



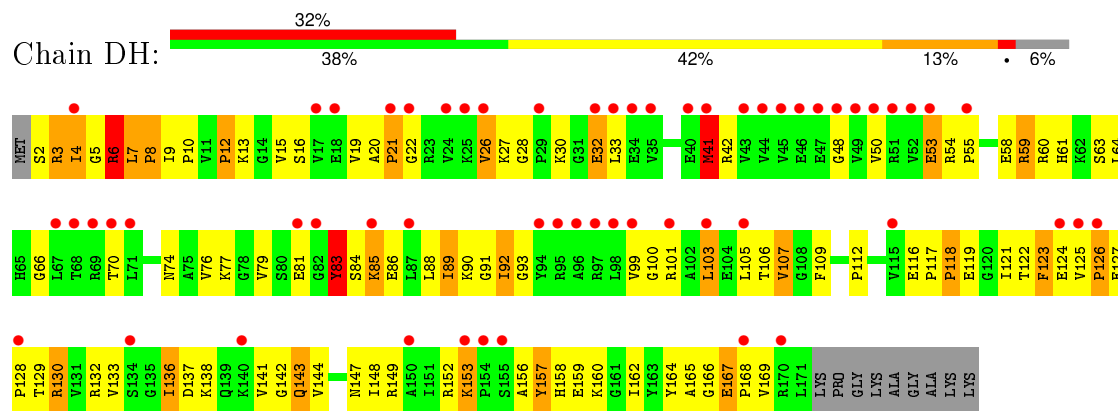
- Molecule 30: 50S ribosomal protein L5



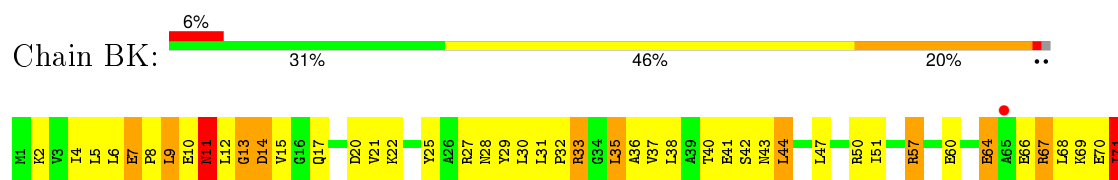
- Molecule 31: 50S ribosomal protein L6

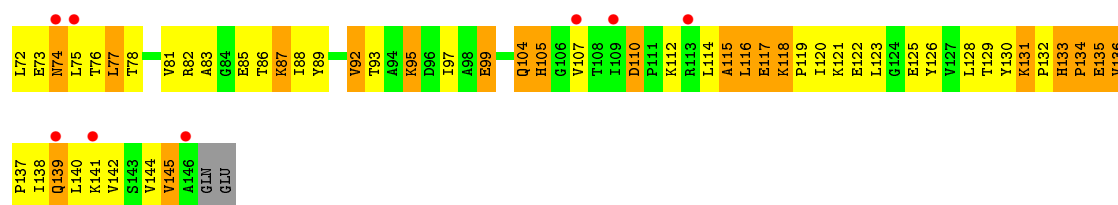


- Molecule 31: 50S ribosomal protein L6

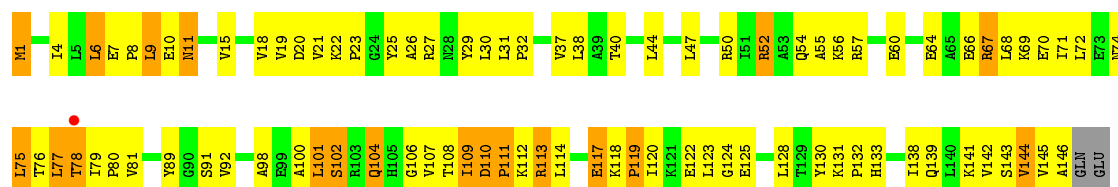


- Molecule 32: 50S ribosomal protein L9

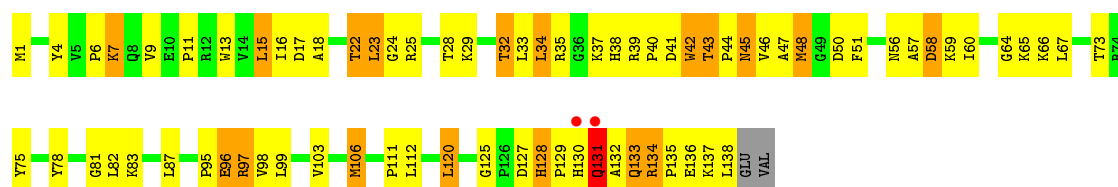




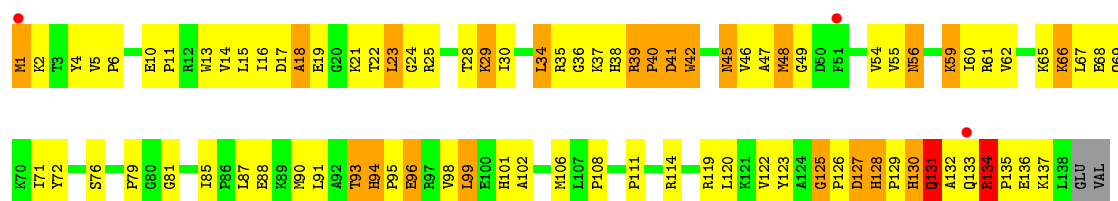
• Molecule 32: 50S ribosomal protein L9



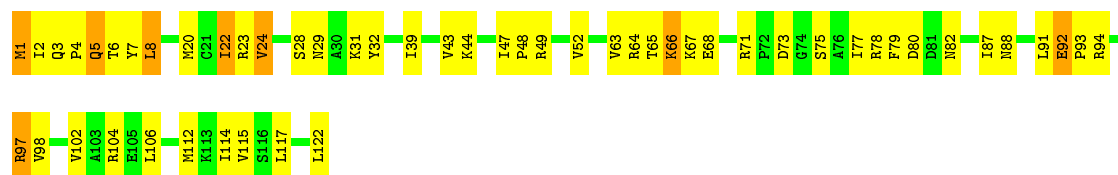
• Molecule 33: 50S ribosomal protein L13



• Molecule 33: 50S ribosomal protein L13

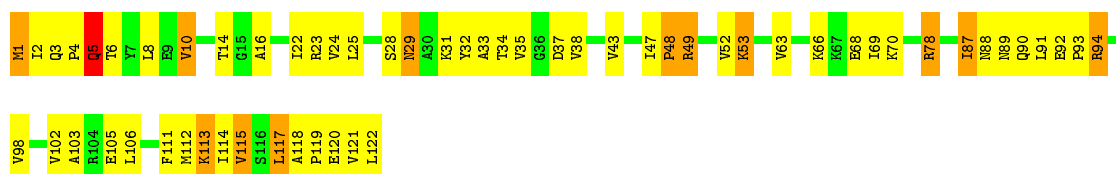


• Molecule 34: 50S ribosomal protein L14

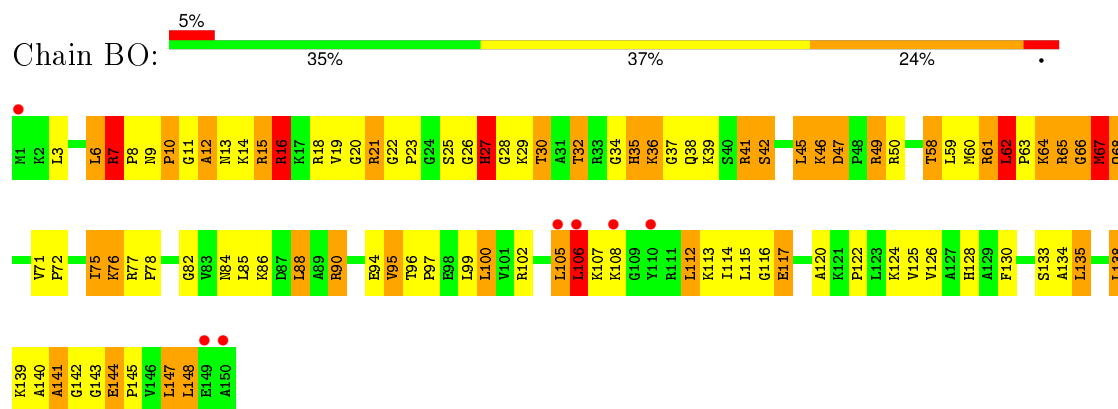


• Molecule 34: 50S ribosomal protein L14

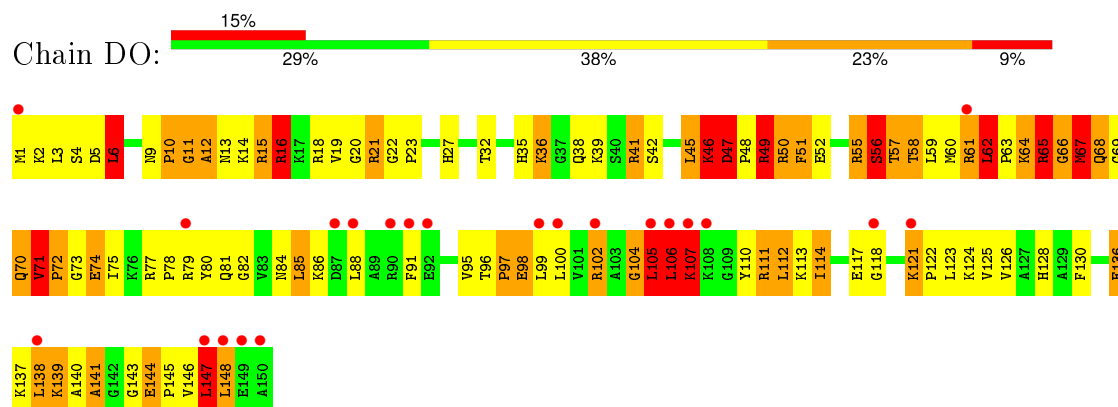




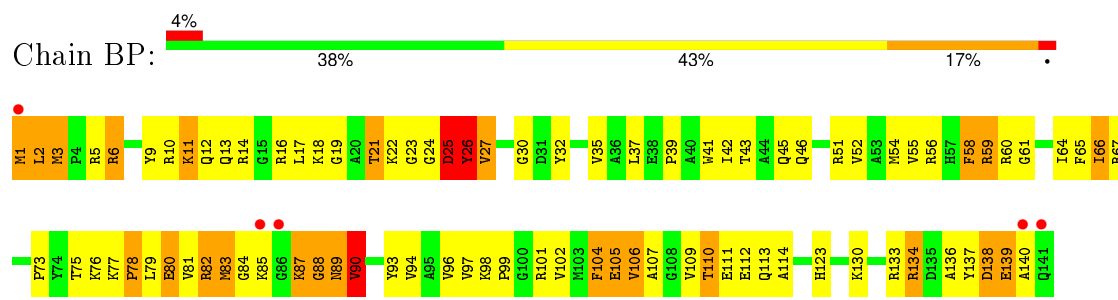
• Molecule 35: 50S ribosomal protein L15



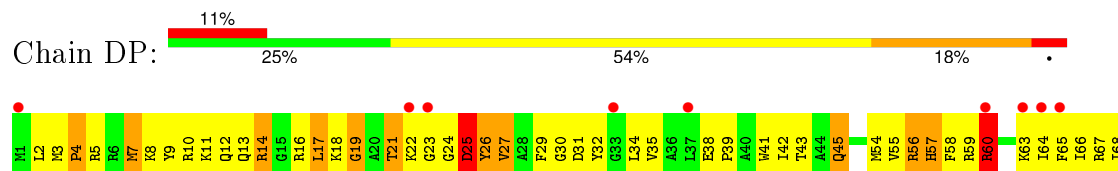
• Molecule 35: 50S ribosomal protein L15

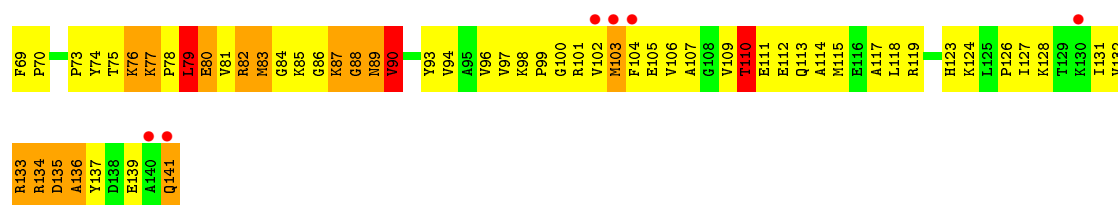


• Molecule 36: 50S ribosomal protein L16



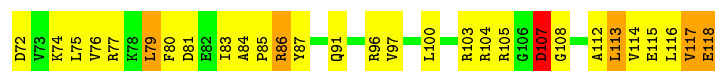
• Molecule 36: 50S ribosomal protein L16





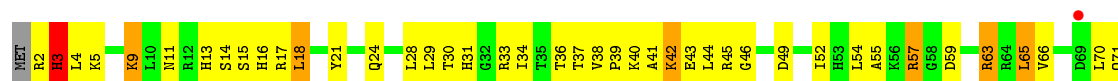
- Molecule 37: 50S ribosomal protein L17

Chain B0: 40% 46% 13%



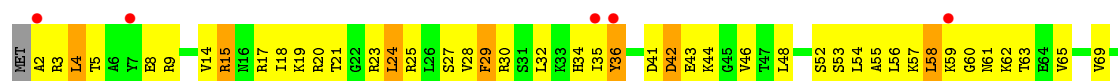
- Molecule 37: 50S ribosomal protein L17

Chain D0: 39% 49% 10%



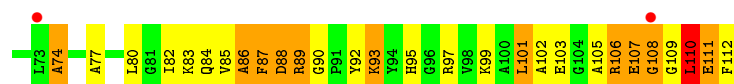
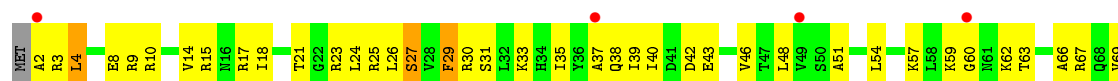
- Molecule 38: 50S ribosomal protein L18

Chain BQ: 9% 38% 48% 13%

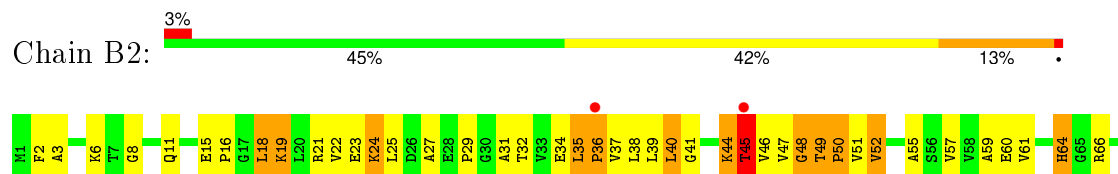


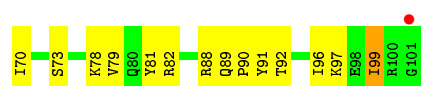
- Molecule 38: 50S ribosomal protein L18

Chain DQ: 5% 39% 46% 13%

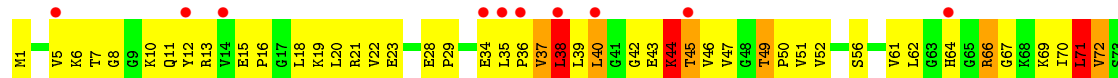


- Molecule 39: 50S ribosomal protein L19





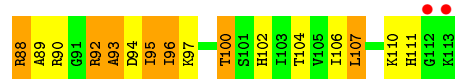
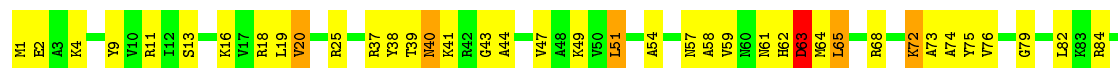
- Molecule 41: 50S ribosomal protein L21



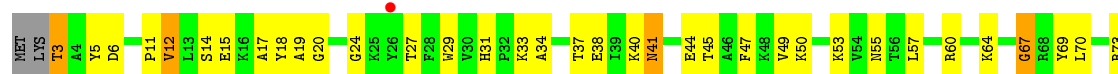
- Molecule 42: 50S ribosomal protein L22



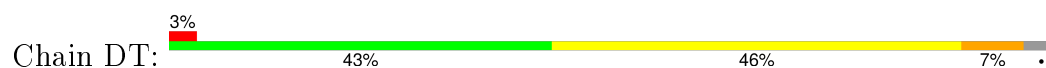
- Molecule 42: 50S ribosomal protein L22

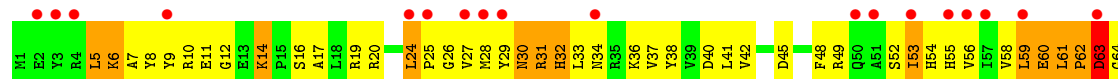


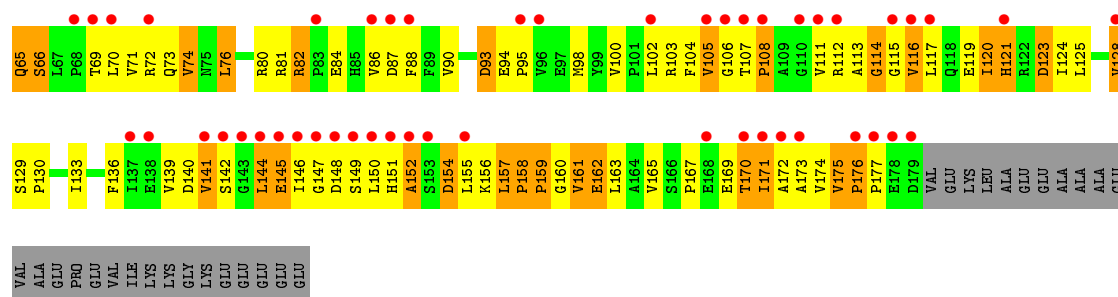
- Molecule 43: 50S ribosomal protein L23



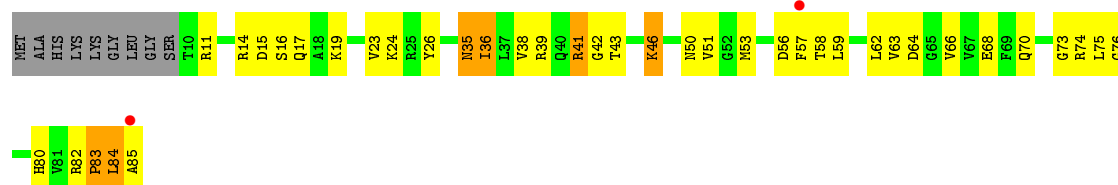
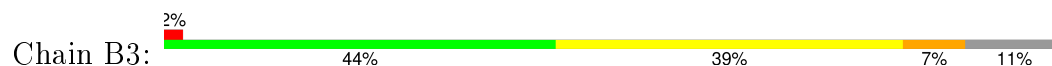
- Molecule 43: 50S ribosomal protein L23



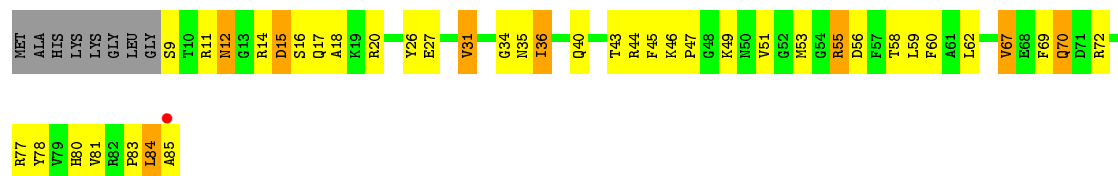
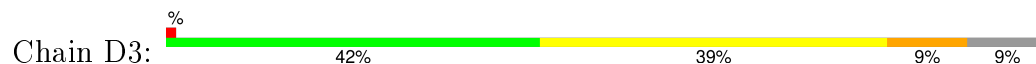




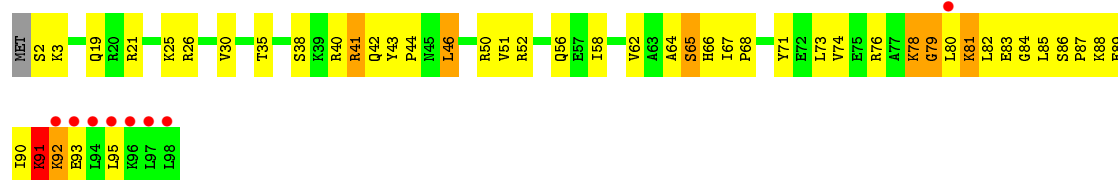
- Molecule 46: 50S ribosomal protein L27



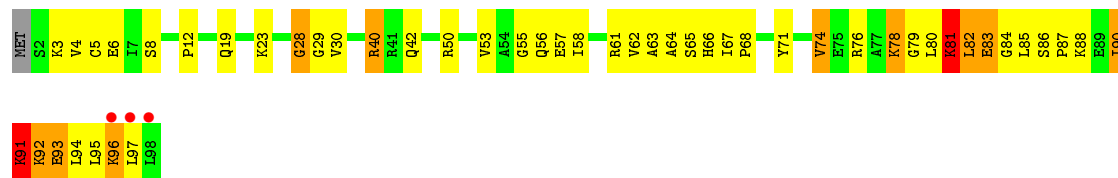
- Molecule 46: 50S ribosomal protein L27



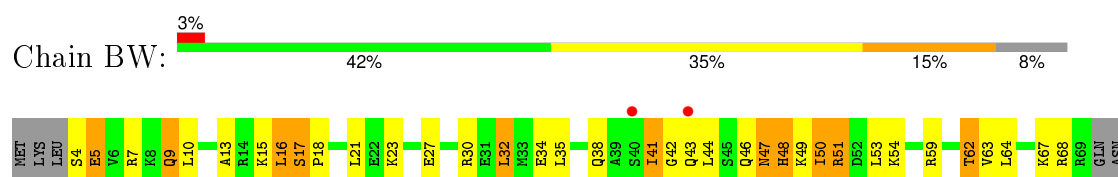
- Molecule 47: 50S ribosomal protein L28



- Molecule 47: 50S ribosomal protein L28

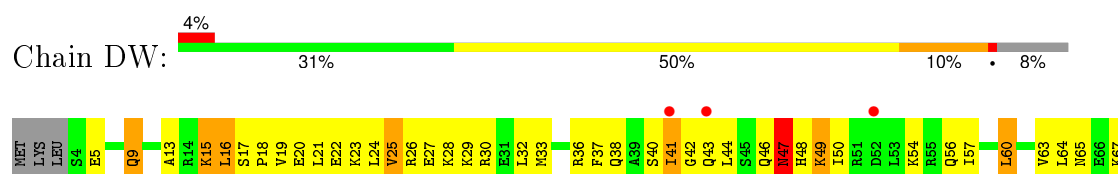


- Molecule 48: 50S ribosomal protein L29

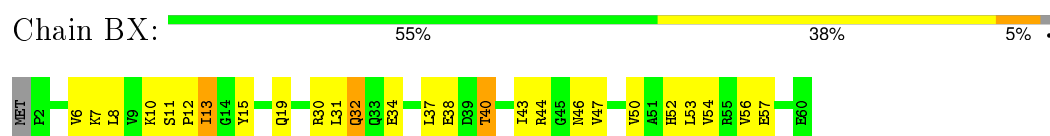


ALA

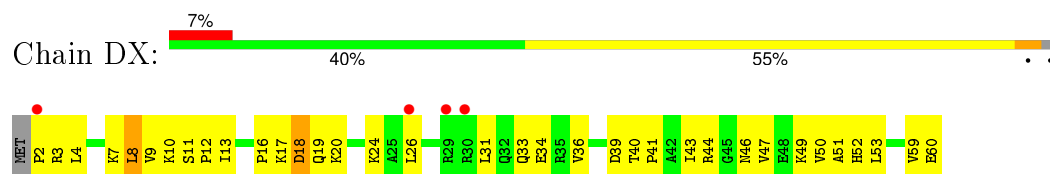
- Molecule 48: 50S ribosomal protein L29



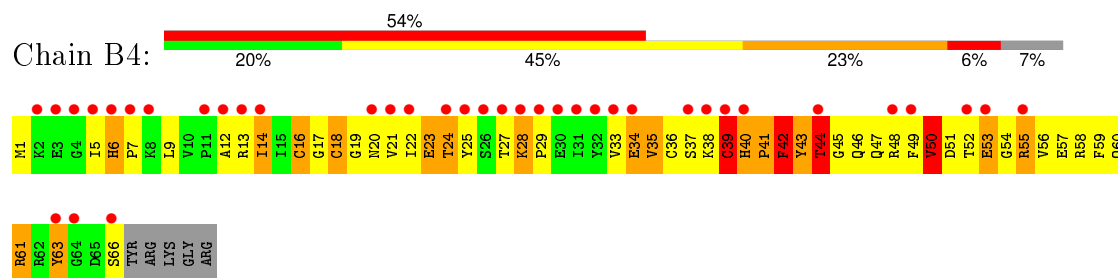
- Molecule 49: 50S ribosomal protein L30



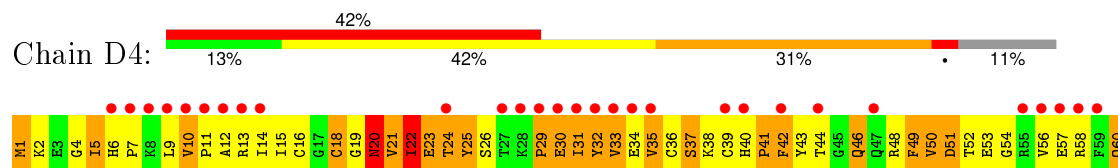
- Molecule 49: 50S ribosomal protein L30



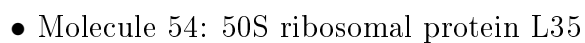
- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31







