



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:38 PM GMT

PDB ID : 1VY7
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in the pre-attack state of peptide bond formation containing short substrate-mimic Cytidine-Cytidine-Puromycin in the A site and acylated tRNA in the P site.
Authors : Polikanov, Y.S.; Steitz, T.A.; Innis, C.A.
Deposited on : 2014-05-13
Resolution : 2.80 Å(reported)

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

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

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

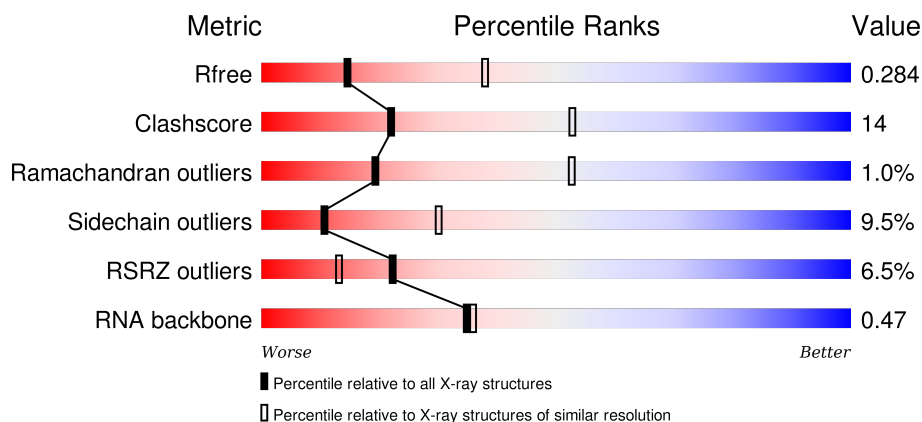
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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

Mol	Chain	Length	Quality of chain
1	AA	1521	<div> <div>38%</div> <div>43%</div> <div>16%</div> <div>..</div> </div>
1	CA	1521	<div> <div>2%</div> <div>33%</div> <div>47%</div> <div>17%</div> <div>..</div> </div>
2	AB	256	<div> <div>6%</div> <div>50%</div> <div>32%</div> <div>8%</div> <div>10%</div> </div>
2	CB	256	<div> <div>43%</div> <div>49%</div> <div>32%</div> <div>8%</div> <div>10%</div> </div>

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	24	
22	CV	24	
23	AW	3	
23	CW	3	
24	AX	77	
24	CX	77	
25	AY	76	
25	CY	76	
26	BA	2915	
26	DA	2915	
27	BB	121	
27	DB	121	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BD	276	% 69% 29% .
28	DD	276	72% 25% .
29	BE	206	68% 25% 6% .
29	DE	206	67% 26% 5% ..
30	BF	210	% 64% 28% . .
30	DF	210	61% 32% . .
31	BG	182	4% 67% 29% . .
31	DG	182	29% 48% 42% 8% ..
32	BH	180	% 69% 27% . .
32	DH	180	22% 58% 34% . .
33	BI	148	9% 66% 24% 8% .
33	DI	148	54% 57% 32% 9% ..
34	BN	140	% 72% 25% .
34	DN	140	% 72% 24% .
35	BO	122	% 71% 25% .
35	DO	122	63% 34% .
36	BP	150	% 69% 27% . .
36	DP	150	5% 61% 31% 7% .
37	BQ	141	66% 31% . .
37	DQ	141	12% 70% 26% .
38	BR	118	62% 30% 8%
38	DR	118	55% 36% 8%
39	BS	112	% 69% 24% . .
39	DS	112	10% 61% 34% . .
40	BT	146	58% 27% . 10%

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	3024	-	-	-	X
57	MG	AA	3030	-	-	-	X
57	MG	AA	3055	-	-	-	X
57	MG	AA	3074	-	-	-	X
57	MG	AA	3083	-	-	-	X
57	MG	AA	3089	-	-	-	X
57	MG	AA	3090	-	-	-	X
57	MG	AA	3091	-	-	-	X
57	MG	AA	3113	-	-	-	X
57	MG	AA	3116	-	-	-	X
57	MG	AA	3144	-	-	-	X
57	MG	AA	3155	-	-	-	X
57	MG	AA	3172	-	-	-	X
57	MG	AA	3204	-	-	-	X
57	MG	AX	3007	-	-	-	X
57	MG	B7	102	-	-	-	X
57	MG	BA	3026	-	-	-	X
57	MG	BA	3027	-	-	-	X
57	MG	BA	3036	-	-	-	X
57	MG	BA	3041	-	-	-	X
57	MG	BA	3053	-	-	-	X
57	MG	BA	3054	-	-	-	X
57	MG	BA	3067	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3101	-	-	-	X
57	MG	BA	3105	-	-	-	X
57	MG	BA	3111	-	-	-	X
57	MG	BA	3114	-	-	-	X
57	MG	BA	3118	-	-	-	X
57	MG	BA	3125	-	-	-	X
57	MG	BA	3131	-	-	-	X
57	MG	BA	3133	-	-	-	X
57	MG	BA	3148	-	-	-	X
57	MG	BA	3150	-	-	-	X
57	MG	BA	3152	-	-	-	X
57	MG	BA	3160	-	-	-	X
57	MG	BA	3183	-	-	-	X
57	MG	BA	3185	-	-	-	X
57	MG	BA	3190	-	-	-	X
57	MG	BA	3193	-	-	-	X
57	MG	BA	3200	-	-	-	X
57	MG	BA	3212	-	-	-	X
57	MG	BA	3226	-	-	-	X
57	MG	BA	3244	-	-	-	X
57	MG	BA	3245	-	-	-	X
57	MG	BA	3246	-	-	-	X
57	MG	BA	3253	-	-	-	X
57	MG	BA	3257	-	-	-	X
57	MG	BA	3259	-	-	-	X
57	MG	BA	3267	-	-	-	X
57	MG	BA	3271	-	-	-	X
57	MG	BA	3277	-	-	-	X
57	MG	BA	3281	-	-	-	X
57	MG	BA	3283	-	-	-	X
57	MG	BA	3294	-	-	-	X
57	MG	BA	3303	-	-	-	X
57	MG	BA	3310	-	-	-	X
57	MG	BA	3314	-	-	-	X
57	MG	BA	3366	-	-	-	X
57	MG	BA	3384	-	-	-	X
57	MG	BA	3385	-	-	-	X
57	MG	BA	3391	-	-	-	X
57	MG	BA	3396	-	-	-	X
57	MG	BA	3401	-	-	-	X
57	MG	BA	3403	-	-	-	X
57	MG	BA	3405	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3412	-	-	-	X
57	MG	BA	3423	-	-	-	X
57	MG	BA	3431	-	-	-	X
57	MG	BA	3432	-	-	-	X
57	MG	BA	3436	-	-	-	X
57	MG	BA	3437	-	-	-	X
57	MG	BA	3443	-	-	-	X
57	MG	BA	3461	-	-	-	X
57	MG	BA	3490	-	-	-	X
57	MG	BA	3498	-	-	-	X
57	MG	BA	3508	-	-	-	X
57	MG	BA	3509	-	-	-	X
57	MG	BA	3514	-	-	-	X
57	MG	BA	3529	-	-	-	X
57	MG	BA	3530	-	-	-	X
57	MG	BA	3532	-	-	-	X
57	MG	BA	3533	-	-	-	X
57	MG	BA	3534	-	-	-	X
57	MG	BA	3545	-	-	-	X
57	MG	BA	3546	-	-	-	X
57	MG	BA	3602	-	-	-	X
57	MG	BA	3651	-	-	-	X
57	MG	BA	3663	-	-	-	X
57	MG	BA	3677	-	-	-	X
57	MG	BA	3686	-	-	-	X
57	MG	BA	3698	-	-	-	X
57	MG	BA	3705	-	-	-	X
57	MG	BA	3706	-	-	-	X
57	MG	BA	3707	-	-	-	X
57	MG	BA	3709	-	-	-	X
57	MG	BD	301	-	-	-	X
57	MG	BD	303	-	-	-	X
57	MG	BD	306	-	-	-	X
57	MG	BD	308	-	-	-	X
57	MG	BD	310	-	-	-	X
57	MG	BD	311	-	-	-	X
57	MG	BE	3001	-	-	-	X
57	MG	BE	3002	-	-	-	X
57	MG	BF	304	-	-	-	X
57	MG	BF	307	-	-	-	X
57	MG	BN	3001	-	-	-	X
57	MG	BN	3004	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BN	3006	-	-	-	X
57	MG	BP	3001	-	-	-	X
57	MG	BQ	3001	-	-	-	X
57	MG	BQ	3002	-	-	-	X
57	MG	BQ	3003	-	-	-	X
57	MG	BR	203	-	-	-	X
57	MG	BU	204	-	-	-	X
57	MG	BU	206	-	-	-	X
57	MG	BU	208	-	-	-	X
57	MG	BW	202	-	-	-	X
57	MG	CA	3017	-	-	-	X
57	MG	CA	3047	-	-	-	X
57	MG	CA	3054	-	-	-	X
57	MG	CA	3058	-	-	-	X
57	MG	CA	3070	-	-	-	X
57	MG	CA	3074	-	-	-	X
57	MG	CA	3095	-	-	-	X
57	MG	CA	3097	-	-	-	X
57	MG	CA	3116	-	-	-	X
57	MG	CA	3126	-	-	-	X
57	MG	DA	3001	-	-	-	X
57	MG	DA	3004	-	-	-	X
57	MG	DA	3015	-	-	-	X
57	MG	DA	3017	-	-	-	X
57	MG	DA	3020	-	-	-	X
57	MG	DA	3023	-	-	-	X
57	MG	DA	3030	-	-	-	X
57	MG	DA	3039	-	-	-	X
57	MG	DA	3042	-	-	-	X
57	MG	DA	3044	-	-	-	X
57	MG	DA	3058	-	-	-	X
57	MG	DA	3059	-	-	-	X
57	MG	DA	3061	-	-	-	X
57	MG	DA	3096	-	-	-	X
57	MG	DA	3100	-	-	-	X
57	MG	DA	3103	-	-	-	X
57	MG	DA	3106	-	-	-	X
57	MG	DA	3116	-	-	-	X
57	MG	DA	3119	-	-	-	X
57	MG	DA	3127	-	-	-	X
57	MG	DA	3141	-	-	-	X
57	MG	DA	3145	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3152	-	-	-	X
57	MG	DA	3161	-	-	-	X
57	MG	DA	3162	-	-	-	X
57	MG	DA	3166	-	-	-	X
57	MG	DA	3170	-	-	-	X
57	MG	DA	3171	-	-	-	X
57	MG	DA	3173	-	-	-	X
57	MG	DA	3174	-	-	-	X
57	MG	DA	3177	-	-	-	X
57	MG	DA	3183	-	-	-	X
57	MG	DA	3185	-	-	-	X
57	MG	DA	3192	-	-	-	X
57	MG	DA	3207	-	-	-	X
57	MG	DA	3210	-	-	-	X
57	MG	DA	3216	-	-	-	X
57	MG	DA	3228	-	-	-	X
57	MG	DA	3230	-	-	-	X
57	MG	DA	3234	-	-	-	X
57	MG	DA	3238	-	-	-	X
57	MG	DA	3242	-	-	-	X
57	MG	DA	3243	-	-	-	X
57	MG	DA	3251	-	-	-	X
57	MG	DA	3255	-	-	-	X
57	MG	DA	3257	-	-	-	X
57	MG	DA	3258	-	-	-	X
57	MG	DA	3267	-	-	-	X
57	MG	DA	3274	-	-	-	X
57	MG	DA	3277	-	-	-	X
57	MG	DA	3291	-	-	-	X
57	MG	DA	3307	-	-	-	X
57	MG	DA	3312	-	-	-	X
57	MG	DA	3319	-	-	-	X
57	MG	DA	3348	-	-	-	X
57	MG	DA	3350	-	-	-	X
57	MG	DA	3351	-	-	-	X
57	MG	DA	3363	-	-	-	X
57	MG	DA	3369	-	-	-	X
57	MG	DA	3371	-	-	-	X
57	MG	DA	3373	-	-	-	X
57	MG	DA	3376	-	-	-	X
57	MG	DA	3382	-	-	-	X
57	MG	DA	3387	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	3410	-	-	-	X
57	MG	DA	3417	-	-	-	X
57	MG	DA	3426	-	-	-	X
57	MG	DA	3430	-	-	-	X
57	MG	DA	3440	-	-	-	X
57	MG	DA	3441	-	-	-	X
57	MG	DA	3444	-	-	-	X
57	MG	DA	3448	-	-	-	X
57	MG	DA	3453	-	-	-	X
57	MG	DA	3456	-	-	-	X
57	MG	DA	3462	-	-	-	X
57	MG	DA	3466	-	-	-	X
57	MG	DA	3471	-	-	-	X
57	MG	DA	3473	-	-	-	X
57	MG	DA	3474	-	-	-	X
57	MG	DA	3475	-	-	-	X
57	MG	DA	3483	-	-	-	X
57	MG	DA	3501	-	-	-	X
57	MG	DA	3533	-	-	-	X
57	MG	DA	3537	-	-	-	X
57	MG	DA	3538	-	-	-	X
57	MG	DA	3552	-	-	-	X
57	MG	DA	3559	-	-	-	X
57	MG	DA	3579	-	-	-	X
57	MG	DA	3594	-	-	-	X
57	MG	DA	3602	-	-	-	X
57	MG	DA	3609	-	-	-	X
57	MG	DA	3614	-	-	-	X
57	MG	DA	3619	-	-	-	X
57	MG	DA	3621	-	-	-	X
57	MG	DA	3624	-	-	-	X
57	MG	DA	3628	-	-	-	X
57	MG	DB	3005	-	-	-	X
57	MG	DD	303	-	-	-	X
57	MG	DD	305	-	-	-	X
57	MG	DD	306	-	-	-	X
57	MG	DE	302	-	-	-	X
57	MG	DF	3004	-	-	-	X
57	MG	DP	202	-	-	-	X
57	MG	DU	3001	-	-	-	X
57	MG	DV	201	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 290205 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
22	CV	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

- Molecule 23 is a RNA chain called Cytidine-Puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
23	CW	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0	0
			1633	730	296	529	76	2			
24	CX	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	5	Total	C	N	O	P	0	0	0
			104	47	19	33	5			
25	CY	5	Total	C	N	O	P	0	0	0
			104	47	19	33	5			

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			
51	D4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BA	720	Total	Mg	0	0
			720	720		
57	AK	1	Total	Mg	0	0
			1	1		
57	DQ	3	Total	Mg	0	0
			3	3		
57	D3	1	Total	Mg	0	0
			1	1		
57	DF	4	Total	Mg	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B8	1	Total 1	Mg 1	0	0
57	BE	7	Total 7	Mg 7	0	0
57	AW	1	Total 1	Mg 1	0	0
57	DU	4	Total 4	Mg 4	0	0
57	B1	1	Total 1	Mg 1	0	0
57	AN	2	Total 2	Mg 2	0	0
57	BP	4	Total 4	Mg 4	0	0
57	AX	11	Total 11	Mg 11	0	0
57	DN	1	Total 1	Mg 1	0	0
57	AS	1	Total 1	Mg 1	0	0
57	CA	160	Total 160	Mg 160	0	0
57	B5	2	Total 2	Mg 2	0	0
57	BB	20	Total 20	Mg 20	0	0
57	AJ	1	Total 1	Mg 1	0	0
57	D8	2	Total 2	Mg 2	0	0
57	AE	2	Total 2	Mg 2	0	0
57	DG	1	Total 1	Mg 1	0	0
57	B9	1	Total 1	Mg 1	0	0
57	BF	10	Total 10	Mg 10	0	0
57	AV	1	Total 1	Mg 1	0	0
57	BX	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

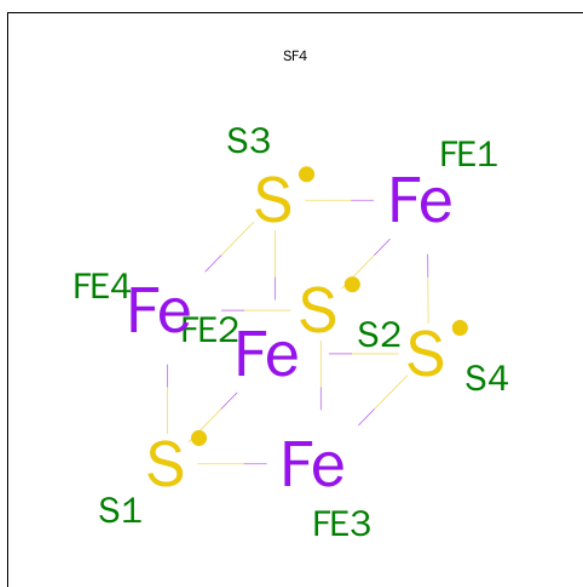
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B2	1	Total 1	Mg 1	0	0
57	AA	207	Total 207	Mg 207	0	0
57	BQ	5	Total 5	Mg 5	0	0
57	CX	2	Total 2	Mg 2	0	0
57	DV	2	Total 2	Mg 2	0	0
57	AM	1	Total 1	Mg 1	0	0
57	BU	8	Total 8	Mg 8	0	0
57	DR	2	Total 2	Mg 2	0	0
57	AD	2	Total 2	Mg 2	0	0
57	BN	6	Total 6	Mg 6	0	0
57	CT	1	Total 1	Mg 1	0	0
57	BG	2	Total 2	Mg 2	0	0
57	BY	1	Total 1	Mg 1	0	0
57	DE	4	Total 4	Mg 4	0	0
57	B3	2	Total 2	Mg 2	0	0
57	CJ	1	Total 1	Mg 1	0	0
57	BR	3	Total 3	Mg 3	0	0
57	DA	629	Total 629	Mg 629	0	0
57	DP	2	Total 2	Mg 2	0	0
57	DW	2	Total 2	Mg 2	0	0
57	B7	3	Total 3	Mg 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CF	1	Total 1	Mg 1	0	0
57	BV	4	Total 4	Mg 4	0	0
57	DO	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	BZ	1	Total 1	Mg 1	0	0
57	DY	1	Total 1	Mg 1	0	0
57	CW	1	Total 1	Mg 1	0	0
57	D5	1	Total 1	Mg 1	0	0
57	BD	11	Total 11	Mg 11	0	0
57	B0	4	Total 4	Mg 4	0	0
57	CE	1	Total 1	Mg 1	0	0
57	BW	5	Total 5	Mg 5	0	0
57	DD	7	Total 7	Mg 7	0	0
57	CK	1	Total 1	Mg 1	0	0
57	AF	1	Total 1	Mg 1	0	0
57	DB	10	Total 10	Mg 10	0	0

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



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

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

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

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AA	170	Total 170	O 170	0	0
61	AL	2	Total 2	O 2	0	0
61	AO	1	Total 1	O 1	0	0
61	AU	1	Total 1	O 1	0	0
61	AV	2	Total 2	O 2	0	0
61	AW	3	Total 3	O 3	0	0
61	BA	1102	Total 1102	O 1102	0	0
61	BB	36	Total 36	O 36	0	0
61	BD	8	Total 8	O 8	0	0
61	BE	13	Total 13	O 13	0	0
61	BF	4	Total 4	O 4	0	0
61	BG	3	Total 3	O 3	0	0
61	BI	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	BP	15	Total 15	O 15	0	0
61	BQ	3	Total 3	O 3	0	0
61	BR	1	Total 1	O 1	0	0
61	BS	1	Total 1	O 1	0	0
61	BT	3	Total 3	O 3	0	0
61	BU	1	Total 1	O 1	0	0
61	BV	4	Total 4	O 4	0	0
61	BW	2	Total 2	O 2	0	0
61	BX	2	Total 2	O 2	0	0
61	B0	4	Total 4	O 4	0	0
61	B1	1	Total 1	O 1	0	0
61	B3	1	Total 1	O 1	0	0
61	B5	5	Total 5	O 5	0	0
61	B7	1	Total 1	O 1	0	0
61	B8	7	Total 7	O 7	0	0
61	CA	130	Total 130	O 130	0	0
61	CE	1	Total 1	O 1	0	0
61	CJ	2	Total 2	O 2	0	0
61	CN	1	Total 1	O 1	0	0
61	CT	1	Total 1	O 1	0	0
61	CV	1	Total 1	O 1	0	0

Continued on next page...

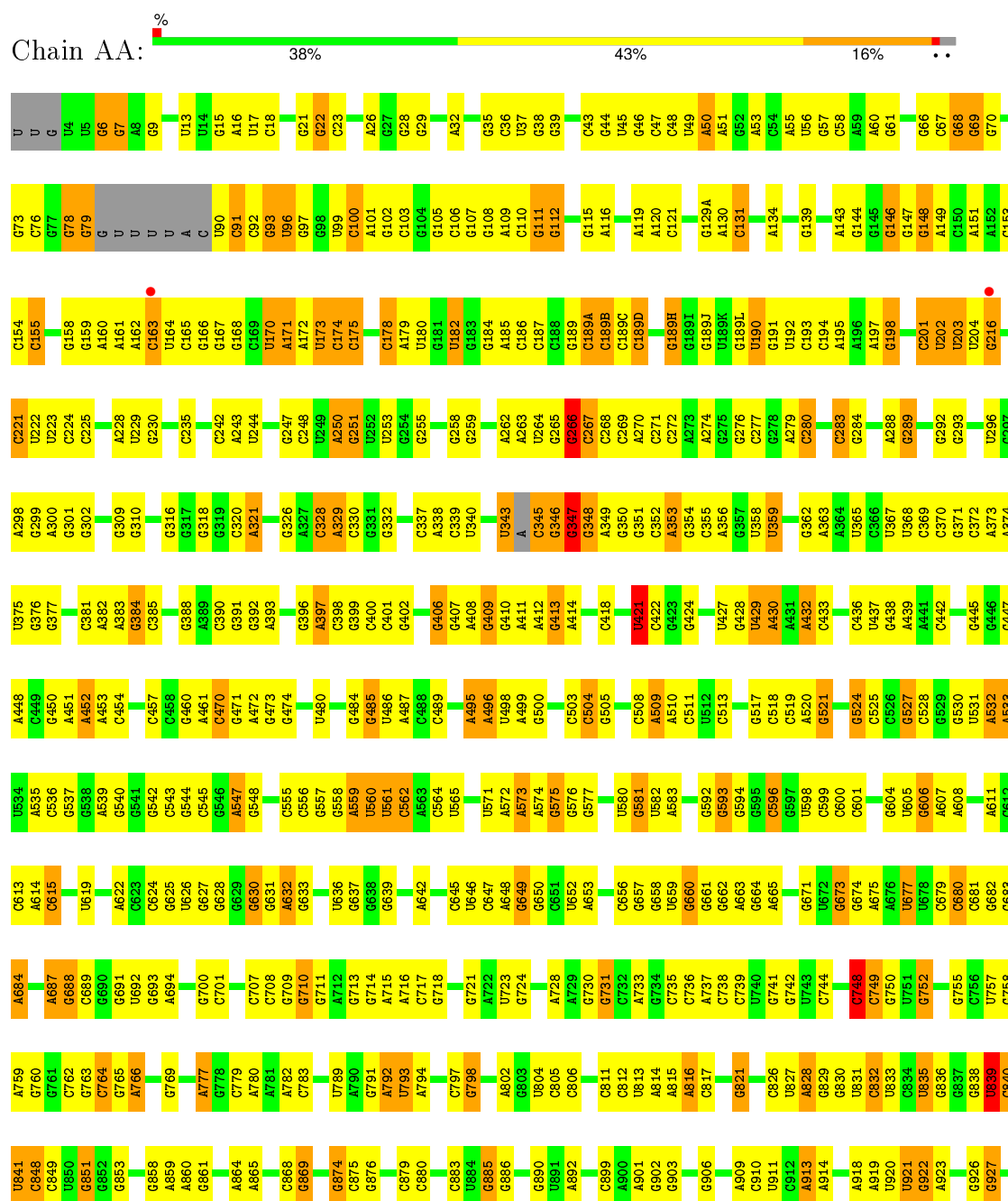
Continued from previous page...