Met1	P2	K3	M4		H7	K8		K12	R13	V14	K15	L16	T17	A18		V22	V23	A24	M25	K26	T27	K28	G29	K30	R31	L32	R33	R34	Q35	K36	S37	G38	K39	E40	I41		L50	K52	P53	E54	A55	E56	R57	I58	K59	L60	L61	LEU	PRO	TRA	GLU
------	----	----	----	--	----	----	--	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.67Å 451.75Å 625.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	154.06 – 3.00 257.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (154.06-3.00) 93.5 (257.02-3.00)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_810)	Depositor
R, R_{free}	0.203 , 0.235 0.202 , 0.231	Depositor DCC
R_{free} test set	2000 reflections (0.18%)	DCC
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 1175691 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	299676	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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: MIA, 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	0.28	0/36139	0.67	20/56406 (0.0%)
1	CA	0.28	0/36142	0.66	20/56410 (0.0%)
2	AE	0.22	0/1959	0.42	0/2642
2	CE	0.22	0/1959	0.42	0/2642
3	AF	0.22	0/1629	0.42	0/2195
3	CF	0.21	0/1636	0.40	0/2205
4	AG	0.29	1/1733 (0.1%)	0.44	0/2318
4	CG	0.27	0/1733	0.47	0/2318
5	AH	0.24	0/1171	0.44	0/1576
5	CH	0.24	0/1171	0.44	0/1576
6	AI	0.24	0/856	0.42	0/1154
6	CI	0.24	0/856	0.42	0/1154
7	AJ	0.22	0/1276	0.40	0/1709
7	CJ	0.22	0/1276	0.38	0/1709
8	AK	0.23	0/1136	0.44	0/1527
8	CK	0.22	0/1136	0.42	0/1527
9	AL	0.23	0/1029	0.41	0/1379
9	CL	0.22	0/1029	0.42	0/1379
10	AM	0.22	0/814	0.42	0/1095
10	CM	0.21	0/814	0.43	0/1095
11	AN	0.24	0/900	0.44	0/1213
11	CN	0.24	0/900	0.43	0/1213
12	AO	0.26	0/991	0.49	0/1327
12	CO	0.25	0/991	0.49	0/1327
13	AP	0.22	0/938	0.45	0/1258
13	CP	0.20	0/943	0.41	0/1265
14	AQ	0.27	0/485	0.47	0/643
14	CQ	0.23	0/485	0.43	0/643
15	AR	0.24	0/745	0.43	0/992
15	CR	0.23	0/745	0.39	0/992
16	AS	0.22	0/721	0.44	0/970
16	CS	0.23	0/721	0.42	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AT	0.23	0/847	0.43	0/1131
17	CT	0.24	0/847	0.42	0/1131
18	AU	0.25	0/596	0.45	0/790
18	CU	0.24	0/596	0.44	0/790
19	AV	0.23	0/638	0.45	0/860
19	CV	0.22	0/638	0.43	0/860
20	AW	0.22	0/765	0.42	0/1007
20	CW	0.23	0/765	0.45	0/1007
21	AX	0.22	0/221	0.41	0/288
21	CX	0.21	0/221	0.40	0/288
22	AB	0.28	0/1992	0.60	0/3099
22	AD	0.21	0/1992	0.50	0/3099
22	CB	0.26	0/1992	0.57	0/3099
22	CD	0.20	0/1992	0.49	0/3099
23	AC	0.25	0/1835	0.59	1/2859 (0.0%)
23	CC	0.24	0/1835	0.57	0/2859
24	A1	0.33	0/389	0.64	0/604
24	C1	0.38	0/389	0.65	0/604
25	BA	0.37	0/70233	0.75	52/109643 (0.0%)
25	DA	0.33	1/70122 (0.0%)	0.70	54/109469 (0.0%)
26	BB	0.33	0/2928	0.80	11/4568 (0.2%)
26	DB	0.29	0/2928	0.74	4/4568 (0.1%)
27	BD	0.32	0/2165	0.58	1/2919 (0.0%)
27	DD	0.29	0/2165	0.52	0/2919
28	BE	0.29	0/1601	0.55	0/2160
28	DE	0.27	0/1601	0.52	0/2160
29	BF	0.28	0/1620	0.50	0/2194
29	DF	0.26	0/1662	0.52	0/2249
30	BG	0.24	0/1499	0.43	0/2016
30	DG	0.21	0/1499	0.42	0/2016
31	BH	0.25	0/1332	0.50	0/1802
31	DH	0.21	0/1332	0.44	0/1802
32	BK	0.24	0/1151	0.49	0/1558
32	DK	0.23	0/1151	0.51	0/1558
33	BM	0.26	0/1131	0.49	0/1525
33	DM	0.23	0/1131	0.44	0/1525
34	BN	0.27	0/943	0.46	0/1269
34	DN	0.26	0/943	0.46	0/1269
35	BO	0.28	0/1162	0.58	0/1544
35	DO	0.24	0/1162	0.45	0/1544
36	BP	0.27	0/1143	0.46	0/1527
36	DP	0.24	0/1143	0.41	0/1527
37	B0	0.26	0/982	0.48	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	D0	0.25	0/974	0.45	0/1302
38	BQ	0.26	0/892	0.50	0/1187
38	DQ	0.23	0/892	0.46	0/1187
39	BR	0.28	0/1155	0.49	0/1542
39	DR	0.25	0/1155	0.44	0/1542
40	B1	0.28	0/982	0.49	0/1306
40	D1	0.24	0/982	0.44	0/1306
41	B2	0.26	0/790	0.48	0/1057
41	D2	0.27	0/790	0.51	0/1057
42	BS	0.27	0/911	0.47	0/1220
42	DS	0.26	0/911	0.44	0/1220
43	BT	0.31	0/739	0.49	0/993
43	DT	0.28	0/739	0.46	0/993
44	BU	0.29	0/798	0.52	0/1064
44	DU	0.26	0/798	0.48	0/1064
45	BV	0.23	0/1427	0.48	1/1935 (0.1%)
45	DV	0.22	0/1460	0.43	0/1982
46	B3	0.28	0/615	0.46	0/819
46	D3	0.26	0/621	0.44	0/827
47	BZ	0.27	0/770	0.50	0/1022
47	DZ	0.26	0/770	0.50	0/1022
48	BW	0.28	0/560	0.52	0/741
48	DW	0.25	0/560	0.45	0/741
49	BX	0.25	0/474	0.42	0/635
49	DX	0.22	0/474	0.41	0/635
50	B4	0.22	0/545	0.49	0/733
50	D4	0.23	0/527	0.51	0/709
51	B5	0.25	0/473	0.51	0/639
51	D5	0.24	0/473	0.54	0/639
52	B6	0.26	0/396	0.46	0/529
52	D6	0.23	0/396	0.51	0/529
53	B7	0.31	0/399	0.44	0/526
53	D7	0.26	0/399	0.44	0/526
54	B8	0.33	0/486	0.55	0/638
54	D8	0.33	0/486	0.67	0/638
All	All	0.30	2/324157 (0.0%)	0.65	164/485451 (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
31	BH	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	DA	2873	A	N7-C5	-5.99	1.35	1.39
4	AG	12	CYS	CB-SG	5.09	1.90	1.82

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	DA	2311	A	N1-C2-N3	12.09	135.35	129.30
25	DA	2311	A	N1-C6-N6	10.02	124.61	118.60
25	BA	673	C	C2-N3-C4	-10.01	114.89	119.90
26	BB	95	U	C5-C4-O4	9.25	131.45	125.90
25	DA	673	C	C2-N3-C4	-9.13	115.33	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	BH	153	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32284	0	16296	1132	1
1	CA	32287	0	16295	1151	1
2	AE	1924	0	1975	160	0
2	CE	1924	0	1975	155	0
3	AF	1605	0	1668	115	0
3	CF	1612	0	1677	117	0
4	AG	1703	0	1763	116	0
4	CG	1703	0	1763	116	0
5	AH	1155	0	1213	75	0
5	CH	1155	0	1213	63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AI	843	0	857	52	0
6	CI	843	0	857	41	0
7	AJ	1257	0	1296	66	0
7	CJ	1257	0	1296	73	0
8	AK	1116	0	1177	76	0
8	CK	1116	0	1177	48	0
9	AL	1010	0	1037	80	0
9	CL	1010	0	1037	112	0
10	AM	801	0	849	76	0
10	CM	801	0	849	83	0
11	AN	885	0	904	58	0
11	CN	885	0	904	38	0
12	AO	975	0	1062	96	0
12	CO	975	0	1062	66	0
13	AP	928	0	987	76	0
13	CP	933	0	992	81	0
14	AQ	476	0	511	42	0
14	CQ	476	0	511	39	0
15	AR	734	0	771	33	0
15	CR	734	0	771	32	0
16	AS	705	0	725	57	0
16	CS	705	0	725	23	0
17	AT	834	0	904	43	0
17	CT	834	0	904	39	0
18	AU	591	0	662	27	0
18	CU	591	0	662	37	0
19	AV	624	0	636	52	0
19	CV	624	0	636	67	0
20	AW	763	0	861	63	0
20	CW	763	0	861	58	0
21	AX	217	0	234	18	0
21	CX	217	0	234	20	0
22	AB	1814	0	932	112	0
22	AD	1814	0	932	110	0
22	CB	1814	0	932	111	0
22	CD	1814	0	932	99	0
23	AC	1643	0	837	41	0
23	CC	1643	0	837	38	0
24	A1	346	0	174	19	0
24	C1	346	0	174	17	0
25	BA	62707	0	31614	1935	0
25	DA	62607	0	31565	2087	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	BB	2617	0	1328	89	0
26	DB	2617	0	1328	108	0
27	BD	2115	0	2195	197	0
27	DD	2115	0	2195	189	0
28	BE	1568	0	1634	146	0
28	DE	1568	0	1634	183	0
29	BF	1585	0	1632	111	0
29	DF	1627	0	1680	162	0
30	BG	1474	0	1535	129	0
30	DG	1474	0	1535	101	0
31	BH	1307	0	1382	147	0
31	DH	1307	0	1382	101	1
32	BK	1136	0	1223	102	0
32	DK	1136	0	1223	79	0
33	BM	1104	0	1180	75	0
33	DM	1104	0	1180	82	0
34	BN	933	0	996	51	0
34	DN	933	0	996	55	0
35	BO	1145	0	1228	176	0
35	DO	1145	0	1228	299	0
36	BP	1122	0	1179	140	0
36	DP	1122	0	1179	166	0
37	B0	968	0	1033	75	0
37	D0	960	0	1021	66	0
38	BQ	882	0	943	84	0
38	DQ	882	0	943	79	0
39	BR	1141	0	1202	98	0
39	DR	1141	0	1202	94	0
40	B1	964	0	1022	74	0
40	D1	964	0	1022	84	0
41	B2	779	0	852	72	0
41	D2	779	0	852	114	0
42	BS	900	0	964	41	0
42	DS	900	0	964	52	0
43	BT	725	0	778	48	0
43	DT	725	0	778	50	0
44	BU	785	0	878	99	0
44	DU	785	0	878	91	0
45	BV	1397	0	1430	138	0
45	DV	1428	0	1454	125	0
46	B3	607	0	628	41	0
46	D3	613	0	633	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BZ	763	0	848	50	0
47	DZ	763	0	848	48	0
48	BW	558	0	610	38	0
48	DW	558	0	610	43	0
49	BX	469	0	518	21	0
49	DX	469	0	518	24	0
50	B4	533	0	522	128	0
50	D4	515	0	510	71	0
51	B5	459	0	480	92	0
51	D5	459	0	476	39	0
52	B6	389	0	404	80	0
52	D6	389	0	404	51	0
53	B7	391	0	432	17	0
53	D7	391	0	432	25	0
54	B8	480	0	549	116	0
54	D8	480	0	549	81	0
55	A1	1	0	0	0	0
55	AA	220	0	0	0	0
55	AB	4	0	0	0	0
55	AC	8	0	0	0	0
55	AD	3	0	0	0	0
55	AG	2	0	0	0	0
55	AN	1	0	0	0	0
55	AR	1	0	0	0	0
55	AS	1	0	0	0	0
55	B0	1	0	0	0	0
55	B1	2	0	0	0	0
55	B2	1	0	0	0	0
55	B3	3	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B7	1	0	0	0	0
55	BA	568	0	0	0	0
55	BB	18	0	0	0	0
55	BD	1	0	0	0	0
55	BE	3	0	0	0	0
55	BF	3	0	0	0	0
55	BO	2	0	0	0	0
55	BW	1	0	0	0	0
55	CA	219	0	0	0	0
55	CB	4	0	0	0	0
55	CC	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	CD	1	0	0	0	0
55	CG	2	0	0	0	0
55	CK	1	0	0	0	0
55	CR	1	0	0	0	0
55	D0	1	0	0	0	0
55	D1	1	0	0	0	0
55	D3	1	0	0	0	0
55	D5	2	0	0	0	0
55	D7	1	0	0	0	0
55	D8	1	0	0	0	0
55	DA	488	0	0	0	0
55	DB	20	0	0	0	0
55	DD	3	0	0	0	0
55	DE	1	0	0	0	0
55	DO	1	0	0	0	0
56	AG	1	0	0	0	0
56	AQ	1	0	0	0	0
56	CG	1	0	0	0	0
56	CQ	1	0	0	0	0
All	All	299676	0	200977	13379	2

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 27.

The worst 5 of 13379 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)
35:DO:46:LYS:HD3	35:DO:51:PHE:CD1	1.38	1.55
54:B8:34:TRP:CB	54:B8:35:GLN:HB2	1.34	1.55
50:B4:37:SER:HB3	50:B4:42:PHE:CD1	1.40	1.52
35:DO:71:VAL:HG13	35:DO:72:PRO:CD	1.44	1.47
35:BO:19:VAL:HG23	35:BO:27:HIS:CB	1.45	1.46

All (2) 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)
1:AA:85:U:O2'	31:DH:100:GLY:O[3_555]	1.97	0.23
1:CA:86:U:O2'	25:DA:276:A:OP2[3_545]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AE	235/256 (92%)	170 (72%)	44 (19%)	21 (9%)	1	4
2	CE	235/256 (92%)	161 (68%)	48 (20%)	26 (11%)	0	2
3	AF	203/239 (85%)	157 (77%)	36 (18%)	10 (5%)	3	16
3	CF	204/239 (85%)	151 (74%)	40 (20%)	13 (6%)	2	9
4	AG	206/208 (99%)	169 (82%)	29 (14%)	8 (4%)	4	21
4	CG	206/208 (99%)	167 (81%)	24 (12%)	15 (7%)	1	6
5	AH	149/162 (92%)	128 (86%)	16 (11%)	5 (3%)	5	25
5	CH	149/162 (92%)	129 (87%)	18 (12%)	2 (1%)	15	53
6	AI	99/101 (98%)	88 (89%)	8 (8%)	3 (3%)	5	29
6	CI	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
7	AJ	153/156 (98%)	127 (83%)	21 (14%)	5 (3%)	5	26
7	CJ	153/156 (98%)	131 (86%)	16 (10%)	6 (4%)	4	21
8	AK	136/138 (99%)	113 (83%)	15 (11%)	8 (6%)	2	11
8	CK	136/138 (99%)	116 (85%)	17 (12%)	3 (2%)	8	38
9	AL	125/128 (98%)	90 (72%)	26 (21%)	9 (7%)	1	7
9	CL	125/128 (98%)	86 (69%)	30 (24%)	9 (7%)	1	7
10	AM	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	5	28
10	CM	97/105 (92%)	79 (81%)	13 (13%)	5 (5%)	2	15
11	AN	117/129 (91%)	101 (86%)	11 (9%)	5 (4%)	3	19
11	CN	117/129 (91%)	97 (83%)	16 (14%)	4 (3%)	5	25
12	AO	123/132 (93%)	104 (85%)	7 (6%)	12 (10%)	1	3
12	CO	123/132 (93%)	96 (78%)	21 (17%)	6 (5%)	3	16
13	AP	114/126 (90%)	76 (67%)	26 (23%)	12 (10%)	1	3
13	CP	115/126 (91%)	83 (72%)	18 (16%)	14 (12%)	0	2
14	AQ	56/61 (92%)	37 (66%)	7 (12%)	12 (21%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CQ	56/61 (92%)	39 (70%)	9 (16%)	8 (14%)	0	1
15	AR	86/89 (97%)	68 (79%)	14 (16%)	4 (5%)	3	17
15	CR	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	8	36
16	AS	82/88 (93%)	64 (78%)	13 (16%)	5 (6%)	2	11
16	CS	82/88 (93%)	72 (88%)	10 (12%)	0	100	100
17	AT	98/105 (93%)	83 (85%)	9 (9%)	6 (6%)	2	11
17	CT	98/105 (93%)	85 (87%)	10 (10%)	3 (3%)	5	28
18	AU	70/88 (80%)	53 (76%)	13 (19%)	4 (6%)	2	12
18	CU	70/88 (80%)	60 (86%)	7 (10%)	3 (4%)	3	19
19	AV	76/93 (82%)	56 (74%)	12 (16%)	8 (10%)	1	3
19	CV	76/93 (82%)	53 (70%)	16 (21%)	7 (9%)	1	4
20	AW	97/106 (92%)	75 (77%)	14 (14%)	8 (8%)	1	5
20	CW	97/106 (92%)	72 (74%)	16 (16%)	9 (9%)	1	4
21	AX	23/27 (85%)	19 (83%)	2 (9%)	2 (9%)	1	4
21	CX	23/27 (85%)	18 (78%)	2 (9%)	3 (13%)	0	1
27	BD	270/276 (98%)	227 (84%)	30 (11%)	13 (5%)	3	17
27	DD	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	3	18
28	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	0	2
28	DE	203/206 (98%)	134 (66%)	40 (20%)	29 (14%)	0	1
29	BF	200/210 (95%)	177 (88%)	14 (7%)	9 (4%)	3	18
29	DF	206/210 (98%)	153 (74%)	30 (15%)	23 (11%)	0	2
30	BG	179/182 (98%)	139 (78%)	27 (15%)	13 (7%)	1	6
30	DG	179/182 (98%)	140 (78%)	28 (16%)	11 (6%)	2	11
31	BH	168/180 (93%)	113 (67%)	20 (12%)	35 (21%)	0	0
31	DH	168/180 (93%)	108 (64%)	36 (21%)	24 (14%)	0	1
32	BK	144/148 (97%)	90 (62%)	39 (27%)	15 (10%)	1	3
32	DK	144/148 (97%)	98 (68%)	36 (25%)	10 (7%)	1	7
33	BM	136/140 (97%)	107 (79%)	21 (15%)	8 (6%)	2	11
33	DM	136/140 (97%)	106 (78%)	16 (12%)	14 (10%)	1	3
34	BN	120/122 (98%)	114 (95%)	4 (3%)	2 (2%)	11	46
34	DN	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	5	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	BO	148/150 (99%)	99 (67%)	29 (20%)	20 (14%)	0	1
35	DO	148/150 (99%)	92 (62%)	25 (17%)	31 (21%)	0	0
36	BP	139/141 (99%)	102 (73%)	19 (14%)	18 (13%)	0	1
36	DP	139/141 (99%)	92 (66%)	31 (22%)	16 (12%)	0	2
37	B0	116/118 (98%)	97 (84%)	11 (10%)	8 (7%)	1	7
37	D0	115/118 (98%)	95 (83%)	15 (13%)	5 (4%)	3	19
38	BQ	109/112 (97%)	85 (78%)	17 (16%)	7 (6%)	2	9
38	DQ	109/112 (97%)	73 (67%)	26 (24%)	10 (9%)	1	4
39	BR	135/146 (92%)	105 (78%)	21 (16%)	9 (7%)	1	8
39	DR	135/146 (92%)	108 (80%)	18 (13%)	9 (7%)	1	8
40	B1	115/118 (98%)	102 (89%)	8 (7%)	5 (4%)	3	19
40	D1	115/118 (98%)	91 (79%)	18 (16%)	6 (5%)	2	15
41	B2	99/101 (98%)	81 (82%)	12 (12%)	6 (6%)	2	11
41	D2	99/101 (98%)	68 (69%)	17 (17%)	14 (14%)	0	1
42	BS	111/113 (98%)	92 (83%)	13 (12%)	6 (5%)	2	14
42	DS	111/113 (98%)	92 (83%)	15 (14%)	4 (4%)	4	24
43	BT	90/96 (94%)	81 (90%)	5 (6%)	4 (4%)	3	18
43	DT	90/96 (94%)	72 (80%)	13 (14%)	5 (6%)	2	13
44	BU	100/110 (91%)	65 (65%)	21 (21%)	14 (14%)	0	1
44	DU	100/110 (91%)	62 (62%)	19 (19%)	19 (19%)	0	0
45	BV	173/206 (84%)	112 (65%)	32 (18%)	29 (17%)	0	1
45	DV	177/206 (86%)	109 (62%)	39 (22%)	29 (16%)	0	1
46	B3	74/85 (87%)	65 (88%)	6 (8%)	3 (4%)	3	20
46	D3	75/85 (88%)	64 (85%)	8 (11%)	3 (4%)	4	21
47	BZ	95/98 (97%)	79 (83%)	12 (13%)	4 (4%)	3	20
47	DZ	95/98 (97%)	76 (80%)	11 (12%)	8 (8%)	1	5
48	BW	64/72 (89%)	53 (83%)	6 (9%)	5 (8%)	1	6
48	DW	64/72 (89%)	54 (84%)	6 (9%)	4 (6%)	2	9
49	BX	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	11	45
49	DX	57/60 (95%)	49 (86%)	5 (9%)	3 (5%)	2	14
50	B4	64/71 (90%)	36 (56%)	12 (19%)	16 (25%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	D4	61/71 (86%)	22 (36%)	22 (36%)	17 (28%)	0	0
51	B5	57/60 (95%)	44 (77%)	6 (10%)	7 (12%)	0	2
51	D5	57/60 (95%)	46 (81%)	8 (14%)	3 (5%)	2	14
52	B6	43/54 (80%)	24 (56%)	12 (28%)	7 (16%)	0	1
52	D6	43/54 (80%)	26 (60%)	8 (19%)	9 (21%)	0	0
53	B7	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
53	D7	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
54	B8	58/65 (89%)	42 (72%)	8 (14%)	8 (14%)	0	1
54	D8	58/65 (89%)	37 (64%)	13 (22%)	8 (14%)	0	1
All	All	11319/12052 (94%)	8735 (77%)	1671 (15%)	913 (8%)	1	5

5 of 913 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AE	195	ASP
2	AE	236	TYR
2	AE	237	ALA
3	AF	4	LYS
3	AF	12	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AE	205/220 (93%)	165 (80%)	40 (20%)	2	9
2	CE	205/220 (93%)	180 (88%)	25 (12%)	6	25
3	AF	159/188 (85%)	141 (89%)	18 (11%)	7	28
3	CF	160/188 (85%)	143 (89%)	17 (11%)	8	31
4	AG	180/180 (100%)	160 (89%)	20 (11%)	8	29
4	CG	180/180 (100%)	160 (89%)	20 (11%)	8	29
5	AH	116/123 (94%)	97 (84%)	19 (16%)	3	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CH	116/123 (94%)	102 (88%)	14 (12%)	6	25
6	AI	90/90 (100%)	80 (89%)	10 (11%)	8	29
6	CI	90/90 (100%)	81 (90%)	9 (10%)	9	34
7	AJ	126/127 (99%)	106 (84%)	20 (16%)	3	15
7	CJ	126/127 (99%)	105 (83%)	21 (17%)	3	13
8	AK	119/119 (100%)	106 (89%)	13 (11%)	8	30
8	CK	119/119 (100%)	111 (93%)	8 (7%)	20	57
9	AL	98/99 (99%)	86 (88%)	12 (12%)	6	25
9	CL	98/99 (99%)	81 (83%)	17 (17%)	2	12
10	AM	89/92 (97%)	79 (89%)	10 (11%)	7	29
10	CM	89/92 (97%)	78 (88%)	11 (12%)	6	24
11	AN	90/99 (91%)	79 (88%)	11 (12%)	6	25
11	CN	90/99 (91%)	85 (94%)	5 (6%)	26	65
12	AO	104/109 (95%)	95 (91%)	9 (9%)	13	43
12	CO	104/109 (95%)	94 (90%)	10 (10%)	10	38
13	AP	94/101 (93%)	87 (93%)	7 (7%)	17	52
13	CP	94/101 (93%)	83 (88%)	11 (12%)	7	27
14	AQ	48/50 (96%)	42 (88%)	6 (12%)	6	24
14	CQ	48/50 (96%)	44 (92%)	4 (8%)	14	46
15	AR	79/80 (99%)	73 (92%)	6 (8%)	16	51
15	CR	79/80 (99%)	67 (85%)	12 (15%)	3	16
16	AS	72/74 (97%)	68 (94%)	4 (6%)	26	65
16	CS	72/74 (97%)	64 (89%)	8 (11%)	8	29
17	AT	95/97 (98%)	85 (90%)	10 (10%)	8	32
17	CT	95/97 (98%)	92 (97%)	3 (3%)	46	82
18	AU	63/77 (82%)	57 (90%)	6 (10%)	11	38
18	CU	63/77 (82%)	51 (81%)	12 (19%)	2	10
19	AV	67/80 (84%)	55 (82%)	12 (18%)	2	11
19	CV	67/80 (84%)	58 (87%)	9 (13%)	5	21
20	AW	76/82 (93%)	68 (90%)	8 (10%)	8	32
20	CW	76/82 (93%)	66 (87%)	10 (13%)	5	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	AX	20/22 (91%)	20 (100%)	0	100	100
21	CX	20/22 (91%)	20 (100%)	0	100	100
27	BD	214/218 (98%)	178 (83%)	36 (17%)	2	13
27	DD	214/218 (98%)	181 (85%)	33 (15%)	3	16
28	BE	165/166 (99%)	135 (82%)	30 (18%)	2	11
28	DE	165/166 (99%)	139 (84%)	26 (16%)	3	15
29	BF	161/166 (97%)	141 (88%)	20 (12%)	6	24
29	DF	165/166 (99%)	140 (85%)	25 (15%)	3	16
30	BG	155/156 (99%)	135 (87%)	20 (13%)	5	23
30	DG	155/156 (99%)	139 (90%)	16 (10%)	9	33
31	BH	142/148 (96%)	122 (86%)	20 (14%)	4	19
31	DH	142/148 (96%)	124 (87%)	18 (13%)	5	23
32	BK	122/124 (98%)	101 (83%)	21 (17%)	2	12
32	DK	122/124 (98%)	106 (87%)	16 (13%)	5	22
33	BM	117/119 (98%)	98 (84%)	19 (16%)	3	14
33	DM	117/119 (98%)	97 (83%)	20 (17%)	2	12
34	BN	100/100 (100%)	92 (92%)	8 (8%)	15	47
34	DN	100/100 (100%)	87 (87%)	13 (13%)	5	22
35	BO	116/116 (100%)	84 (72%)	32 (28%)	0	2
35	DO	116/116 (100%)	80 (69%)	36 (31%)	0	2
36	BP	111/111 (100%)	94 (85%)	17 (15%)	3	16
36	DP	111/111 (100%)	89 (80%)	22 (20%)	1	8
37	B0	101/101 (100%)	85 (84%)	16 (16%)	3	15
37	D0	100/101 (99%)	82 (82%)	18 (18%)	2	11
38	BQ	87/88 (99%)	73 (84%)	14 (16%)	3	14
38	DQ	87/88 (99%)	79 (91%)	8 (9%)	11	40
39	BR	120/127 (94%)	99 (82%)	21 (18%)	2	12
39	DR	120/127 (94%)	102 (85%)	18 (15%)	3	17
40	B1	93/94 (99%)	85 (91%)	8 (9%)	13	44
40	D1	93/94 (99%)	82 (88%)	11 (12%)	6	26
41	B2	82/82 (100%)	70 (85%)	12 (15%)	4	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	D2	82/82 (100%)	69 (84%)	13 (16%)	3	15
42	BS	92/92 (100%)	79 (86%)	13 (14%)	4	19
42	DS	92/92 (100%)	76 (83%)	16 (17%)	2	12
43	BT	74/78 (95%)	65 (88%)	9 (12%)	6	25
43	DT	74/78 (95%)	63 (85%)	11 (15%)	4	17
44	BU	85/91 (93%)	72 (85%)	13 (15%)	3	16
44	DU	85/91 (93%)	67 (79%)	18 (21%)	1	6
45	BV	154/179 (86%)	126 (82%)	28 (18%)	2	11
45	DV	158/179 (88%)	138 (87%)	20 (13%)	5	23
46	B3	61/67 (91%)	57 (93%)	4 (7%)	21	57
46	D3	62/67 (92%)	55 (89%)	7 (11%)	7	28
47	BZ	82/83 (99%)	69 (84%)	13 (16%)	3	15
47	DZ	82/83 (99%)	68 (83%)	14 (17%)	2	12
48	BW	62/67 (92%)	51 (82%)	11 (18%)	2	11
48	DW	62/67 (92%)	51 (82%)	11 (18%)	2	11
49	BX	51/52 (98%)	46 (90%)	5 (10%)	10	36
49	DX	51/52 (98%)	48 (94%)	3 (6%)	24	63
50	B4	59/63 (94%)	49 (83%)	10 (17%)	2	13
50	D4	57/63 (90%)	46 (81%)	11 (19%)	2	9
51	B5	51/52 (98%)	42 (82%)	9 (18%)	2	12
51	D5	51/52 (98%)	41 (80%)	10 (20%)	1	9
52	B6	44/52 (85%)	34 (77%)	10 (23%)	1	5
52	D6	44/52 (85%)	40 (91%)	4 (9%)	12	41
53	B7	38/42 (90%)	33 (87%)	5 (13%)	5	22
53	D7	38/42 (90%)	33 (87%)	5 (13%)	5	22
54	B8	50/55 (91%)	37 (74%)	13 (26%)	0	3
54	D8	50/55 (91%)	41 (82%)	9 (18%)	2	11
All	All	9565/9996 (96%)	8229 (86%)	1336 (14%)	4	19

5 of 1336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BZ	26	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	CH	75	THR
44	DU	64	GLU
48	BW	50	ILE
2	CE	5	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 282 such sidechains are listed below:

Mol	Chain	Res	Type
47	BZ	56	GLN
5	CH	141	GLN
45	DV	75	ASN
49	BX	19	GLN
54	B8	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1501/1506 (99%)	295 (19%)	43 (2%)
1	CA	1501/1506 (99%)	296 (19%)	49 (3%)
22	AB	83/85 (97%)	38 (45%)	8 (9%)
22	AD	83/85 (97%)	26 (31%)	5 (6%)
22	CB	83/85 (97%)	38 (45%)	9 (10%)
22	CD	83/85 (97%)	25 (30%)	4 (4%)
23	AC	76/77 (98%)	11 (14%)	1 (1%)
23	CC	76/77 (98%)	13 (17%)	3 (3%)
24	A1	15/16 (93%)	6 (40%)	2 (13%)
24	C1	15/16 (93%)	6 (40%)	3 (20%)
25	BA	2911/2912 (99%)	542 (18%)	51 (1%)
25	DA	2905/2912 (99%)	569 (19%)	53 (1%)
26	BB	121/122 (99%)	17 (14%)	0
26	DB	121/122 (99%)	27 (22%)	1 (0%)
All	All	9574/9606 (99%)	1909 (19%)	232 (2%)

5 of 1909 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	13	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	32	A

5 of 232 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2566	A
1	CA	509	A
25	DA	2211	G
25	BA	2689	U
1	CA	201	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	MIA	AB	38	22	21,31,32	0.43	0	26,44,47	1.98	6 (23%)
22	MIA	AD	38	22	21,31,32	0.55	0	26,44,47	2.70	5 (19%)
22	MIA	CB	38	22	21,31,32	0.47	0	26,44,47	2.28	7 (26%)
22	MIA	CD	38	22	21,31,32	0.56	0	26,44,47	2.78	6 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	MIA	AB	38	22	-	0/11/33/34	0/3/3/3
22	MIA	AD	38	22	-	0/11/33/34	0/3/3/3
22	MIA	CB	38	22	-	2/11/33/34	0/3/3/3
22	MIA	CD	38	22	-	0/11/33/34	0/3/3/3

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
22	AD	38	MIA	C12-N6-C6	-4.87	117.36	123.42
22	CD	38	MIA	C12-N6-C6	-4.36	117.99	123.42
22	AB	38	MIA	C12-N6-C6	-4.00	118.44	123.42
22	CB	38	MIA	C4-C5-N7	-3.92	105.87	109.48
22	AB	38	MIA	C4-C5-N7	-3.13	106.60	109.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	CB	38	MIA	N1-C2-S10-C11
22	CB	38	MIA	N3-C2-S10-C11

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AB	38	MIA	1	0
22	AD	38	MIA	3	0
22	CB	38	MIA	3	0
22	CD	38	MIA	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1608 ligands modelled in this entry, 1608 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1502/1506 (99%)	-0.35	5 (0%) 94 84	54, 99, 183, 246	0
1	CA	1502/1506 (99%)	-0.27	13 (0%) 85 64	59, 100, 182, 245	0
2	AE	237/256 (92%)	0.27	12 (5%) 32 12	98, 139, 177, 190	0
2	CE	237/256 (92%)	0.60	19 (8%) 15 5	106, 152, 189, 209	0
3	AF	205/239 (85%)	0.33	8 (3%) 43 18	88, 113, 149, 158	0
3	CF	206/239 (86%)	1.08	34 (16%) 2 1	101, 135, 165, 180	0
4	AG	208/208 (100%)	-0.30	1 (0%) 91 76	81, 107, 131, 143	0
4	CG	208/208 (100%)	0.27	3 (1%) 78 51	75, 95, 123, 135	0
5	AH	151/162 (93%)	0.03	2 (1%) 79 53	78, 99, 125, 164	0
5	CH	151/162 (93%)	0.22	2 (1%) 79 53	84, 106, 131, 167	0
6	AI	101/101 (100%)	0.47	5 (4%) 32 13	67, 99, 115, 141	0
6	CI	101/101 (100%)	-0.05	0 100 100	76, 96, 115, 153	0
7	AJ	155/156 (99%)	0.44	13 (8%) 14 5	96, 114, 143, 161	0
7	CJ	155/156 (99%)	0.08	8 (5%) 31 12	100, 119, 147, 158	0
8	AK	138/138 (100%)	-0.26	0 100 100	81, 103, 117, 132	0
8	CK	138/138 (100%)	0.04	1 (0%) 89 70	81, 109, 125, 136	0
9	AL	127/128 (99%)	0.55	14 (11%) 7 3	83, 138, 159, 166	0
9	CL	127/128 (99%)	0.12	6 (4%) 35 14	95, 147, 165, 171	0
10	AM	99/105 (94%)	0.81	14 (14%) 4 1	81, 140, 167, 178	0
10	CM	99/105 (94%)	0.88	13 (13%) 5 2	103, 154, 174, 180	0
11	AN	119/129 (92%)	0.81	15 (12%) 5 2	62, 95, 130, 161	0
11	CN	119/129 (92%)	0.24	2 (1%) 73 45	74, 99, 133, 164	0
12	AO	125/132 (94%)	-0.20	2 (1%) 74 47	59, 75, 107, 162	0
12	CO	125/132 (94%)	0.66	15 (12%) 6 2	63, 91, 126, 166	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AP	116/126 (92%)	0.26	6 (5%) 31 12	75, 124, 143, 155	0
13	CP	117/126 (92%)	0.22	7 (5%) 25 9	91, 145, 161, 169	0
14	AQ	58/61 (95%)	-0.13	0 100 100	87, 103, 120, 127	0
14	CQ	58/61 (95%)	1.22	10 (17%) 2 1	108, 125, 150, 154	0
15	AR	88/89 (98%)	-0.12	0 100 100	70, 94, 116, 120	0
15	CR	88/89 (98%)	-0.04	0 100 100	67, 96, 124, 136	0
16	AS	84/88 (95%)	-0.34	0 100 100	87, 109, 134, 174	0
16	CS	84/88 (95%)	0.35	2 (2%) 62 32	76, 91, 118, 157	0
17	AT	100/105 (95%)	-0.34	2 (2%) 68 39	80, 102, 118, 129	0
17	CT	100/105 (95%)	0.06	2 (2%) 68 39	75, 100, 126, 144	0
18	AU	72/88 (81%)	0.60	7 (9%) 10 4	77, 97, 135, 164	0
18	CU	72/88 (81%)	0.20	2 (2%) 56 27	85, 103, 149, 172	0
19	AV	78/93 (83%)	0.15	2 (2%) 59 29	97, 120, 145, 156	0
19	CV	78/93 (83%)	0.59	5 (6%) 23 8	128, 152, 178, 186	0
20	AW	99/106 (93%)	-0.15	0 100 100	97, 121, 148, 153	0
20	CW	99/106 (93%)	0.24	2 (2%) 68 39	86, 106, 141, 153	0
21	AX	25/27 (92%)	0.25	1 (4%) 42 17	97, 107, 121, 153	0
21	CX	25/27 (92%)	0.82	2 (8%) 15 5	101, 129, 150, 171	0
22	AB	84/85 (98%)	0.78	15 (17%) 2 1	76, 148, 167, 178	0
22	AD	84/85 (98%)	0.33	11 (13%) 5 2	70, 147, 206, 218	0
22	CB	84/85 (98%)	1.67	31 (36%) 0 0	92, 155, 171, 179	0
22	CD	84/85 (98%)	-0.63	0 100 100	74, 147, 207, 212	0
23	AC	77/77 (100%)	-0.41	0 100 100	66, 91, 135, 155	0
23	CC	77/77 (100%)	-0.59	0 100 100	79, 104, 143, 165	0
24	A1	16/16 (100%)	-0.20	0 100 100	66, 97, 168, 177	0
24	C1	16/16 (100%)	-0.16	0 100 100	75, 107, 176, 183	0
25	BA	2912/2912 (100%)	-0.02	45 (1%) 76 49	39, 68, 206, 243	0
25	DA	2907/2912 (99%)	-0.16	66 (2%) 64 33	49, 82, 226, 247	0
26	BB	122/122 (100%)	-0.26	1 (0%) 87 67	65, 92, 113, 183	0
26	DB	122/122 (100%)	-0.45	2 (1%) 74 47	78, 110, 139, 198	0
27	BD	272/276 (98%)	0.05	1 (0%) 93 80	39, 59, 82, 104	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DD	272/276 (98%)	-0.06	1 (0%) 93 80	45, 67, 87, 120	0
28	BE	205/206 (99%)	0.13	5 (2%) 62 32	44, 77, 125, 150	0
28	DE	205/206 (99%)	0.09	9 (4%) 38 16	56, 93, 144, 157	0
29	BF	202/210 (96%)	0.11	2 (0%) 84 60	42, 75, 110, 127	0
29	DF	208/210 (99%)	0.88	27 (12%) 5 2	53, 93, 155, 185	0
30	BG	181/182 (99%)	0.99	35 (19%) 2 1	79, 105, 136, 146	0
30	DG	181/182 (99%)	0.41	9 (4%) 32 13	96, 128, 157, 168	0
31	BH	170/180 (94%)	0.15	4 (2%) 62 32	71, 105, 126, 151	0
31	DH	170/180 (94%)	1.62	58 (34%) 0 0	143, 193, 217, 231	0
32	BK	146/148 (98%)	0.49	9 (6%) 24 9	72, 120, 141, 153	0
32	DK	146/148 (98%)	-0.19	1 (0%) 89 70	73, 120, 147, 151	0
33	BM	138/140 (98%)	0.11	2 (1%) 78 51	58, 79, 115, 136	0
33	DM	138/140 (98%)	0.15	3 (2%) 65 35	72, 104, 137, 147	0
34	BN	122/122 (100%)	-0.05	0 100 100	55, 71, 87, 93	0
34	DN	122/122 (100%)	0.06	0 100 100	66, 85, 103, 110	0
35	BO	150/150 (100%)	0.35	7 (4%) 35 14	45, 82, 109, 167	0
35	DO	150/150 (100%)	0.89	22 (14%) 3 1	45, 93, 136, 174	0
36	BP	141/141 (100%)	0.20	5 (3%) 48 21	55, 77, 105, 140	0
36	DP	141/141 (100%)	0.46	15 (10%) 8 3	58, 100, 130, 154	0
37	B0	118/118 (100%)	0.03	0 100 100	53, 74, 96, 106	0
37	D0	117/118 (99%)	0.05	1 (0%) 85 64	62, 81, 100, 117	0
38	BQ	111/112 (99%)	0.77	10 (9%) 12 4	71, 91, 116, 130	0
38	DQ	111/112 (99%)	0.27	6 (5%) 29 11	73, 109, 135, 157	0
39	BR	137/146 (93%)	0.17	4 (2%) 55 26	66, 85, 135, 167	0
39	DR	137/146 (93%)	0.10	3 (2%) 65 35	73, 94, 154, 184	0
40	B1	117/118 (99%)	0.03	2 (1%) 73 45	50, 70, 98, 140	0
40	D1	117/118 (99%)	0.52	10 (8%) 13 5	60, 99, 137, 155	0
41	B2	101/101 (100%)	0.11	3 (2%) 54 25	46, 91, 116, 128	0
41	D2	101/101 (100%)	1.02	14 (13%) 4 1	63, 122, 139, 150	0
42	BS	113/113 (100%)	-0.03	1 (0%) 85 64	44, 67, 99, 152	0
42	DS	113/113 (100%)	0.18	2 (1%) 71 43	61, 75, 109, 161	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
43	BT	92/96 (95%)	0.38	3 (3%)	50	22	54, 69, 95, 112	0
43	DT	92/96 (95%)	0.25	3 (3%)	50	22	65, 81, 109, 122	0
44	BU	102/110 (92%)	0.52	6 (5%)	26	10	70, 94, 144, 165	0
44	DU	102/110 (92%)	1.53	29 (28%)	1	0	78, 111, 162, 172	0
45	BV	175/206 (84%)	1.34	39 (22%)	1	1	79, 120, 189, 194	0
45	DV	179/206 (86%)	1.94	66 (36%)	0	0	111, 152, 207, 219	0
46	B3	76/85 (89%)	0.19	2 (2%)	59	29	51, 72, 92, 125	0
46	D3	77/85 (90%)	-0.02	1 (1%)	79	53	64, 87, 110, 151	0
47	BZ	97/98 (98%)	0.47	8 (8%)	14	5	48, 71, 115, 155	0
47	DZ	97/98 (98%)	-0.05	3 (3%)	52	24	54, 74, 126, 152	0
48	BW	66/72 (91%)	0.39	2 (3%)	54	25	59, 79, 95, 127	0
48	DW	66/72 (91%)	0.43	3 (4%)	37	15	75, 99, 121, 134	0
49	BX	59/60 (98%)	-0.01	0	100	100	61, 77, 112, 131	0
49	DX	59/60 (98%)	0.62	4 (6%)	20	7	76, 103, 136, 159	0
50	B4	66/71 (92%)	2.50	38 (57%)	0	0	112, 153, 176, 181	0
50	D4	63/71 (88%)	2.05	30 (47%)	0	0	141, 181, 191, 201	0
51	B5	59/60 (98%)	0.42	6 (10%)	9	3	43, 81, 156, 165	0
51	D5	59/60 (98%)	0.87	8 (13%)	4	1	61, 84, 169, 188	0
52	B6	45/54 (83%)	6.11	45 (100%)	0	0	117, 148, 164, 173	0
52	D6	45/54 (83%)	2.68	25 (55%)	0	0	131, 164, 181, 185	0
53	B7	45/49 (91%)	-0.00	0	100	100	38, 48, 68, 85	0
53	D7	45/49 (91%)	0.03	0	100	100	52, 59, 74, 94	0
54	B8	60/65 (92%)	0.38	2 (3%)	50	22	51, 68, 88, 115	0
54	D8	60/65 (92%)	0.37	3 (5%)	32	13	64, 80, 106, 132	0
All	All	21100/21658 (97%)	0.15	1025 (4%)	33	13	38, 95, 177, 247	0