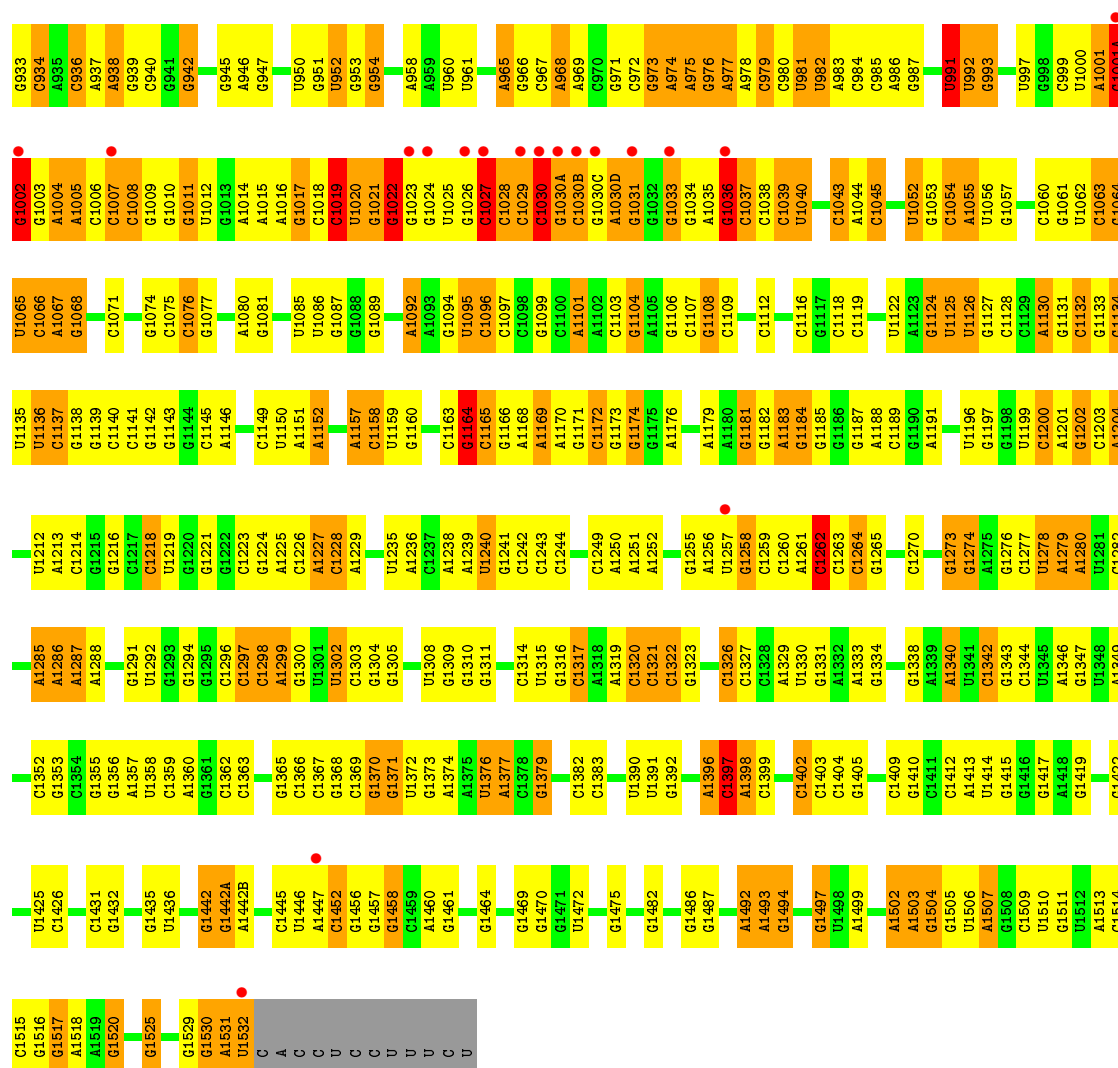
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CW	1	Total 1	O 1	0	0
61	CX	1	Total 1	O 1	0	0
61	DA	767	Total 767	O 767	0	0
61	DB	9	Total 9	O 9	0	0
61	DD	9	Total 9	O 9	0	0
61	DE	5	Total 5	O 5	0	0
61	DF	6	Total 6	O 6	0	0
61	DN	2	Total 2	O 2	0	0
61	DP	12	Total 12	O 12	0	0
61	DR	2	Total 2	O 2	0	0
61	DT	1	Total 1	O 1	0	0
61	DU	2	Total 2	O 2	0	0
61	DV	1	Total 1	O 1	0	0
61	DX	2	Total 2	O 2	0	0
61	DY	1	Total 1	O 1	0	0
61	D0	5	Total 5	O 5	0	0
61	D1	1	Total 1	O 1	0	0
61	D3	2	Total 2	O 2	0	0
61	D7	1	Total 1	O 1	0	0
61	D8	4	Total 4	O 4	0	0

3 Residue-property plots

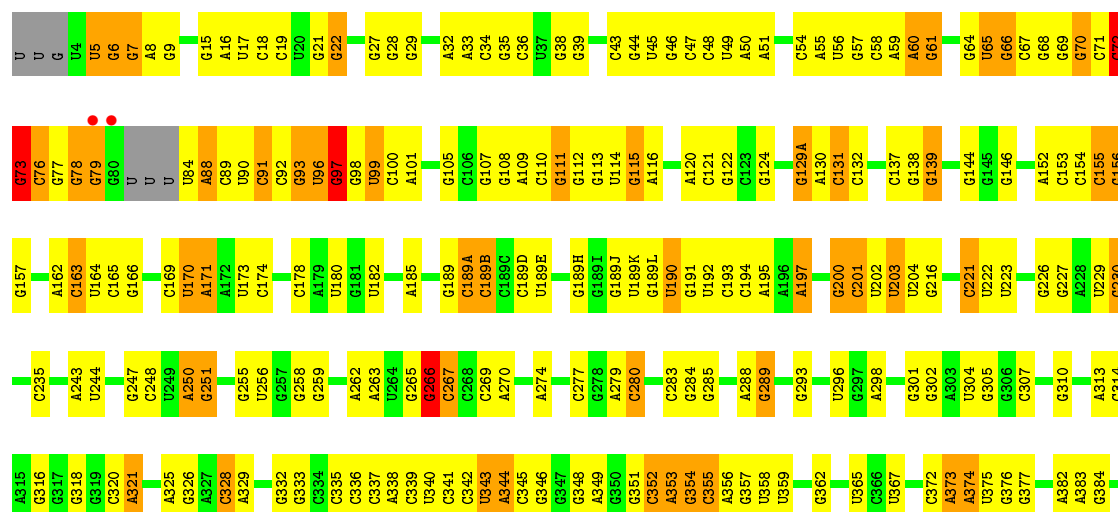
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S Ribosomal RNA

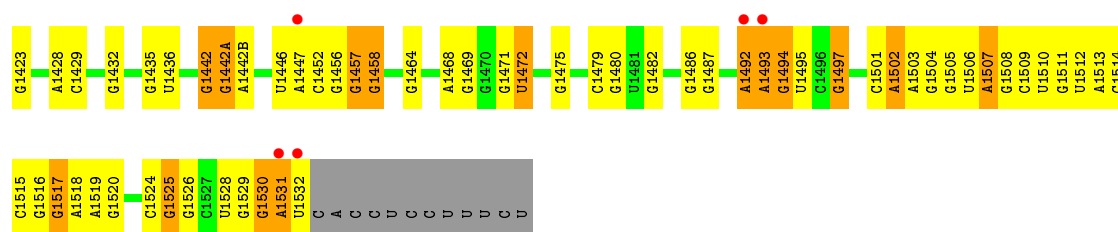




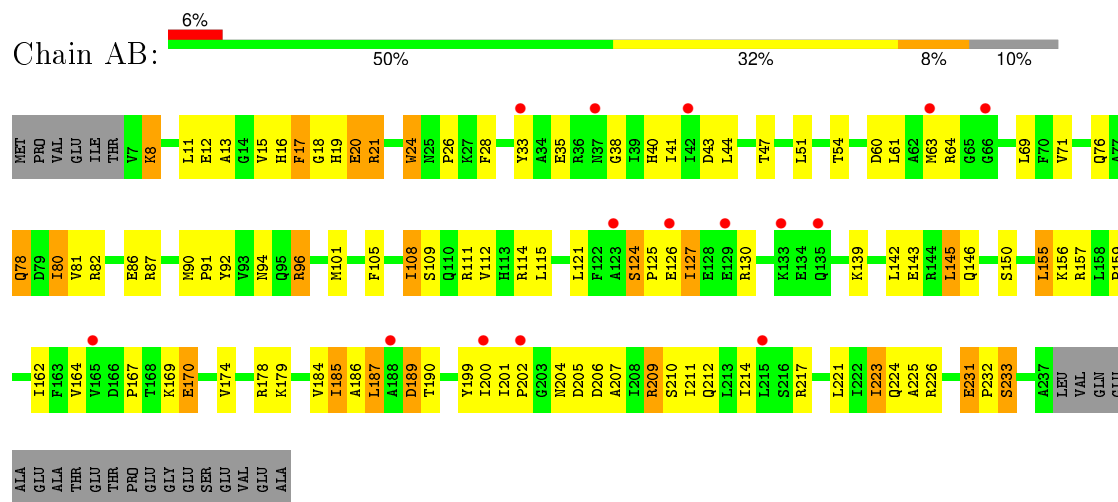
• Molecule 1: 16S Ribosomal RNA



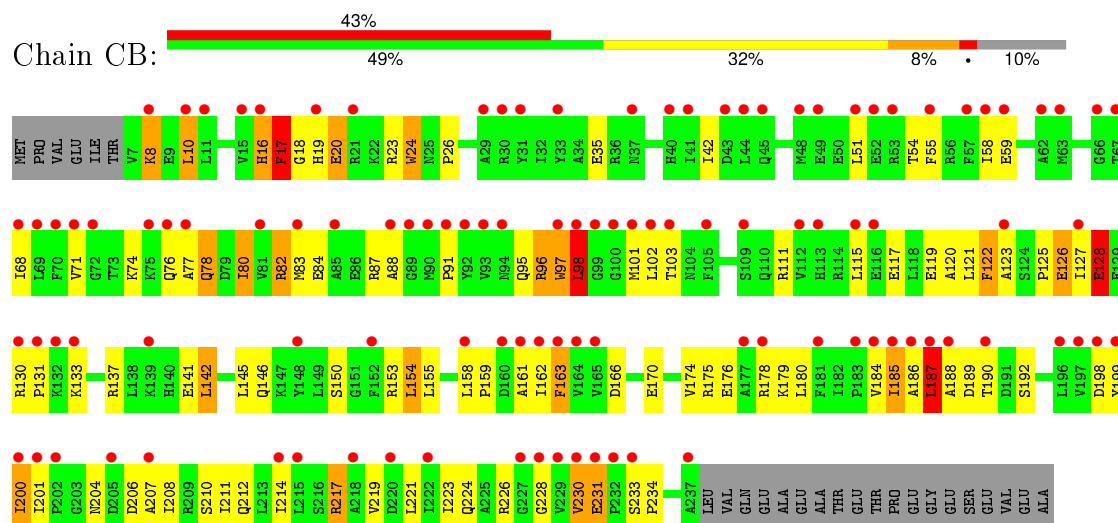
A1357	G1293	C1226	G1160	G1034	C979	G829	U751	A684	G615	G544	G460	U387
U1358	G1294	A1227	G1161	A1035	C980	G830	G752	G685	G616	C545	A461	C390
C1359	G1228	C1228	G1162	G1036	U981	U831	A753	U686	G617	G546	C470	C391
A1360	A1229	C1229	C1037	A909	C982	C832	C754	A687	G618	G547	G471	G392
G1361	C1297	G1230	G1104	G1038	A983	U833	G755	G688	U619	G548	A472	A393
C1362	C1298	G1231	G1105	C1039	C984	C834	G756	C689	U620	C549	G473	
C1363	A1299		U1040	U1040	C985	U835	G757	G690	A621	G550	G474	
A1363A	G1300	U1235	A1170	A1041	A986	G836	G758	G691	G623	U552	G475	A397
U1364	U1301	A1236	G1171	G1108	C987	G837	A759	U692	G624	C556	G476	C398
G1365	U1302	C1237	C1172	C1043	C988	U838	G760	G693	G625			G399
C1366	G1303	A1238	A1109	A1044	C989	U839	G761	A694	G626		G484	G400
C1367	G1304	A1239	G1174	C1045	C990	C840	G762	A695	U626		G485	C401
G1368	G1305	U1240	A1175	A1046	U991	U841	C763	A696	G627		U486	
C1369	A1176		G1047	G992	U992	C848	C764	U697	G628		A487	
G1370	G1177			U1052	A993	C849	G765	G698	G629		C488	U405
G1371	G1178			G1053	A994	U850	A766	C699	G630		G407	
U1372	A1179			C1054	C995	G851	A767	G700	G631		U498	A408
G1373	A1180			A1055	A996	G852	G768	C701	A632		U494	A409
A1374	G1181			U1056	U997	G853	G769	A702	G633		A495	G410
A1375	G1182			C998					G634		A496	A411
U1376	A1183			G999		C857	G775	C707	G635		U498	A412
U1377	G1184			U1000		G858	G776	C708	U636		A499	G413
A1377	G1185			A1001		A859	A777	G709	G637		G500	A414
C1378	G1316			C996		A860	G778	G710	G638		C501	
G1379	C1317			A937		G861	C779	G711	G639		G502	
U1380	A1318			A938		G861	A780	A712			C503	
U1381	A1319			C999					A642		C504	
C1382	C1320			G942		A864	G786	G714	G645		C505	
C1383	C1321			A1005		A865		G715	C646		U420	
	C1322			C1006		C866		A716	U646		U421	
G1386	U1194			G944		G867	U789	A717	C647		C508	
	G1195			U943		C868	A790	C717	A648		A509	
G1392	U1196			G945		C869	A791	G718	U582		A510	
U1393	G1263			A946		U870	A792	C719	A649		C511	
C1394	C1264			U947			G793	G720	G584		U512	
A1394	G1265			C948		U871	A794	C721	G585		C514	
C1395	G1266			U950		A873		A722			U429	
A1396	C1200			A874		G874	G797	U723	G566		A430	
U1397	A1201			U952			G798	G724	G657		U516	
G1398	G1202			G953		C877	G799		G658		G517	
A1398	C1203			G954		G878	G800	A728	U659		C518	
C1399	G1204			U954		C879	U801	A729	G660		C433	
C1400	A1204			C1018		C880	A802	G730	G661		C519	
G1401	U1205			C1019		C881	G803	G731	G662		A520	
A1402	G1273			U958		G885	U804	G732	A663		G521	
C1403	G1274			A959		G886	C805	C733	G664		C436	
A1404	C1276			U960		G887	C806	A734	A665		C522	
G1405	C1277			U961		C888	C811	C735	G666		A523	
U1406				G1021		G890	C812	G736	G667		C524	
				G1022		U891	U813	A737	U603		C525	
C1409	G1338			G1085		A892	A814	C738	G671		C442	
G1410	A1339			U1086		A893	A815	G741	U672		C443	
C1411	G1342			G1087		C970	A816	G742	G673		G445	
A1412	U1210			U1088		A894	C817	G743	G674		A532	
C1413	G1284			G1089		G895			A608		A533	
U1414	A1279			U1090		C899	A817	C745	A609		G538	
A1415	C1217			U1091		A900	A746	G746	A610		A539	
G1416	A1285			A1092		A901	C747	G747	A611		A540	
C1417	A1286			C1030		G902	U826	C748	G612		C457	
G1417	A1350			A1093		G903	U827	C749	G613		G458	
A1418	U1351			G1094		C899	G821		G683			
G1418	A1287			G1095		A900						
C1419	U1220			C1096		A901						
A1419	G1221			C1097		G902						
	C1222			U1098		G903						
	G1354			G1099		G1033						
	G1355											
	G1356											



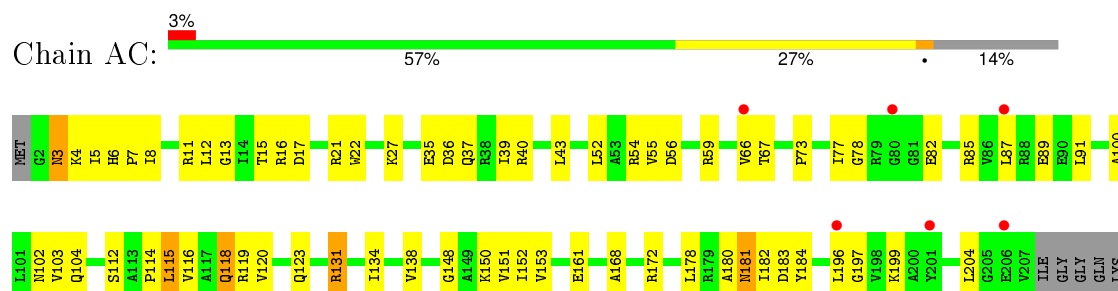
• Molecule 2: 30S ribosomal protein S2



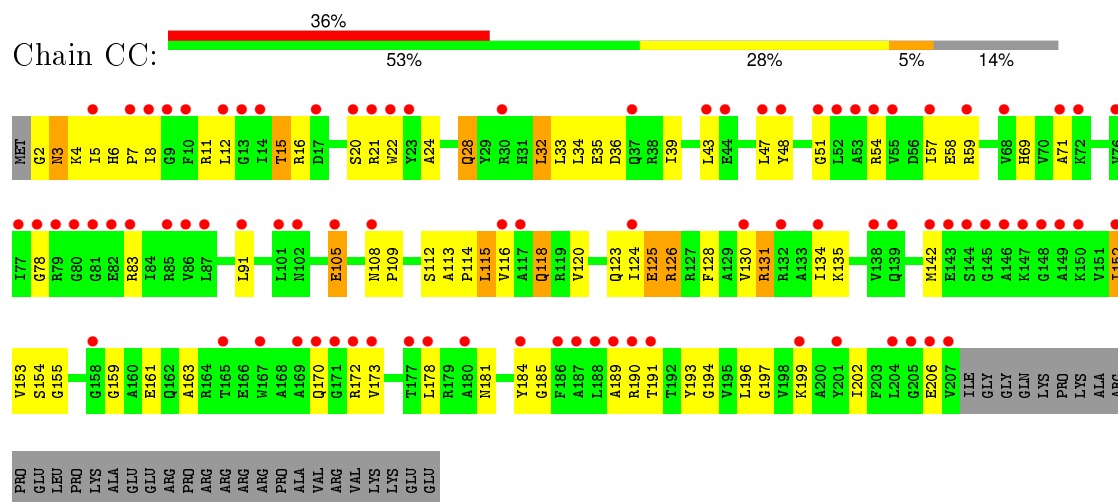
• Molecule 2: 30S ribosomal protein S2



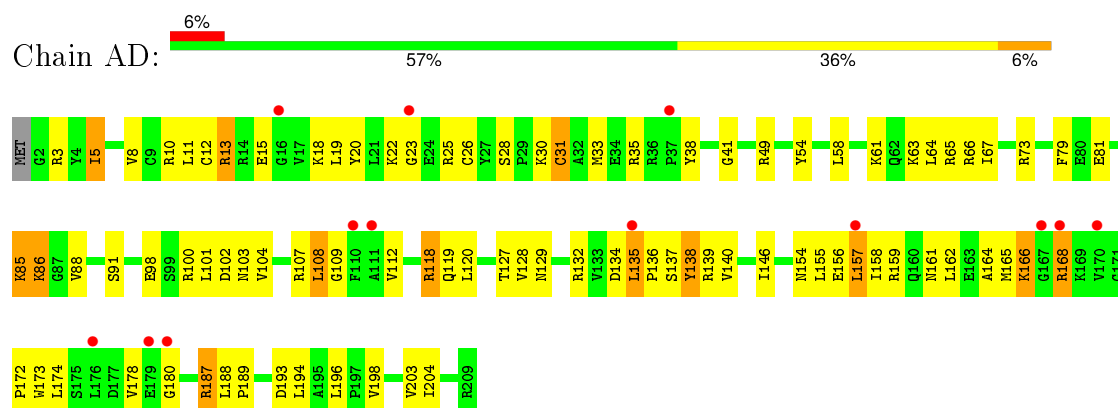
• Molecule 3: 30S ribosomal protein S3



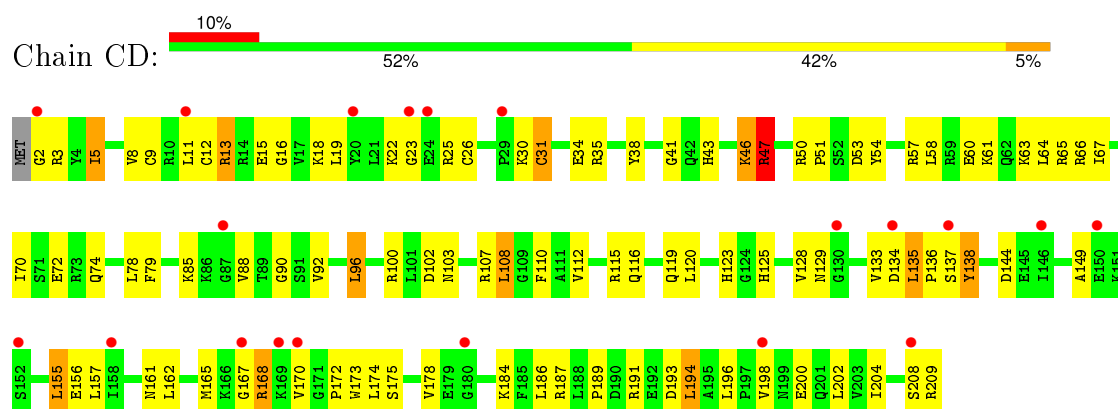
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

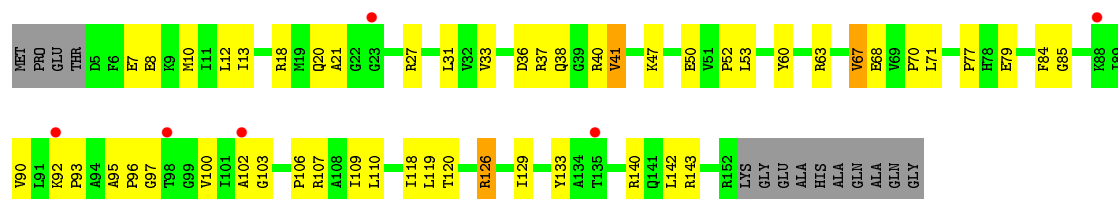


- Molecule 4: 30S ribosomal protein S4

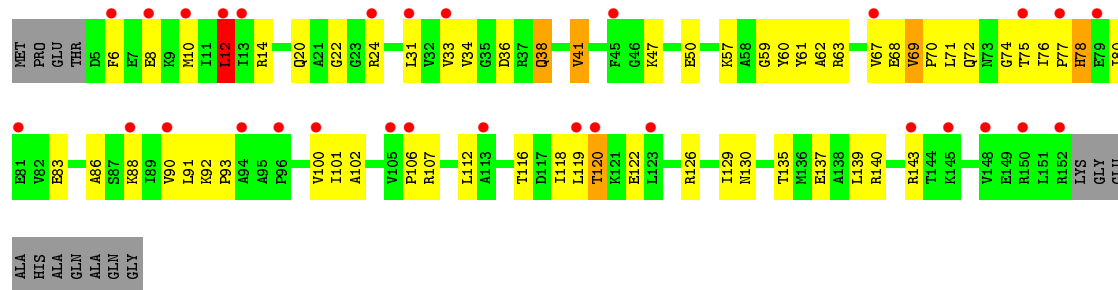


- Molecule 5: 30S ribosomal protein S5

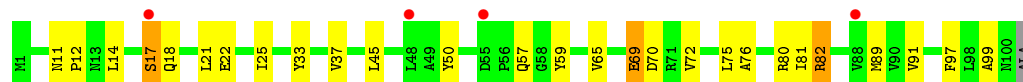
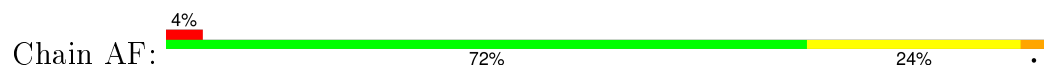




• Molecule 5: 30S ribosomal protein S5



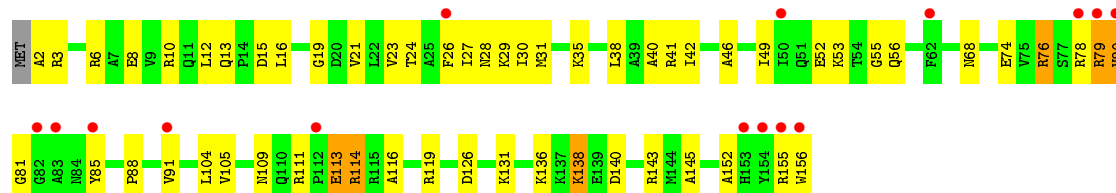
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

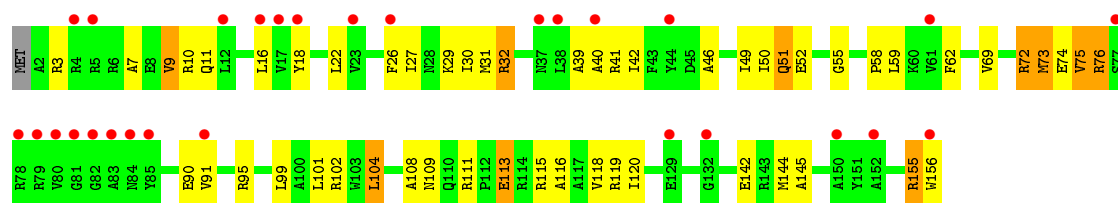


• Molecule 7: 30S ribosomal protein S7

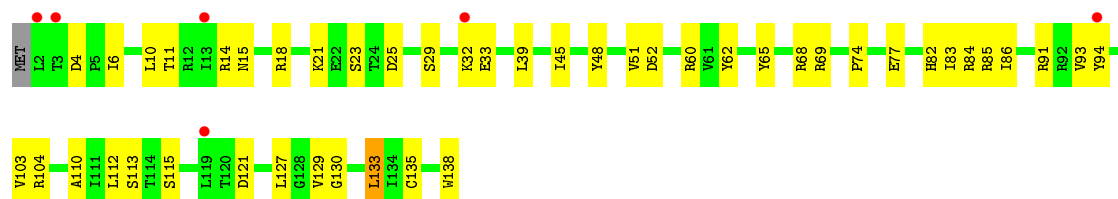


• Molecule 7: 30S ribosomal protein S7

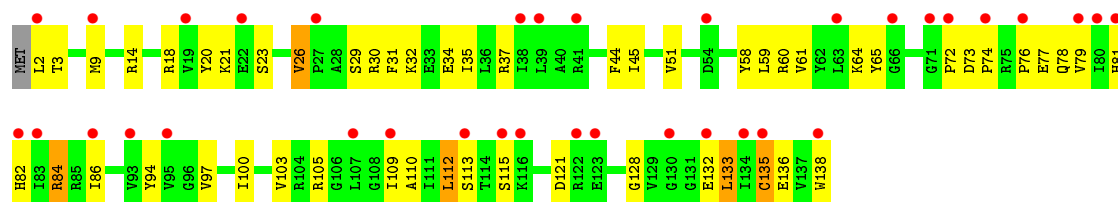




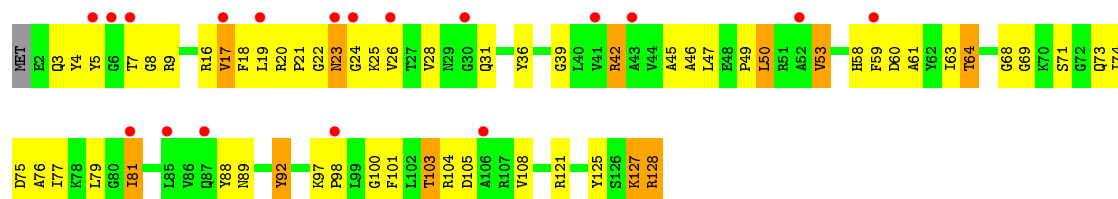
• Molecule 8: 30S ribosomal protein S8



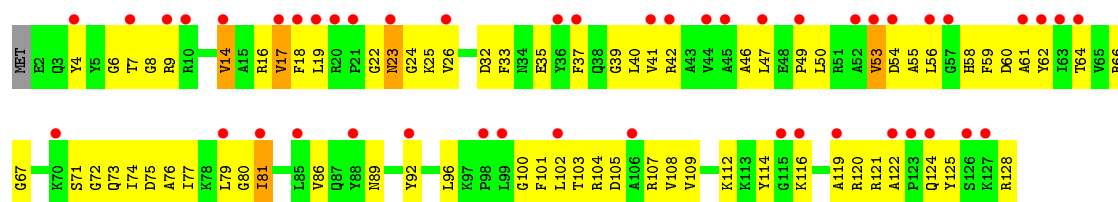
• Molecule 8: 30S ribosomal protein S8



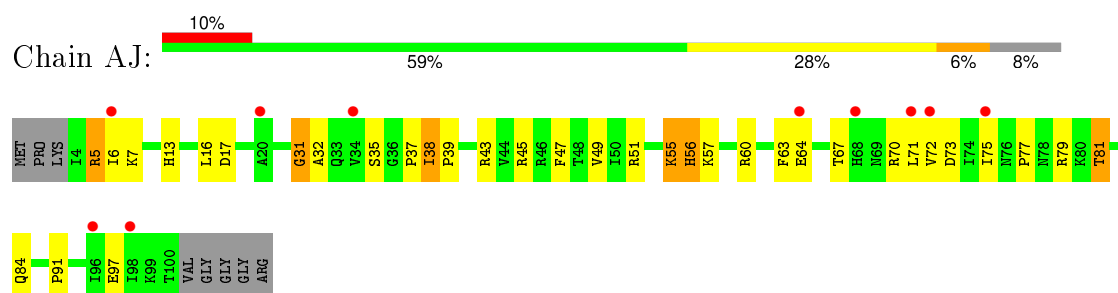
• Molecule 9: 30S ribosomal protein S9



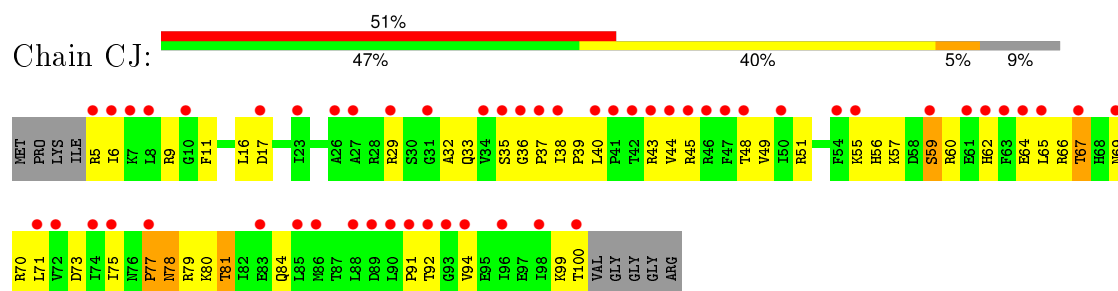
• Molecule 9: 30S ribosomal protein S9



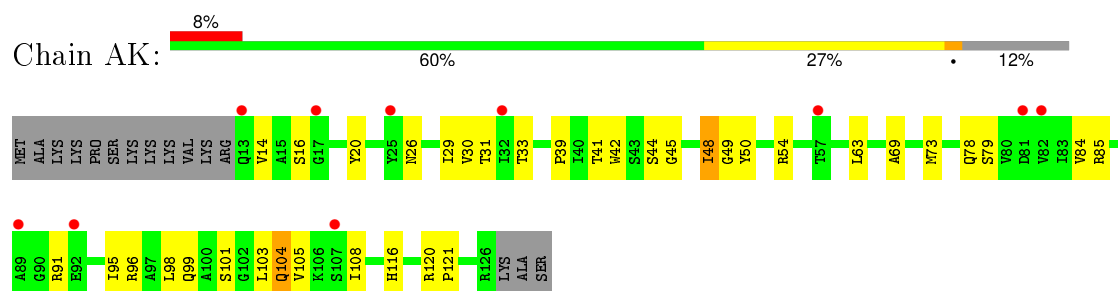
• Molecule 10: 30S ribosomal protein S10



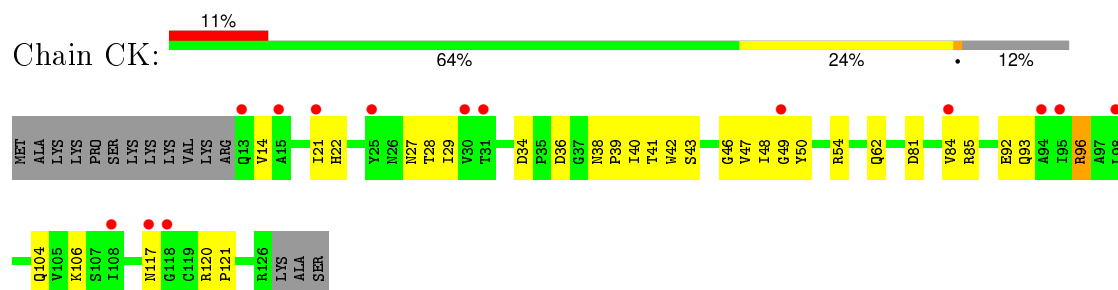
- Molecule 10: 30S ribosomal protein S10



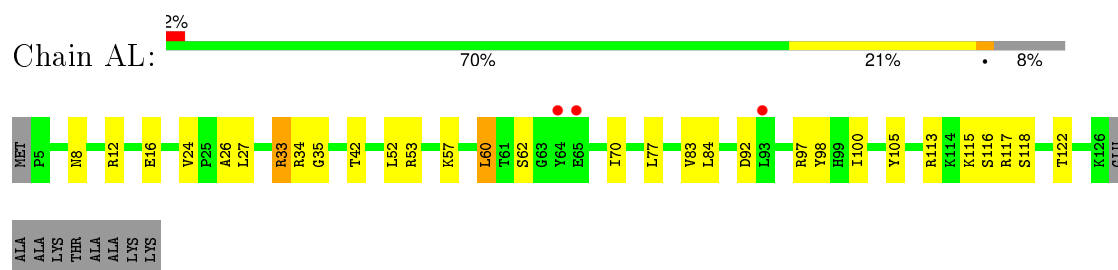
- Molecule 11: 30S ribosomal protein S11



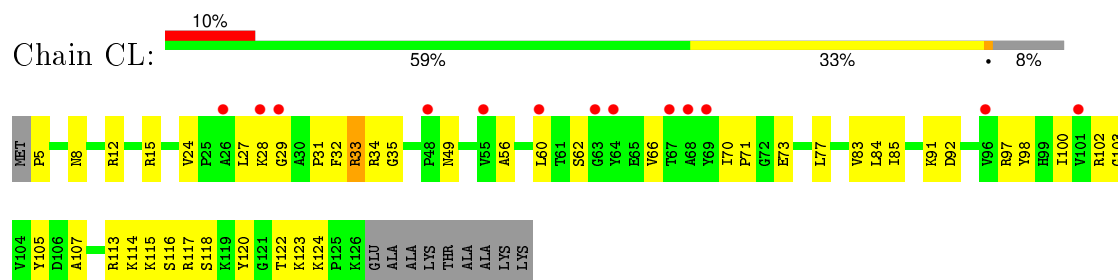
- Molecule 11: 30S ribosomal protein S11



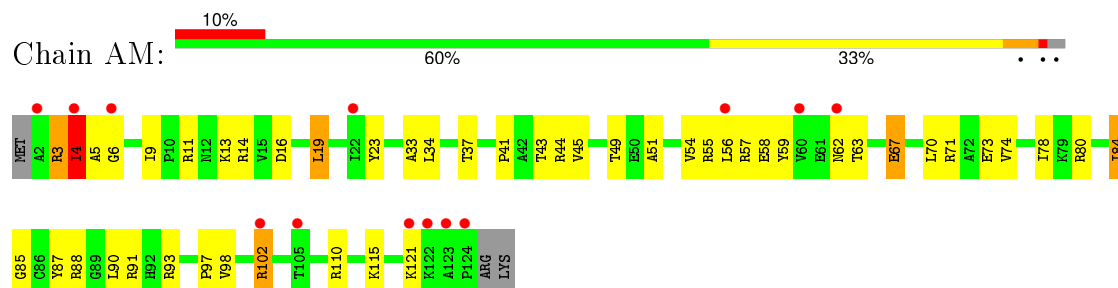
- Molecule 12: 30S ribosomal protein S12



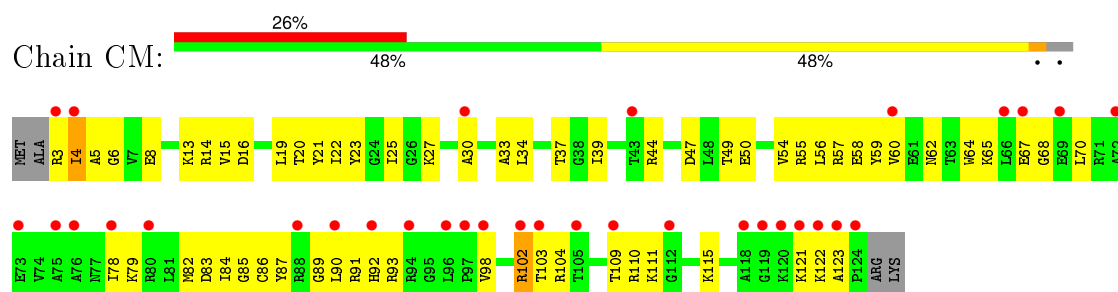
- Molecule 12: 30S ribosomal protein S12



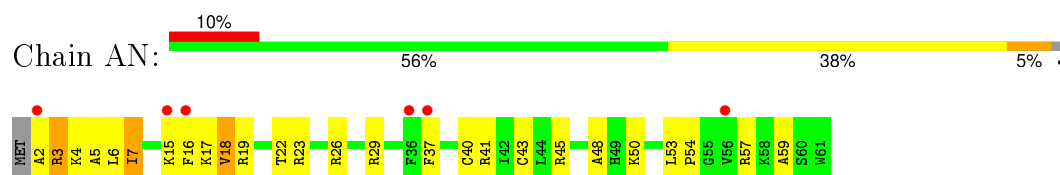
- Molecule 13: 30S ribosomal protein S13



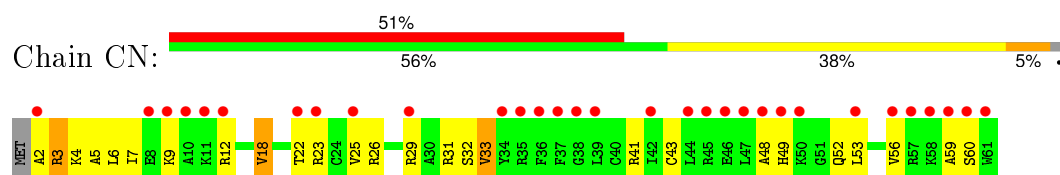
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z

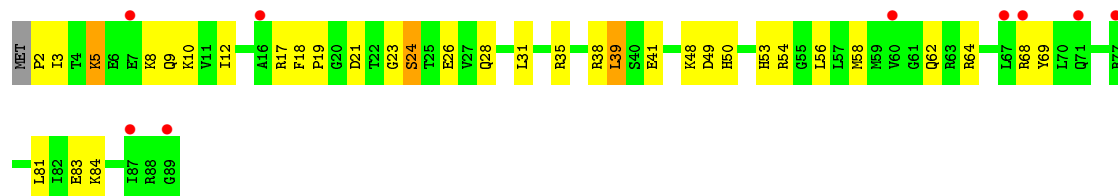


- Molecule 15: 30S ribosomal protein S15





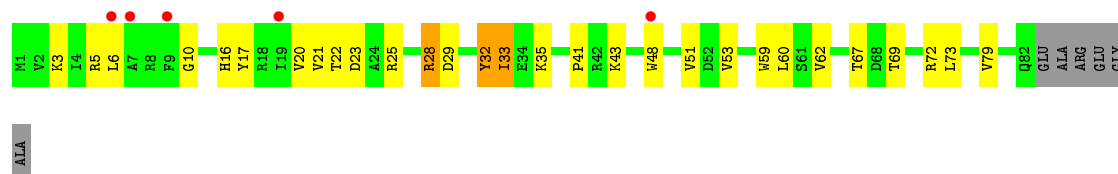
- Molecule 15: 30S ribosomal protein S15



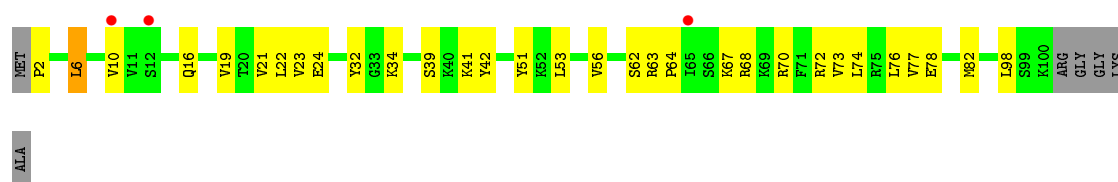
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16

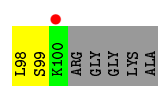


- Molecule 17: 30S ribosomal protein S17

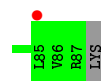
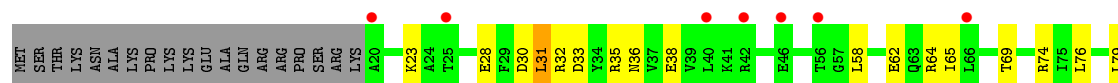


- Molecule 17: 30S ribosomal protein S17

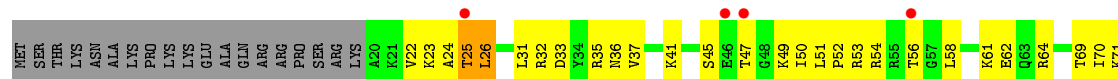
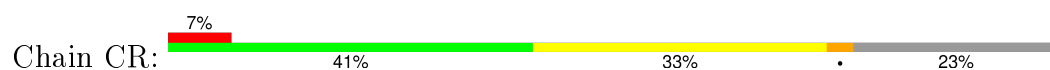




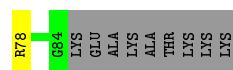
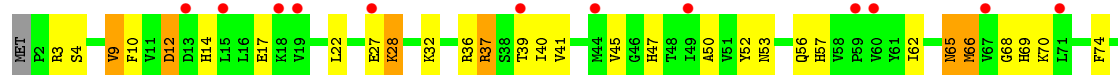
- Molecule 18: 30S ribosomal protein S18



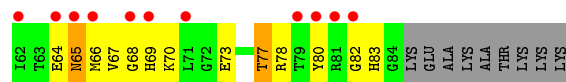
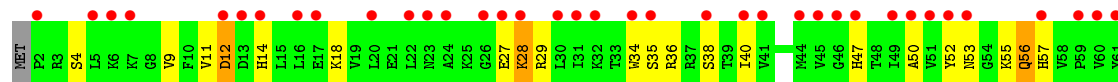
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

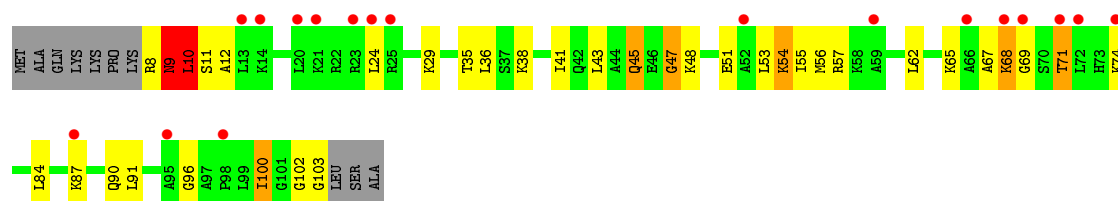


- Molecule 19: 30S ribosomal protein S19

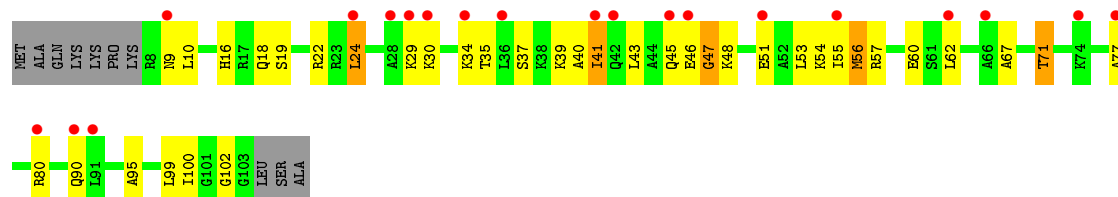


- Molecule 20: 30S ribosomal protein S20





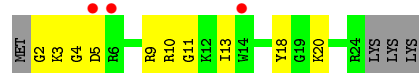
- Molecule 20: 30S ribosomal protein S20



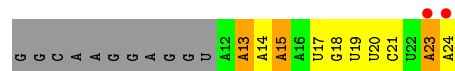
- Molecule 21: 30S ribosomal protein Thx



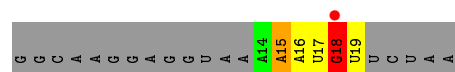
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: mRNA



- Molecule 22: mRNA



- Molecule 23: Cytidine-Puromycin





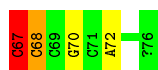
- Molecule 23: Cytidine-Puromycin

Chain CW: 33% 67%



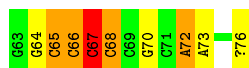
- Molecule 24: P-site tRNA

Chain AX: 32% 45% 19% ..