The worst 5 of 1025 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	DA	654(J)	A	20.4
29	DF	1	MET	19.0
25	DA	654(L)	G	16.2
25	BA	654(J)	A	15.4
25	DA	654(K)	C	14.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
22	MIA	CB	38	29/30	0.94	0.19	-	63,95,112,126	0
22	MIA	AB	38	29/30	0.96	0.18	-	65,78,90,93	0
22	MIA	AD	38	29/30	0.92	0.18	-	98,122,141,145	0
22	MIA	CD	38	29/30	0.94	0.21	-	101,121,146,154	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	BA	3492	1/1	0.97	0.39	37.87	54,54,54,54	0
55	MG	BA	3300	1/1	0.78	0.43	36.77	80,80,80,80	0
55	MG	AA	1683	1/1	0.78	0.41	35.48	87,87,87,87	0
55	MG	AA	1740	1/1	0.91	0.45	35.39	76,76,76,76	0
55	MG	BA	3540	1/1	0.74	0.43	35.31	83,83,83,83	0
55	MG	AA	1681	1/1	0.89	0.39	34.94	72,72,72,72	0
55	MG	AA	1698	1/1	0.97	0.48	31.98	76,76,76,76	0
55	MG	CA	1742	1/1	0.47	0.92	29.22	108,108,108,108	0
55	MG	BA	3184	1/1	0.91	0.46	29.10	46,46,46,46	0
55	MG	BA	3522	1/1	0.92	0.42	28.63	45,45,45,45	0
55	MG	BA	3546	1/1	0.64	0.47	28.56	101,101,101,101	0
55	MG	BA	3144	1/1	0.97	0.42	28.19	39,39,39,39	0
55	MG	AA	1652	1/1	0.95	0.43	27.94	72,72,72,72	0
55	MG	DA	3318	1/1	0.81	0.28	27.54	77,77,77,77	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	3182	1/1	0.96	0.50	27.23	45,45,45,45	0
55	MG	BA	3499	1/1	0.96	0.48	26.35	38,38,38,38	0
55	MG	CA	1720	1/1	0.90	0.35	26.25	68,68,68,68	0
55	MG	BA	3454	1/1	0.90	0.54	26.24	80,80,80,80	0
55	MG	DA	3123	1/1	0.93	0.42	23.66	50,50,50,50	0
55	MG	BA	3346	1/1	0.84	0.53	23.44	69,69,69,69	0
55	MG	DA	3089	1/1	0.85	0.43	22.52	60,60,60,60	0
55	MG	DA	3362	1/1	0.85	0.31	22.35	150,150,150,150	0
55	MG	BA	3116	1/1	0.94	0.47	22.28	50,50,50,50	0
55	MG	BA	3161	1/1	0.99	0.44	21.78	45,45,45,45	0
55	MG	BA	3010	1/1	0.93	0.38	21.68	45,45,45,45	0
55	MG	CA	1639	1/1	0.94	0.38	21.12	59,59,59,59	0
55	MG	CA	1638	1/1	0.78	0.33	20.84	68,68,68,68	0
55	MG	BA	3083	1/1	0.89	0.50	20.64	47,47,47,47	0
55	MG	BA	3172	1/1	0.84	0.44	20.38	74,74,74,74	0
55	MG	BA	3157	1/1	0.96	0.50	20.37	50,50,50,50	0
55	MG	DA	3430	1/1	0.96	0.42	19.33	52,52,52,52	0
55	MG	BA	3389	1/1	0.96	0.31	19.26	56,56,56,56	0
55	MG	BA	3150	1/1	0.93	0.49	19.14	49,49,49,49	0
55	MG	DA	3059	1/1	0.98	0.30	19.12	61,61,61,61	0
55	MG	BA	3006	1/1	0.97	0.44	18.78	58,58,58,58	0
55	MG	DA	3453	1/1	0.93	0.41	18.49	65,65,65,65	0
55	MG	DA	3115	1/1	0.92	0.45	18.44	64,64,64,64	0
55	MG	DA	3307	1/1	0.80	0.32	18.43	99,99,99,99	0
55	MG	BA	3167	1/1	0.95	0.39	18.30	45,45,45,45	0
55	MG	BA	3055	1/1	0.95	0.34	18.04	78,78,78,78	0
55	MG	BA	3549	1/1	0.96	0.45	17.86	55,55,55,55	0
55	MG	BA	3088	1/1	0.97	0.43	17.67	57,57,57,57	0
55	MG	BA	3127	1/1	0.83	0.42	17.58	73,73,73,73	0
55	MG	BA	3059	1/1	0.98	0.32	17.18	63,63,63,63	0
55	MG	BA	3352	1/1	0.74	0.39	17.16	75,75,75,75	0
55	MG	DA	3071	1/1	0.89	0.39	17.14	57,57,57,57	0
55	MG	BA	3004	1/1	0.98	0.36	16.42	36,36,36,36	0
55	MG	BA	3337	1/1	0.92	0.45	16.32	52,52,52,52	0
55	MG	BA	3490	1/1	0.98	0.37	16.29	36,36,36,36	0
55	MG	BA	3124	1/1	0.95	0.34	16.27	66,66,66,66	0
55	MG	DA	3056	1/1	0.95	0.44	16.23	52,52,52,52	0
55	MG	DA	3107	1/1	0.95	0.38	16.19	55,55,55,55	0
55	MG	BA	3223	1/1	0.96	0.48	16.12	56,56,56,56	0
55	MG	DA	3470	1/1	0.98	0.33	16.10	54,54,54,54	0
55	MG	DA	3174	1/1	0.95	0.38	15.83	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	CA	1744	1/1	0.84	0.28	15.74	73,73,73,73	0
55	MG	AA	1659	1/1	0.97	0.40	15.54	46,46,46,46	0
55	MG	BA	3129	1/1	0.92	0.41	15.24	50,50,50,50	0
55	MG	CA	1776	1/1	0.69	0.31	14.75	118,118,118,118	0
55	MG	BA	3518	1/1	0.97	0.49	14.72	36,36,36,36	0
55	MG	DA	3202	1/1	0.89	0.34	14.59	67,67,67,67	0
55	MG	BA	3435	1/1	0.99	0.46	14.31	49,49,49,49	0
55	MG	BA	3131	1/1	0.94	0.38	14.16	41,41,41,41	0
55	MG	BA	3087	1/1	0.95	0.35	14.13	38,38,38,38	0
55	MG	DA	3045	1/1	0.98	0.43	14.02	71,71,71,71	0
55	MG	AA	1788	1/1	0.27	0.27	13.88	98,98,98,98	0
55	MG	AA	1811	1/1	0.94	0.47	13.65	65,65,65,65	0
55	MG	BA	3016	1/1	0.98	0.36	13.56	48,48,48,48	0
55	MG	BA	3202	1/1	0.08	0.33	13.39	97,97,97,97	0
55	MG	DA	3144	1/1	0.97	0.47	13.21	66,66,66,66	0
55	MG	BA	3528	1/1	0.89	0.38	13.11	32,32,32,32	0
55	MG	DA	3433	1/1	0.96	0.37	13.10	50,50,50,50	0
55	MG	DA	3098	1/1	0.96	0.32	13.03	48,48,48,48	0
55	MG	DA	3119	1/1	0.90	0.38	12.89	65,65,65,65	0
55	MG	BA	3460	1/1	0.87	0.36	12.77	97,97,97,97	0
55	MG	BA	3524	1/1	0.90	0.34	12.74	43,43,43,43	0
55	MG	BA	3392	1/1	0.89	0.32	12.72	78,78,78,78	0
55	MG	CA	1657	1/1	0.91	0.34	12.68	68,68,68,68	0
55	MG	CA	1806	1/1	0.47	0.27	12.58	103,103,103,103	0
55	MG	DA	3370	1/1	0.65	0.31	12.58	81,81,81,81	0
55	MG	AA	1646	1/1	0.98	0.42	12.55	60,60,60,60	0
55	MG	AA	1739	1/1	0.86	0.36	12.54	82,82,82,82	0
55	MG	BA	3012	1/1	0.97	0.39	12.47	45,45,45,45	0
55	MG	BA	3498	1/1	0.84	0.27	12.41	40,40,40,40	0
55	MG	CA	1634	1/1	0.98	0.45	12.32	58,58,58,58	0
55	MG	AC	107	1/1	0.20	0.43	12.23	124,124,124,124	0
55	MG	DA	3131	1/1	0.96	0.34	12.14	48,48,48,48	0
55	MG	DA	3084	1/1	0.89	0.37	12.14	57,57,57,57	0
55	MG	AA	1628	1/1	0.97	0.46	12.09	77,77,77,77	0
55	MG	BA	3486	1/1	0.87	0.28	12.07	42,42,42,42	0
55	MG	CA	1603	1/1	0.97	0.30	11.90	60,60,60,60	0
55	MG	DA	3439	1/1	0.58	0.36	11.87	107,107,107,107	0
55	MG	BA	3021	1/1	0.96	0.28	11.86	42,42,42,42	0
55	MG	BA	3169	1/1	0.97	0.37	11.75	45,45,45,45	0
55	MG	CA	1602	1/1	0.94	0.35	11.71	64,64,64,64	0
55	MG	DA	3006	1/1	0.97	0.29	11.56	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	3289	1/1	0.91	0.39	11.37	62,62,62,62	0
55	MG	DA	3061	1/1	0.97	0.34	11.37	53,53,53,53	0
55	MG	BA	3262	1/1	0.62	0.40	11.32	87,87,87,87	0
55	MG	AA	1709	1/1	0.88	0.24	11.16	56,56,56,56	0
55	MG	BA	3110	1/1	0.87	0.30	11.15	69,69,69,69	0
55	MG	AA	1625	1/1	0.78	0.28	11.14	68,68,68,68	0
55	MG	CA	1656	1/1	0.88	0.32	11.10	72,72,72,72	0
55	MG	BA	3109	1/1	0.97	0.36	11.10	81,81,81,81	0
55	MG	BA	3332	1/1	0.87	0.37	11.08	76,76,76,76	0
55	MG	DB	212	1/1	0.57	0.33	11.00	120,120,120,120	0
55	MG	DA	3009	1/1	0.97	0.34	10.96	53,53,53,53	0
55	MG	DA	3450	1/1	0.96	0.32	10.90	54,54,54,54	0
55	MG	DA	3387	1/1	0.78	0.26	10.87	102,102,102,102	0
55	MG	BA	3044	1/1	0.95	0.26	10.73	68,68,68,68	0
55	MG	BA	3117	1/1	0.95	0.40	10.73	52,52,52,52	0
55	MG	DD	301	1/1	0.97	0.38	10.65	51,51,51,51	0
55	MG	CA	1676	1/1	0.96	0.36	10.64	76,76,76,76	0
55	MG	BA	3160	1/1	0.97	0.31	10.60	44,44,44,44	0
55	MG	DA	3270	1/1	0.75	0.36	10.55	76,76,76,76	0
55	MG	BA	3264	1/1	0.98	0.41	10.41	61,61,61,61	0
55	MG	BA	3241	1/1	0.95	0.31	10.38	62,62,62,62	0
55	MG	DA	3241	1/1	0.92	0.32	10.36	75,75,75,75	0
55	MG	DA	3055	1/1	0.98	0.41	10.36	52,52,52,52	0
55	MG	AA	1610	1/1	0.95	0.34	10.31	58,58,58,58	0
55	MG	DA	3220	1/1	0.93	0.31	10.21	64,64,64,64	0
55	MG	BA	3070	1/1	0.94	0.28	10.21	68,68,68,68	0
55	MG	DA	3432	1/1	0.93	0.29	10.15	64,64,64,64	0
55	MG	BA	3002	1/1	0.95	0.38	10.09	40,40,40,40	0
55	MG	CA	1651	1/1	0.92	0.35	10.07	77,77,77,77	0
55	MG	BA	3497	1/1	0.95	0.28	10.01	30,30,30,30	0
55	MG	DA	3456	1/1	0.97	0.29	9.95	57,57,57,57	0
55	MG	DA	3247	1/1	0.96	0.34	9.89	58,58,58,58	0
55	MG	DA	3044	1/1	0.97	0.34	9.85	66,66,66,66	0
55	MG	BA	3493	1/1	0.93	0.35	9.78	51,51,51,51	0
55	MG	BA	3287	1/1	0.83	0.28	9.78	60,60,60,60	0
55	MG	DA	3212	1/1	0.83	0.31	9.67	121,121,121,121	0
55	MG	BA	3084	1/1	0.97	0.37	9.67	37,37,37,37	0
55	MG	BA	3001	1/1	0.98	0.50	9.66	55,55,55,55	0
55	MG	BA	3495	1/1	0.94	0.39	9.64	75,75,75,75	0
55	MG	BA	3130	1/1	0.98	0.43	9.59	50,50,50,50	0
55	MG	DA	3187	1/1	0.75	0.30	9.47	101,101,101,101	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	3014	1/1	0.98	0.41	9.24	43,43,43,43	0
55	MG	AA	1669	1/1	0.77	0.27	9.22	77,77,77,77	0
55	MG	AA	1620	1/1	0.92	0.28	9.01	69,69,69,69	0
55	MG	BA	3299	1/1	0.83	0.26	8.96	66,66,66,66	0
55	MG	CC	101	1/1	0.90	0.33	8.94	77,77,77,77	0
55	MG	DA	3124	1/1	0.98	0.29	8.91	47,47,47,47	0
55	MG	CA	1616	1/1	0.96	0.23	8.90	87,87,87,87	0
55	MG	BA	3024	1/1	0.98	0.39	8.83	44,44,44,44	0
55	MG	AA	1639	1/1	0.87	0.28	8.74	84,84,84,84	0
55	MG	AA	1790	1/1	0.90	0.27	8.70	79,79,79,79	0
55	MG	AA	1648	1/1	0.25	0.36	8.69	115,115,115,115	0
55	MG	BA	3286	1/1	0.97	0.51	8.66	46,46,46,46	0
55	MG	BA	3283	1/1	0.93	0.25	8.60	56,56,56,56	0
55	MG	BA	3534	1/1	0.93	0.24	8.58	69,69,69,69	0
55	MG	DA	3129	1/1	0.96	0.38	8.52	65,65,65,65	0
55	MG	BA	3134	1/1	0.90	0.33	8.51	59,59,59,59	0
55	MG	BA	3027	1/1	0.97	0.24	8.49	41,41,41,41	0
55	MG	CA	1814	1/1	0.80	0.19	8.37	83,83,83,83	0
55	MG	BA	3042	1/1	0.96	0.38	8.36	75,75,75,75	0
55	MG	DA	3043	1/1	0.97	0.28	8.29	69,69,69,69	0
55	MG	CC	109	1/1	0.80	0.29	8.24	114,114,114,114	0
55	MG	DE	301	1/1	0.95	0.28	8.04	59,59,59,59	0
55	MG	DA	3057	1/1	0.93	0.31	8.03	56,56,56,56	0
55	MG	BA	3076	1/1	0.93	0.39	7.98	81,81,81,81	0
55	MG	DA	3474	1/1	0.97	0.28	7.92	60,60,60,60	0
55	MG	BA	3018	1/1	0.94	0.41	7.90	44,44,44,44	0
55	MG	DA	3018	1/1	0.91	0.25	7.89	46,46,46,46	0
55	MG	BB	210	1/1	0.74	0.30	7.80	81,81,81,81	0
55	MG	AA	1601	1/1	0.95	0.30	7.77	60,60,60,60	0
55	MG	DA	3010	1/1	0.97	0.31	7.73	53,53,53,53	0
55	MG	DA	3068	1/1	0.94	0.31	7.62	54,54,54,54	0
55	MG	CA	1617	1/1	0.94	0.37	7.54	83,83,83,83	0
55	MG	CA	1695	1/1	0.94	0.30	7.48	69,69,69,69	0
55	MG	BA	3368	1/1	0.85	0.29	7.46	59,59,59,59	0
55	MG	BA	3507	1/1	0.92	0.29	7.44	79,79,79,79	0
55	MG	DA	3428	1/1	0.95	0.33	7.43	59,59,59,59	0
55	MG	DA	3075	1/1	0.89	0.31	7.39	57,57,57,57	0
55	MG	BA	3140	1/1	0.97	0.28	7.34	67,67,67,67	0
55	MG	BA	3488	1/1	0.89	0.30	7.32	137,137,137,137	0
55	MG	BA	3020	1/1	0.96	0.30	7.29	29,29,29,29	0
55	MG	DA	3058	1/1	0.92	0.34	7.29	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3207	1/1	0.80	0.44	7.23	83,83,83,83	0
55	MG	BA	3101	1/1	0.98	0.33	7.23	66,66,66,66	0
55	MG	BA	3415	1/1	0.87	0.21	7.14	65,65,65,65	0
55	MG	DA	3282	1/1	0.82	0.30	7.14	64,64,64,64	0
55	MG	BA	3056	1/1	0.93	0.30	7.06	57,57,57,57	0
55	MG	DA	3173	1/1	0.88	0.27	7.05	90,90,90,90	0
55	MG	DA	3008	1/1	0.94	0.32	7.05	57,57,57,57	0
55	MG	BA	3048	1/1	0.91	0.24	7.03	60,60,60,60	0
55	MG	BA	3039	1/1	0.96	0.28	6.95	55,55,55,55	0
55	MG	AA	1710	1/1	0.97	0.22	6.84	56,56,56,56	0
55	MG	DA	3002	1/1	0.96	0.36	6.73	48,48,48,48	0
55	MG	BA	3147	1/1	0.84	0.32	6.70	47,47,47,47	0
55	MG	AA	1636	1/1	0.94	0.27	6.65	95,95,95,95	0
55	MG	CA	1811	1/1	0.90	0.35	6.60	69,69,69,69	0
55	MG	DA	3159	1/1	0.70	0.31	6.53	68,68,68,68	0
55	MG	DA	3106	1/1	0.93	0.33	6.45	57,57,57,57	0
55	MG	DA	3116	1/1	0.95	0.35	6.38	61,61,61,61	0
55	MG	BA	3086	1/1	0.90	0.32	6.37	56,56,56,56	0
55	MG	CA	1813	1/1	0.52	0.24	6.21	108,108,108,108	0
55	MG	BA	3080	1/1	0.89	0.29	6.18	64,64,64,64	0
55	MG	CA	1793	1/1	0.34	0.23	6.18	110,110,110,110	0
55	MG	AA	1608	1/1	0.89	0.29	6.18	65,65,65,65	0
55	MG	AC	101	1/1	0.95	0.30	6.13	55,55,55,55	0
55	MG	DA	3250	1/1	0.71	0.24	6.12	62,62,62,62	0
55	MG	DA	3028	1/1	0.94	0.30	6.08	73,73,73,73	0
55	MG	DA	3236	1/1	0.91	0.39	6.08	62,62,62,62	0
55	MG	DA	3408	1/1	0.98	0.23	6.06	66,66,66,66	0
55	MG	CA	1601	1/1	0.96	0.26	5.98	67,67,67,67	0
55	MG	BA	3240	1/1	0.88	0.30	5.86	73,73,73,73	0
55	MG	DA	3015	1/1	0.96	0.33	5.85	64,64,64,64	0
55	MG	BA	3145	1/1	0.81	0.27	5.78	54,54,54,54	0
55	MG	DB	208	1/1	0.61	0.30	5.77	99,99,99,99	0
55	MG	AA	1605	1/1	0.89	0.26	5.70	75,75,75,75	0
55	MG	CA	1615	1/1	0.76	0.27	5.68	106,106,106,106	0
55	MG	CA	1767	1/1	0.66	0.19	5.66	87,87,87,87	0
55	MG	DA	3341	1/1	0.96	0.33	5.66	56,56,56,56	0
55	MG	B1	201	1/1	0.86	0.27	5.65	71,71,71,71	0
55	MG	DA	3162	1/1	0.96	0.34	5.59	58,58,58,58	0
55	MG	CC	108	1/1	0.82	0.22	5.53	95,95,95,95	0
55	MG	BA	3290	1/1	0.67	0.24	5.46	75,75,75,75	0
55	MG	AA	1602	1/1	0.95	0.28	5.35	71,71,71,71	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	3458	1/1	0.81	0.34	5.35	75,75,75,75	0
55	MG	BA	3174	1/1	0.93	0.38	5.34	46,46,46,46	0
55	MG	DA	3240	1/1	0.90	0.18	5.33	55,55,55,55	0
55	MG	CA	1613	1/1	0.93	0.25	5.24	84,84,84,84	0
55	MG	BA	3553	1/1	0.92	0.27	5.16	49,49,49,49	0
55	MG	CA	1631	1/1	0.93	0.27	5.12	65,65,65,65	0
55	MG	AA	1662	1/1	0.95	0.23	5.04	41,41,41,41	0
55	MG	BA	3328	1/1	0.83	0.22	4.98	52,52,52,52	0
55	MG	BA	3356	1/1	0.91	0.32	4.98	60,60,60,60	0
55	MG	BA	3090	1/1	0.87	0.26	4.86	40,40,40,40	0
55	MG	AA	1619	1/1	0.95	0.38	4.73	58,58,58,58	0
55	MG	BA	3215	1/1	0.95	0.24	4.72	44,44,44,44	0
55	MG	BA	3334	1/1	0.69	0.28	4.68	67,67,67,67	0
55	MG	DA	3094	1/1	0.92	0.26	4.65	48,48,48,48	0
55	MG	BA	3272	1/1	0.92	0.22	4.63	59,59,59,59	0
55	MG	BA	3407	1/1	0.94	0.26	4.59	73,73,73,73	0
55	MG	BA	3054	1/1	0.94	0.30	4.58	52,52,52,52	0
55	MG	DA	3197	1/1	0.87	0.27	4.47	48,48,48,48	0
55	MG	BA	3231	1/1	0.81	0.35	4.40	46,46,46,46	0
55	MG	AA	1632	1/1	0.94	0.23	4.37	55,55,55,55	0
55	MG	DA	3235	1/1	0.88	0.33	4.37	69,69,69,69	0
55	MG	DA	3030	1/1	0.81	0.20	4.22	85,85,85,85	0
55	MG	DA	3200	1/1	0.95	0.37	4.18	55,55,55,55	0
55	MG	BA	3496	1/1	0.98	0.28	4.18	45,45,45,45	0
55	MG	DA	3190	1/1	0.84	0.32	3.95	66,66,66,66	0
55	MG	BA	3248	1/1	0.95	0.21	3.92	34,34,34,34	0
55	MG	DA	3463	1/1	0.97	0.22	3.86	84,84,84,84	0
55	MG	BA	3469	1/1	0.90	0.36	3.86	124,124,124,124	0
55	MG	CA	1645	1/1	0.94	0.25	3.81	84,84,84,84	0
55	MG	BA	3330	1/1	0.84	0.24	3.79	61,61,61,61	0
55	MG	AD	103	1/1	0.53	0.23	3.79	89,89,89,89	0
55	MG	DA	3222	1/1	0.74	0.16	3.78	75,75,75,75	0
55	MG	BA	3555	1/1	0.98	0.24	3.76	47,47,47,47	0
55	MG	BA	3186	1/1	0.97	0.29	3.69	45,45,45,45	0
55	MG	BA	3448	1/1	0.44	0.24	3.66	104,104,104,104	0
55	MG	DA	3070	1/1	0.97	0.33	3.63	49,49,49,49	0
55	MG	BA	3313	1/1	0.91	0.23	3.56	74,74,74,74	0
55	MG	DA	3383	1/1	0.59	0.20	3.54	107,107,107,107	0
55	MG	DA	3196	1/1	0.95	0.22	3.52	45,45,45,45	0
55	MG	BA	3539	1/1	0.96	0.25	3.33	35,35,35,35	0
55	MG	BA	3538	1/1	0.94	0.23	3.29	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	3020	1/1	0.94	0.21	3.22	45,45,45,45	0
55	MG	BA	3026	1/1	0.90	0.31	3.09	43,43,43,43	0
55	MG	BB	215	1/1	0.82	0.23	3.08	91,91,91,91	0
55	MG	DA	3435	1/1	0.91	0.20	3.01	51,51,51,51	0
55	MG	BA	3521	1/1	0.95	0.24	2.98	45,45,45,45	0
55	MG	BA	3047	1/1	0.93	0.20	2.91	46,46,46,46	0
55	MG	DA	3471	1/1	0.97	0.22	2.90	60,60,60,60	0
55	MG	BA	3057	1/1	0.93	0.21	2.87	46,46,46,46	0
55	MG	BA	3074	1/1	0.90	0.17	2.81	91,91,91,91	0
55	MG	DA	3233	1/1	0.85	0.32	2.67	90,90,90,90	0
55	MG	BA	3475	1/1	0.67	0.32	2.66	212,212,212,212	0
55	MG	BA	3095	1/1	0.91	0.26	2.54	79,79,79,79	0
55	MG	DA	3321	1/1	0.60	0.16	2.52	112,112,112,112	0
55	MG	AA	1706	1/1	0.54	0.21	2.43	91,91,91,91	0
55	MG	B1	202	1/1	0.70	0.33	2.42	86,86,86,86	0
55	MG	BB	202	1/1	0.90	0.22	2.36	74,74,74,74	0
55	MG	AG	301	1/1	0.85	0.23	2.32	98,98,98,98	0
55	MG	BA	3232	1/1	0.85	0.22	2.31	57,57,57,57	0
55	MG	BA	3520	1/1	0.96	0.38	2.29	40,40,40,40	0
55	MG	DA	3137	1/1	0.95	0.23	2.25	53,53,53,53	0
55	MG	DA	3017	1/1	0.90	0.26	2.23	90,90,90,90	0
55	MG	BA	3505	1/1	0.82	0.23	2.23	61,61,61,61	0
55	MG	DB	213	1/1	0.88	0.15	2.21	99,99,99,99	0
55	MG	DA	3063	1/1	0.97	0.25	2.21	45,45,45,45	0
55	MG	DA	3390	1/1	0.67	0.21	2.14	92,92,92,92	0
55	MG	BA	3506	1/1	0.90	0.24	1.97	73,73,73,73	0
55	MG	BA	3060	1/1	0.96	0.22	1.93	51,51,51,51	0
55	MG	DA	3156	1/1	0.90	0.27	1.90	78,78,78,78	0
55	MG	AC	108	1/1	0.90	0.15	1.83	82,82,82,82	0
55	MG	B0	201	1/1	0.98	0.32	1.77	46,46,46,46	0
55	MG	AA	1795	1/1	0.65	0.37	1.76	113,113,113,113	0
55	MG	CA	1653	1/1	0.74	0.26	1.64	97,97,97,97	0
55	MG	AA	1664	1/1	0.92	0.21	1.56	53,53,53,53	0
55	MG	BA	3128	1/1	0.72	0.23	1.55	71,71,71,71	0
55	MG	AA	1686	1/1	0.70	0.18	1.54	91,91,91,91	0
55	MG	CA	1605	1/1	0.91	0.18	1.49	90,90,90,90	0
56	ZN	AG	303	1/1	0.97	0.35	1.46	100,100,100,100	0
55	MG	BA	3398	1/1	0.91	0.17	1.32	57,57,57,57	0
55	MG	DA	3434	1/1	0.86	0.18	1.30	73,73,73,73	0
55	MG	BA	3541	1/1	0.94	0.21	1.27	66,66,66,66	0