- Molecule 24: P-site tRNA

Chain CX: 22% 43% 31% ..



- Molecule 25: E-site tRNA

Chain AY: 93%



- Molecule 25: E-site tRNA

Chain CY: 5% 93%

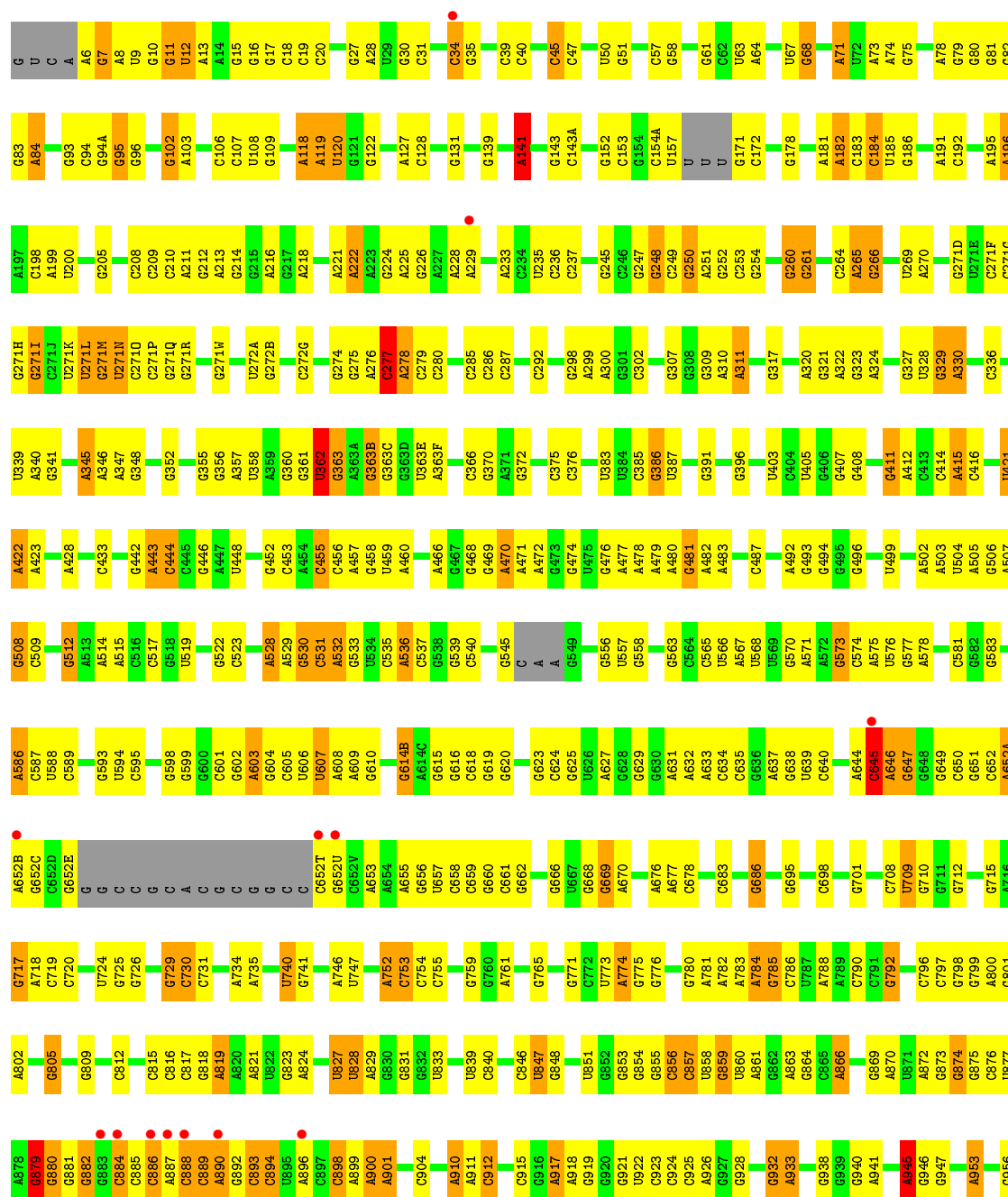


- Molecule 26: 23S Ribosomal RNA

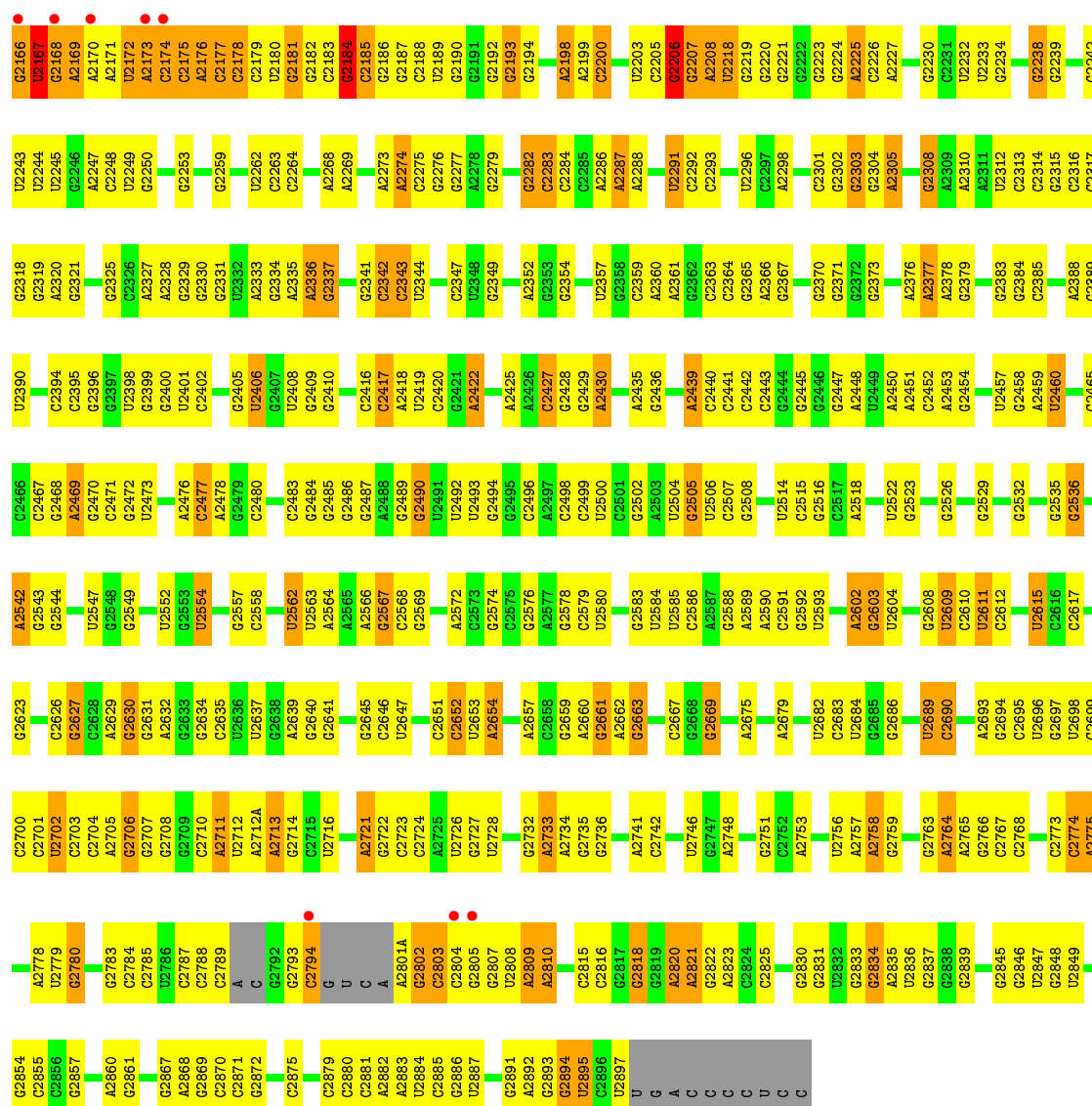
Chain BA: 51% 36% 9% ..





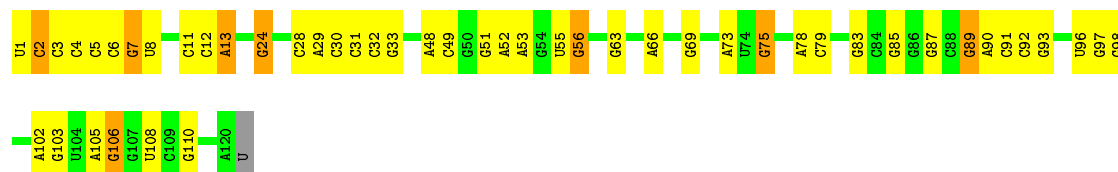






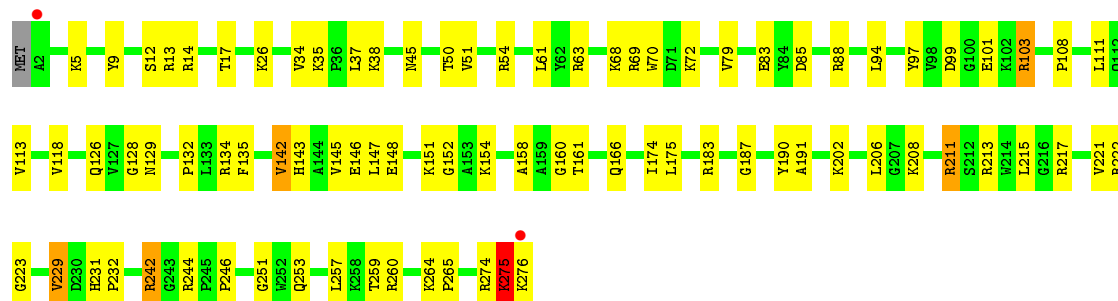
• Molecule 27: 5S Ribosomal RNA

Chain BB: 59% 34% 7%

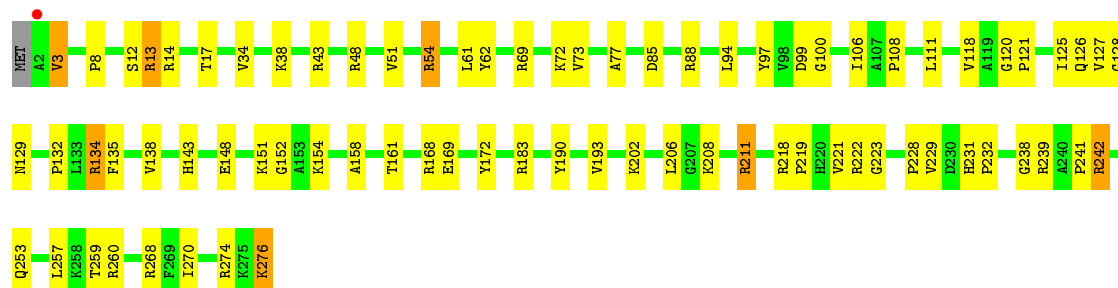




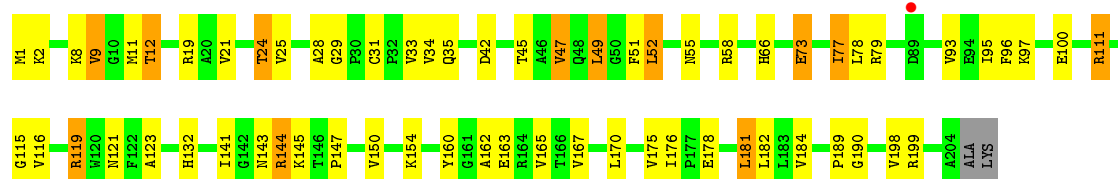
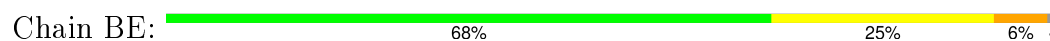
• Molecule 28: 50S ribosomal protein L2