55	MG	BA	3097	1/1	0.81	0.20	1.25	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	DA	3437	1/1	0.74	0.18	1.19	66,66,66,66	0
55	MG	DA	3357	1/1	0.87	0.16	1.00	87,87,87,87	0
55	MG	CA	1705	1/1	0.91	0.20	0.89	101,101,101,101	0
55	MG	BA	3531	1/1	0.97	0.20	0.87	31,31,31,31	0
55	MG	AA	1718	1/1	0.79	0.18	0.80	82,82,82,82	0
55	MG	BA	3348	1/1	0.82	0.18	0.76	96,96,96,96	0
55	MG	DA	3126	1/1	0.84	0.17	0.72	63,63,63,63	0
55	MG	BA	3166	1/1	0.94	0.23	0.71	28,28,28,28	0
55	MG	AA	1817	1/1	0.76	0.17	0.59	61,61,61,61	0
55	MG	BA	3143	1/1	0.97	0.19	0.41	43,43,43,43	0
55	MG	BA	3226	1/1	0.94	0.18	0.37	69,69,69,69	0
55	MG	AA	1712	1/1	0.94	0.17	0.29	73,73,73,73	0
55	MG	CA	1632	1/1	0.91	0.17	0.27	53,53,53,53	0
55	MG	DA	3031	1/1	0.87	0.17	0.21	70,70,70,70	0
55	MG	CA	1789	1/1	0.87	0.14	0.12	71,71,71,71	0
55	MG	D0	201	1/1	0.93	0.21	0.02	63,63,63,63	0
55	MG	AA	1682	1/1	0.80	0.22	-0.06	93,93,93,93	0
55	MG	BA	3361	1/1	0.95	0.17	-0.14	70,70,70,70	0
55	MG	CA	1630	1/1	0.23	0.18	-0.14	149,149,149,149	0
55	MG	DA	3364	1/1	0.85	0.12	-0.15	93,93,93,93	0
56	ZN	CG	303	1/1	0.98	0.30	-0.21	109,109,109,109	0
55	MG	CA	1650	1/1	0.84	0.17	-0.22	78,78,78,78	0
55	MG	CA	1618	1/1	0.86	0.18	-0.41	95,95,95,95	0
55	MG	CA	1783	1/1	0.84	0.13	-0.59	87,87,87,87	0
55	MG	DA	3199	1/1	0.61	0.16	-0.69	85,85,85,85	0
55	MG	B6	101	1/1	0.51	0.32	-0.70	102,102,102,102	0
55	MG	DD	303	1/1	0.20	0.16	-0.74	69,69,69,69	0
56	ZN	CQ	101	1/1	0.97	0.17	-0.75	118,118,118,118	0
55	MG	AA	1711	1/1	0.85	0.17	-0.77	97,97,97,97	0
55	MG	D8	101	1/1	0.72	0.16	-0.81	88,88,88,88	0
56	ZN	AQ	101	1/1	0.98	0.14	-0.83	142,142,142,142	0
55	MG	CA	1666	1/1	0.78	0.16	-0.83	90,90,90,90	0
55	MG	CA	1624	1/1	0.92	0.17	-0.90	93,93,93,93	0
55	MG	CA	1641	1/1	0.94	0.15	-0.91	64,64,64,64	0
55	MG	CA	1607	1/1	0.94	0.13	-0.94	70,70,70,70	0
55	MG	CA	1718	1/1	0.98	0.13	-1.07	64,64,64,64	0
55	MG	BA	3308	1/1	0.93	0.12	-1.20	63,63,63,63	0
55	MG	DA	3062	1/1	0.94	0.17	-1.44	39,39,39,39	0
55	MG	DA	3181	1/1	0.92	0.16	-1.44	50,50,50,50	0
55	MG	DA	3037	1/1	0.92	0.12	-1.67	71,71,71,71	0
55	MG	DA	3276	1/1	0.93	0.13	-1.74	81,81,81,81	0
55	MG	BF	301	1/1	0.95	0.14	-1.76	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	AA	1645	1/1	0.93	0.13	-1.85	65,65,65,65	0
55	MG	DA	3232	1/1	0.87	0.13	-1.88	56,56,56,56	0
55	MG	BA	3185	1/1	0.88	0.17	-1.89	46,46,46,46	0
55	MG	DA	3401	1/1	0.79	0.12	-2.06	75,75,75,75	0
55	MG	DA	3242	1/1	0.58	0.11	-2.09	81,81,81,81	0
55	MG	CG	302	1/1	0.83	0.12	-2.09	89,89,89,89	0
55	MG	DA	3025	1/1	0.91	0.13	-2.10	70,70,70,70	0
55	MG	DB	202	1/1	0.95	0.14	-2.21	91,91,91,91	0
55	MG	BA	3204	1/1	0.91	0.16	-2.42	56,56,56,56	0
55	MG	AN	201	1/1	0.96	0.07	-2.46	67,67,67,67	0
55	MG	DA	3258	1/1	0.81	0.13	-2.55	87,87,87,87	0
55	MG	DA	3347	1/1	0.95	0.12	-2.60	91,91,91,91	0
55	MG	DA	3204	1/1	0.96	0.13	-2.70	48,48,48,48	0
55	MG	DB	203	1/1	0.86	0.09	-2.72	111,111,111,111	0
55	MG	BE	301	1/1	0.84	0.12	-3.02	57,57,57,57	0
55	MG	BA	3193	1/1	0.93	0.13	-3.18	46,46,46,46	0
55	MG	DA	3023	1/1	0.96	0.10	-3.49	47,47,47,47	0
55	MG	CA	1637	1/1	0.96	0.10	-3.74	70,70,70,70	0
55	MG	DA	3335	1/1	0.89	0.11	-4.01	80,80,80,80	0
55	MG	DA	3304	1/1	0.88	0.12	-4.34	77,77,77,77	0
55	MG	AA	1731	1/1	0.79	0.11	-5.68	90,90,90,90	0
55	MG	BA	3527	1/1	0.96	0.12	-5.82	40,40,40,40	0
55	MG	AA	1820	1/1	0.89	0.12	-6.37	82,82,82,82	0
55	MG	CA	1794	1/1	0.90	0.10	-9.62	67,67,67,67	0
55	MG	AA	1606	1/1	0.96	0.07	-11.36	77,77,77,77	0
55	MG	CA	1775	1/1	0.83	0.45	-	69,69,69,69	0
55	MG	DA	3306	1/1	0.81	0.34	-	96,96,96,96	0
55	MG	BA	3386	1/1	0.23	0.42	-	115,115,115,115	0
55	MG	AC	102	1/1	0.64	0.37	-	106,106,106,106	0
55	MG	BA	3175	1/1	0.90	0.30	-	62,62,62,62	0
55	MG	BA	3307	1/1	0.85	0.47	-	79,79,79,79	0
55	MG	BA	3075	1/1	0.77	0.40	-	75,75,75,75	0
55	MG	BA	3529	1/1	0.99	0.49	-	42,42,42,42	0
55	MG	BA	3103	1/1	0.95	0.49	-	76,76,76,76	0
55	MG	BA	3366	1/1	0.91	0.20	-	91,91,91,91	0
55	MG	CC	103	1/1	0.49	0.23	-	114,114,114,114	0
55	MG	AA	1713	1/1	0.68	0.35	-	98,98,98,98	0
55	MG	CA	1633	1/1	0.96	0.37	-	61,61,61,61	0
55	MG	DA	3478	1/1	0.90	0.15	-	89,89,89,89	0
55	MG	BA	3406	1/1	0.41	1.36	-	182,182,182,182	0
55	MG	DA	3170	1/1	0.98	0.39	-	59,59,59,59	0
55	MG	DA	3443	1/1	0.58	0.26	-	94,94,94,94	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	3322	1/1	0.81	0.38	-	81,81,81,81	0
55	MG	DA	3353	1/1	0.61	0.24	-	102,102,102,102	0
55	MG	BA	3100	1/1	0.53	0.41	-	93,93,93,93	0
55	MG	CA	1625	1/1	0.85	0.23	-	104,104,104,104	0
55	MG	DA	3351	1/1	0.28	0.22	-	151,151,151,151	0
55	MG	DA	3257	1/1	0.82	0.41	-	77,77,77,77	0
55	MG	BA	3421	1/1	0.79	0.89	-	97,97,97,97	0
55	MG	BA	3369	1/1	0.65	0.19	-	92,92,92,92	0
55	MG	AA	1752	1/1	0.92	0.37	-	67,67,67,67	0
55	MG	DA	3169	1/1	0.92	0.26	-	92,92,92,92	0
55	MG	BA	3171	1/1	0.48	0.46	-	96,96,96,96	0
55	MG	CA	1658	1/1	0.72	0.33	-	90,90,90,90	0
55	MG	DA	3467	1/1	0.72	0.13	-	103,103,103,103	0
55	MG	BA	3197	1/1	0.95	0.40	-	57,57,57,57	0
55	MG	CA	1665	1/1	0.93	0.32	-	70,70,70,70	0
55	MG	BA	3470	1/1	0.94	0.48	-	83,83,83,83	0
55	MG	DA	3033	1/1	0.87	0.26	-	83,83,83,83	0
55	MG	BA	3304	1/1	0.90	0.36	-	80,80,80,80	0
55	MG	BA	3125	1/1	0.35	0.32	-	107,107,107,107	0
55	MG	BA	3146	1/1	0.95	0.36	-	62,62,62,62	0
55	MG	DA	3147	1/1	0.86	0.22	-	87,87,87,87	0
55	MG	AA	1759	1/1	0.77	0.14	-	66,66,66,66	0
55	MG	DA	3163	1/1	0.61	0.37	-	75,75,75,75	0
55	MG	AA	1722	1/1	-	-	-	62,62,62,62	1
55	MG	AA	1638	1/1	0.86	0.36	-	105,105,105,105	0
55	MG	DA	3120	1/1	0.77	0.43	-	73,73,73,73	0
55	MG	DA	3323	1/1	0.88	0.92	-	104,104,104,104	0
55	MG	BA	3207	1/1	0.90	0.55	-	70,70,70,70	0
55	MG	DA	3029	1/1	0.92	0.32	-	82,82,82,82	0
55	MG	DA	3185	1/1	0.75	0.15	-	78,78,78,78	0
55	MG	DA	3122	1/1	0.91	0.41	-	69,69,69,69	0
55	MG	CA	1604	1/1	0.94	0.20	-	60,60,60,60	0
55	MG	DA	3457	1/1	0.97	0.28	-	48,48,48,48	0
55	MG	CA	1769	1/1	0.95	0.30	-	67,67,67,67	0
55	MG	DA	3374	1/1	0.79	0.19	-	92,92,92,92	0
55	MG	BA	3245	1/1	0.74	0.46	-	107,107,107,107	0
55	MG	AA	1675	1/1	0.80	0.20	-	81,81,81,81	0
55	MG	CA	1627	1/1	0.82	0.17	-	140,140,140,140	0
55	MG	AA	1708	1/1	0.64	0.14	-	77,77,77,77	0
55	MG	DA	3081	1/1	0.78	0.32	-	84,84,84,84	0
55	MG	BA	3011	1/1	0.96	0.41	-	40,40,40,40	0
55	MG	AA	1617	1/1	0.68	0.35	-	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	1655	1/1	0.94	0.41	-	78,78,78,78	0
55	MG	CA	1737	1/1	0.43	0.23	-	122,122,122,122	0
55	MG	DA	3422	1/1	0.78	0.20	-	75,75,75,75	0
55	MG	DA	3109	1/1	0.96	0.36	-	55,55,55,55	0
55	MG	DA	3261	1/1	0.61	0.22	-	78,78,78,78	0
55	MG	DA	3464	1/1	0.86	0.31	-	90,90,90,90	0
55	MG	CA	1655	1/1	0.80	0.11	-	85,85,85,85	0
55	MG	DA	3110	1/1	0.94	0.14	-	61,61,61,61	0
55	MG	BA	3164	1/1	0.96	0.40	-	47,47,47,47	0
55	MG	BA	3563	1/1	0.77	0.24	-	100,100,100,100	0
55	MG	AA	1819	1/1	0.53	0.32	-	126,126,126,126	0
55	MG	AA	1719	1/1	0.96	0.23	-	80,80,80,80	0
55	MG	DA	3226	1/1	0.93	0.28	-	85,85,85,85	0
55	MG	AA	1755	1/1	0.64	0.30	-	88,88,88,88	0
55	MG	CA	1764	1/1	0.57	0.22	-	117,117,117,117	0
55	MG	AA	1742	1/1	0.90	0.27	-	88,88,88,88	0
55	MG	DA	3245	1/1	0.79	0.16	-	91,91,91,91	0
55	MG	BA	3325	1/1	0.85	0.22	-	81,81,81,81	0
55	MG	AA	1793	1/1	0.93	0.20	-	87,87,87,87	0
55	MG	CA	1660	1/1	0.80	0.13	-	85,85,85,85	0
55	MG	DA	3049	1/1	0.95	0.41	-	55,55,55,55	0
55	MG	AA	1730	1/1	0.39	0.29	-	113,113,113,113	0
55	MG	DA	3011	1/1	0.97	0.34	-	50,50,50,50	0
55	MG	DA	3108	1/1	0.96	0.41	-	54,54,54,54	0
55	MG	CA	1735	1/1	0.88	0.41	-	119,119,119,119	0
55	MG	DA	3278	1/1	0.79	0.25	-	100,100,100,100	0
55	MG	BA	3219	1/1	0.86	0.33	-	68,68,68,68	0
55	MG	DA	3314	1/1	0.75	0.15	-	95,95,95,95	0
55	MG	DA	3193	1/1	0.97	0.50	-	48,48,48,48	0
55	MG	AA	1654	1/1	0.82	0.28	-	77,77,77,77	0
55	MG	CA	1782	1/1	0.90	0.14	-	113,113,113,113	0
55	MG	BA	3151	1/1	0.82	0.57	-	97,97,97,97	0
55	MG	BA	3062	1/1	0.56	0.36	-	79,79,79,79	0
55	MG	CA	1784	1/1	0.86	0.11	-	92,92,92,92	0
55	MG	BA	3423	1/1	0.94	0.38	-	90,90,90,90	0
55	MG	CA	1734	1/1	0.77	0.13	-	80,80,80,80	0
55	MG	CA	1717	1/1	0.90	0.39	-	73,73,73,73	0
55	MG	BA	3073	1/1	0.94	0.29	-	65,65,65,65	0
55	MG	DA	3466	1/1	0.85	0.17	-	81,81,81,81	0
55	MG	AA	1785	1/1	0.27	2.26	-	125,125,125,125	0
55	MG	DA	3384	1/1	0.77	0.38	-	97,97,97,97	0
55	MG	DA	3431	1/1	0.92	0.24	-	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	BA	3188	1/1	0.97	0.35	-	64,64,64,64	0
55	MG	DA	3326	1/1	0.79	0.33	-	109,109,109,109	0
55	MG	AA	1687	1/1	0.71	0.26	-	108,108,108,108	0
55	MG	BA	3261	1/1	0.98	0.47	-	57,57,57,57	0
55	MG	AA	1672	1/1	0.96	0.52	-	67,67,67,67	0
55	MG	AA	1685	1/1	0.82	0.34	-	85,85,85,85	0
55	MG	AA	1692	1/1	0.84	0.24	-	73,73,73,73	0
55	MG	BA	3051	1/1	0.66	0.32	-	103,103,103,103	0
55	MG	BA	3072	1/1	0.96	0.35	-	67,67,67,67	0
55	MG	DA	3112	1/1	0.96	0.28	-	63,63,63,63	0
55	MG	AA	1697	1/1	0.62	0.29	-	101,101,101,101	0
55	MG	BA	3149	1/1	0.97	0.36	-	41,41,41,41	0
55	MG	DA	3273	1/1	0.81	0.10	-	77,77,77,77	0
55	MG	DA	3296	1/1	0.68	0.17	-	93,93,93,93	0
55	MG	AA	1766	1/1	0.75	0.32	-	98,98,98,98	0
55	MG	BA	3251	1/1	0.85	0.43	-	80,80,80,80	0
55	MG	DA	3067	1/1	0.98	0.17	-	50,50,50,50	0
55	MG	BA	3437	1/1	0.84	0.32	-	97,97,97,97	0
55	MG	DA	3182	1/1	0.94	0.26	-	47,47,47,47	0
55	MG	DA	3284	1/1	0.90	0.19	-	90,90,90,90	0
55	MG	BA	3067	1/1	0.93	0.27	-	79,79,79,79	0
55	MG	AA	1737	1/1	0.86	0.26	-	81,81,81,81	0
55	MG	CA	1809	1/1	0.44	0.35	-	93,93,93,93	0
55	MG	DA	3050	1/1	0.35	0.27	-	90,90,90,90	0
55	MG	DA	3042	1/1	0.97	0.38	-	51,51,51,51	0
55	MG	AA	1736	1/1	0.65	0.56	-	108,108,108,108	0
55	MG	BA	3210	1/1	0.76	0.25	-	99,99,99,99	0
55	MG	BA	3121	1/1	0.84	0.33	-	72,72,72,72	0
55	MG	BA	3244	1/1	0.95	0.16	-	34,34,34,34	0
55	MG	CA	1622	1/1	0.80	0.65	-	110,110,110,110	0
55	MG	B3	101	1/1	0.86	0.42	-	81,81,81,81	0
55	MG	AA	1607	1/1	0.95	0.20	-	86,86,86,86	0
55	MG	BA	3227	1/1	0.91	0.43	-	64,64,64,64	0
55	MG	DA	3134	1/1	0.76	0.19	-	93,93,93,93	0
55	MG	BA	3526	1/1	0.97	0.39	-	41,41,41,41	0
55	MG	AA	1791	1/1	0.64	0.47	-	90,90,90,90	0
55	MG	BA	3052	1/1	0.91	0.24	-	66,66,66,66	0
55	MG	DA	3149	1/1	0.84	0.22	-	93,93,93,93	0
55	MG	BB	204	1/1	0.67	0.32	-	91,91,91,91	0
55	MG	BA	3388	1/1	0.87	0.39	-	76,76,76,76	0
55	MG	CA	1748	1/1	0.67	0.31	-	76,76,76,76	0
55	MG	BA	3324	1/1	0.73	0.43	-	105,105,105,105	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	3119	1/1	0.96	0.39	-	61,61,61,61	0
55	MG	BA	3284	1/1	0.91	0.43	-	75,75,75,75	0
55	MG	CA	1749	1/1	0.67	0.25	-	117,117,117,117	0
55	MG	BA	3266	1/1	0.70	0.41	-	71,71,71,71	0
55	MG	DA	3014	1/1	0.93	0.35	-	76,76,76,76	0
55	MG	DA	3287	1/1	0.87	0.46	-	120,120,120,120	0
55	MG	DA	3076	1/1	0.34	0.33	-	107,107,107,107	0
55	MG	DA	3026	1/1	0.93	0.28	-	73,73,73,73	0
55	MG	DA	3080	1/1	0.95	0.27	-	73,73,73,73	0
55	MG	DA	3074	1/1	0.90	0.35	-	65,65,65,65	0
55	MG	BA	3481	1/1	0.91	0.21	-	97,97,97,97	0
55	MG	DA	3345	1/1	0.88	0.24	-	85,85,85,85	0
55	MG	BE	303	1/1	0.80	0.39	-	105,105,105,105	0
55	MG	BA	3568	1/1	0.67	0.20	-	106,106,106,106	0
55	MG	DA	3160	1/1	0.94	0.34	-	59,59,59,59	0
55	MG	DA	3329	1/1	0.86	0.26	-	71,71,71,71	0
55	MG	BA	3229	1/1	0.83	0.38	-	65,65,65,65	0
55	MG	DB	220	1/1	0.84	0.13	-	121,121,121,121	0
55	MG	BA	3139	1/1	0.98	0.47	-	43,43,43,43	0
55	MG	CC	107	1/1	0.81	0.22	-	123,123,123,123	0
55	MG	BA	3478	1/1	0.92	0.33	-	61,61,61,61	0
55	MG	DA	3365	1/1	0.50	0.48	-	112,112,112,112	0
55	MG	BB	217	1/1	0.72	0.31	-	104,104,104,104	0
55	MG	DB	204	1/1	0.66	0.37	-	94,94,94,94	0
55	MG	BA	3427	1/1	0.83	0.45	-	97,97,97,97	0
55	MG	AA	1613	1/1	0.04	0.48	-	116,116,116,116	0
55	MG	BA	3362	1/1	0.90	0.21	-	84,84,84,84	0
55	MG	BA	3173	1/1	0.99	0.40	-	58,58,58,58	0
55	MG	BA	3472	1/1	0.58	0.62	-	133,133,133,133	0
55	MG	DA	3298	1/1	0.84	0.28	-	80,80,80,80	0
55	MG	CA	1755	1/1	0.83	0.34	-	104,104,104,104	0
55	MG	DA	3363	1/1	0.83	0.21	-	78,78,78,78	0
55	MG	DA	3228	1/1	0.66	0.54	-	103,103,103,103	0
55	MG	CA	1729	1/1	0.48	0.38	-	102,102,102,102	0
55	MG	BA	3402	1/1	0.89	0.25	-	76,76,76,76	0
55	MG	AA	1702	1/1	0.71	0.36	-	89,89,89,89	0
55	MG	DA	3376	1/1	0.75	0.25	-	107,107,107,107	0
55	MG	BA	3316	1/1	0.67	0.39	-	87,87,87,87	0
55	MG	DA	3297	1/1	0.90	0.42	-	82,82,82,82	0
55	MG	DA	3412	1/1	0.83	0.28	-	92,92,92,92	0
55	MG	BA	3480	1/1	0.76	0.34	-	76,76,76,76	0
55	MG	AB	103	1/1	0.85	0.34	-	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	1784	1/1	0.61	0.22	-	112,112,112,112	0
55	MG	DA	3481	1/1	0.74	0.14	-	79,79,79,79	0
55	MG	BA	3461	1/1	0.79	0.34	-	98,98,98,98	0
55	MG	CA	1725	1/1	0.91	0.35	-	86,86,86,86	0
55	MG	BA	3112	1/1	0.86	0.48	-	73,73,73,73	0
55	MG	DB	215	1/1	0.16	0.29	-	129,129,129,129	0
55	MG	DA	3482	1/1	0.73	0.37	-	83,83,83,83	0
55	MG	BA	3459	1/1	0.82	0.35	-	81,81,81,81	0
55	MG	DA	3366	1/1	0.05	0.35	-	105,105,105,105	0
55	MG	DA	3183	1/1	0.97	0.29	-	75,75,75,75	0
55	MG	BA	3378	1/1	0.52	0.25	-	140,140,140,140	0
55	MG	CA	1745	1/1	0.46	0.30	-	159,159,159,159	0
55	MG	AA	1647	1/1	0.85	0.31	-	81,81,81,81	0
55	MG	BA	3178	1/1	0.36	0.38	-	96,96,96,96	0
55	MG	DA	3224	1/1	0.86	0.20	-	75,75,75,75	0
55	MG	AA	1748	1/1	0.37	0.29	-	116,116,116,116	0
55	MG	DA	3302	1/1	0.88	0.31	-	69,69,69,69	0
55	MG	BA	3049	1/1	0.90	0.23	-	75,75,75,75	0
55	MG	DA	3382	1/1	0.62	0.48	-	121,121,121,121	0
55	MG	DA	3331	1/1	0.89	0.31	-	91,91,91,91	0
55	MG	BA	3447	1/1	0.86	0.42	-	72,72,72,72	0
55	MG	CA	1620	1/1	0.94	0.14	-	64,64,64,64	0
55	MG	DA	3090	1/1	0.91	0.27	-	71,71,71,71	0
55	MG	AA	1627	1/1	0.96	0.34	-	62,62,62,62	0
55	MG	CA	1781	1/1	0.30	0.21	-	172,172,172,172	0
55	MG	BA	3114	1/1	0.97	0.23	-	37,37,37,37	0
55	MG	BA	3474	1/1	0.78	0.37	-	72,72,72,72	0
55	MG	DA	3426	1/1	0.61	0.32	-	103,103,103,103	0
55	MG	BA	3523	1/1	0.97	0.41	-	36,36,36,36	0
55	MG	BA	3484	1/1	0.64	0.36	-	87,87,87,87	0
55	MG	DA	3024	1/1	0.53	0.34	-	104,104,104,104	0
55	MG	CA	1712	1/1	0.88	0.42	-	76,76,76,76	0
55	MG	BB	207	1/1	0.84	0.19	-	109,109,109,109	0
55	MG	BA	3104	1/1	0.90	0.31	-	82,82,82,82	0
55	MG	CA	1768	1/1	-0.04	0.43	-	138,138,138,138	0
55	MG	DA	3371	1/1	0.83	0.22	-	122,122,122,122	0
55	MG	BA	3414	1/1	0.82	0.36	-	100,100,100,100	0
55	MG	AA	1814	1/1	0.47	0.33	-	107,107,107,107	0
55	MG	DA	3445	1/1	0.73	0.15	-	118,118,118,118	0
55	MG	DA	3334	1/1	0.72	0.31	-	87,87,87,87	0
55	MG	DA	3424	1/1	0.91	0.24	-	83,83,83,83	0
55	MG	BA	3405	1/1	0.88	0.21	-	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	BA	3093	1/1	0.91	0.35	-	57,57,57,57	0
55	MG	DA	3400	1/1	0.76	0.14	-	115,115,115,115	0
55	MG	CA	1686	1/1	0.85	0.24	-	77,77,77,77	0
55	MG	BA	3445	1/1	0.63	0.27	-	82,82,82,82	0
55	MG	DA	3372	1/1	0.05	0.68	-	125,125,125,125	0
55	MG	DA	3194	1/1	0.52	0.33	-	104,104,104,104	0
55	MG	CA	1647	1/1	0.53	0.40	-	96,96,96,96	0
55	MG	DA	3066	1/1	0.79	0.30	-	76,76,76,76	0
55	MG	BA	3277	1/1	0.79	0.34	-	79,79,79,79	0
55	MG	BA	3288	1/1	0.67	0.26	-	75,75,75,75	0
55	MG	BA	3257	1/1	0.91	0.29	-	87,87,87,87	0
55	MG	BA	3270	1/1	0.78	0.36	-	96,96,96,96	0
55	MG	AA	1728	1/1	0.73	0.46	-	99,99,99,99	0
55	MG	BA	3238	1/1	0.78	0.32	-	75,75,75,75	0
55	MG	CA	1714	1/1	0.94	0.24	-	87,87,87,87	0
55	MG	BA	3017	1/1	0.97	0.41	-	58,58,58,58	0
55	MG	CA	1700	1/1	0.61	0.33	-	96,96,96,96	0
55	MG	DA	3310	1/1	0.72	0.29	-	105,105,105,105	0
55	MG	BA	3122	1/1	0.50	0.53	-	106,106,106,106	0
55	MG	DB	218	1/1	0.72	0.13	-	107,107,107,107	0
55	MG	AA	1744	1/1	0.81	0.38	-	79,79,79,79	0
55	MG	CA	1728	1/1	0.97	0.45	-	58,58,58,58	0
55	MG	BA	3221	1/1	0.98	0.39	-	59,59,59,59	0
55	MG	DA	3385	1/1	0.94	0.17	-	86,86,86,86	0
55	MG	DA	3103	1/1	0.93	0.36	-	60,60,60,60	0
55	MG	DA	3369	1/1	0.74	0.35	-	108,108,108,108	0
55	MG	CB	102	1/1	0.51	0.19	-	102,102,102,102	0
55	MG	DA	3411	1/1	0.41	0.37	-	144,144,144,144	0
55	MG	BA	3007	1/1	0.93	0.31	-	36,36,36,36	0
55	MG	DA	3192	1/1	0.45	0.17	-	90,90,90,90	0
55	MG	DA	3354	1/1	0.77	0.24	-	83,83,83,83	0
55	MG	DA	3395	1/1	0.48	0.28	-	87,87,87,87	0
55	MG	DA	3060	1/1	0.90	0.33	-	67,67,67,67	0
55	MG	DA	3128	1/1	0.91	0.30	-	47,47,47,47	0
55	MG	BA	3292	1/1	0.95	0.27	-	63,63,63,63	0
55	MG	DA	3065	1/1	0.96	0.38	-	75,75,75,75	0
55	MG	AA	1703	1/1	0.33	0.31	-	106,106,106,106	0
55	MG	BA	3404	1/1	0.63	0.35	-	100,100,100,100	0
55	MG	AA	1624	1/1	0.80	0.21	-	94,94,94,94	0
55	MG	AA	1794	1/1	0.84	0.49	-	112,112,112,112	0
55	MG	DA	3392	1/1	0.77	0.22	-	126,126,126,126	0
55	MG	BA	3281	1/1	0.58	0.28	-	78,78,78,78	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	216	1/1	0.90	0.41	-	63,63,63,63	0
55	MG	DA	3239	1/1	0.89	0.33	-	92,92,92,92	0
55	MG	BA	3053	1/1	0.82	0.10	-	106,106,106,106	0
55	MG	AA	1792	1/1	0.80	0.29	-	97,97,97,97	0
55	MG	DA	3285	1/1	0.89	0.37	-	79,79,79,79	0
55	MG	CA	1772	1/1	0.95	0.17	-	107,107,107,107	0
55	MG	BA	3372	1/1	0.71	0.46	-	76,76,76,76	0
55	MG	BA	3410	1/1	0.80	0.23	-	84,84,84,84	0
55	MG	DA	3032	1/1	0.95	0.29	-	77,77,77,77	0
55	MG	BA	3396	1/1	0.58	0.55	-	87,87,87,87	0
55	MG	BA	3411	1/1	0.64	0.30	-	102,102,102,102	0
55	MG	CA	1754	1/1	0.91	0.37	-	92,92,92,92	0
55	MG	DA	3230	1/1	0.91	0.32	-	74,74,74,74	0
55	MG	CA	1708	1/1	0.70	0.18	-	124,124,124,124	0
55	MG	CA	1701	1/1	0.55	1.26	-	108,108,108,108	0
55	MG	BA	3105	1/1	0.92	0.18	-	71,71,71,71	0
55	MG	BA	3487	1/1	0.78	0.49	-	100,100,100,100	0
55	MG	BA	3390	1/1	0.88	0.38	-	98,98,98,98	0
55	MG	BA	3294	1/1	0.79	0.34	-	61,61,61,61	0
55	MG	DA	3348	1/1	0.94	0.19	-	56,56,56,56	0
55	MG	BA	3557	1/1	0.58	0.33	-	94,94,94,94	0
55	MG	AR	101	1/1	0.63	0.19	-	114,114,114,114	0
55	MG	BA	3263	1/1	0.73	0.45	-	80,80,80,80	0
55	MG	BA	3329	1/1	0.87	0.63	-	67,67,67,67	0
55	MG	BA	3385	1/1	0.76	0.18	-	86,86,86,86	0
55	MG	BA	3156	1/1	0.95	0.35	-	61,61,61,61	0
55	MG	DA	3338	1/1	0.87	0.33	-	69,69,69,69	0
55	MG	BA	3383	1/1	0.76	0.18	-	94,94,94,94	0
55	MG	BA	3363	1/1	0.96	0.37	-	57,57,57,57	0
55	MG	DA	3367	1/1	0.89	0.32	-	82,82,82,82	0
55	MG	BA	3102	1/1	0.84	0.26	-	68,68,68,68	0
55	MG	BA	3298	1/1	0.93	0.39	-	66,66,66,66	0
55	MG	DA	3139	1/1	0.82	0.28	-	53,53,53,53	0
55	MG	BA	3426	1/1	0.71	0.47	-	86,86,86,86	0
55	MG	AA	1816	1/1	0.75	0.25	-	95,95,95,95	0
55	MG	DA	3064	1/1	0.91	0.32	-	70,70,70,70	0
55	MG	BW	101	1/1	0.97	0.21	-	64,64,64,64	0
55	MG	AA	1772	1/1	0.79	0.58	-	131,131,131,131	0
55	MG	DA	3154	1/1	0.96	0.22	-	77,77,77,77	0
55	MG	CC	106	1/1	0.71	0.35	-	94,94,94,94	0
55	MG	CA	1736	1/1	0.80	1.03	-	143,143,143,143	0
55	MG	BA	3351	1/1	0.89	0.25	-	88,88,88,88	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	3556	1/1	0.88	0.23	-	98,98,98,98	0
55	MG	AA	1665	1/1	0.96	0.17	-	52,52,52,52	0
55	MG	BA	3500	1/1	0.93	0.49	-	64,64,64,64	0
55	MG	B3	102	1/1	0.63	0.35	-	107,107,107,107	0
55	MG	BA	3420	1/1	-0.24	0.26	-	114,114,114,114	0
55	MG	DA	3465	1/1	0.90	0.20	-	112,112,112,112	0
55	MG	BA	3217	1/1	0.82	0.34	-	40,40,40,40	0
55	MG	DA	3145	1/1	0.94	0.29	-	54,54,54,54	0
55	MG	BA	3417	1/1	0.91	0.58	-	86,86,86,86	0
55	MG	BA	3489	1/1	0.81	0.41	-	95,95,95,95	0
55	MG	CA	1681	1/1	0.92	0.35	-	89,89,89,89	0
55	MG	BA	3256	1/1	0.84	0.44	-	80,80,80,80	0
55	MG	CA	1685	1/1	0.87	0.36	-	91,91,91,91	0
55	MG	CA	1808	1/1	-0.23	0.55	-	153,153,153,153	0
55	MG	BA	3535	1/1	0.87	0.32	-	82,82,82,82	0
55	MG	DA	3180	1/1	0.96	0.25	-	48,48,48,48	0
55	MG	BA	3275	1/1	0.76	0.35	-	60,60,60,60	0
55	MG	CA	1785	1/1	0.87	0.40	-	155,155,155,155	0
55	MG	BA	3170	1/1	0.95	0.30	-	54,54,54,54	0
55	MG	AA	1762	1/1	0.67	0.18	-	121,121,121,121	0
55	MG	BA	3550	1/1	0.41	1.21	-	131,131,131,131	0
55	MG	DA	3472	1/1	0.97	0.24	-	53,53,53,53	0
55	MG	DA	3454	1/1	0.99	0.35	-	52,52,52,52	0
55	MG	DA	3237	1/1	0.95	0.26	-	79,79,79,79	0
55	MG	DA	3319	1/1	0.70	0.21	-	95,95,95,95	0
55	MG	DA	3420	1/1	0.75	0.14	-	108,108,108,108	0
55	MG	DA	3484	1/1	0.63	0.22	-	84,84,84,84	0
55	MG	BA	3022	1/1	0.95	0.31	-	46,46,46,46	0
55	MG	BA	3098	1/1	0.88	0.38	-	88,88,88,88	0
55	MG	BA	3357	1/1	0.85	0.41	-	78,78,78,78	0
55	MG	DA	3046	1/1	0.95	0.10	-	100,100,100,100	0
55	MG	CA	1752	1/1	0.97	0.44	-	80,80,80,80	0
55	MG	DA	3083	1/1	0.94	0.10	-	65,65,65,65	0
55	MG	CA	1773	1/1	0.19	0.62	-	139,139,139,139	0
55	MG	DA	3117	1/1	0.90	0.25	-	61,61,61,61	0
55	MG	AA	1668	1/1	0.92	0.43	-	68,68,68,68	0
55	MG	DA	3175	1/1	0.95	0.38	-	60,60,60,60	0
55	MG	AA	1699	1/1	0.83	0.16	-	99,99,99,99	0
55	MG	DB	217	1/1	0.66	0.28	-	97,97,97,97	0
55	MG	AA	1733	1/1	0.77	0.31	-	101,101,101,101	0
55	MG	DA	3203	1/1	0.91	0.30	-	74,74,74,74	0
55	MG	BF	302	1/1	0.81	0.53	-	88,88,88,88	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	3412	1/1	0.67	0.38	-	89,89,89,89	0
55	MG	CA	1747	1/1	0.26	0.34	-	109,109,109,109	0
55	MG	D3	101	1/1	0.81	0.13	-	91,91,91,91	0
55	MG	DA	3078	1/1	0.96	0.35	-	76,76,76,76	0
55	MG	BA	3565	1/1	0.62	0.38	-	105,105,105,105	0
55	MG	AA	1637	1/1	0.62	0.23	-	112,112,112,112	0
55	MG	BA	3444	1/1	0.66	0.21	-	87,87,87,87	0
55	MG	BA	3148	1/1	0.94	0.13	-	56,56,56,56	0
55	MG	CA	1703	1/1	0.98	0.43	-	72,72,72,72	0
55	MG	BA	3029	1/1	0.93	0.22	-	57,57,57,57	0
55	MG	DA	3205	1/1	0.82	0.26	-	110,110,110,110	0
55	MG	BA	3176	1/1	0.69	0.27	-	78,78,78,78	0
55	MG	BD	301	1/1	0.59	0.21	-	80,80,80,80	0
55	MG	DA	3034	1/1	0.93	0.28	-	76,76,76,76	0
55	MG	CA	1699	1/1	0.79	0.33	-	87,87,87,87	0
55	MG	DA	3039	1/1	0.51	0.23	-	101,101,101,101	0
55	MG	DA	3359	1/1	0.54	0.14	-	111,111,111,111	0
55	MG	BA	3365	1/1	0.73	0.22	-	81,81,81,81	0
55	MG	AA	1640	1/1	0.86	0.34	-	71,71,71,71	0
55	MG	DA	3153	1/1	0.76	0.09	-	88,88,88,88	0
55	MG	DA	3448	1/1	0.71	0.19	-	129,129,129,129	0
55	MG	CA	1758	1/1	0.93	0.24	-	107,107,107,107	0
55	MG	AA	1693	1/1	0.84	0.31	-	72,72,72,72	0
55	MG	BA	3077	1/1	0.95	0.27	-	83,83,83,83	0
55	MG	AA	1810	1/1	0.26	0.28	-	148,148,148,148	0
55	MG	BA	3532	1/1	0.94	0.40	-	54,54,54,54	0
55	MG	CA	1690	1/1	0.89	0.16	-	90,90,90,90	0
55	MG	BA	3162	1/1	0.80	0.28	-	67,67,67,67	0
55	MG	BA	3511	1/1	0.87	0.14	-	83,83,83,83	0
55	MG	AA	1609	1/1	0.90	0.39	-	88,88,88,88	0
55	MG	DA	3104	1/1	0.86	0.34	-	62,62,62,62	0
55	MG	BA	3198	1/1	0.84	0.18	-	74,74,74,74	0
55	MG	BA	3453	1/1	0.55	0.20	-	75,75,75,75	0
55	MG	BA	3155	1/1	0.65	0.98	-	114,114,114,114	0
55	MG	DA	3151	1/1	0.94	0.33	-	78,78,78,78	0
55	MG	DA	3214	1/1	0.91	0.30	-	76,76,76,76	0
55	MG	DA	3253	1/1	0.95	0.28	-	77,77,77,77	0
55	MG	BA	3327	1/1	0.96	0.30	-	69,69,69,69	0
55	MG	DA	3004	1/1	0.98	0.23	-	39,39,39,39	0
55	MG	BA	3243	1/1	0.68	0.26	-	79,79,79,79	0
55	MG	DB	205	1/1	0.87	0.33	-	73,73,73,73	0
55	MG	BA	3483	1/1	0.60	0.35	-	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	AA	1779	1/1	0.05	0.26	-	119,119,119,119	0
55	MG	DA	3475	1/1	0.89	0.27	-	62,62,62,62	0
55	MG	DA	3003	1/1	0.96	0.24	-	58,58,58,58	0
55	MG	DA	3051	1/1	0.83	0.13	-	87,87,87,87	0
55	MG	DA	3087	1/1	0.89	0.26	-	85,85,85,85	0
55	MG	CA	1746	1/1	0.77	0.20	-	87,87,87,87	0
55	MG	DA	3333	1/1	0.85	0.30	-	95,95,95,95	0
55	MG	AA	1801	1/1	0.64	0.19	-	130,130,130,130	0
55	MG	DA	3255	1/1	0.69	0.15	-	82,82,82,82	0
55	MG	DB	210	1/1	0.33	0.80	-	128,128,128,128	0
55	MG	AA	1679	1/1	0.93	0.42	-	83,83,83,83	0
55	MG	DA	3218	1/1	0.52	0.27	-	86,86,86,86	0
55	MG	CA	1649	1/1	0.87	0.42	-	77,77,77,77	0
55	MG	BA	3220	1/1	0.88	0.28	-	70,70,70,70	0
55	MG	DA	3249	1/1	0.95	0.07	-	81,81,81,81	0
55	MG	AB	104	1/1	0.80	0.43	-	97,97,97,97	0
55	MG	CA	1762	1/1	0.72	0.45	-	108,108,108,108	0
55	MG	CA	1635	1/1	0.92	0.29	-	72,72,72,72	0
55	MG	DA	3105	1/1	0.95	0.34	-	37,37,37,37	0
55	MG	AA	1616	1/1	0.93	0.10	-	110,110,110,110	0
55	MG	CA	1730	1/1	0.86	0.15	-	79,79,79,79	0
55	MG	CA	1765	1/1	0.90	0.22	-	115,115,115,115	0
55	MG	BA	3339	1/1	0.94	0.37	-	74,74,74,74	0
55	MG	CA	1818	1/1	0.84	0.40	-	81,81,81,81	0
55	MG	DA	3164	1/1	0.94	0.26	-	67,67,67,67	0
55	MG	CA	1796	1/1	0.60	0.18	-	146,146,146,146	0
55	MG	CA	1687	1/1	0.64	0.29	-	99,99,99,99	0
55	MG	DA	3259	1/1	0.79	0.29	-	92,92,92,92	0
55	MG	DA	3095	1/1	0.87	0.27	-	89,89,89,89	0
55	MG	DA	3308	1/1	0.59	0.30	-	99,99,99,99	0
55	MG	DA	3243	1/1	0.79	0.25	-	97,97,97,97	0
55	MG	DA	3127	1/1	0.83	0.36	-	73,73,73,73	0
55	MG	DA	3096	1/1	0.93	0.44	-	47,47,47,47	0
55	MG	AA	1813	1/1	0.82	0.36	-	85,85,85,85	0
55	MG	BA	3211	1/1	0.97	0.37	-	55,55,55,55	0
55	MG	DA	3488	1/1	0.79	0.23	-	100,100,100,100	0
55	MG	AA	1745	1/1	0.89	0.28	-	83,83,83,83	0
55	MG	DA	3339	1/1	0.86	0.43	-	104,104,104,104	0
55	MG	BA	3246	1/1	0.87	0.23	-	89,89,89,89	0
55	MG	AA	1815	1/1	0.40	0.41	-	114,114,114,114	0
55	MG	CA	1771	1/1	0.78	0.19	-	117,117,117,117	0
55	MG	BA	3543	1/1	0.60	0.39	-	101,101,101,101	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	3045	1/1	0.85	0.35	-	105,105,105,105	0
55	MG	DA	3143	1/1	0.90	0.31	-	74,74,74,74	0
55	MG	DA	3485	1/1	0.90	0.34	-	84,84,84,84	0
55	MG	BA	3373	1/1	0.40	0.48	-	92,92,92,92	0
55	MG	BB	212	1/1	0.90	0.45	-	74,74,74,74	0
55	MG	CA	1691	1/1	0.87	0.19	-	90,90,90,90	0
55	MG	AA	1809	1/1	-0.06	0.49	-	204,204,204,204	0
55	MG	CA	1646	1/1	0.78	0.25	-	88,88,88,88	0
55	MG	DA	3332	1/1	0.76	0.17	-	84,84,84,84	0
55	MG	BA	3418	1/1	0.85	0.28	-	82,82,82,82	0
55	MG	DA	3021	1/1	0.91	0.20	-	77,77,77,77	0
55	MG	BA	3037	1/1	0.57	0.34	-	105,105,105,105	0
55	MG	BA	3295	1/1	0.80	0.19	-	92,92,92,92	0
55	MG	DA	3001	1/1	0.96	0.30	-	46,46,46,46	0
55	MG	DA	3179	1/1	0.72	0.33	-	88,88,88,88	0
55	MG	AA	1778	1/1	0.80	0.10	-	143,143,143,143	0
55	MG	AA	1635	1/1	0.78	0.18	-	81,81,81,81	0
55	MG	BA	3456	1/1	-0.34	0.48	-	168,168,168,168	0
55	MG	DA	3227	1/1	0.13	2.16	-	118,118,118,118	0
55	MG	BA	3142	1/1	0.98	0.13	-	49,49,49,49	0
55	MG	BA	3058	1/1	0.67	0.30	-	88,88,88,88	0
55	MG	CA	1766	1/1	0.90	0.17	-	114,114,114,114	0
55	MG	DB	219	1/1	0.74	0.12	-	94,94,94,94	0
55	MG	CA	1731	1/1	0.96	0.36	-	97,97,97,97	0
55	MG	BB	213	1/1	0.92	0.24	-	101,101,101,101	0
55	MG	CA	1795	1/1	0.94	0.41	-	73,73,73,73	0
55	MG	CA	1740	1/1	0.31	0.56	-	122,122,122,122	0
55	MG	DA	3215	1/1	0.84	0.31	-	83,83,83,83	0
55	MG	BA	3137	1/1	0.60	0.44	-	88,88,88,88	0
55	MG	DA	3136	1/1	0.98	0.39	-	73,73,73,73	0
55	MG	AA	1799	1/1	0.73	0.21	-	101,101,101,101	0
55	MG	BA	3111	1/1	0.94	0.21	-	55,55,55,55	0
55	MG	AA	1641	1/1	0.96	0.31	-	56,56,56,56	0
55	MG	BA	3440	1/1	0.63	0.56	-	96,96,96,96	0
55	MG	BA	3108	1/1	0.94	0.38	-	58,58,58,58	0
55	MG	BB	211	1/1	0.77	0.22	-	109,109,109,109	0
55	MG	BA	3152	1/1	0.98	0.42	-	58,58,58,58	0
55	MG	B3	103	1/1	0.70	0.32	-	83,83,83,83	0
55	MG	AA	1621	1/1	0.41	0.28	-	102,102,102,102	0
55	MG	BE	302	1/1	0.99	0.42	-	40,40,40,40	0
55	MG	D5	102	1/1	0.65	0.24	-	104,104,104,104	0
55	MG	BA	3305	1/1	0.93	0.50	-	94,94,94,94	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	209	1/1	0.47	0.33	-	130,130,130,130	0
55	MG	BA	3136	1/1	0.95	0.15	-	53,53,53,53	0
55	MG	AA	1780	1/1	0.56	0.23	-	103,103,103,103	0
55	MG	AA	1673	1/1	0.82	0.31	-	75,75,75,75	0
55	MG	BA	3477	1/1	0.74	0.57	-	77,77,77,77	0
55	MG	DA	3244	1/1	0.92	0.38	-	80,80,80,80	0
55	MG	AA	1729	1/1	0.65	0.29	-	84,84,84,84	0
55	MG	BB	205	1/1	0.93	0.29	-	71,71,71,71	0
55	MG	DA	3399	1/1	0.72	0.59	-	117,117,117,117	0
55	MG	BA	3343	1/1	0.35	0.32	-	114,114,114,114	0
55	MG	DA	3208	1/1	0.76	0.29	-	91,91,91,91	0
55	MG	DA	3135	1/1	0.78	0.17	-	87,87,87,87	0
55	MG	AA	1734	1/1	0.91	0.44	-	93,93,93,93	0
55	MG	BA	3138	1/1	0.81	0.46	-	86,86,86,86	0
55	MG	DA	3271	1/1	0.82	0.20	-	71,71,71,71	0
55	MG	BA	3364	1/1	0.80	0.32	-	72,72,72,72	0
55	MG	DA	3414	1/1	0.64	0.30	-	111,111,111,111	0
55	MG	DA	3425	1/1	0.69	0.42	-	88,88,88,88	0
55	MG	CC	102	1/1	0.91	0.31	-	85,85,85,85	0
55	MG	DA	3409	1/1	0.65	0.51	-	124,124,124,124	0
55	MG	DA	3479	1/1	0.61	0.17	-	97,97,97,97	0
55	MG	BA	3310	1/1	0.85	0.29	-	76,76,76,76	0
55	MG	DA	3317	1/1	0.90	0.32	-	58,58,58,58	0
55	MG	AA	1623	1/1	0.81	0.34	-	63,63,63,63	0
55	MG	BA	3393	1/1	-0.01	0.34	-	118,118,118,118	0
55	MG	BA	3242	1/1	0.79	0.26	-	116,116,116,116	0
55	MG	DA	3277	1/1	0.74	0.16	-	78,78,78,78	0
55	MG	BA	3233	1/1	0.81	0.36	-	66,66,66,66	0
55	MG	CA	1608	1/1	0.96	0.23	-	74,74,74,74	0
55	MG	B7	101	1/1	0.76	0.32	-	72,72,72,72	0
55	MG	BA	3554	1/1	0.89	0.27	-	48,48,48,48	0
55	MG	DA	3418	1/1	0.83	0.17	-	85,85,85,85	0
55	MG	CA	1679	1/1	0.95	0.23	-	80,80,80,80	0
55	MG	DA	3216	1/1	0.91	0.33	-	90,90,90,90	0
55	MG	BA	3191	1/1	0.81	0.39	-	89,89,89,89	0
55	MG	DA	3447	1/1	0.92	0.27	-	92,92,92,92	0
55	MG	DA	3388	1/1	0.26	0.21	-	138,138,138,138	0
55	MG	CA	1671	1/1	0.64	0.21	-	100,100,100,100	0
55	MG	BA	3312	1/1	-	-	-	62,62,62,62	1
55	MG	CA	1788	1/1	0.69	0.24	-	132,132,132,132	0
55	MG	DA	3355	1/1	0.88	0.38	-	83,83,83,83	0
55	MG	AA	1727	1/1	0.67	0.22	-	95,95,95,95	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	1661	1/1	0.88	0.23	-	92,92,92,92	0
55	MG	CB	101	1/1	0.72	0.18	-	106,106,106,106	0
55	MG	BA	3078	1/1	0.28	0.52	-	101,101,101,101	0
55	MG	BA	3379	1/1	0.80	0.45	-	78,78,78,78	0
55	MG	CA	1810	1/1	0.65	0.27	-	101,101,101,101	0
55	MG	DA	3209	1/1	0.77	0.35	-	96,96,96,96	0
55	MG	AA	1649	1/1	0.80	0.21	-	95,95,95,95	0
55	MG	BA	3107	1/1	0.82	0.19	-	81,81,81,81	0
55	MG	DA	3252	1/1	0.73	0.17	-	99,99,99,99	0
55	MG	BA	3274	1/1	0.65	0.47	-	108,108,108,108	0
55	MG	DA	3288	1/1	0.92	0.09	-	101,101,101,101	0
55	MG	BA	3354	1/1	0.96	0.43	-	73,73,73,73	0
55	MG	CA	1719	1/1	0.91	0.26	-	91,91,91,91	0
55	MG	BA	3205	1/1	0.90	0.18	-	59,59,59,59	0
55	MG	DA	3380	1/1	0.82	0.19	-	80,80,80,80	0
55	MG	BA	3501	1/1	0.71	0.35	-	86,86,86,86	0
55	MG	BA	3259	1/1	0.75	0.24	-	109,109,109,109	0
55	MG	AA	1812	1/1	0.97	0.46	-	69,69,69,69	0
55	MG	DA	3415	1/1	0.85	0.34	-	85,85,85,85	0
55	MG	DA	3427	1/1	0.99	0.29	-	56,56,56,56	0
55	MG	CA	1800	1/1	0.84	0.28	-	99,99,99,99	0
55	MG	AB	101	1/1	0.88	0.18	-	92,92,92,92	0
55	MG	DB	207	1/1	0.89	0.33	-	69,69,69,69	0
55	MG	DA	3210	1/1	0.74	0.38	-	77,77,77,77	0
55	MG	DA	3150	1/1	0.86	0.49	-	77,77,77,77	0
55	MG	BA	3126	1/1	0.88	0.63	-	95,95,95,95	0
55	MG	BA	3545	1/1	0.82	0.23	-	82,82,82,82	0
55	MG	BA	3282	1/1	0.89	0.44	-	103,103,103,103	0
55	MG	BA	3432	1/1	0.75	0.24	-	106,106,106,106	0
55	MG	BA	3567	1/1	0.88	0.21	-	99,99,99,99	0
55	MG	DA	3268	1/1	0.89	0.26	-	77,77,77,77	0
55	MG	BA	3302	1/1	0.85	0.23	-	83,83,83,83	0
55	MG	DA	3140	1/1	0.81	0.30	-	76,76,76,76	0
55	MG	DA	3404	1/1	0.74	0.26	-	119,119,119,119	0
55	MG	B5	101	1/1	0.81	0.18	-	49,49,49,49	0
55	MG	BA	3429	1/1	0.24	0.55	-	146,146,146,146	0
55	MG	DA	3446	1/1	0.60	0.43	-	166,166,166,166	0
55	MG	BA	3015	1/1	0.97	0.39	-	35,35,35,35	0
55	MG	BA	3387	1/1	0.96	0.10	-	88,88,88,88	0
55	MG	DA	3352	1/1	0.86	0.27	-	122,122,122,122	0
55	MG	BA	3032	1/1	0.98	0.31	-	41,41,41,41	0
55	MG	BA	3403	1/1	0.90	0.39	-	71,71,71,71	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	3455	1/1	0.69	0.78	-	89,89,89,89	0
55	MG	BA	3512	1/1	0.79	0.32	-	90,90,90,90	0
55	MG	BA	3265	1/1	0.85	0.14	-	89,89,89,89	0
55	MG	CA	1815	1/1	0.65	0.20	-	95,95,95,95	0
55	MG	BA	3120	1/1	0.97	0.37	-	42,42,42,42	0
55	MG	DA	3281	1/1	0.62	0.23	-	90,90,90,90	0
55	MG	DA	3048	1/1	0.93	0.36	-	76,76,76,76	0
55	MG	BA	3276	1/1	0.84	0.22	-	92,92,92,92	0
55	MG	DA	3138	1/1	0.91	0.35	-	54,54,54,54	0
55	MG	CA	1672	1/1	0.53	0.17	-	119,119,119,119	0
55	MG	BA	3562	1/1	0.91	0.42	-	91,91,91,91	0
55	MG	BA	3408	1/1	0.90	0.14	-	82,82,82,82	0
55	MG	BA	3419	1/1	0.85	0.49	-	80,80,80,80	0
55	MG	BA	3247	1/1	0.84	0.32	-	97,97,97,97	0
55	MG	BA	3422	1/1	0.26	0.70	-	110,110,110,110	0
55	MG	AA	1770	1/1	0.75	0.25	-	80,80,80,80	0
55	MG	BA	3267	1/1	0.81	0.36	-	62,62,62,62	0
55	MG	BA	3333	1/1	0.67	0.52	-	80,80,80,80	0
55	MG	CA	1779	1/1	0.85	0.27	-	109,109,109,109	0
55	MG	CA	1694	1/1	0.73	0.16	-	80,80,80,80	0
55	MG	DD	302	1/1	0.83	0.27	-	82,82,82,82	0
55	MG	DA	3166	1/1	0.81	0.25	-	90,90,90,90	0