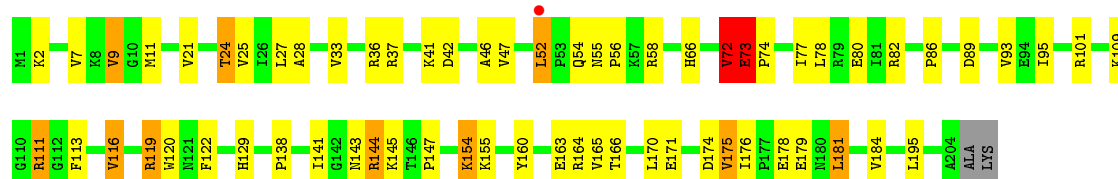
• Molecule 28: 50S ribosomal protein L2



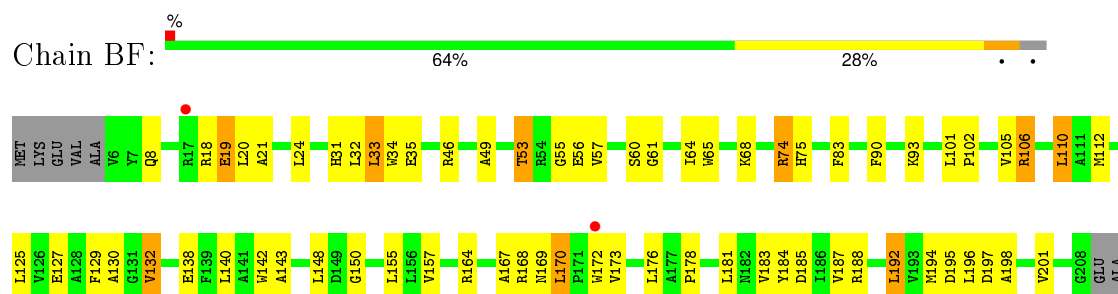
• Molecule 29: 50S ribosomal protein L3



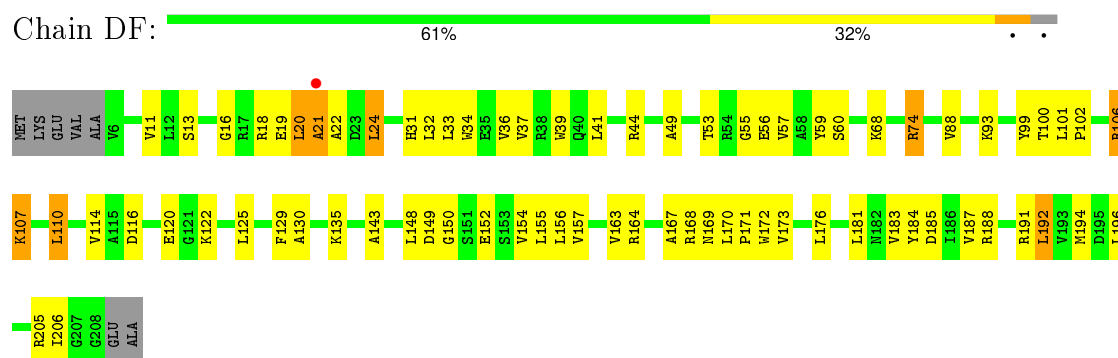
• Molecule 29: 50S ribosomal protein L3



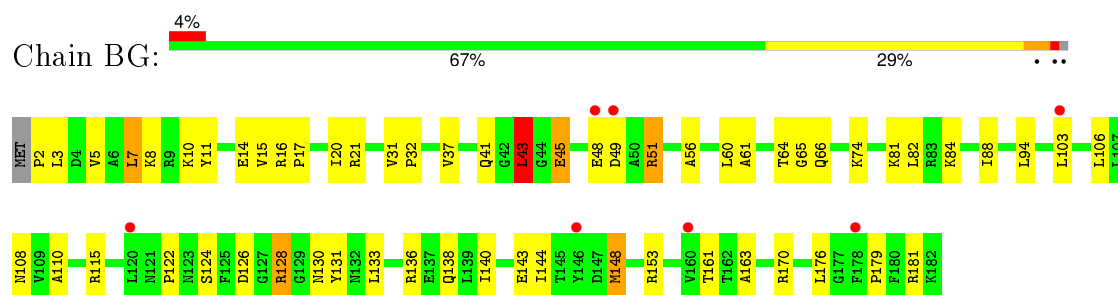
- Molecule 30: 50S ribosomal protein L4



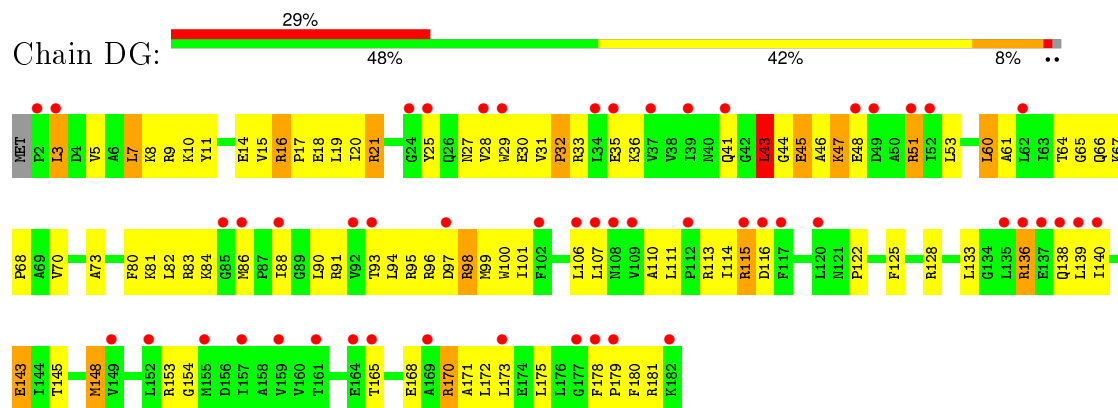
- Molecule 30: 50S ribosomal protein L4



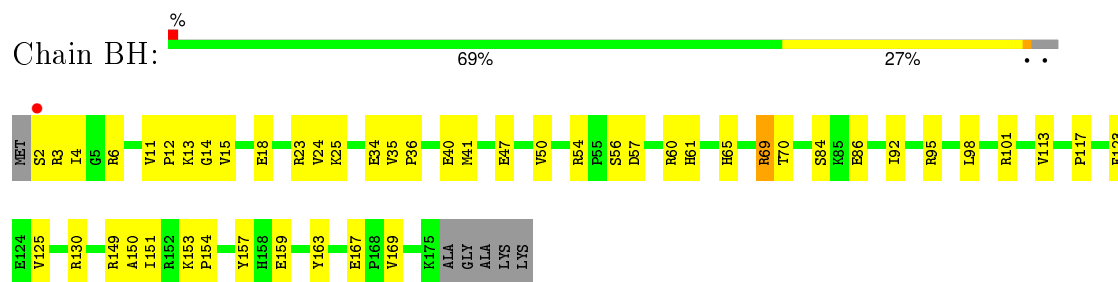
- Molecule 31: 50S ribosomal protein L5



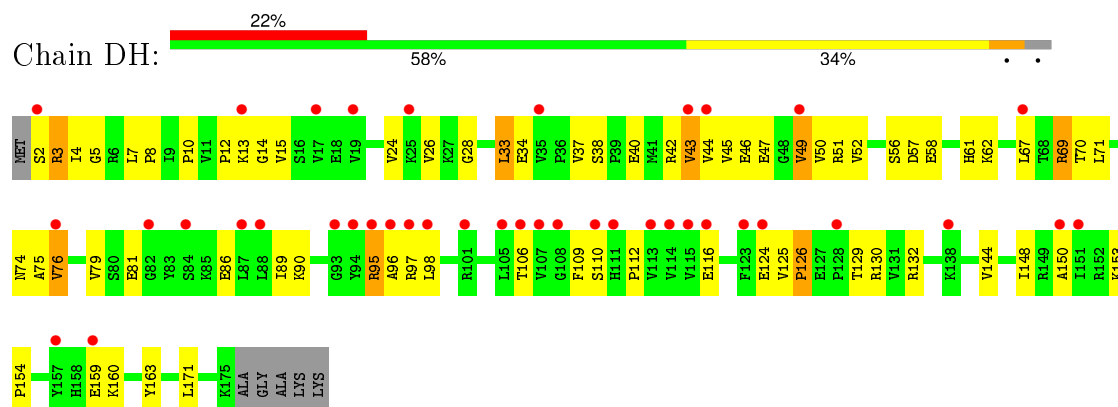
- Molecule 31: 50S ribosomal protein L5



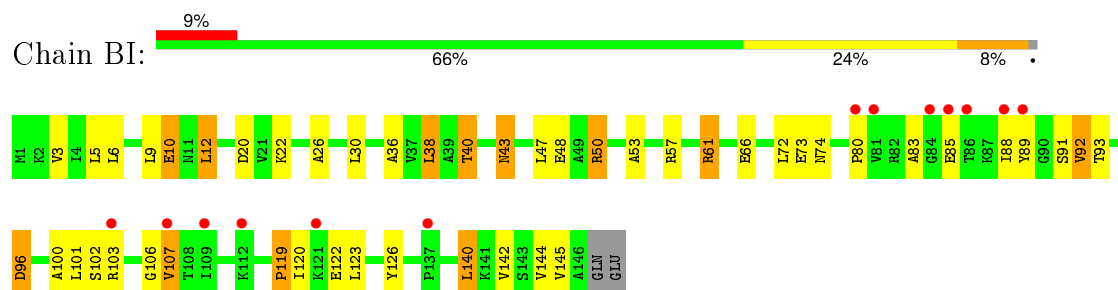
- Molecule 32: 50S ribosomal protein L6



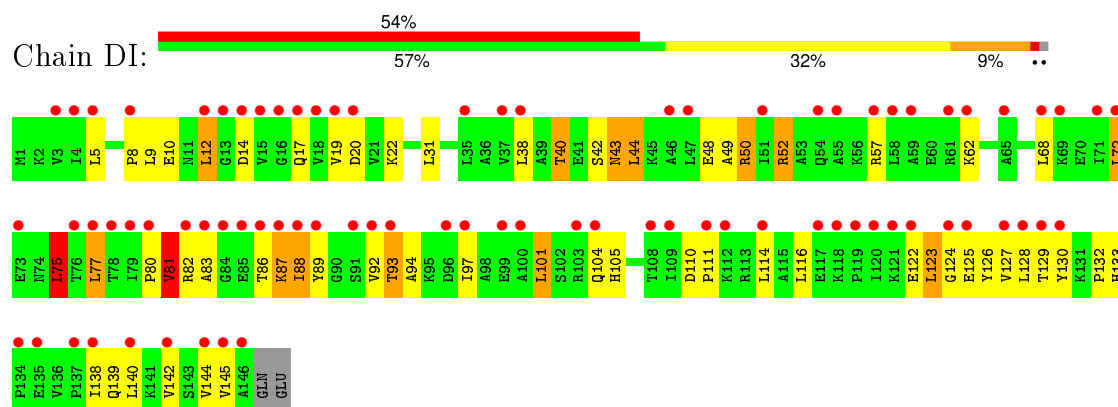
• Molecule 32: 50S ribosomal protein L6



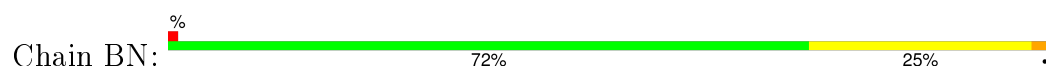
• Molecule 33: 50S ribosomal protein L9

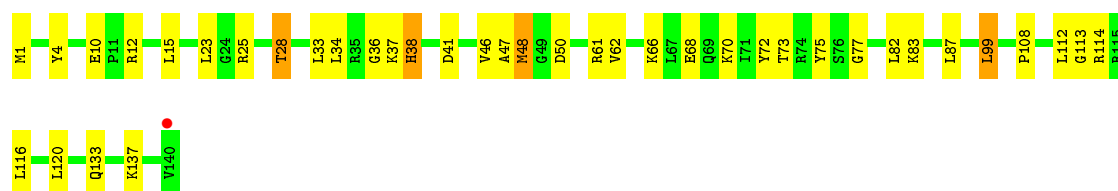


• Molecule 33: 50S ribosomal protein L9

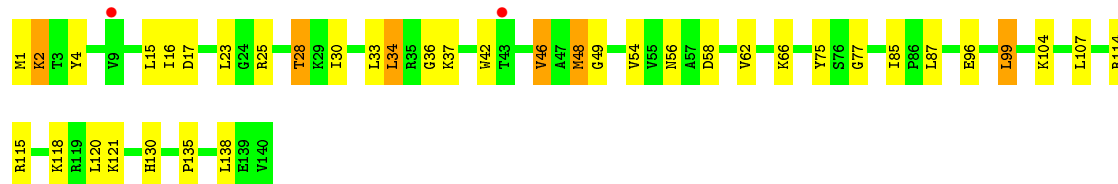
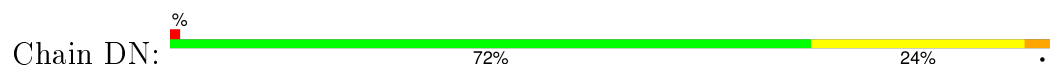


• Molecule 34: 50S ribosomal protein L13

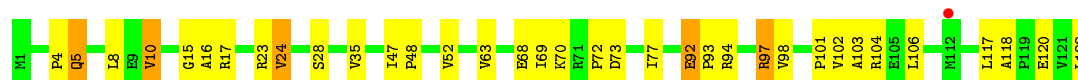
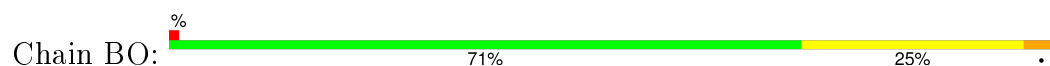




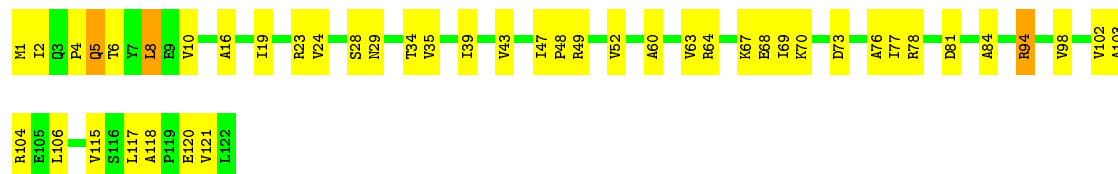
- Molecule 34: 50S ribosomal protein L13



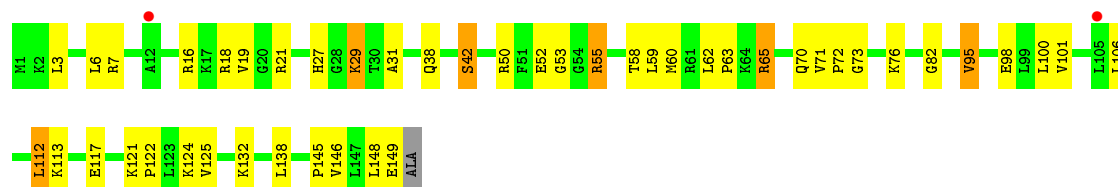
- Molecule 35: 50S ribosomal protein L14



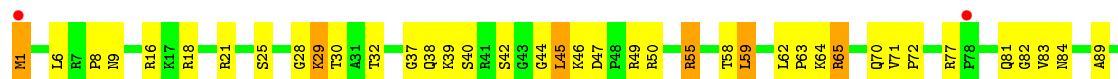
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15



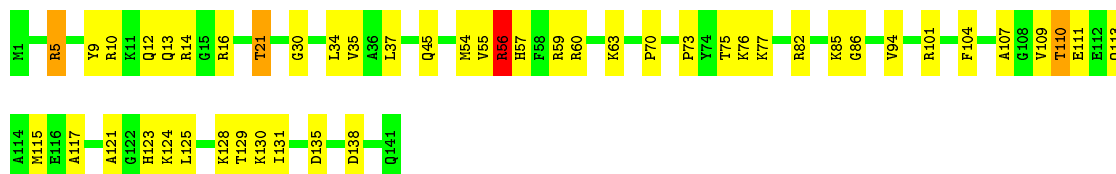
- Molecule 36: 50S ribosomal protein L15





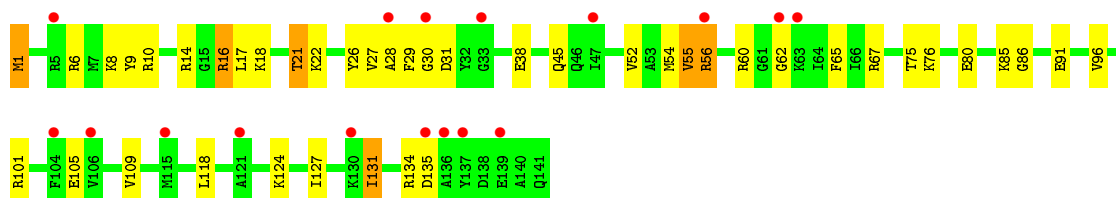
- Molecule 37: 50S ribosomal protein L16

Chain BQ: 66% 31% ..



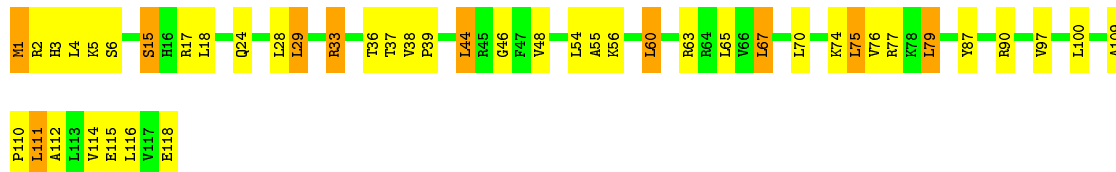
- Molecule 37: 50S ribosomal protein L16

Chain DQ: 12% 70% 26% .



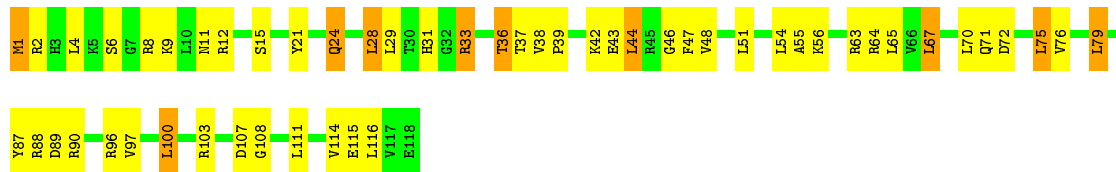
- Molecule 38: 50S ribosomal protein L17

Chain BR: 62% 30% 8%



- Molecule 38: 50S ribosomal protein L17

Chain DR: 55% 36% 8%

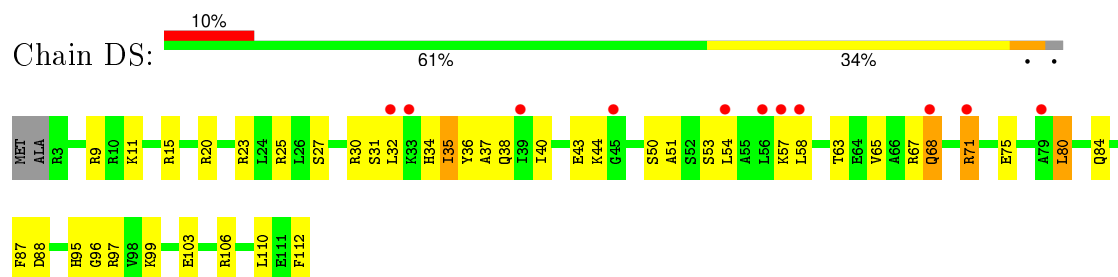


- Molecule 39: 50S ribosomal protein L18

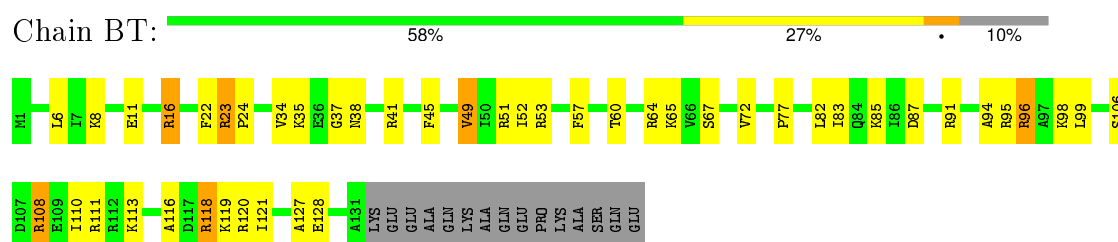
Chain BS: 69% 24% . . .



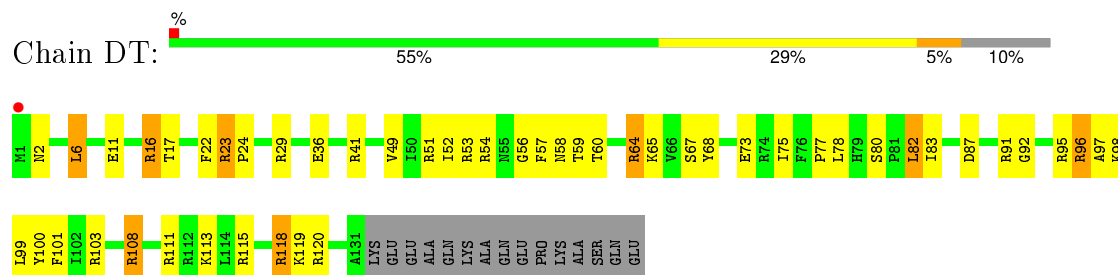
- Molecule 39: 50S ribosomal protein L18



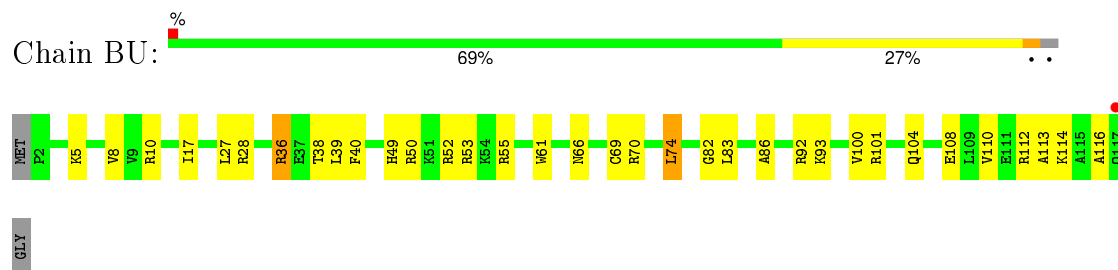
- Molecule 40: 50S ribosomal protein L19



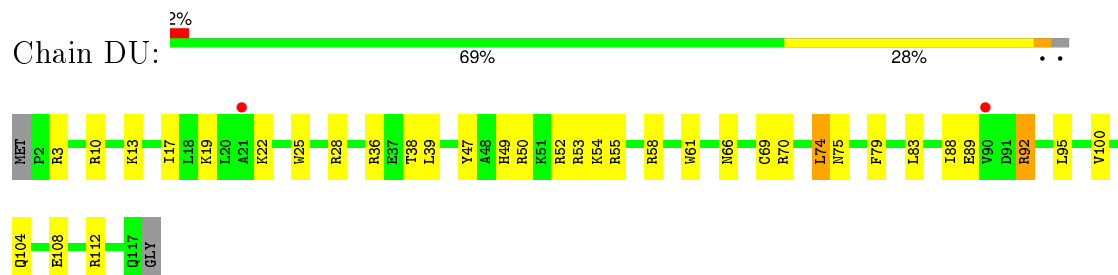
- Molecule 40: 50S ribosomal protein L19



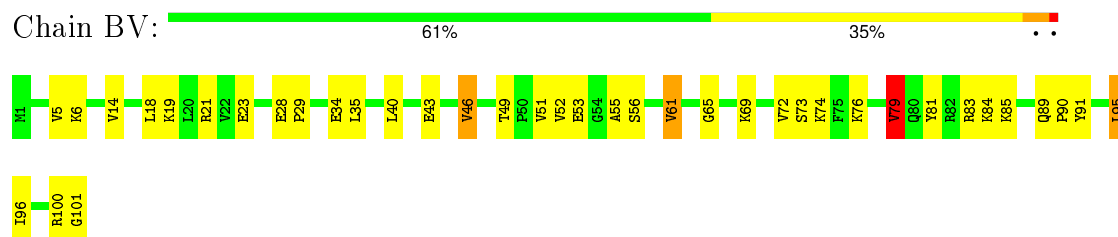
- Molecule 41: 50S ribosomal protein L20



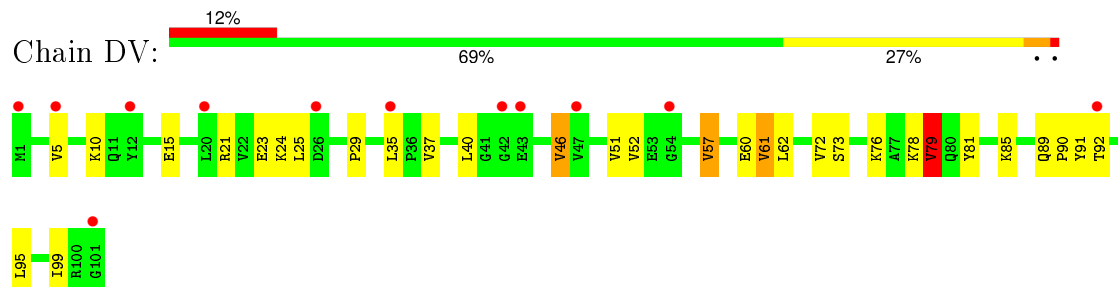
- Molecule 41: 50S ribosomal protein L20



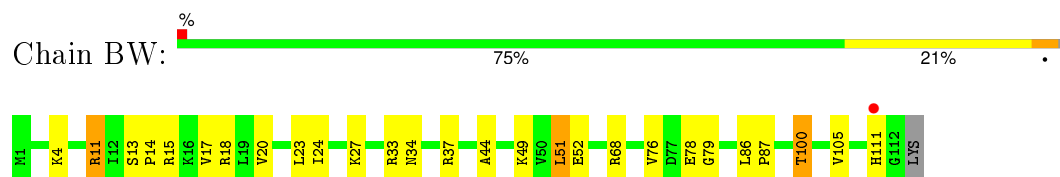
- Molecule 42: 50S ribosomal protein L21



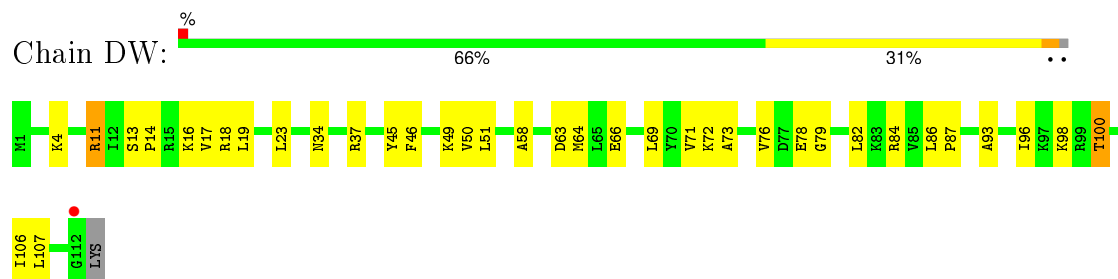
- Molecule 42: 50S ribosomal protein L21



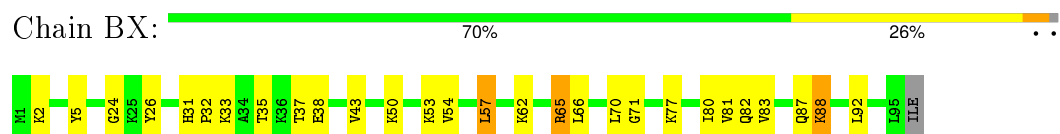
- Molecule 43: 50S ribosomal protein L22



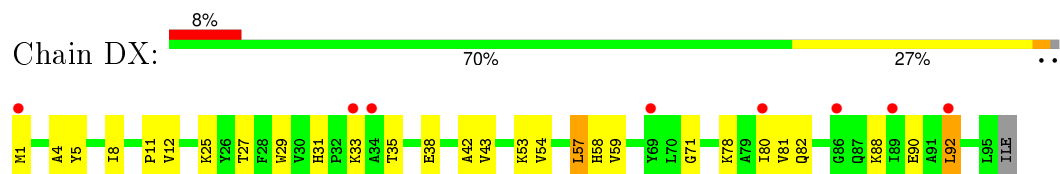
- Molecule 43: 50S ribosomal protein L22



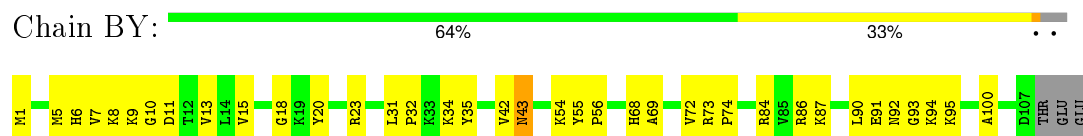
- Molecule 44: 50S ribosomal protein L23



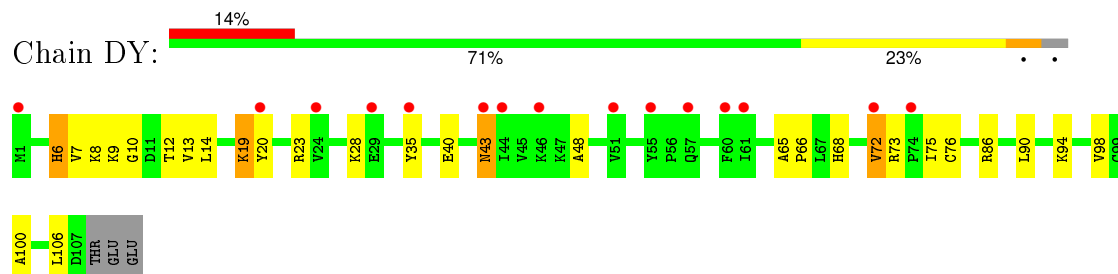
- Molecule 44: 50S ribosomal protein L23



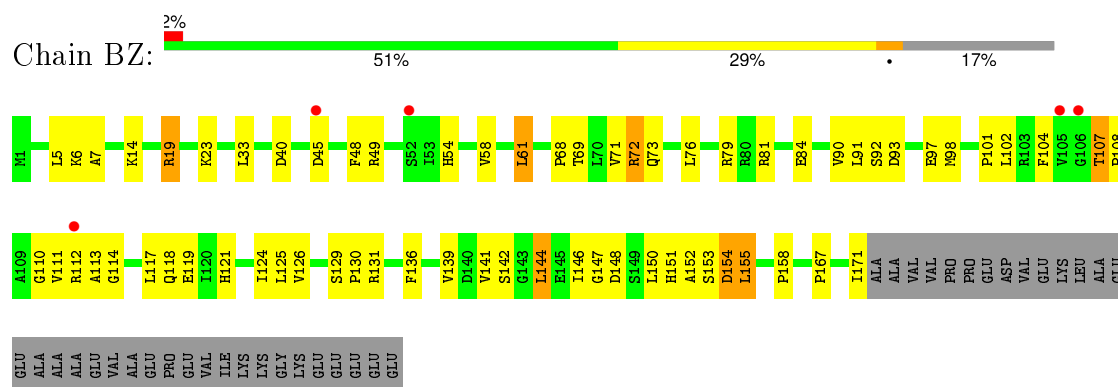
- Molecule 45: 50S ribosomal protein L24



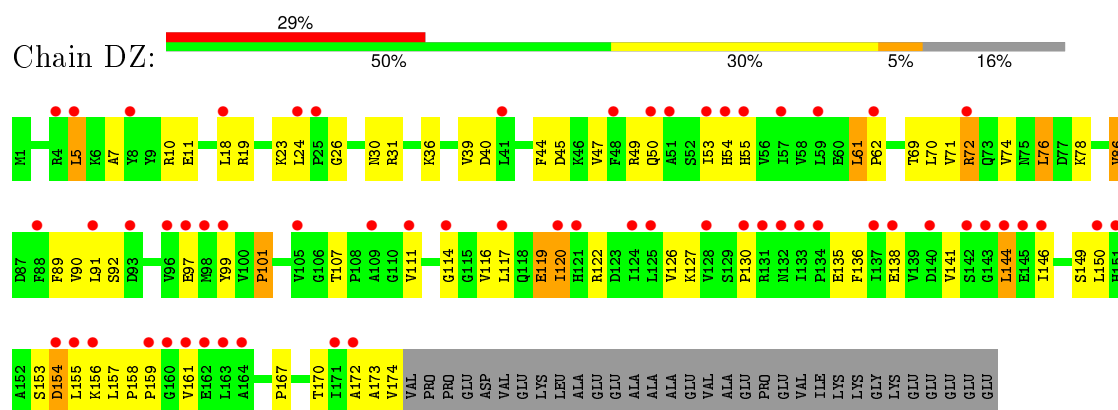
- Molecule 45: 50S ribosomal protein L24



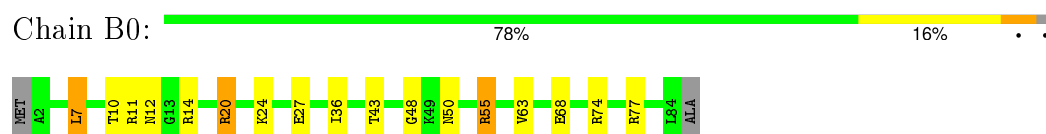
- Molecule 46: 50S ribosomal protein L25



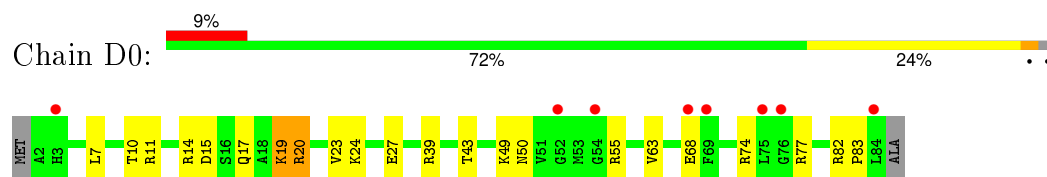
- Molecule 46: 50S ribosomal protein L25



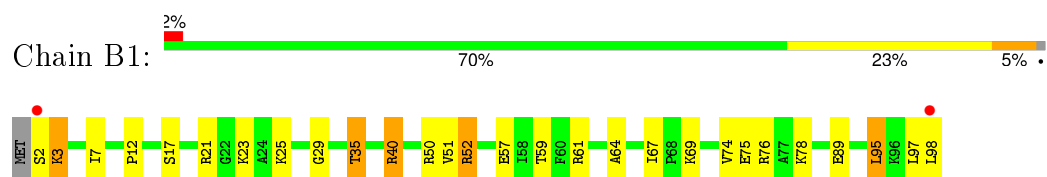
- Molecule 47: 50S ribosomal protein L27



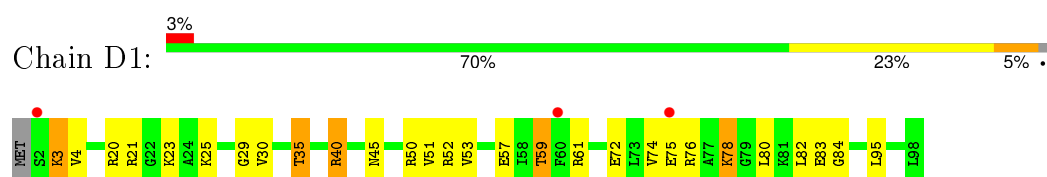
- Molecule 47: 50S ribosomal protein L27



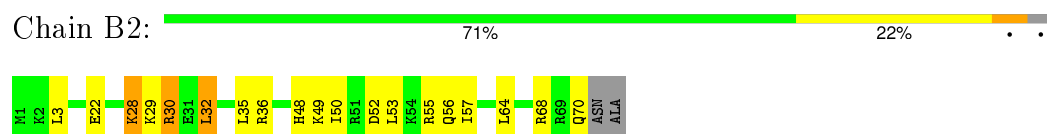
- Molecule 48: 50S ribosomal protein L28



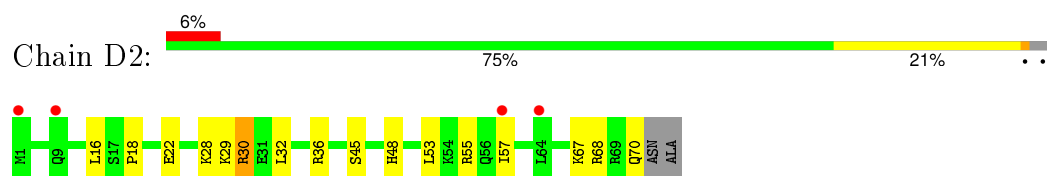
- Molecule 48: 50S ribosomal protein L28



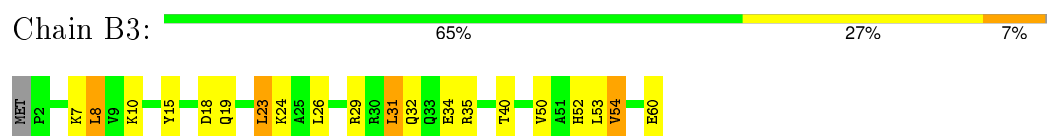
- Molecule 49: 50S ribosomal protein L29



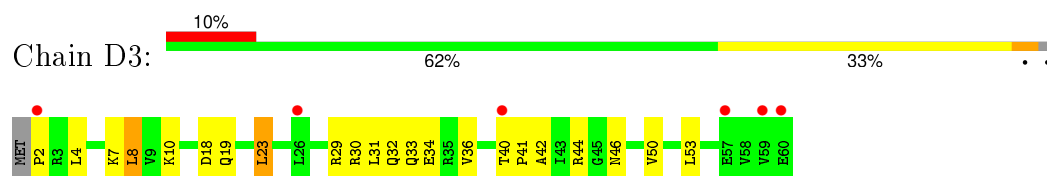
- Molecule 49: 50S ribosomal protein L29



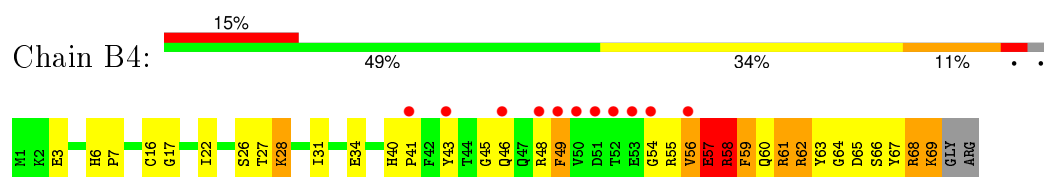
- Molecule 50: 50S ribosomal protein L30



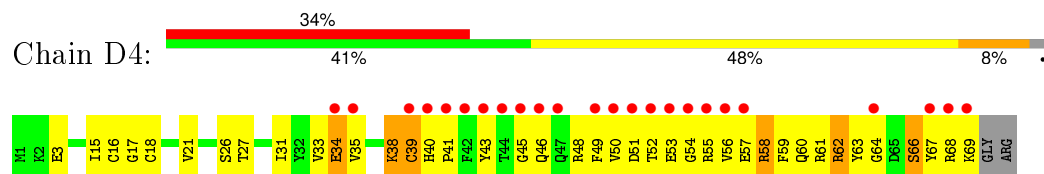
- Molecule 50: 50S ribosomal protein L30



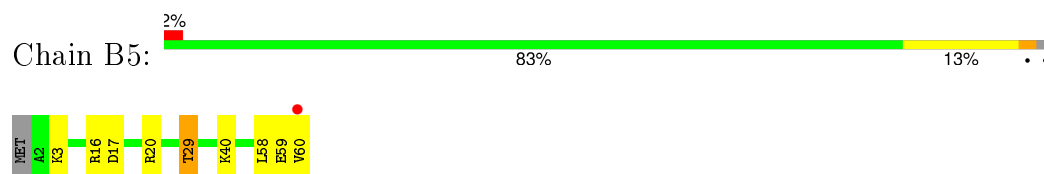
- Molecule 51: 50S ribosomal protein L31



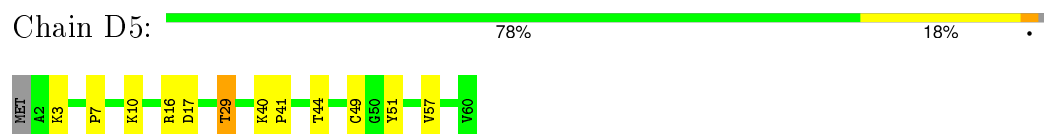
- Molecule 51: 50S ribosomal protein L31



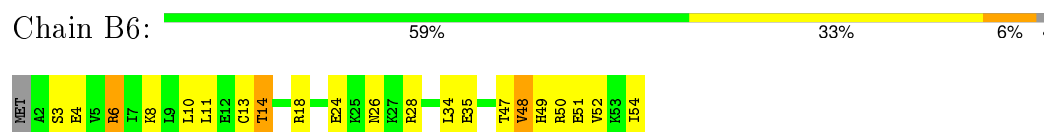
- Molecule 52: 50S ribosomal protein L32



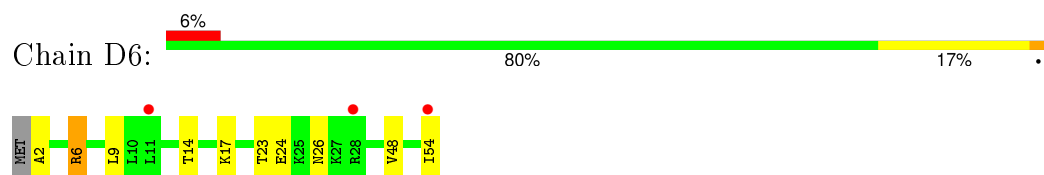
- Molecule 52: 50S ribosomal protein L32



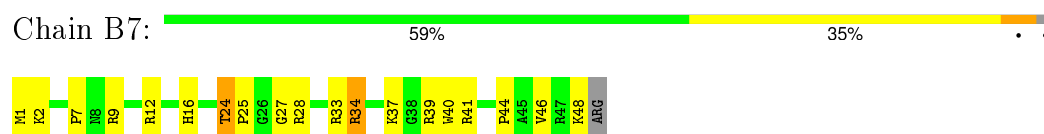
- Molecule 53: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L33

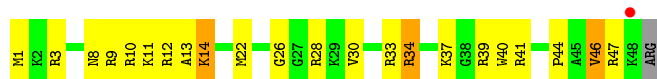


- Molecule 54: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L34

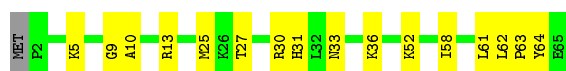
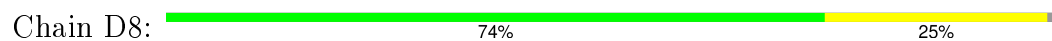




- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.56Å 444.23Å 613.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	150.38 – 2.80 150.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (150.38-2.80) 98.0 (150.38-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.234 , 0.280 0.239 , 0.284	Depositor DCC
R_{free} test set	67651 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 1345521 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	290205	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, PPU, K, ZN, 31H, 5MC, 4SU, SF4, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.41	4/36049 (0.0%)	0.98	71/56261 (0.1%)
1	CA	0.42	7/36170 (0.0%)	1.05	147/56452 (0.3%)
2	AB	0.29	0/1881	0.59	0/2542
2	CB	0.33	0/1860	0.68	3/2518 (0.1%)
3	AC	0.28	0/1576	0.52	0/2130
3	CC	0.30	0/1566	0.58	0/2119
4	AD	0.28	0/1689	0.55	0/2267
4	CD	0.30	0/1704	0.56	0/2284
5	AE	0.29	0/1145	0.52	0/1543
5	CE	0.30	0/1149	0.58	1/1548 (0.1%)
6	AF	0.29	0/819	0.50	0/1111
6	CF	0.30	0/829	0.49	0/1123
7	AG	0.27	0/1250	0.51	0/1679
7	CG	0.29	0/1254	0.53	0/1683
8	AH	0.27	0/1108	0.51	0/1494
8	CH	0.27	0/1108	0.55	0/1494
9	AI	0.28	0/1002	0.54	0/1346
9	CI	0.30	0/997	0.56	0/1343
10	AJ	0.27	0/722	0.60	0/982
10	CJ	0.30	0/727	0.57	0/988
11	AK	0.29	0/844	0.50	0/1145
11	CK	0.27	0/848	0.50	0/1149
12	AL	0.29	0/946	0.51	0/1274
12	CL	0.29	0/946	0.56	0/1274
13	AM	0.28	0/969	0.58	0/1302
13	CM	0.29	0/961	0.57	0/1291
14	AN	0.30	0/501	0.55	0/664
14	CN	0.32	0/501	0.55	0/664
15	AO	0.27	0/739	0.53	0/985
15	CO	0.30	0/739	0.54	0/985
16	AP	0.29	0/697	0.53	0/939
16	CP	0.28	0/693	0.54	0/935

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.29	0/836	0.55	0/1117
17	CQ	0.29	0/836	0.53	0/1117
18	AR	0.27	0/560	0.48	0/746
18	CR	0.28	0/560	0.52	0/746
19	AS	0.28	0/667	0.54	0/900
19	CS	0.30	0/661	0.68	0/893
20	AT	0.27	0/730	0.58	0/965
20	CT	0.27	0/729	0.52	0/965
21	AU	0.29	0/203	0.56	0/266
21	CU	0.32	0/203	0.48	0/266
22	AV	0.49	0/310	0.95	1/480 (0.2%)
22	CV	1.15	3/144 (2.1%)	3.12	11/222 (5.0%)
23	AW	0.45	0/40	1.07	0/60
23	CW	0.35	0/40	1.09	0/60
24	AX	0.53	2/1700 (0.1%)	1.24	23/2650 (0.9%)
24	CX	0.54	0/1700	1.36	19/2650 (0.7%)
25	AY	0.33	0/115	0.82	0/176
25	CY	0.29	0/115	0.95	0/176
26	BA	0.50	4/68013 (0.0%)	0.93	70/106165 (0.1%)
26	DA	0.42	0/67542	0.94	88/105428 (0.1%)
27	BB	0.41	0/2878	0.91	2/4490 (0.0%)
27	DB	0.41	0/2878	1.00	8/4490 (0.2%)
28	BD	0.37	0/2186	0.57	0/2944
28	DD	0.34	0/2186	0.56	0/2944
29	BE	0.36	0/1592	0.53	0/2149
29	DE	0.34	0/1592	0.59	1/2149 (0.0%)
30	BF	0.35	0/1619	0.53	0/2193
30	DF	0.33	0/1615	0.56	0/2188
31	BG	0.29	0/1450	0.54	0/1959
31	DG	0.32	0/1449	0.57	0/1958
32	BH	0.30	0/1356	0.51	0/1834
32	DH	0.29	0/1356	0.51	0/1834
33	BI	0.31	0/1100	0.59	0/1501
33	DI	0.37	0/1076	0.78	4/1471 (0.3%)
34	BN	0.34	0/1144	0.54	0/1543
34	DN	0.31	0/1144	0.52	0/1543
35	BO	0.34	0/943	0.56	0/1269
35	DO	0.33	0/943	0.55	1/1269 (0.1%)
36	BP	0.35	0/1152	0.57	0/1533
36	DP	0.32	0/1152	0.63	0/1533
37	BQ	0.35	0/1143	0.59	1/1527 (0.1%)
37	DQ	0.32	0/1143	0.54	0/1527
38	BR	0.36	0/982	0.57	0/1312

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.29	0/982	0.55	0/1312
39	BS	0.32	0/887	0.57	1/1180 (0.1%)
39	DS	0.29	0/880	0.57	0/1172
40	BT	0.34	0/1105	0.61	0/1477
40	DT	0.30	0/1097	0.53	0/1468
41	BU	0.35	0/977	0.53	0/1301
41	DU	0.28	0/977	0.50	0/1301
42	BV	0.36	0/782	0.55	0/1049
42	DV	0.29	0/782	0.54	0/1049
43	BW	0.35	0/897	0.53	0/1205
43	DW	0.30	0/897	0.49	0/1205
44	BX	0.39	0/764	0.58	1/1025 (0.1%)
44	DX	0.32	0/764	0.53	1/1025 (0.1%)
45	BY	0.34	0/819	0.59	0/1095
45	DY	0.30	0/819	0.55	0/1095
46	BZ	0.32	0/1379	0.58	0/1873
46	DZ	0.29	0/1390	0.54	0/1890
47	B0	0.36	0/662	0.60	0/881
47	D0	0.30	0/662	0.50	0/881
48	B1	0.32	0/762	0.53	0/1014
48	D1	0.31	0/762	0.53	0/1014
49	B2	0.32	0/590	0.57	0/781
49	D2	0.26	0/590	0.49	0/781
50	B3	0.35	0/474	0.52	0/635
50	D3	0.31	0/469	0.54	0/630
51	B4	0.34	0/565	0.70	0/761
51	D4	0.32	0/545	0.67	0/737
52	B5	0.37	0/469	0.62	1/635 (0.2%)
52	D5	0.32	0/469	0.54	0/635
53	B6	0.36	0/460	0.53	0/613
53	D6	0.34	0/456	0.51	0/608
54	B7	0.36	0/426	0.56	0/561
54	D7	0.34	0/426	0.49	0/561
55	B8	0.37	0/519	0.54	0/684
55	D8	0.31	0/525	0.50	0/691
56	B9	0.43	0/310	0.65	0/407
56	D9	0.33	0/310	0.59	0/407
All	All	0.41	20/310421 (0.0%)	0.88	455/464361 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	AB	0	1
7	AG	0	1
20	AT	0	1
29	DE	0	1
33	DI	0	1
39	BS	0	1
46	BZ	0	1
51	B4	0	2
51	D4	0	1
All	All	0	10

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1154	G	C6-N1	-12.37	1.30	1.39
1	AA	1172	C	N3-C4	-10.50	1.26	1.33
1	CA	1154	G	N1-C2	-10.41	1.29	1.37
1	AA	1172	C	C2-N3	-8.49	1.28	1.35
1	AA	1164	G	N1-C2	-6.91	1.32	1.37