55	MG	CA	1702	1/1	0.06	0.29	-	106,106,106,106	0
55	MG	DA	3299	1/1	0.63	0.19	-	84,84,84,84	0
55	MG	CA	1673	1/1	-0.10	0.64	-	136,136,136,136	0
55	MG	DA	3394	1/1	0.88	0.29	-	101,101,101,101	0
55	MG	AA	1747	1/1	0.76	0.20	-	98,98,98,98	0
55	MG	DB	214	1/1	0.91	0.10	-	95,95,95,95	0
55	MG	BA	3213	1/1	0.96	0.41	-	41,41,41,41	0
55	MG	CA	1799	1/1	0.72	0.18	-	81,81,81,81	0
55	MG	AC	106	1/1	0.80	0.39	-	102,102,102,102	0
55	MG	DA	3102	1/1	0.90	0.35	-	72,72,72,72	0
55	MG	CA	1732	1/1	0.89	0.36	-	105,105,105,105	0
55	MG	AA	1633	1/1	0.81	0.39	-	102,102,102,102	0
55	MG	CA	1662	1/1	0.90	0.42	-	84,84,84,84	0
55	MG	BA	3301	1/1	0.66	0.26	-	84,84,84,84	0
55	MG	AS	101	1/1	0.86	0.23	-	96,96,96,96	0
55	MG	DA	3305	1/1	0.84	0.15	-	93,93,93,93	0
55	MG	CA	1760	1/1	0.84	0.24	-	105,105,105,105	0
55	MG	DA	3141	1/1	0.90	0.29	-	101,101,101,101	0
55	MG	BA	3424	1/1	0.80	0.47	-	84,84,84,84	0
55	MG	BA	3552	1/1	0.98	0.38	-	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	AA	1761	1/1	0.89	0.32	-	77,77,77,77	0
55	MG	BA	3165	1/1	0.96	0.32	-	60,60,60,60	0
55	MG	CA	1707	1/1	0.68	0.31	-	109,109,109,109	0
55	MG	DA	3167	1/1	0.46	0.17	-	95,95,95,95	0
55	MG	DA	3148	1/1	0.92	0.14	-	111,111,111,111	0
55	MG	BA	3451	1/1	0.28	0.50	-	101,101,101,101	0
55	MG	CA	1805	1/1	0.52	0.18	-	102,102,102,102	0
55	MG	BA	3434	1/1	0.89	0.39	-	69,69,69,69	0
55	MG	CA	1750	1/1	0.81	0.26	-	86,86,86,86	0
55	MG	DA	3468	1/1	0.77	0.15	-	101,101,101,101	0
55	MG	CA	1659	1/1	0.94	0.41	-	75,75,75,75	0
55	MG	DA	3052	1/1	0.90	0.16	-	78,78,78,78	0
55	MG	DA	3142	1/1	0.77	0.37	-	81,81,81,81	0
55	MG	BA	3458	1/1	0.90	0.32	-	91,91,91,91	0
55	MG	CA	1684	1/1	0.74	0.26	-	101,101,101,101	0
55	MG	BA	3374	1/1	0.79	0.26	-	93,93,93,93	0
55	MG	DA	3327	1/1	0.77	0.23	-	93,93,93,93	0
55	MG	DA	3286	1/1	0.80	0.33	-	78,78,78,78	0
55	MG	BA	3433	1/1	0.60	0.42	-	99,99,99,99	0
55	MG	DA	3100	1/1	0.33	0.44	-	116,116,116,116	0
55	MG	BA	3441	1/1	0.93	0.29	-	84,84,84,84	0
55	MG	DA	3451	1/1	0.66	0.23	-	92,92,92,92	0
55	MG	BA	3159	1/1	0.96	0.36	-	57,57,57,57	0
55	MG	BA	3353	1/1	0.62	0.45	-	77,77,77,77	0
55	MG	AA	1604	1/1	0.97	0.35	-	52,52,52,52	0
55	MG	DA	3221	1/1	0.56	1.31	-	154,154,154,154	0
55	MG	DA	3274	1/1	0.51	0.25	-	85,85,85,85	0
55	MG	CA	1693	1/1	0.68	0.26	-	103,103,103,103	0
55	MG	AA	1760	1/1	0.88	0.35	-	77,77,77,77	0
55	MG	BA	3236	1/1	0.91	0.38	-	67,67,67,67	0
55	MG	DA	3188	1/1	0.25	0.26	-	113,113,113,113	0
55	MG	BA	3189	1/1	-0.07	0.67	-	108,108,108,108	0
55	MG	CA	1626	1/1	0.93	0.31	-	69,69,69,69	0
55	MG	DA	3035	1/1	0.28	0.32	-	124,124,124,124	0
55	MG	CA	1621	1/1	0.45	0.19	-	97,97,97,97	0
55	MG	DA	3219	1/1	0.71	0.26	-	128,128,128,128	0
55	MG	DA	3155	1/1	0.93	0.14	-	90,90,90,90	0
55	MG	CA	1709	1/1	0.67	0.34	-	110,110,110,110	0
55	MG	BA	3559	1/1	0.88	0.26	-	86,86,86,86	0
55	MG	DA	3449	1/1	0.94	0.27	-	66,66,66,66	0
55	MG	DA	3054	1/1	0.64	0.41	-	108,108,108,108	0
55	MG	DA	3213	1/1	0.86	0.18	-	103,103,103,103	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	3291	1/1	0.17	0.48	-	149,149,149,149	0
55	MG	DA	3092	1/1	0.67	0.17	-	87,87,87,87	0
55	MG	AA	1660	1/1	0.92	0.42	-	77,77,77,77	0
55	MG	BA	3089	1/1	0.97	0.35	-	61,61,61,61	0
55	MG	AA	1700	1/1	0.85	0.17	-	136,136,136,136	0
55	MG	AA	1691	1/1	0.75	0.27	-	88,88,88,88	0
55	MG	BA	3335	1/1	0.57	0.34	-	102,102,102,102	0
55	MG	BA	3260	1/1	0.97	0.43	-	65,65,65,65	0
55	MG	DA	3072	1/1	0.93	0.39	-	65,65,65,65	0
55	MG	AA	1769	1/1	0.92	0.18	-	95,95,95,95	0
55	MG	CK	201	1/1	0.72	1.47	-	124,124,124,124	0
55	MG	AA	1746	1/1	0.73	0.32	-	93,93,93,93	0
55	MG	CA	1726	1/1	0.85	0.10	-	73,73,73,73	0
55	MG	CA	1812	1/1	0.78	1.05	-	176,176,176,176	0
55	MG	BA	3183	1/1	0.86	0.45	-	84,84,84,84	0
55	MG	CA	1819	1/1	0.63	0.45	-	134,134,134,134	0
55	MG	DA	3416	1/1	0.83	0.49	-	77,77,77,77	0
55	MG	DA	3269	1/1	0.82	0.30	-	78,78,78,78	0
55	MG	AA	1782	1/1	0.85	0.12	-	118,118,118,118	0
55	MG	AA	1680	1/1	0.82	0.49	-	97,97,97,97	0
55	MG	DA	3342	1/1	0.57	0.93	-	122,122,122,122	0
55	MG	BA	3208	1/1	0.96	0.55	-	55,55,55,55	0
55	MG	CA	1696	1/1	0.62	0.20	-	104,104,104,104	0
55	MG	DA	3290	1/1	0.62	0.17	-	99,99,99,99	0
55	MG	DA	3077	1/1	0.89	0.38	-	72,72,72,72	0
55	MG	BA	3081	1/1	0.93	0.49	-	91,91,91,91	0
55	MG	DA	3452	1/1	0.91	0.29	-	52,52,52,52	0
55	MG	CA	1780	1/1	0.72	0.21	-	88,88,88,88	0
55	MG	CA	1751	1/1	0.82	0.24	-	90,90,90,90	0
55	MG	BO	202	1/1	0.73	0.20	-	98,98,98,98	0
55	MG	CC	105	1/1	0.57	0.13	-	94,94,94,94	0
55	MG	BA	3446	1/1	0.15	0.41	-	121,121,121,121	0
55	MG	DA	3356	1/1	0.88	0.36	-	76,76,76,76	0
55	MG	AA	1674	1/1	0.96	0.32	-	56,56,56,56	0
55	MG	BA	3431	1/1	0.88	0.18	-	66,66,66,66	0
55	MG	DA	3487	1/1	0.92	0.21	-	85,85,85,85	0
55	MG	CA	1753	1/1	0.45	0.24	-	103,103,103,103	0
55	MG	AD	102	1/1	0.52	0.23	-	125,125,125,125	0
55	MG	BA	3513	1/1	0.72	0.29	-	92,92,92,92	0
55	MG	B2	201	1/1	0.71	0.36	-	91,91,91,91	0
55	MG	BA	3467	1/1	0.55	0.25	-	69,69,69,69	0
55	MG	BA	3533	1/1	0.90	0.33	-	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	BA	3135	1/1	0.87	0.41	-	69,69,69,69	0
55	MG	AA	1667	1/1	0.82	0.56	-	78,78,78,78	0
55	MG	AA	1753	1/1	0.77	0.19	-	97,97,97,97	0
55	MG	BA	3465	1/1	0.95	0.51	-	61,61,61,61	0
55	MG	AA	1789	1/1	0.92	0.34	-	63,63,63,63	0
55	MG	DA	3337	1/1	0.91	0.28	-	86,86,86,86	0
55	MG	AA	1806	1/1	0.72	0.40	-	85,85,85,85	0
55	MG	BA	3222	1/1	0.78	0.47	-	68,68,68,68	0
55	MG	CA	1698	1/1	0.96	0.23	-	79,79,79,79	0
55	MG	CA	1614	1/1	0.94	0.29	-	79,79,79,79	0
55	MG	CA	1678	1/1	0.78	0.50	-	83,83,83,83	0
55	MG	BA	3038	1/1	0.97	0.23	-	33,33,33,33	0
55	MG	DB	216	1/1	0.69	0.16	-	100,100,100,100	0
55	MG	BA	3153	1/1	0.94	0.47	-	78,78,78,78	0
55	MG	AA	1818	1/1	0.61	0.47	-	124,124,124,124	0
55	MG	BB	208	1/1	0.66	0.42	-	117,117,117,117	0
55	MG	DA	3013	1/1	0.94	0.25	-	51,51,51,51	0
55	MG	DA	3279	1/1	-0.02	0.53	-	135,135,135,135	0
55	MG	BA	3494	1/1	0.95	0.36	-	76,76,76,76	0
55	MG	BA	3218	1/1	0.91	0.26	-	64,64,64,64	0
55	MG	BA	3345	1/1	0.92	0.26	-	46,46,46,46	0
55	MG	AA	1614	1/1	0.93	0.29	-	92,92,92,92	0
55	MG	BA	3194	1/1	0.81	0.27	-	74,74,74,74	0
55	MG	DA	3223	1/1	0.91	0.16	-	81,81,81,81	0
55	MG	AA	1650	1/1	0.89	0.30	-	80,80,80,80	0
55	MG	BA	3065	1/1	0.77	0.31	-	82,82,82,82	0
55	MG	BA	3239	1/1	0.82	0.20	-	69,69,69,69	0
55	MG	BA	3311	1/1	0.96	0.38	-	68,68,68,68	0
55	MG	CA	1817	1/1	0.56	0.44	-	106,106,106,106	0
55	MG	DA	3114	1/1	0.74	0.38	-	91,91,91,91	0
55	MG	CA	1692	1/1	0.71	0.10	-	157,157,157,157	0
55	MG	BA	3508	1/1	0.87	0.33	-	77,77,77,77	0
55	MG	BA	3115	1/1	0.97	0.44	-	41,41,41,41	0
55	MG	BA	3179	1/1	0.89	0.40	-	72,72,72,72	0
55	MG	DA	3460	1/1	0.93	0.26	-	116,116,116,116	0
55	MG	AA	1808	1/1	0.82	0.31	-	88,88,88,88	0
55	MG	CA	1654	1/1	0.85	0.25	-	78,78,78,78	0
55	MG	BA	3525	1/1	0.94	0.31	-	51,51,51,51	0
55	MG	DA	3328	1/1	0.61	0.27	-	84,84,84,84	0
55	MG	BA	3028	1/1	0.93	0.33	-	52,52,52,52	0
55	MG	BA	3350	1/1	0.88	0.48	-	92,92,92,92	0
55	MG	CA	1680	1/1	0.40	0.20	-	99,99,99,99	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	1626	1/1	0.65	0.32	-	91,91,91,91	0
55	MG	DA	3121	1/1	0.69	0.20	-	104,104,104,104	0
55	MG	CA	1774	1/1	0.84	0.22	-	75,75,75,75	0
55	MG	BA	3192	1/1	0.53	0.47	-	92,92,92,92	0
55	MG	DA	3022	1/1	0.93	0.27	-	74,74,74,74	0
55	MG	BA	3154	1/1	0.86	0.50	-	87,87,87,87	0
55	MG	AA	1631	1/1	0.65	0.24	-	84,84,84,84	0
55	MG	DA	3469	1/1	0.42	0.31	-	109,109,109,109	0
55	MG	DA	3101	1/1	0.98	0.33	-	76,76,76,76	0
55	MG	BA	3273	1/1	0.97	0.34	-	73,73,73,73	0
55	MG	D7	101	1/1	0.55	0.34	-	86,86,86,86	0
55	MG	AA	1656	1/1	0.96	0.41	-	87,87,87,87	0
55	MG	BA	3285	1/1	0.89	0.41	-	102,102,102,102	0
55	MG	DA	3231	1/1	0.74	0.27	-	101,101,101,101	0
55	MG	BA	3443	1/1	0.85	0.23	-	125,125,125,125	0
55	MG	BB	214	1/1	0.85	0.31	-	76,76,76,76	0
55	MG	DA	3480	1/1	0.77	0.20	-	109,109,109,109	0
55	MG	BA	3036	1/1	0.96	0.35	-	58,58,58,58	0
55	MG	DA	3292	1/1	0.87	0.39	-	98,98,98,98	0
55	MG	BA	3355	1/1	0.84	0.25	-	95,95,95,95	0
55	MG	BA	3491	1/1	0.99	0.35	-	41,41,41,41	0
55	MG	BA	3094	1/1	0.94	0.37	-	68,68,68,68	0
55	MG	CA	1675	1/1	0.43	0.39	-	111,111,111,111	0
55	MG	AA	1749	1/1	0.81	0.44	-	110,110,110,110	0
55	MG	DA	3377	1/1	0.78	0.28	-	87,87,87,87	0
55	MG	BA	3023	1/1	0.91	0.48	-	64,64,64,64	0
55	MG	AA	1642	1/1	0.93	0.38	-	70,70,70,70	0
55	MG	DA	3047	1/1	0.95	0.34	-	67,67,67,67	0
55	MG	BA	3003	1/1	0.97	0.34	-	50,50,50,50	0
55	MG	BA	3409	1/1	0.87	0.38	-	98,98,98,98	0
55	MG	BA	3252	1/1	0.81	0.42	-	107,107,107,107	0
55	MG	DA	3088	1/1	0.74	0.26	-	62,62,62,62	0
55	MG	DA	3177	1/1	0.76	0.12	-	129,129,129,129	0
55	MG	DA	3260	1/1	0.93	0.34	-	73,73,73,73	0
55	MG	BA	3237	1/1	0.61	0.36	-	102,102,102,102	0
55	MG	DA	3238	1/1	0.49	0.40	-	105,105,105,105	0
55	MG	DA	3361	1/1	0.92	0.10	-	89,89,89,89	0
55	MG	CA	1763	1/1	0.46	0.16	-	100,100,100,100	0
55	MG	DA	3350	1/1	0.70	0.33	-	120,120,120,120	0
55	MG	BA	3249	1/1	0.85	0.17	-	82,82,82,82	0
55	MG	BA	3370	1/1	0.92	0.26	-	78,78,78,78	0
55	MG	AA	1677	1/1	0.90	0.42	-	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	AA	1723	1/1	0.82	0.20	-	93,93,93,93	0
55	MG	CA	1611	1/1	0.83	0.35	-	82,82,82,82	0
55	MG	DA	3251	1/1	0.88	0.34	-	79,79,79,79	0
55	MG	DA	3375	1/1	0.86	0.13	-	86,86,86,86	0
55	MG	DA	3016	1/1	0.89	0.28	-	78,78,78,78	0
55	MG	CA	1802	1/1	0.93	0.24	-	73,73,73,73	0
55	MG	DA	3069	1/1	0.94	0.42	-	76,76,76,76	0
55	MG	BA	3255	1/1	0.94	0.41	-	50,50,50,50	0
55	MG	AA	1721	1/1	0.82	0.29	-	60,60,60,60	0
55	MG	DA	3358	1/1	0.76	0.45	-	90,90,90,90	0
55	MG	DA	3012	1/1	0.97	0.34	-	50,50,50,50	0
55	MG	AA	1803	1/1	0.76	0.28	-	89,89,89,89	0
55	MG	AC	105	1/1	0.51	0.36	-	102,102,102,102	0
55	MG	DA	3398	1/1	-0.01	0.34	-	101,101,101,101	0
55	MG	DA	3444	1/1	0.59	0.23	-	109,109,109,109	0
55	MG	BF	303	1/1	0.89	0.45	-	78,78,78,78	0
55	MG	AA	1630	1/1	0.80	0.34	-	112,112,112,112	0
55	MG	BA	3450	1/1	0.80	0.30	-	82,82,82,82	0
55	MG	BA	3360	1/1	0.88	0.37	-	81,81,81,81	0
55	MG	DA	3442	1/1	0.76	0.30	-	98,98,98,98	0
55	MG	BA	3509	1/1	0.58	0.46	-	97,97,97,97	0
55	MG	CA	1724	1/1	0.94	0.18	-	87,87,87,87	0
55	MG	AA	1798	1/1	0.82	0.31	-	84,84,84,84	0
55	MG	DB	211	1/1	0.55	0.22	-	111,111,111,111	0
55	MG	AA	1763	1/1	0.65	0.21	-	92,92,92,92	0
55	MG	BA	3397	1/1	0.05	0.34	-	131,131,131,131	0
55	MG	BA	3123	1/1	0.86	0.33	-	81,81,81,81	0
55	MG	DA	3393	1/1	0.25	0.20	-	116,116,116,116	0
55	MG	DA	3111	1/1	0.95	0.23	-	45,45,45,45	0
55	MG	BA	3457	1/1	0.80	0.17	-	85,85,85,85	0
55	MG	AA	1743	1/1	0.56	0.25	-	107,107,107,107	0
55	MG	DA	3391	1/1	0.12	0.35	-	102,102,102,102	0
55	MG	AA	1750	1/1	0.69	0.45	-	134,134,134,134	0
55	MG	CA	1801	1/1	0.88	0.23	-	81,81,81,81	0
55	MG	BA	3542	1/1	0.91	0.36	-	85,85,85,85	0
55	MG	BB	201	1/1	0.64	0.28	-	97,97,97,97	0
55	MG	BA	3471	1/1	0.63	0.38	-	126,126,126,126	0
55	MG	CA	1648	1/1	0.74	0.28	-	113,113,113,113	0
55	MG	BA	3019	1/1	0.95	0.31	-	45,45,45,45	0
55	MG	AA	1773	1/1	0.71	0.35	-	130,130,130,130	0
55	MG	BA	3008	1/1	0.97	0.38	-	44,44,44,44	0
55	MG	BA	3514	1/1	0.83	0.35	-	113,113,113,113	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	3403	1/1	0.85	0.32	-	107,107,107,107	0
55	MG	BA	3375	1/1	0.88	0.23	-	87,87,87,87	0
55	MG	BA	3297	1/1	0.85	0.21	-	86,86,86,86	0
55	MG	BA	3479	1/1	0.58	0.55	-	146,146,146,146	0
55	MG	AA	1676	1/1	0.92	0.35	-	89,89,89,89	0
55	MG	BA	3309	1/1	0.75	0.45	-	77,77,77,77	0
55	MG	CA	1704	1/1	0.71	0.37	-	88,88,88,88	0
55	MG	DA	3486	1/1	0.61	0.20	-	101,101,101,101	0
55	MG	CA	1757	1/1	0.66	0.28	-	95,95,95,95	0
55	MG	BA	3395	1/1	0.76	0.29	-	90,90,90,90	0
55	MG	AA	1612	1/1	0.78	0.26	-	88,88,88,88	0
55	MG	BA	3280	1/1	0.91	0.40	-	80,80,80,80	0
55	MG	DA	3256	1/1	0.77	0.19	-	91,91,91,91	0
55	MG	DA	3027	1/1	0.95	0.13	-	47,47,47,47	0
55	MG	BA	3206	1/1	0.83	0.26	-	68,68,68,68	0
55	MG	CA	1606	1/1	0.94	0.19	-	65,65,65,65	0
55	MG	BA	3201	1/1	0.89	0.41	-	64,64,64,64	0
55	MG	CB	104	1/1	-0.32	0.35	-	147,147,147,147	0
55	MG	DA	3079	1/1	0.64	0.25	-	103,103,103,103	0
55	MG	CA	1716	1/1	0.39	0.31	-	103,103,103,103	0
55	MG	DA	3217	1/1	0.90	0.15	-	125,125,125,125	0
55	MG	AA	1768	1/1	0.79	0.48	-	71,71,71,71	0
55	MG	BA	3228	1/1	0.92	0.54	-	82,82,82,82	0
55	MG	DA	3406	1/1	0.71	0.34	-	129,129,129,129	0
55	MG	AA	1724	1/1	0.27	0.20	-	78,78,78,78	0
55	MG	DA	3191	1/1	0.96	0.46	-	55,55,55,55	0
55	MG	DA	3005	1/1	0.94	0.28	-	48,48,48,48	0
55	MG	DA	3113	1/1	0.95	0.23	-	80,80,80,80	0
55	MG	BA	3516	1/1	0.82	0.37	-	88,88,88,88	0
55	MG	BA	3377	1/1	0.97	0.41	-	64,64,64,64	0
55	MG	BA	3033	1/1	0.91	0.37	-	77,77,77,77	0
55	MG	BA	3214	1/1	0.92	0.42	-	58,58,58,58	0
55	MG	DA	3440	1/1	0.89	0.09	-	81,81,81,81	0
55	MG	CA	1628	1/1	0.86	0.21	-	123,123,123,123	0
55	MG	DA	3132	1/1	0.83	0.20	-	77,77,77,77	0
55	MG	CA	1787	1/1	0.86	0.45	-	84,84,84,84	0
55	MG	AA	1800	1/1	0.78	0.43	-	131,131,131,131	0
55	MG	CA	1798	1/1	0.79	0.39	-	74,74,74,74	0
55	MG	BA	3141	1/1	0.91	0.29	-	78,78,78,78	0
55	MG	DA	3423	1/1	0.66	0.87	-	118,118,118,118	0
55	MG	CA	1778	1/1	0.64	0.24	-	133,133,133,133	0
55	MG	AA	1696	1/1	0.60	0.39	-	112,112,112,112	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	3322	1/1	0.77	0.32	-	99,99,99,99	0
55	MG	BA	3106	1/1	0.78	0.22	-	89,89,89,89	0
55	MG	AA	1690	1/1	0.75	0.18	-	98,98,98,98	0
55	MG	DA	3082	1/1	0.51	0.21	-	91,91,91,91	0
55	MG	BA	3041	1/1	0.57	0.48	-	80,80,80,80	0
55	MG	DA	3086	1/1	0.87	0.47	-	75,75,75,75	0
55	MG	DA	3130	1/1	0.98	0.24	-	49,49,49,49	0
55	MG	BA	3400	1/1	0.83	0.53	-	108,108,108,108	0
55	MG	BA	3113	1/1	0.91	0.31	-	47,47,47,47	0
55	MG	DA	3477	1/1	0.75	0.34	-	88,88,88,88	0
55	MG	BA	3278	1/1	0.88	0.69	-	92,92,92,92	0
55	MG	CG	301	1/1	0.80	0.40	-	107,107,107,107	0
55	MG	CA	1682	1/1	0.67	0.13	-	100,100,100,100	0
55	MG	AA	1717	1/1	0.86	0.42	-	73,73,73,73	0
55	MG	BA	3452	1/1	0.58	0.35	-	103,103,103,103	0
55	MG	DA	3441	1/1	0.77	0.17	-	89,89,89,89	0
55	MG	CA	1677	1/1	0.81	0.19	-	107,107,107,107	0
55	MG	BA	3225	1/1	0.89	0.37	-	68,68,68,68	0
55	MG	BA	3336	1/1	0.87	0.20	-	78,78,78,78	0
55	MG	AA	1732	1/1	0.88	0.32	-	95,95,95,95	0
55	MG	BA	3384	1/1	0.95	0.65	-	85,85,85,85	0
55	MG	BA	3177	1/1	0.88	0.22	-	34,34,34,34	0
55	MG	AB	102	1/1	0.46	0.29	-	96,96,96,96	0
55	MG	DA	3041	1/1	0.97	0.41	-	47,47,47,47	0
55	MG	DA	3099	1/1	0.77	0.51	-	83,83,83,83	0
55	MG	DA	3340	1/1	0.84	0.27	-	75,75,75,75	0
55	MG	AA	1765	1/1	0.60	0.28	-	149,149,149,149	0
55	MG	BA	3547	1/1	0.74	0.29	-	77,77,77,77	0
55	MG	CA	1711	1/1	0.79	0.18	-	101,101,101,101	0
55	MG	AA	1670	1/1	0.95	0.38	-	75,75,75,75	0
55	MG	BA	3381	1/1	0.83	0.52	-	87,87,87,87	0
55	MG	BA	3394	1/1	0.85	0.43	-	80,80,80,80	0
55	MG	DA	3320	1/1	0.73	0.29	-	87,87,87,87	0
55	MG	DA	3413	1/1	0.71	0.37	-	86,86,86,86	0
55	MG	DA	3172	1/1	0.44	0.42	-	122,122,122,122	0
55	MG	DA	3360	1/1	0.59	0.15	-	97,97,97,97	0
55	MG	AA	1603	1/1	0.94	0.25	-	65,65,65,65	0
55	MG	BA	3254	1/1	0.81	0.44	-	89,89,89,89	0
55	MG	DA	3178	1/1	0.89	0.25	-	88,88,88,88	0
55	MG	DA	3316	1/1	0.74	0.17	-	102,102,102,102	0
55	MG	BA	3566	1/1	0.60	0.33	-	83,83,83,83	0
55	MG	DA	3264	1/1	0.88	0.40	-	88,88,88,88	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	3235	1/1	0.94	0.38	-	39,39,39,39	0
55	MG	BB	206	1/1	0.87	0.19	-	79,79,79,79	0
55	MG	BA	3216	1/1	0.89	0.26	-	53,53,53,53	0
55	MG	DA	3461	1/1	0.75	0.24	-	97,97,97,97	0
55	MG	AA	1705	1/1	0.93	0.31	-	81,81,81,81	0
55	MG	DA	3459	1/1	0.65	0.28	-	76,76,76,76	0
55	MG	BA	3537	1/1	0.60	0.47	-	73,73,73,73	0
55	MG	DA	3085	1/1	0.78	0.44	-	81,81,81,81	0
55	MG	DA	3038	1/1	0.84	0.21	-	73,73,73,73	0
55	MG	DA	3007	1/1	0.95	0.24	-	55,55,55,55	0
55	MG	BA	3391	1/1	0.13	0.52	-	112,112,112,112	0
55	MG	AA	1774	1/1	0.91	0.52	-	69,69,69,69	0
55	MG	BA	3199	1/1	0.87	0.27	-	65,65,65,65	0