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1172	C	N1-C2-O2	39.76	142.76	118.90
1	CA	1119	C	N1-C2-O2	26.84	135.00	118.90
1	AA	1172	C	N3-C2-O2	-25.31	104.18	121.90
1	CA	1154	G	C5-C6-O6	24.22	143.13	128.60
1	CA	1154	G	N1-C2-N2	-23.61	94.95	116.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	8	LYS	Peptide
7	AG	79	ARG	Peptide
20	AT	9	ASN	Peptide
39	BS	58	LEU	Peptide
46	BZ	158	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32205	0	16255	743	1
1	CA	32312	0	16307	964	1
2	AB	1846	0	1867	74	0
2	CB	1825	0	1828	76	0
3	AC	1552	0	1546	49	0
3	CC	1542	0	1517	58	0
4	AD	1659	0	1676	74	0
4	CD	1674	0	1714	83	0
5	AE	1129	0	1184	33	0
5	CE	1133	0	1191	39	0
6	AF	806	0	793	16	0
6	CF	816	0	808	23	0
7	AG	1231	0	1238	37	0
7	CG	1235	0	1249	38	0
8	AH	1088	0	1126	35	0
8	CH	1088	0	1126	40	0
9	AI	983	0	986	48	0
9	CI	978	0	966	53	0
10	AJ	709	0	650	35	0
10	CJ	714	0	672	38	0
11	AK	829	0	825	23	0
11	CK	833	0	836	20	0
12	AL	930	0	980	21	0
12	CL	930	0	980	33	0
13	AM	958	0	1002	37	0
13	CM	950	0	988	47	0
14	AN	492	0	529	27	0
14	CN	492	0	529	23	0
15	AO	728	0	760	22	0
15	CO	728	0	760	27	0
16	AP	681	0	697	27	0
16	CP	677	0	686	26	0
17	AQ	823	0	891	23	0
17	CQ	823	0	891	18	0
18	AR	555	0	618	11	0
18	CR	555	0	618	23	0
19	AS	652	0	662	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	CS	646	0	644	40	0
20	AT	728	0	798	27	0
20	CT	727	0	796	23	0
21	AU	199	0	208	5	0
21	CU	199	0	208	8	0
22	AV	277	0	140	7	0
22	CV	129	0	65	16	0
23	AW	74	0	51	5	0
23	CW	74	0	51	11	0
24	AX	1633	0	836	35	0
24	CX	1635	0	838	83	0
25	AY	104	0	56	3	0
25	CY	104	0	56	2	0
26	BA	60729	0	30620	950	0
26	DA	60311	0	30412	1223	1
27	BB	2573	0	1306	32	0
27	DB	2573	0	1306	87	0
28	BD	2136	0	2218	67	0
28	DD	2136	0	2218	74	0
29	BE	1559	0	1618	43	0
29	DE	1559	0	1618	56	0
30	BF	1584	0	1625	49	0
30	DF	1580	0	1619	55	0
31	BG	1425	0	1443	37	0
31	DG	1424	0	1434	73	0
32	BH	1330	0	1407	29	0
32	DH	1330	0	1407	44	0
33	BI	1085	0	1114	28	1
33	DI	1061	0	1080	50	0
34	BN	1117	0	1184	21	0
34	DN	1117	0	1184	29	0
35	BO	933	0	996	27	0
35	DO	933	0	996	38	0
36	BP	1135	0	1212	53	0
36	DP	1135	0	1212	61	0
37	BQ	1122	0	1179	38	0
37	DQ	1122	0	1179	33	0
38	BR	968	0	1033	26	1
38	DR	968	0	1033	36	0
39	BS	877	0	938	28	0
39	DS	870	0	923	29	0
40	BT	1091	0	1151	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	DT	1083	0	1136	39	0
41	BU	959	0	1019	24	0
41	DU	959	0	1018	29	0
42	BV	771	0	830	21	1
42	DV	771	0	830	24	0
43	BW	886	0	940	15	0
43	DW	886	0	940	20	0
44	BX	750	0	814	24	0
44	DX	750	0	814	19	0
45	BY	806	0	881	24	0
45	DY	806	0	881	19	0
46	BZ	1349	0	1355	38	0
46	DZ	1360	0	1363	47	0
47	B0	653	0	674	20	0
47	D0	653	0	674	19	0
48	B1	755	0	826	19	0
48	D1	755	0	826	20	0
49	B2	588	0	643	8	0
49	D2	588	0	643	9	0
50	B3	469	0	518	15	0
50	D3	464	0	514	15	0
51	B4	552	0	533	32	0
51	D4	532	0	503	28	0
52	B5	455	0	465	8	0
52	D5	455	0	465	10	0
53	B6	453	0	473	13	0
53	D6	449	0	469	6	0
54	B7	418	0	467	19	0
54	D7	418	0	467	15	0
55	B8	511	0	571	29	0
55	D8	517	0	582	14	0
56	B9	307	0	335	8	0
56	D9	307	0	335	10	0
57	AA	207	0	0	0	0
57	AD	2	0	0	0	0
57	AE	2	0	0	0	0
57	AF	1	0	0	0	0
57	AJ	1	0	0	0	0
57	AK	1	0	0	0	0
57	AM	1	0	0	0	0
57	AN	2	0	0	0	0
57	AS	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AV	1	0	0	0	0
57	AW	1	0	0	0	0
57	AX	11	0	0	0	0
57	B0	4	0	0	0	0
57	B1	1	0	0	0	0
57	B2	1	0	0	0	0
57	B3	2	0	0	0	0
57	B5	2	0	0	0	0
57	B7	3	0	0	0	0
57	B8	1	0	0	0	0
57	B9	1	0	0	0	0
57	BA	720	0	0	0	0
57	BB	20	0	0	0	0
57	BD	11	0	0	0	0
57	BE	7	0	0	0	0
57	BF	10	0	0	0	0
57	BG	2	0	0	0	0
57	BN	6	0	0	0	0
57	BO	1	0	0	0	0
57	BP	4	0	0	0	0
57	BQ	5	0	0	0	0
57	BR	3	0	0	0	0
57	BU	8	0	0	0	0
57	BV	4	0	0	0	0
57	BW	5	0	0	0	0
57	BX	1	0	0	0	0
57	BY	1	0	0	0	0
57	BZ	1	0	0	0	0
57	CA	160	0	0	0	0
57	CE	1	0	0	0	0
57	CF	1	0	0	0	0
57	CJ	1	0	0	0	0
57	CK	1	0	0	0	0
57	CT	1	0	0	0	0
57	CW	1	0	0	0	0
57	CX	2	0	0	0	0
57	D3	1	0	0	0	0
57	D5	1	0	0	0	0
57	D8	2	0	0	0	0
57	DA	629	0	0	0	0
57	DB	10	0	0	0	0
57	DD	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DE	4	0	0	0	0
57	DF	4	0	0	0	0
57	DG	1	0	0	0	0
57	DN	1	0	0	0	0
57	DO	1	0	0	0	0
57	DP	2	0	0	0	0
57	DQ	3	0	0	0	0
57	DR	2	0	0	0	0
57	DU	4	0	0	0	0
57	DV	2	0	0	0	0
57	DW	2	0	0	0	0
57	DY	1	0	0	0	0
58	AD	8	0	0	1	0
58	CD	8	0	0	1	0
59	AN	1	0	0	0	0
59	B4	1	0	0	0	0
59	B5	1	0	0	0	0
59	B6	1	0	0	0	0
59	B9	1	0	0	0	0
59	BY	1	0	0	0	0
59	CN	1	0	0	0	0
59	D4	1	0	0	0	0
59	D5	1	0	0	0	0
59	D6	1	0	0	0	0
59	D9	1	0	0	0	0
59	DY	1	0	0	0	0
60	AX	1	0	0	0	0
60	CX	1	0	0	0	0
61	AA	170	0	0	16	0
61	AL	2	0	0	1	0
61	AO	1	0	0	0	0
61	AU	1	0	0	1	0
61	AV	2	0	0	0	0
61	AW	3	0	0	0	0
61	B0	4	0	0	0	0
61	B1	1	0	0	0	0
61	B3	1	0	0	0	0
61	B5	5	0	0	0	0
61	B7	1	0	0	1	0
61	B8	7	0	0	0	0
61	BA	1102	0	0	59	0
61	BB	36	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	BD	8	0	0	1	0
61	BE	13	0	0	5	0
61	BF	4	0	0	0	0
61	BG	3	0	0	0	0
61	BI	1	0	0	0	0
61	BP	15	0	0	1	0
61	BQ	3	0	0	0	0
61	BR	1	0	0	1	0
61	BS	1	0	0	0	0
61	BT	3	0	0	0	0
61	BU	1	0	0	1	0
61	BV	4	0	0	0	0
61	BW	2	0	0	0	0
61	BX	2	0	0	0	0
61	CA	130	0	0	8	0
61	CE	1	0	0	0	0
61	CJ	2	0	0	0	0
61	CN	1	0	0	0	0
61	CT	1	0	0	0	0
61	CV	1	0	0	0	0
61	CW	1	0	0	0	0
61	CX	1	0	0	1	0
61	D0	5	0	0	1	0
61	D1	1	0	0	0	0
61	D3	2	0	0	0	0
61	D7	1	0	0	0	0
61	D8	4	0	0	0	0
61	DA	767	0	0	55	0
61	DB	9	0	0	0	0
61	DD	9	0	0	3	0
61	DE	5	0	0	0	0
61	DF	6	0	0	0	0
61	DN	2	0	0	0	0
61	DP	12	0	0	3	0
61	DR	2	0	0	1	0
61	DT	1	0	0	0	0
61	DU	2	0	0	0	0
61	DV	1	0	0	1	0
61	DX	2	0	0	0	0
61	DY	1	0	0	1	0
All	All	290205	0	193167	6242	3

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 14.

The worst 5 of 6242 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:1002:G:H1	1:CA:1038:C:N4	1.48	1.11
26:DA:2121:G:H1	26:DA:2177:C:N4	1.52	1.06
1:AA:1164:G:N2	1:AA:1165:C:C5	2.24	1.06
1:CA:72:C:N4	1:CA:97:G:N1	2.04	1.05
26:DA:2139:C:N4	26:DA:2152:G:H1	1.55	1.04

All (3) 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:1043:C:O2'	26:DA:2137:C:O2'[2_655]	2.08	0.12
33:BI:89:TYR:O	1:CA:357:G:O2'[3_654]	2.10	0.10
38:BR:33:ARG:NH2	42:BV:53:GLU:OE2[4_445]	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	AB	229/256 (90%)	204 (89%)	21 (9%)	4 (2%)	11	36
2	CB	229/256 (90%)	204 (89%)	14 (6%)	11 (5%)	3	9
3	AC	204/239 (85%)	189 (93%)	13 (6%)	2 (1%)	19	52
3	CC	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	34	69
4	AD	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	34	69
4	CD	206/209 (99%)	196 (95%)	7 (3%)	3 (2%)	13	40
5	AE	146/162 (90%)	136 (93%)	9 (6%)	1 (1%)	26	62
5	CE	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	26	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AF	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
6	CF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	AG	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	9	30
7	CG	153/156 (98%)	143 (94%)	9 (6%)	1 (1%)	26	62
8	AH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
8	CH	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	26	62
9	AI	125/128 (98%)	118 (94%)	7 (6%)	0	100	100
9	CI	125/128 (98%)	118 (94%)	6 (5%)	1 (1%)	24	58
10	AJ	95/105 (90%)	83 (87%)	5 (5%)	7 (7%)	1	3
10	CJ	94/105 (90%)	83 (88%)	6 (6%)	5 (5%)	2	7
11	AK	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	21	55
11	CK	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	21	55
12	AL	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
12	CL	120/132 (91%)	113 (94%)	7 (6%)	0	100	100
13	AM	121/126 (96%)	113 (93%)	6 (5%)	2 (2%)	11	36
13	CM	120/126 (95%)	110 (92%)	9 (8%)	1 (1%)	24	58
14	AN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	CN	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	AO	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
15	CO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	AP	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
16	CP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	AQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	CQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	AR	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
18	CR	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
19	AS	81/93 (87%)	70 (86%)	11 (14%)	0	100	100
19	CS	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	7	24
20	AT	94/106 (89%)	85 (90%)	3 (3%)	6 (6%)	2	4
20	CT	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	3	10
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
28	BD	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	39	74
28	DD	273/276 (99%)	261 (96%)	10 (4%)	2 (1%)	26	62
29	BE	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	34	69
29	DE	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	19	52
30	BF	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	34	69
30	DF	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	19	52
31	BG	179/182 (98%)	166 (93%)	9 (5%)	4 (2%)	8	28
31	DG	179/182 (98%)	166 (93%)	9 (5%)	4 (2%)	8	28
32	BH	172/180 (96%)	161 (94%)	9 (5%)	2 (1%)	16	47
32	DH	172/180 (96%)	163 (95%)	7 (4%)	2 (1%)	16	47
33	BI	144/148 (97%)	132 (92%)	9 (6%)	3 (2%)	9	29
33	DI	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	14	42
34	BN	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
34	DN	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	26	62
35	BO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	24	58
35	DO	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	24	58
36	BP	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	26	62
36	DP	147/150 (98%)	133 (90%)	13 (9%)	1 (1%)	26	62
37	BQ	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
37	DQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
38	BR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
38	DR	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
39	BS	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
39	DS	108/112 (96%)	104 (96%)	3 (3%)	1 (1%)	21	55
40	BT	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
40	DT	129/146 (88%)	125 (97%)	3 (2%)	1 (1%)	24	58
41	BU	114/118 (97%)	114 (100%)	0	0	100	100
41	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
42	BV	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	19	52
42	DV	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	19	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	BW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
43	DW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
44	BX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
44	DX	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
45	BY	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
45	DY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
46	BZ	169/206 (82%)	148 (88%)	19 (11%)	2 (1%)	16	47
46	DZ	172/206 (84%)	156 (91%)	14 (8%)	2 (1%)	16	47
47	B0	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
47	D0	81/85 (95%)	77 (95%)	4 (5%)	0	100	100
48	B1	95/98 (97%)	94 (99%)	0	1 (1%)	17	50
48	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	50
49	B2	68/72 (94%)	68 (100%)	0	0	100	100
49	D2	68/72 (94%)	68 (100%)	0	0	100	100
50	B3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
50	D3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	B4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	3
51	D4	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	2	5
52	B5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
52	D5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
53	B6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
53	D6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
54	B7	46/49 (94%)	46 (100%)	0	0	100	100
54	D7	46/49 (94%)	45 (98%)	0	1 (2%)	8	28
55	B8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
55	D8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
56	B9	35/37 (95%)	35 (100%)	0	0	100	100
56	D9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11409/12128 (94%)	10783 (94%)	516 (4%)	110 (1%)	19	52

5 of 110 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	231	GLU
4	AD	166	LYS
7	AG	80	VAL
10	AJ	55	LYS
20	AT	10	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	192/220 (87%)	161 (84%)	31 (16%)	3	9
2	CB	187/220 (85%)	161 (86%)	26 (14%)	4	13
3	AC	143/188 (76%)	131 (92%)	12 (8%)	14	37
3	CC	140/188 (74%)	127 (91%)	13 (9%)	11	32
4	AD	170/181 (94%)	153 (90%)	17 (10%)	9	27
4	CD	173/181 (96%)	157 (91%)	16 (9%)	11	32
5	AE	113/123 (92%)	106 (94%)	7 (6%)	23	54
5	CE	114/123 (93%)	105 (92%)	9 (8%)	15	40
6	AF	83/90 (92%)	78 (94%)	5 (6%)	24	56
6	CF	85/90 (94%)	79 (93%)	6 (7%)	18	46
7	AG	119/127 (94%)	107 (90%)	12 (10%)	9	27
7	CG	120/127 (94%)	108 (90%)	12 (10%)	9	27
8	AH	114/119 (96%)	109 (96%)	5 (4%)	35	69
8	CH	114/119 (96%)	106 (93%)	8 (7%)	19	47
9	AI	90/99 (91%)	76 (84%)	14 (16%)	3	9
9	CI	89/99 (90%)	78 (88%)	11 (12%)	6	17
10	AJ	66/92 (72%)	60 (91%)	6 (9%)	12	33
10	CJ	69/92 (75%)	63 (91%)	6 (9%)	13	35
11	AK	82/99 (83%)	76 (93%)	6 (7%)	17	44
11	CK	83/99 (84%)	79 (95%)	4 (5%)	31	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	AL	97/109 (89%)	91 (94%)	6 (6%)	23	54
12	CL	97/109 (89%)	94 (97%)	3 (3%)	47	81
13	AM	93/101 (92%)	82 (88%)	11 (12%)	6	19
13	CM	92/101 (91%)	81 (88%)	11 (12%)	6	19
14	AN	49/50 (98%)	43 (88%)	6 (12%)	6	18
14	CN	49/50 (98%)	43 (88%)	6 (12%)	6	18
15	AO	78/80 (98%)	66 (85%)	12 (15%)	3	10
15	CO	78/80 (98%)	70 (90%)	8 (10%)	9	26
16	AP	69/74 (93%)	60 (87%)	9 (13%)	5	15
16	CP	68/74 (92%)	62 (91%)	6 (9%)	12	35
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	46	80
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	17	43
18	AR	59/77 (77%)	54 (92%)	5 (8%)	13	36
18	CR	59/77 (77%)	54 (92%)	5 (8%)	13	36
19	AS	69/80 (86%)	61 (88%)	8 (12%)	7	20
19	CS	67/80 (84%)	62 (92%)	5 (8%)	17	43
20	AT	70/82 (85%)	60 (86%)	10 (14%)	4	12
20	CT	70/82 (85%)	63 (90%)	7 (10%)	9	27
21	AU	18/22 (82%)	16 (89%)	2 (11%)	8	23
21	CU	18/22 (82%)	17 (94%)	1 (6%)	26	59
28	BD	215/218 (99%)	201 (94%)	14 (6%)	21	52
28	DD	215/218 (99%)	200 (93%)	15 (7%)	19	47
29	BE	164/166 (99%)	144 (88%)	20 (12%)	6	18
29	DE	164/166 (99%)	147 (90%)	17 (10%)	9	25
30	BF	160/166 (96%)	145 (91%)	15 (9%)	11	31
30	DF	159/166 (96%)	146 (92%)	13 (8%)	14	38
31	BG	143/156 (92%)	128 (90%)	15 (10%)	8	24
31	DG	142/156 (91%)	122 (86%)	20 (14%)	4	12
32	BH	144/148 (97%)	138 (96%)	6 (4%)	36	71
32	DH	144/148 (97%)	132 (92%)	12 (8%)	14	38
33	BI	110/124 (89%)	90 (82%)	20 (18%)	2	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DI	104/124 (84%)	87 (84%)	17 (16%)	3	8
34	BN	118/119 (99%)	103 (87%)	15 (13%)	5	16
34	DN	118/119 (99%)	108 (92%)	10 (8%)	13	36
35	BO	100/100 (100%)	94 (94%)	6 (6%)	24	56
35	DO	100/100 (100%)	96 (96%)	4 (4%)	38	73
36	BP	115/116 (99%)	105 (91%)	10 (9%)	13	35
36	DP	115/116 (99%)	103 (90%)	12 (10%)	9	25
37	BQ	111/111 (100%)	100 (90%)	11 (10%)	10	28
37	DQ	111/111 (100%)	100 (90%)	11 (10%)	10	28
38	BR	101/101 (100%)	82 (81%)	19 (19%)	2	6
38	DR	101/101 (100%)	84 (83%)	17 (17%)	2	8
39	BS	87/88 (99%)	79 (91%)	8 (9%)	11	32
39	DS	85/88 (97%)	75 (88%)	10 (12%)	6	19
40	BT	115/127 (91%)	106 (92%)	9 (8%)	16	41
40	DT	113/127 (89%)	103 (91%)	10 (9%)	12	35
41	BU	93/94 (99%)	86 (92%)	7 (8%)	17	43
41	DU	93/94 (99%)	88 (95%)	5 (5%)	27	60
42	BV	80/82 (98%)	68 (85%)	12 (15%)	3	11
42	DV	80/82 (98%)	72 (90%)	8 (10%)	9	27
43	BW	90/92 (98%)	84 (93%)	6 (7%)	20	50
43	DW	90/92 (98%)	82 (91%)	8 (9%)	12	34
44	BX	77/78 (99%)	74 (96%)	3 (4%)	39	74
44	DX	77/78 (99%)	72 (94%)	5 (6%)	21	52
45	BY	85/91 (93%)	77 (91%)	8 (9%)	11	31
45	DY	85/91 (93%)	78 (92%)	7 (8%)	14	38
46	BZ	145/179 (81%)	131 (90%)	14 (10%)	10	29
46	DZ	145/179 (81%)	127 (88%)	18 (12%)	6	17
47	B0	65/67 (97%)	62 (95%)	3 (5%)	33	67
47	D0	65/67 (97%)	62 (95%)	3 (5%)	33	67
48	B1	80/83 (96%)	72 (90%)	8 (10%)	9	27
48	D1	80/83 (96%)	73 (91%)	7 (9%)	12	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	B2	65/67 (97%)	56 (86%)	9 (14%)	4	13
49	D2	65/67 (97%)	59 (91%)	6 (9%)	11	32
50	B3	51/52 (98%)	45 (88%)	6 (12%)	6	19
50	D3	50/52 (96%)	47 (94%)	3 (6%)	24	56
51	B4	59/63 (94%)	47 (80%)	12 (20%)	1	4
51	D4	53/63 (84%)	46 (87%)	7 (13%)	5	14
52	B5	50/52 (96%)	48 (96%)	2 (4%)	38	73
52	D5	50/52 (96%)	48 (96%)	2 (4%)	38	73
53	B6	51/52 (98%)	44 (86%)	7 (14%)	4	13
53	D6	50/52 (96%)	48 (96%)	2 (4%)	38	73
54	B7	41/42 (98%)	38 (93%)	3 (7%)	17	44
54	D7	41/42 (98%)	38 (93%)	3 (7%)	17	44
55	B8	53/55 (96%)	49 (92%)	4 (8%)	17	43
55	D8	54/55 (98%)	53 (98%)	1 (2%)	65	91
56	B9	34/34 (100%)	31 (91%)	3 (9%)	12	35
56	D9	34/34 (100%)	33 (97%)	1 (3%)	50	83
All	All	9319/10066 (93%)	8433 (90%)	886 (10%)	11	30

5 of 886 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BZ	136	PHE
3	CC	115	LEU
43	DW	51	LEU
48	B1	75	GLU
53	B6	28	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
41	BU	117	GLN
2	CB	40	HIS
38	DR	71	GLN
45	BY	6	HIS
49	B2	48	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1495/1521 (98%)	407 (27%)	26 (1%)
1	CA	1501/1521 (98%)	413 (27%)	28 (1%)
22	AV	12/24 (50%)	7 (58%)	0
22	CV	5/24 (20%)	4 (80%)	0
23	AW	1/3 (33%)	0	0
23	CW	1/3 (33%)	0	0
24	AX	74/77 (96%)	26 (35%)	2 (2%)
24	CX	74/77 (96%)	31 (41%)	4 (5%)
25	AY	4/76 (5%)	1 (25%)	0
25	CY	4/76 (5%)	1 (25%)	0
26	BA	2811/2915 (96%)	529 (18%)	30 (1%)
26	DA	2791/2915 (95%)	595 (21%)	30 (1%)
27	BB	120/121 (99%)	16 (13%)	2 (1%)
27	DB	119/121 (98%)	31 (26%)	0
All	All	9012/9474 (95%)	2061 (22%)	122 (1%)

5 of 2061 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	9	G
1	AA	15	G
1	AA	22	G

5 of 122 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2689	U
1	CA	509	A
26	DA	2104	G
26	BA	2756	U
1	CA	65	U

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PPU	AW	76	26,23	30,40,41	0.97	1 (3%)	37,57,60	1.90	10 (27%)
24	5MC	AX	32	24	13,22,23	1.32	1 (7%)	15,32,35	1.03	1 (6%)
24	5MU	AX	54	24	12,22,23	0.30	0	14,32,35	2.18	2 (14%)
24	PSU	AX	55	24	13,21,22	1.22	1 (7%)	18,30,33	3.26	6 (33%)
24	31H	AX	76	24,57	23,32,35	1.07	2 (8%)	24,45,50	3.07	5 (20%)
24	4SU	AX	8	24	11,21,22	1.20	1 (9%)	13,30,33	1.72	1 (7%)
23	PPU	CW	76	26,23	30,40,41	0.92	1 (3%)	37,57,60	2.01	11 (29%)
24	5MC	CX	32	24	13,22,23	1.35	1 (7%)	15,32,35	1.03	1 (6%)
24	5MU	CX	54	24	12,22,23	0.34	0	14,32,35	2.20	2 (14%)
24	PSU	CX	55	24	13,21,22	1.35	1 (7%)	18,30,33	3.45	6 (33%)
24	31H	CX	76	24,60,57	25,34,35	1.19	3 (12%)	26,47,50	3.07	7 (26%)
24	4SU	CX	8	24	11,21,22	1.22	1 (9%)	13,30,33	1.29	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PPU	AW	76	26,23	-	0/21/43/44	0/4/4/4
24	5MC	AX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	AX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
24	31H	AX	76	24,57	-	0/15/37/41	0/3/3/3
24	4SU	AX	8	24	-	0/3/25/26	0/2/2/2
23	PPU	CW	76	26,23	-	0/21/43/44	0/4/4/4
24	5MC	CX	32	24	-	0/3/25/26	0/2/2/2
24	5MU	CX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	CX	55	24	-	0/7/25/26	0/2/2/2
24	31H	CX	76	24,60,57	-	1/18/40/41	0/3/3/3
24	4SU	CX	8	24	-	0/3/25/26	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CX	55	PSU	C5-C1'	-4.39	1.48	1.52
24	AX	55	PSU	C5-C1'	-3.84	1.48	1.52
24	CX	8	4SU	C4-S4	-3.84	1.60	1.67
24	AX	8	4SU	C4-S4	-3.79	1.60	1.67
24	CX	76	31H	C5-C4	-3.19	1.33	1.40

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	76	31H	N3-C2-N1	-12.05	119.67	128.89
24	CX	76	31H	N3-C2-N1	-11.87	119.81	128.89
24	CX	55	PSU	N1-C2-N3	-10.74	121.48	128.33
24	AX	55	PSU	N1-C2-N3	-10.14	121.86	128.33
24	AX	8	4SU	C5-C4-N3	-5.67	118.07	123.63

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	CX	76	31H	OCN-CN-N-CA

There are no ring outliers.