55	MG	BA	3323	1/1	0.74	0.59	-	73,73,73,73	0
55	MG	BA	3279	1/1	0.72	0.40	-	75,75,75,75	0
55	MG	AA	1787	1/1	0.90	0.33	-	101,101,101,101	0
55	MG	BA	3061	1/1	0.91	0.33	-	73,73,73,73	0
55	MG	CA	1668	1/1	0.88	0.42	-	72,72,72,72	0
55	MG	AA	1629	1/1	0.83	0.12	-	95,95,95,95	0
55	MG	DA	3386	1/1	0.72	0.23	-	130,130,130,130	0
55	MG	BA	3082	1/1	0.51	0.36	-	100,100,100,100	0
55	MG	DA	3152	1/1	0.94	0.28	-	63,63,63,63	0
55	MG	DA	3378	1/1	0.77	0.28	-	88,88,88,88	0
55	MG	DA	3309	1/1	0.81	0.46	-	116,116,116,116	0
55	MG	BA	3399	1/1	0.64	0.32	-	99,99,99,99	0
55	MG	DA	3146	1/1	0.84	0.10	-	89,89,89,89	0
55	MG	BA	3195	1/1	0.13	0.64	-	97,97,97,97	0
55	MG	DA	3195	1/1	0.93	0.28	-	82,82,82,82	0
55	MG	AA	1757	1/1	0.49	0.40	-	101,101,101,101	0
55	MG	BA	3321	1/1	0.90	0.46	-	88,88,88,88	0
55	MG	D5	101	1/1	0.95	0.27	-	58,58,58,58	0
55	MG	BA	3043	1/1	0.95	0.39	-	78,78,78,78	0
55	MG	DA	3091	1/1	0.82	0.15	-	74,74,74,74	0
55	MG	BA	3158	1/1	0.95	0.40	-	66,66,66,66	0
55	MG	AA	1741	1/1	0.60	0.22	-	98,98,98,98	0
55	MG	CA	1761	1/1	0.25	0.55	-	143,143,143,143	0
55	MG	BA	3342	1/1	0.87	0.24	-	66,66,66,66	0
55	MG	BA	3200	1/1	0.84	0.24	-	81,81,81,81	0
55	MG	BA	3464	1/1	0.81	0.15	-	91,91,91,91	0
55	MG	BB	218	1/1	0.87	0.21	-	98,98,98,98	0
55	MG	BA	3551	1/1	0.97	0.30	-	64,64,64,64	0
55	MG	AA	1738	1/1	0.58	0.26	-	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	CA	1792	1/1	0.38	0.18	-	104,104,104,104	0
55	MG	AA	1653	1/1	0.74	0.30	-	95,95,95,95	0
55	MG	DA	3396	1/1	0.87	0.28	-	76,76,76,76	0
55	MG	AA	1764	1/1	-0.01	0.33	-	146,146,146,146	0
55	MG	AA	1644	1/1	0.87	0.35	-	94,94,94,94	0
55	MG	DA	3429	1/1	0.93	0.31	-	54,54,54,54	0
55	MG	BA	3449	1/1	0.83	0.39	-	100,100,100,100	0
55	MG	BA	3473	1/1	0.73	0.29	-	92,92,92,92	0
55	MG	BA	3359	1/1	0.84	0.49	-	78,78,78,78	0
55	MG	CA	1610	1/1	0.31	0.24	-	118,118,118,118	0
55	MG	DA	3419	1/1	0.83	0.22	-	87,87,87,87	0
55	MG	DA	3325	1/1	0.77	0.17	-	97,97,97,97	0
55	MG	AA	1775	1/1	0.74	0.45	-	129,129,129,129	0
55	MG	DA	3225	1/1	0.76	0.45	-	102,102,102,102	0
55	MG	CB	103	1/1	0.48	1.49	-	147,147,147,147	0
55	MG	BA	3091	1/1	0.83	0.43	-	73,73,73,73	0
55	MG	DA	3283	1/1	0.73	0.25	-	88,88,88,88	0
55	MG	CA	1790	1/1	0.70	0.51	-	142,142,142,142	0
55	MG	BA	3341	1/1	0.86	0.42	-	89,89,89,89	0
55	MG	CA	1710	1/1	0.53	0.17	-	118,118,118,118	0
55	MG	DA	3455	1/1	0.97	0.13	-	44,44,44,44	0
55	MG	AA	1776	1/1	0.96	0.31	-	67,67,67,67	0
55	MG	BA	3253	1/1	0.81	0.47	-	92,92,92,92	0
55	MG	BA	3376	1/1	0.67	0.27	-	83,83,83,83	0
55	MG	DA	3211	1/1	0.86	0.35	-	79,79,79,79	0
55	MG	CA	1770	1/1	0.90	0.38	-	82,82,82,82	0
55	MG	CA	1741	1/1	0.93	0.21	-	85,85,85,85	0
55	MG	A1	101	1/1	0.35	0.20	-	102,102,102,102	0
55	MG	BA	3536	1/1	0.89	0.12	-	37,37,37,37	0
55	MG	AA	1704	1/1	0.77	0.24	-	110,110,110,110	0
55	MG	DA	3040	1/1	0.74	0.23	-	118,118,118,118	0
55	MG	DA	3336	1/1	0.15	0.60	-	115,115,115,115	0
55	MG	DA	3402	1/1	0.50	0.20	-	124,124,124,124	0
55	MG	DA	3266	1/1	0.93	0.44	-	82,82,82,82	0
55	MG	BA	3085	1/1	0.98	0.42	-	38,38,38,38	0
55	MG	DA	3201	1/1	0.88	0.32	-	76,76,76,76	0
55	MG	AA	1695	1/1	0.75	0.20	-	128,128,128,128	0
55	MG	DA	3315	1/1	0.79	0.14	-	91,91,91,91	0
55	MG	CA	1629	1/1	0.89	0.21	-	115,115,115,115	0
55	MG	CA	1721	1/1	0.91	0.19	-	82,82,82,82	0
55	MG	DA	3346	1/1	0.72	0.22	-	102,102,102,102	0
55	MG	DA	3473	1/1	0.89	0.14	-	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1807	1/1	0.97	0.34	-	95,95,95,95	0
55	MG	CC	104	1/1	0.70	0.21	-	98,98,98,98	0
55	MG	CA	1667	1/1	0.69	0.21	-	98,98,98,98	0
55	MG	DB	201	1/1	0.92	0.18	-	92,92,92,92	0
55	MG	CD	101	1/1	0.86	0.13	-	145,145,145,145	0
55	MG	DA	3165	1/1	0.88	0.45	-	73,73,73,73	0
55	MG	CA	1797	1/1	0.72	0.36	-	85,85,85,85	0
55	MG	BA	3442	1/1	0.79	0.30	-	90,90,90,90	0
55	MG	DA	3368	1/1	0.73	0.20	-	97,97,97,97	0
55	MG	DA	3263	1/1	0.43	0.29	-	96,96,96,96	0
55	MG	BA	3502	1/1	0.82	0.30	-	78,78,78,78	0
55	MG	DA	3300	1/1	0.70	0.34	-	75,75,75,75	0
55	MG	BA	3196	1/1	0.93	0.22	-	103,103,103,103	0
55	MG	CA	1642	1/1	0.91	0.20	-	83,83,83,83	0
55	MG	DA	3118	1/1	0.98	0.36	-	55,55,55,55	0
55	MG	BA	3034	1/1	0.97	0.29	-	40,40,40,40	0
55	MG	DA	3436	1/1	0.88	0.16	-	66,66,66,66	0
55	MG	DA	3421	1/1	0.63	0.32	-	84,84,84,84	0
55	MG	BA	3315	1/1	0.82	0.44	-	93,93,93,93	0
55	MG	DA	3293	1/1	0.97	0.48	-	89,89,89,89	0
55	MG	BA	3517	1/1	0.88	0.37	-	69,69,69,69	0
55	MG	DA	3248	1/1	0.75	0.19	-	95,95,95,95	0
55	MG	BA	3468	1/1	0.90	0.38	-	78,78,78,78	0
55	MG	BA	3069	1/1	0.77	0.42	-	93,93,93,93	0
55	MG	CA	1738	1/1	0.90	0.40	-	113,113,113,113	0
55	MG	BA	3344	1/1	0.70	0.68	-	84,84,84,84	0
55	MG	BA	3269	1/1	0.74	0.29	-	79,79,79,79	0
55	MG	DA	3313	1/1	0.94	0.24	-	84,84,84,84	0
55	MG	BA	3510	1/1	0.66	0.48	-	108,108,108,108	0
55	MG	DA	3133	1/1	0.77	0.17	-	91,91,91,91	0
55	MG	AA	1678	1/1	0.73	0.37	-	115,115,115,115	0
55	MG	DA	3280	1/1	0.81	0.41	-	91,91,91,91	0
55	MG	BA	3071	1/1	0.87	0.26	-	63,63,63,63	0
55	MG	DB	206	1/1	0.58	0.31	-	89,89,89,89	0
55	MG	DA	3389	1/1	0.68	0.28	-	97,97,97,97	0
55	MG	BA	3291	1/1	-	-	-	56,56,56,56	1
55	MG	AA	1797	1/1	0.76	0.27	-	79,79,79,79	0
55	MG	BA	3133	1/1	0.92	0.26	-	42,42,42,42	0
55	MG	BA	3319	1/1	0.93	0.54	-	64,64,64,64	0
55	MG	AA	1622	1/1	0.95	0.22	-	87,87,87,87	0
55	MG	AA	1715	1/1	0.68	0.37	-	101,101,101,101	0
55	MG	BA	3463	1/1	0.67	0.81	-	101,101,101,101	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	1796	1/1	0.91	0.42	-	102,102,102,102	0
55	MG	BA	3064	1/1	0.85	0.31	-	87,87,87,87	0
55	MG	AG	302	1/1	0.83	0.34	-	109,109,109,109	0
55	MG	CA	1715	1/1	0.90	0.30	-	89,89,89,89	0
55	MG	DA	3093	1/1	0.96	0.32	-	52,52,52,52	0
55	MG	BA	3230	1/1	0.97	0.43	-	48,48,48,48	0
55	MG	BA	3326	1/1	0.89	0.32	-	67,67,67,67	0
55	MG	AA	1701	1/1	0.85	0.57	-	87,87,87,87	0
55	MG	BA	3063	1/1	0.89	0.19	-	80,80,80,80	0
55	MG	BA	3031	1/1	0.88	0.39	-	54,54,54,54	0
55	MG	AA	1611	1/1	0.71	0.27	-	94,94,94,94	0
55	MG	BA	3485	1/1	0.81	0.27	-	98,98,98,98	0
55	MG	CA	1683	1/1	0.63	0.30	-	121,121,121,121	0
55	MG	BA	3544	1/1	0.65	0.33	-	82,82,82,82	0
55	MG	BA	3118	1/1	0.94	0.41	-	49,49,49,49	0
55	MG	DA	3275	1/1	0.73	0.21	-	85,85,85,85	0
55	MG	CA	1816	1/1	0.44	0.30	-	102,102,102,102	0
55	MG	DA	3036	1/1	0.49	0.20	-	100,100,100,100	0
55	MG	DA	3189	1/1	0.54	0.18	-	86,86,86,86	0
55	MG	BA	3212	1/1	0.91	0.34	-	68,68,68,68	0
55	MG	CA	1743	1/1	0.79	0.28	-	106,106,106,106	0
55	MG	DA	3125	1/1	0.69	0.40	-	74,74,74,74	0
55	MG	AC	104	1/1	0.88	0.38	-	64,64,64,64	0
55	MG	AA	1618	1/1	0.64	0.22	-	91,91,91,91	0
55	MG	BA	3068	1/1	0.98	0.41	-	56,56,56,56	0
55	MG	AA	1751	1/1	0.79	0.29	-	105,105,105,105	0
55	MG	BA	3203	1/1	0.79	0.23	-	106,106,106,106	0
55	MG	AA	1735	1/1	0.49	0.20	-	102,102,102,102	0
55	MG	BA	3096	1/1	0.93	0.43	-	63,63,63,63	0
55	MG	AA	1663	1/1	0.92	0.36	-	72,72,72,72	0
55	MG	BA	3317	1/1	0.84	0.42	-	70,70,70,70	0
55	MG	BA	3558	1/1	0.79	0.34	-	85,85,85,85	0
55	MG	CA	1640	1/1	0.85	0.31	-	89,89,89,89	0
55	MG	AA	1643	1/1	0.42	0.53	-	127,127,127,127	0
55	MG	DA	3158	1/1	0.90	0.38	-	80,80,80,80	0
55	MG	DO	201	1/1	0.71	0.15	-	98,98,98,98	0
55	MG	DA	3272	1/1	0.94	0.45	-	68,68,68,68	0
55	MG	BA	3168	1/1	0.89	0.36	-	47,47,47,47	0
55	MG	BA	3320	1/1	0.81	0.42	-	85,85,85,85	0
55	MG	BA	3416	1/1	0.60	0.30	-	98,98,98,98	0
55	MG	DA	3186	1/1	0.90	0.27	-	60,60,60,60	0
55	MG	CA	1643	1/1	0.94	0.37	-	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	3548	1/1	0.87	0.34	-	95,95,95,95	0
55	MG	AA	1758	1/1	-0.20	0.45	-	165,165,165,165	0
55	MG	CA	1644	1/1	0.57	0.17	-	101,101,101,101	0
55	MG	BA	3306	1/1	0.86	0.30	-	84,84,84,84	0
55	MG	DA	3438	1/1	0.90	0.34	-	79,79,79,79	0
55	MG	DA	3373	1/1	0.87	0.45	-	88,88,88,88	0
55	MG	BA	3347	1/1	0.83	0.60	-	79,79,79,79	0
55	MG	CA	1739	1/1	0.88	0.23	-	80,80,80,80	0
55	MG	CA	1652	1/1	0.86	0.13	-	94,94,94,94	0
55	MG	BA	3503	1/1	0.48	0.46	-	111,111,111,111	0
55	MG	BA	3438	1/1	0.77	0.51	-	84,84,84,84	0
55	MG	DA	3303	1/1	0.90	0.19	-	76,76,76,76	0
55	MG	DA	3312	1/1	0.89	0.33	-	75,75,75,75	0
55	MG	BA	3476	1/1	0.95	0.40	-	47,47,47,47	0
55	MG	DA	3379	1/1	0.83	0.25	-	87,87,87,87	0
55	MG	DA	3019	1/1	0.94	0.25	-	79,79,79,79	0
55	MG	DA	3206	1/1	0.61	0.29	-	109,109,109,109	0
55	MG	BA	3296	1/1	0.85	0.36	-	60,60,60,60	0
55	MG	DA	3311	1/1	0.88	0.20	-	109,109,109,109	0
55	MG	BA	3358	1/1	0.68	0.33	-	98,98,98,98	0
55	MG	BA	3504	1/1	0.75	0.51	-	88,88,88,88	0
55	MG	AA	1666	1/1	0.47	0.43	-	103,103,103,103	0
55	MG	BA	3564	1/1	0.91	0.23	-	112,112,112,112	0
55	MG	CA	1609	1/1	0.90	0.34	-	71,71,71,71	0
55	MG	AA	1777	1/1	0.73	0.27	-	115,115,115,115	0
55	MG	BA	3413	1/1	0.64	0.44	-	83,83,83,83	0
55	MG	AA	1714	1/1	0.92	0.23	-	89,89,89,89	0
55	MG	AA	1807	1/1	0.91	0.24	-	88,88,88,88	0
55	MG	BA	3224	1/1	0.69	0.32	-	78,78,78,78	0
55	MG	BA	3462	1/1	0.61	0.21	-	116,116,116,116	0
55	MG	BA	3303	1/1	0.92	0.38	-	73,73,73,73	0
55	MG	CA	1688	1/1	0.80	0.21	-	95,95,95,95	0
55	MG	AA	1720	1/1	0.96	0.35	-	83,83,83,83	0
55	MG	DA	3198	1/1	0.95	0.35	-	48,48,48,48	0
55	MG	AA	1756	1/1	0.85	0.26	-	85,85,85,85	0
55	MG	BA	3318	1/1	0.81	0.37	-	102,102,102,102	0
55	MG	AA	1657	1/1	0.83	0.35	-	76,76,76,76	0
55	MG	CA	1674	1/1	0.83	0.35	-	88,88,88,88	0
55	MG	CA	1669	1/1	0.72	0.28	-	85,85,85,85	0
55	MG	BA	3258	1/1	0.81	0.47	-	76,76,76,76	0
55	MG	DA	3246	1/1	0.77	0.28	-	89,89,89,89	0
55	MG	BA	3040	1/1	0.86	0.37	-	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
55	MG	CA	1756	1/1	0.83	0.29	-	83,83,83,83	0
55	MG	BA	3530	1/1	0.90	0.31	-	71,71,71,71	0
55	MG	BA	3092	1/1	0.85	0.31	-	67,67,67,67	0
55	MG	DA	3397	1/1	0.36	0.19	-	105,105,105,105	0
55	MG	BA	3436	1/1	0.53	0.18	-	107,107,107,107	0
55	MG	BA	3025	1/1	0.96	0.46	-	46,46,46,46	0
55	MG	CA	1619	1/1	0.93	0.12	-	68,68,68,68	0
55	MG	CA	1623	1/1	0.93	0.35	-	75,75,75,75	0
55	MG	BA	3560	1/1	0.94	0.38	-	69,69,69,69	0
55	MG	DA	3234	1/1	0.90	0.44	-	73,73,73,73	0
55	MG	DA	3407	1/1	-0.01	0.23	-	103,103,103,103	0
55	MG	DA	3343	1/1	0.76	0.34	-	91,91,91,91	0
55	MG	DA	3267	1/1	0.83	0.47	-	80,80,80,80	0
55	MG	BA	3035	1/1	0.94	0.42	-	61,61,61,61	0
55	MG	DA	3405	1/1	0.52	0.29	-	135,135,135,135	0
55	MG	AA	1754	1/1	0.73	0.38	-	95,95,95,95	0
55	MG	CA	1663	1/1	0.95	0.44	-	80,80,80,80	0
55	MG	BA	3250	1/1	0.77	0.23	-	90,90,90,90	0
55	MG	AA	1671	1/1	0.80	0.20	-	95,95,95,95	0
55	MG	BA	3271	1/1	0.74	0.20	-	92,92,92,92	0
55	MG	BB	209	1/1	0.86	0.18	-	96,96,96,96	0
55	MG	AA	1767	1/1	0.63	0.22	-	116,116,116,116	0
55	MG	AA	1694	1/1	0.83	0.20	-	142,142,142,142	0
55	MG	CA	1727	1/1	0.71	0.12	-	84,84,84,84	0
55	MG	AA	1802	1/1	0.71	0.21	-	75,75,75,75	0
55	MG	D1	201	1/1	0.31	0.26	-	89,89,89,89	0
55	MG	BA	3401	1/1	0.56	0.29	-	86,86,86,86	0
55	MG	BA	3314	1/1	0.61	0.23	-	83,83,83,83	0
55	MG	DA	3229	1/1	-0.26	0.38	-	118,118,118,118	0
55	MG	BA	3132	1/1	0.79	0.21	-	76,76,76,76	0
55	MG	AA	1661	1/1	0.89	0.35	-	56,56,56,56	0
55	MG	BA	3430	1/1	0.78	0.27	-	105,105,105,105	0
55	MG	DA	3053	1/1	0.95	0.28	-	72,72,72,72	0
55	MG	BA	3382	1/1	0.67	0.52	-	93,93,93,93	0
55	MG	BA	3079	1/1	0.59	0.27	-	103,103,103,103	0
55	MG	AA	1786	1/1	0.84	0.28	-	89,89,89,89	0
55	MG	AA	1689	1/1	0.51	0.32	-	107,107,107,107	0
55	MG	BA	3371	1/1	0.91	0.20	-	83,83,83,83	0
55	MG	BA	3293	1/1	0.79	0.35	-	96,96,96,96	0
55	MG	BA	3013	1/1	0.92	0.30	-	52,52,52,52	0
55	MG	BA	3234	1/1	0.60	0.26	-	107,107,107,107	0
55	MG	CA	1733	1/1	0.52	0.37	-	103,103,103,103	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	3425	1/1	0.77	0.24	-	87,87,87,87	0
55	MG	DA	3184	1/1	0.85	0.36	-	78,78,78,78	0
55	MG	AC	103	1/1	0.91	0.35	-	66,66,66,66	0
55	MG	AA	1804	1/1	0.46	0.43	-	113,113,113,113	0
55	MG	CA	1636	1/1	0.92	0.31	-	53,53,53,53	0
55	MG	CA	1803	1/1	0.19	0.24	-	103,103,103,103	0
55	MG	DA	3476	1/1	0.73	0.23	-	104,104,104,104	0
55	MG	AA	1726	1/1	0.71	0.45	-	94,94,94,94	0
55	MG	DA	3410	1/1	0.61	0.31	-	103,103,103,103	0
55	MG	DA	3262	1/1	0.79	0.68	-	99,99,99,99	0
55	MG	BA	3349	1/1	0.77	0.34	-	80,80,80,80	0
55	MG	AA	1615	1/1	0.84	0.30	-	90,90,90,90	0
55	MG	CA	1612	1/1	0.84	0.27	-	75,75,75,75	0
55	MG	BA	3340	1/1	0.88	0.37	-	69,69,69,69	0
55	MG	BA	3519	1/1	0.98	0.38	-	24,24,24,24	0
55	MG	DA	3254	1/1	0.87	0.15	-	80,80,80,80	0
55	MG	CR	101	1/1	0.76	0.69	-	135,135,135,135	0
55	MG	AA	1771	1/1	0.89	0.47	-	108,108,108,108	0
55	MG	DA	3171	1/1	0.84	0.16	-	73,73,73,73	0
55	MG	BA	3066	1/1	0.78	0.20	-	99,99,99,99	0
55	MG	BA	3050	1/1	0.96	0.31	-	65,65,65,65	0
55	MG	AA	1725	1/1	0.88	0.31	-	100,100,100,100	0
55	MG	BA	3466	1/1	0.85	0.61	-	92,92,92,92	0
55	MG	BA	3187	1/1	0.95	0.51	-	73,73,73,73	0
55	MG	AA	1651	1/1	0.91	0.47	-	79,79,79,79	0
55	MG	DA	3483	1/1	0.86	0.41	-	82,82,82,82	0
55	MG	BA	3181	1/1	0.91	0.31	-	69,69,69,69	0
55	MG	AA	1688	1/1	0.67	0.15	-	93,93,93,93	0
55	MG	BA	3380	1/1	0.12	0.42	-	98,98,98,98	0
55	MG	BA	3338	1/1	0.50	0.28	-	91,91,91,91	0
55	MG	BA	3005	1/1	0.99	0.40	-	40,40,40,40	0
55	MG	CA	1791	1/1	0.71	0.20	-	80,80,80,80	0
55	MG	BA	3331	1/1	0.57	0.30	-	106,106,106,106	0
55	MG	DA	3330	1/1	0.45	0.66	-	100,100,100,100	0
55	MG	AA	1658	1/1	0.99	0.35	-	56,56,56,56	0
55	MG	CA	1664	1/1	0.97	0.30	-	64,64,64,64	0
55	MG	AA	1805	1/1	0.56	0.73	-	152,152,152,152	0
55	MG	CA	1670	1/1	0.89	0.40	-	67,67,67,67	0
55	MG	BA	3515	1/1	0.94	0.20	-	81,81,81,81	0
55	MG	BA	3367	1/1	0.98	0.54	-	72,72,72,72	0
55	MG	DA	3417	1/1	0.49	0.34	-	135,135,135,135	0
55	MG	DA	3265	1/1	0.87	0.36	-	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	DA	3381	1/1	0.89	0.24	-	90,90,90,90	0
55	MG	CA	1759	1/1	0.75	0.51	-	99,99,99,99	0
55	MG	BA	3268	1/1	0.56	0.25	-	90,90,90,90	0
55	MG	BA	3009	1/1	0.83	0.32	-	58,58,58,58	0
55	MG	BA	3428	1/1	0.74	0.40	-	91,91,91,91	0
55	MG	BA	3046	1/1	0.93	0.38	-	56,56,56,56	0
55	MG	CA	1706	1/1	0.97	0.43	-	79,79,79,79	0
55	MG	BA	3099	1/1	0.93	0.23	-	75,75,75,75	0
55	MG	BA	3030	1/1	0.96	0.35	-	41,41,41,41	0
55	MG	BA	3561	1/1	0.80	0.29	-	84,84,84,84	0
55	MG	AD	101	1/1	0.09	0.32	-	154,154,154,154	0
55	MG	BA	3482	1/1	0.75	0.17	-	82,82,82,82	0
55	MG	AA	1684	1/1	0.89	0.32	-	83,83,83,83	0
55	MG	CA	1804	1/1	0.62	0.40	-	108,108,108,108	0
55	MG	CA	1713	1/1	0.82	0.22	-	82,82,82,82	0
55	MG	DA	3344	1/1	0.59	0.26	-	89,89,89,89	0
55	MG	DA	3294	1/1	0.76	0.38	-	91,91,91,91	0
55	MG	DA	3168	1/1	0.89	0.40	-	87,87,87,87	0
55	MG	DA	3161	1/1	0.98	0.25	-	55,55,55,55	0
55	MG	CA	1777	1/1	0.81	0.13	-	112,112,112,112	0
55	MG	DA	3324	1/1	0.87	0.19	-	91,91,91,91	0
55	MG	DA	3462	1/1	0.56	0.23	-	98,98,98,98	0
55	MG	CA	1786	1/1	0.07	0.27	-	111,111,111,111	0
55	MG	BO	201	1/1	0.89	0.12	-	78,78,78,78	0
55	MG	AA	1783	1/1	0.51	0.36	-	167,167,167,167	0
55	MG	CA	1722	1/1	0.76	0.61	-	106,106,106,106	0
55	MG	BA	3180	1/1	0.84	0.22	-	91,91,91,91	0
55	MG	CA	1723	1/1	0.92	0.20	-	90,90,90,90	0
55	MG	AA	1634	1/1	0.95	0.34	-	67,67,67,67	0
55	MG	CA	1689	1/1	0.92	0.32	-	73,73,73,73	0
55	MG	DA	3157	1/1	0.97	0.28	-	51,51,51,51	0
55	MG	BB	203	1/1	0.77	0.43	-	71,71,71,71	0
55	MG	DA	3176	1/1	0.31	0.54	-	105,105,105,105	0
55	MG	CA	1697	1/1	0.51	0.16	-	84,84,84,84	0
55	MG	BA	3190	1/1	0.95	0.36	-	86,86,86,86	0
55	MG	DA	3349	1/1	0.87	0.24	-	78,78,78,78	0
55	MG	BA	3439	1/1	0.34	0.38	-	115,115,115,115	0
55	MG	BA	3289	1/1	0.70	0.34	-	95,95,95,95	0
55	MG	BA	3163	1/1	0.32	0.34	-	86,86,86,86	0
55	MG	BA	3209	1/1	0.67	0.48	-	78,78,78,78	0
55	MG	DA	3097	1/1	0.98	0.33	-	53,53,53,53	0
55	MG	DA	3295	1/1	0.84	0.34	-	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	1781	1/1	0.61	0.37	-	87,87,87,87	0
55	MG	AA	1716	1/1	0.93	0.25	-	82,82,82,82	0
55	MG	DA	3073	1/1	0.90	0.30	-	84,84,84,84	0
55	MG	DA	3301	1/1	0.90	0.31	-	90,90,90,90	0
55	MG	AA	1707	1/1	0.91	0.18	-	81,81,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.