11 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	76	PPU	5	0
24	AX	32	5MC	2	0
24	AX	54	5MU	1	0
24	AX	55	PSU	1	0
24	AX	8	4SU	2	0
23	CW	76	PPU	11	0
24	CX	32	5MC	3	0
24	CX	54	5MU	2	0
24	CX	55	PSU	1	0
24	CX	76	31H	4	0
24	CX	8	4SU	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1916 ligands modelled in this entry, 1914 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	AD	302	4	0,12,12	0.00	-	0,24,24	0.00	-
58	SF4	CD	501	4	0,12,12	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	AD	302	4	-	0/0/48/48	0/6/5/5
58	SF4	CD	501	4	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AD	302	SF4	1	0
58	CD	501	SF4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1498/1521 (98%)	0.23	20 (1%) 79 71	39, 73, 93, 105	0
1	CA	1503/1521 (98%)	0.17	25 (1%) 73 63	41, 75, 94, 106	0
2	AB	231/256 (90%)	0.53	15 (6%) 22 13	69, 82, 91, 101	0
2	CB	231/256 (90%)	2.20	109 (47%) 0 0	71, 84, 93, 101	0
3	AC	206/239 (86%)	0.47	6 (2%) 55 43	67, 79, 89, 95	0
3	CC	206/239 (86%)	1.91	87 (42%) 0 0	70, 81, 91, 95	0
4	AD	208/209 (99%)	0.59	13 (6%) 23 14	57, 74, 85, 91	0
4	CD	208/209 (99%)	0.81	20 (9%) 10 5	57, 75, 85, 92	0
5	AE	148/162 (91%)	0.52	6 (4%) 41 29	59, 71, 82, 90	0
5	CE	148/162 (91%)	1.04	30 (20%) 1 1	59, 73, 84, 91	0
6	AF	100/101 (99%)	0.45	4 (4%) 42 30	54, 69, 78, 83	0
6	CF	100/101 (99%)	0.27	5 (5%) 32 21	56, 71, 80, 83	0
7	AG	155/156 (99%)	0.58	15 (9%) 10 5	64, 76, 86, 92	0
7	CG	155/156 (99%)	1.10	28 (18%) 2 1	67, 78, 88, 92	0
8	AH	137/138 (99%)	0.43	6 (4%) 38 26	60, 72, 80, 85	0
8	CH	137/138 (99%)	1.38	35 (25%) 1 0	62, 74, 82, 85	0
9	AI	127/128 (99%)	0.85	18 (14%) 4 2	64, 83, 91, 96	0
9	CI	127/128 (99%)	1.64	47 (37%) 0 0	69, 84, 91, 98	0
10	AJ	97/105 (92%)	0.74	10 (10%) 9 4	66, 83, 92, 94	0
10	CJ	96/105 (91%)	2.09	54 (56%) 0 0	69, 85, 93, 94	0
11	AK	114/129 (88%)	0.70	10 (8%) 12 6	46, 70, 81, 85	0
11	CK	114/129 (88%)	0.64	14 (12%) 5 3	50, 71, 82, 85	0
12	AL	122/132 (92%)	0.54	3 (2%) 61 48	50, 64, 73, 81	0
12	CL	122/132 (92%)	0.72	13 (10%) 8 4	52, 65, 75, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	123/126 (97%)	0.66	13 (10%) 8 4	58, 72, 83, 90	0
13	CM	122/126 (96%)	1.51	33 (27%) 1 0	72, 85, 93, 100	0
14	AN	60/61 (98%)	0.65	6 (10%) 9 4	65, 75, 81, 82	0
14	CN	60/61 (98%)	2.24	31 (51%) 0 0	69, 78, 83, 86	0
15	AO	88/89 (98%)	0.77	3 (3%) 49 36	54, 69, 81, 85	0
15	CO	88/89 (98%)	0.61	9 (10%) 9 4	53, 71, 82, 87	0
16	AP	82/88 (93%)	0.82	11 (13%) 4 2	59, 72, 82, 85	0
16	CP	82/88 (93%)	0.53	5 (6%) 25 15	57, 71, 81, 85	0
17	AQ	99/105 (94%)	0.64	3 (3%) 54 41	58, 71, 80, 83	0
17	CQ	99/105 (94%)	1.15	19 (19%) 2 1	56, 72, 81, 83	0
18	AR	68/88 (77%)	0.84	8 (11%) 6 3	59, 70, 80, 84	0
18	CR	68/88 (77%)	0.57	6 (8%) 12 6	60, 71, 82, 85	0
19	AS	83/93 (89%)	0.86	12 (14%) 3 2	72, 82, 89, 93	0
19	CS	83/93 (89%)	2.26	48 (57%) 0 0	73, 84, 91, 95	0
20	AT	96/106 (90%)	1.08	18 (18%) 2 1	60, 71, 83, 85	0
20	CT	96/106 (90%)	1.10	20 (20%) 1 1	56, 71, 83, 85	0
21	AU	23/27 (85%)	0.89	1 (4%) 39 27	69, 74, 79, 85	0
21	CU	23/27 (85%)	0.58	3 (13%) 5 2	71, 76, 84, 86	0
22	AV	13/24 (54%)	1.52	2 (15%) 3 1	56, 88, 93, 97	0
22	CV	6/24 (25%)	1.03	1 (16%) 2 1	59, 76, 95, 96	0
23	AW	2/3 (66%)	0.39	0 100 100	30, 30, 30, 37	0
23	CW	2/3 (66%)	0.73	0 100 100	50, 50, 50, 57	0
24	AX	71/77 (92%)	0.22	0 100 100	27, 70, 84, 92	0
24	CX	71/77 (92%)	0.28	0 100 100	30, 75, 86, 93	0
25	AY	5/76 (6%)	0.10	0 100 100	51, 76, 87, 94	0
25	CY	5/76 (6%)	1.37	1 (20%) 1 1	60, 79, 90, 91	0
26	BA	2819/2915 (96%)	0.24	27 (0%) 84 77	20, 42, 89, 107	0
26	DA	2800/2915 (96%)	-0.00	49 (1%) 71 61	22, 46, 90, 107	0
27	BB	120/121 (99%)	0.10	0 100 100	37, 63, 77, 88	0
27	DB	120/121 (99%)	0.14	5 (4%) 40 28	42, 68, 80, 91	0
28	BD	275/276 (99%)	0.21	2 (0%) 89 84	21, 41, 58, 78	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	275/276 (99%)	0.01	1 (0%) 93 90	23, 43, 61, 80	0
29	BE	204/206 (99%)	0.21	1 (0%) 91 88	21, 46, 65, 82	0
29	DE	204/206 (99%)	-0.05	1 (0%) 91 88	23, 48, 67, 84	0
30	BF	203/210 (96%)	0.23	2 (0%) 84 77	22, 51, 73, 87	0
30	DF	203/210 (96%)	0.07	1 (0%) 91 88	24, 54, 74, 86	0
31	BG	181/182 (99%)	0.37	7 (3%) 43 31	55, 70, 82, 93	0
31	DG	181/182 (99%)	1.36	52 (28%) 1 0	59, 74, 85, 93	0
32	BH	174/180 (96%)	0.14	1 (0%) 90 86	49, 65, 77, 81	0
32	DH	174/180 (96%)	1.25	40 (22%) 1 1	52, 70, 80, 84	0
33	BI	146/148 (98%)	0.73	13 (8%) 12 6	47, 81, 90, 95	0
33	DI	146/148 (98%)	3.04	80 (54%) 0 0	46, 84, 94, 99	0
34	BN	140/140 (100%)	0.27	1 (0%) 89 84	29, 49, 72, 82	0
34	DN	140/140 (100%)	0.09	2 (1%) 78 69	33, 53, 74, 83	0
35	BO	122/122 (100%)	-0.02	1 (0%) 87 81	26, 42, 61, 65	0
35	DO	122/122 (100%)	-0.03	0 100 100	36, 57, 70, 79	0
36	BP	149/150 (99%)	0.33	2 (1%) 79 71	25, 52, 76, 85	0
36	DP	149/150 (99%)	0.54	7 (4%) 35 24	28, 54, 78, 86	0
37	BQ	141/141 (100%)	0.25	0 100 100	29, 51, 65, 78	0
37	DQ	141/141 (100%)	0.71	17 (12%) 6 3	31, 55, 69, 79	0
38	BR	118/118 (100%)	-0.10	0 100 100	23, 37, 56, 63	0
38	DR	118/118 (100%)	0.18	0 100 100	31, 50, 64, 71	0
39	BS	110/112 (98%)	0.19	1 (0%) 85 79	33, 51, 63, 76	0
39	DS	110/112 (98%)	0.80	11 (10%) 9 4	55, 76, 86, 89	0
40	BT	131/146 (89%)	-0.18	0 100 100	27, 44, 73, 86	0
40	DT	131/146 (89%)	0.06	1 (0%) 87 81	42, 59, 78, 86	0
41	BU	116/118 (98%)	-0.06	1 (0%) 85 79	18, 32, 52, 73	0
41	DU	116/118 (98%)	0.28	2 (1%) 73 63	37, 58, 75, 80	0
42	BV	101/101 (100%)	-0.02	0 100 100	20, 43, 61, 76	0
42	DV	101/101 (100%)	0.87	12 (11%) 6 3	36, 67, 81, 87	0
43	BW	112/113 (99%)	0.06	1 (0%) 85 79	20, 33, 51, 84	0
43	DW	112/113 (99%)	0.30	1 (0%) 85 79	32, 47, 65, 100	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	95/96 (98%)	0.12	0 100 100	22, 37, 57, 82	0
44	DX	95/96 (98%)	0.71	8 (8%) 14 6	39, 59, 73, 82	0
45	BY	107/110 (97%)	0.01	0 100 100	32, 48, 70, 81	0
45	DY	107/110 (97%)	0.99	15 (14%) 4 2	48, 68, 78, 89	0
46	BZ	171/206 (83%)	0.48	5 (2%) 55 43	40, 63, 83, 88	0
46	DZ	174/206 (84%)	1.70	60 (34%) 0 0	64, 82, 94, 97	0
47	B0	83/85 (97%)	-0.06	0 100 100	23, 38, 52, 66	0
47	D0	83/85 (97%)	0.77	8 (9%) 10 5	36, 61, 72, 81	0
48	B1	97/98 (98%)	0.03	2 (2%) 67 56	21, 42, 65, 74	0
48	D1	97/98 (98%)	0.43	3 (3%) 52 40	30, 54, 76, 82	0
49	B2	70/72 (97%)	0.12	0 100 100	32, 48, 63, 87	0
49	D2	70/72 (97%)	0.50	4 (5%) 27 17	50, 67, 78, 83	0
50	B3	59/60 (98%)	-0.11	0 100 100	21, 37, 62, 81	0
50	D3	59/60 (98%)	1.01	6 (10%) 9 4	44, 60, 77, 87	0
51	B4	69/71 (97%)	0.64	11 (15%) 3 1	54, 76, 91, 98	0
51	D4	69/71 (97%)	1.58	24 (34%) 0 0	80, 90, 95, 99	0
52	B5	59/60 (98%)	-0.08	1 (1%) 73 63	19, 33, 53, 65	0
52	D5	59/60 (98%)	-0.03	0 100 100	28, 48, 69, 72	0
53	B6	53/54 (98%)	-0.05	0 100 100	28, 40, 60, 64	0
53	D6	53/54 (98%)	0.47	3 (5%) 27 17	43, 59, 72, 82	0
54	B7	48/49 (97%)	-0.05	0 100 100	18, 25, 54, 63	0
54	D7	48/49 (97%)	0.01	1 (2%) 67 56	29, 39, 63, 81	0
55	B8	64/65 (98%)	-0.03	0 100 100	23, 32, 46, 61	0
55	D8	64/65 (98%)	0.44	0 100 100	37, 55, 66, 70	0
56	B9	37/37 (100%)	0.50	1 (2%) 58 45	27, 49, 67, 71	0
56	D9	37/37 (100%)	0.92	5 (13%) 4 2	46, 54, 67, 74	0
All	All	20640/21602 (95%)	0.43	1345 (6%) 22 13	18, 63, 89, 107	0

The worst 5 of 1345 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	DI	119	PRO	11.8
33	DI	65	ALA	11.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	DI	128	LEU	10.9
13	CM	124	PRO	10.8
33	DI	85	GLU	10.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	PPU	AW	76	37/38	0.97	0.20	-	12,29,37,42	0
24	5MC	CX	32	21/22	0.85	0.22	-	68,80,88,99	0
24	PSU	AX	55	20/21	0.93	0.16	-	58,70,77,82	0
24	PSU	CX	55	20/21	0.91	0.16	-	61,72,81,89	0
24	5MU	CX	54	21/22	0.92	0.13	-	71,79,92,107	0
24	5MC	AX	32	21/22	0.95	0.18	-	46,55,75,77	0
24	5MU	AX	54	21/22	0.95	0.16	-	57,67,82,96	0
24	4SU	AX	8	20/21	0.95	0.17	-	47,59,67,84	0
24	31H	AX	76	30/33	0.96	0.26	-	14,31,55,77	8
24	31H	CX	76	32/33	0.95	0.23	-	23,42,61,84	10
24	4SU	CX	8	20/21	0.90	0.17	-	61,80,93,118	0
23	PPU	CW	76	37/38	0.97	0.23	-	27,41,53,63	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3027	1/1	0.89	1.04	67.56	36,36,36,36	0
57	MG	BA	3036	1/1	0.95	0.64	63.42	42,42,42,42	0
57	MG	DA	3238	1/1	0.98	0.43	33.85	31,31,31,31	0
57	MG	DA	3141	1/1	0.87	0.23	28.27	37,37,37,37	0
57	MG	BA	3244	1/1	0.96	0.39	27.78	29,29,29,29	0
57	MG	DA	3039	1/1	0.94	0.39	27.40	48,48,48,48	0
57	MG	CA	3126	1/1	0.83	0.37	25.78	73,73,73,73	0
57	MG	BA	3226	1/1	0.96	0.43	25.58	36,36,36,36	0
57	MG	DA	3001	1/1	0.89	0.37	25.38	45,45,45,45	0
57	MG	DA	3277	1/1	0.95	0.44	23.93	50,50,50,50	0
57	MG	BA	3185	1/1	0.98	0.50	23.04	34,34,34,34	0
57	MG	BA	3401	1/1	0.93	0.28	22.75	31,31,31,31	0
57	MG	DA	3042	1/1	0.95	0.32	22.56	37,37,37,37	0
57	MG	DA	3533	1/1	0.81	0.48	21.51	47,47,47,47	0
57	MG	DA	3173	1/1	0.97	0.34	20.81	42,42,42,42	0
57	MG	BA	3125	1/1	0.98	0.39	20.78	30,30,30,30	0
57	MG	BQ	3003	1/1	0.83	0.73	20.07	68,68,68,68	0
57	MG	DA	3177	1/1	0.94	0.34	19.16	29,29,29,29	0
57	MG	BA	3277	1/1	0.95	0.30	17.04	34,34,34,34	0
57	MG	DA	3210	1/1	0.94	0.44	16.68	57,57,57,57	0
57	MG	DA	3350	1/1	0.93	0.36	16.45	44,44,44,44	0
57	MG	DA	3456	1/1	0.96	0.35	15.88	59,59,59,59	0
57	MG	DA	3351	1/1	0.96	0.34	15.62	45,45,45,45	0
57	MG	DE	302	1/1	0.94	0.60	15.38	51,51,51,51	0
57	MG	DA	3267	1/1	0.89	0.29	14.97	45,45,45,45	0
57	MG	DA	3579	1/1	0.99	0.30	14.29	58,58,58,58	0
57	MG	BA	3533	1/1	0.89	0.28	14.20	45,45,45,45	0
57	MG	BA	3267	1/1	0.95	0.36	13.68	33,33,33,33	0
57	MG	DA	3609	1/1	0.66	0.26	13.56	55,55,55,55	0
57	MG	BA	3602	1/1	0.96	0.34	13.41	65,65,65,65	0
57	MG	BA	3271	1/1	0.95	0.34	13.25	45,45,45,45	0
57	MG	DA	3170	1/1	0.94	0.37	12.80	47,47,47,47	0
57	MG	BA	3131	1/1	0.97	0.38	12.70	31,31,31,31	0
57	MG	BA	3514	1/1	0.87	0.37	12.47	36,36,36,36	0
57	MG	DA	3257	1/1	0.91	0.33	12.38	46,46,46,46	0
57	MG	DA	3619	1/1	0.86	0.43	12.34	63,63,63,63	0
57	MG	BU	204	1/1	0.96	0.33	12.12	38,38,38,38	0
57	MG	BU	208	1/1	0.92	0.44	12.10	39,39,39,39	0
57	MG	BN	3006	1/1	0.95	0.62	11.96	47,47,47,47	0
57	MG	CA	3116	1/1	0.64	0.33	11.89	74,74,74,74	0
57	MG	BW	202	1/1	0.95	0.60	11.83	41,41,41,41	0
57	MG	BA	3384	1/1	0.97	0.29	11.81	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3461	1/1	0.97	0.25	11.68	32,32,32,32	0
57	MG	BA	3412	1/1	0.87	0.40	11.36	44,44,44,44	0
57	MG	AA	3055	1/1	0.91	0.31	11.27	53,53,53,53	0
57	MG	BA	3245	1/1	0.98	0.31	11.21	37,37,37,37	0
57	MG	DA	3373	1/1	0.98	0.23	11.10	43,43,43,43	0
57	MG	BN	3004	1/1	0.95	0.56	10.97	49,49,49,49	0
57	MG	BA	3105	1/1	0.92	0.25	10.92	45,45,45,45	0
57	MG	DA	3614	1/1	0.97	0.49	10.79	56,56,56,56	0
57	MG	DA	3602	1/1	0.86	0.25	10.61	50,50,50,50	0
57	MG	BA	3698	1/1	0.92	0.30	10.21	51,51,51,51	0
57	MG	BE	3001	1/1	0.98	0.34	10.08	48,48,48,48	0
57	MG	BP	3001	1/1	0.94	0.43	10.06	49,49,49,49	0
57	MG	CA	3054	1/1	0.85	0.36	9.90	53,53,53,53	0
57	MG	BE	3002	1/1	0.88	0.44	9.85	50,50,50,50	0
57	MG	CA	3017	1/1	0.85	0.29	9.46	69,69,69,69	0
57	MG	BA	3534	1/1	0.88	0.28	9.43	23,23,23,23	0
57	MG	BA	3101	1/1	0.98	0.29	9.31	29,29,29,29	0
57	MG	DD	306	1/1	0.94	0.38	9.27	44,44,44,44	0
57	MG	BA	3651	1/1	0.81	0.26	9.24	62,62,62,62	0
57	MG	DA	3255	1/1	0.90	0.28	9.20	34,34,34,34	0
57	MG	BD	301	1/1	0.96	0.37	9.11	37,37,37,37	0
57	MG	DA	3559	1/1	0.94	0.21	8.96	31,31,31,31	0
57	MG	DA	3440	1/1	0.95	0.26	8.77	44,44,44,44	0
57	MG	DA	3234	1/1	0.93	0.30	8.73	34,34,34,34	0
57	MG	DA	3258	1/1	0.97	0.26	8.65	32,32,32,32	0
57	MG	DA	3441	1/1	0.95	0.27	8.60	43,43,43,43	0
57	MG	DB	3005	1/1	0.94	0.20	8.57	54,54,54,54	0
57	MG	BD	310	1/1	0.91	0.40	8.46	34,34,34,34	0
57	MG	BA	3663	1/1	0.95	0.24	8.44	36,36,36,36	0
57	MG	DA	3274	1/1	0.95	0.22	8.37	45,45,45,45	0
57	MG	BA	3257	1/1	0.90	0.31	8.22	40,40,40,40	0
57	MG	BA	3111	1/1	0.90	0.29	8.15	51,51,51,51	0
57	MG	BA	3054	1/1	0.93	0.25	8.05	44,44,44,44	0
57	MG	DA	3628	1/1	0.85	0.57	7.85	59,59,59,59	0
57	MG	DA	3426	1/1	0.90	0.34	7.84	38,38,38,38	0
57	MG	AA	3113	1/1	0.87	0.29	7.77	54,54,54,54	0
57	MG	BA	3490	1/1	0.96	0.28	7.65	17,17,17,17	0
57	MG	BA	3707	1/1	0.95	0.36	7.49	34,34,34,34	0
57	MG	DA	3216	1/1	0.92	0.30	7.47	43,43,43,43	0
57	MG	BQ	3001	1/1	0.95	0.32	7.45	51,51,51,51	0
57	MG	DA	3251	1/1	0.93	0.28	7.42	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3259	1/1	0.97	0.29	7.40	40,40,40,40	0
57	MG	BA	3498	1/1	0.97	0.23	7.20	45,45,45,45	0
57	MG	AX	3007	1/1	0.95	0.27	7.01	54,54,54,54	0
57	MG	AA	3024	1/1	0.97	0.24	6.90	49,49,49,49	0
57	MG	BU	206	1/1	0.91	0.35	6.87	39,39,39,39	0
57	MG	DA	3376	1/1	0.93	0.24	6.82	40,40,40,40	0
57	MG	BA	3405	1/1	0.96	0.24	6.71	31,31,31,31	0
57	MG	BA	3283	1/1	0.97	0.23	6.60	22,22,22,22	0
57	MG	DA	3116	1/1	0.90	0.23	6.53	36,36,36,36	0
57	MG	BA	3709	1/1	0.88	0.33	6.52	45,45,45,45	0
57	MG	DU	3001	1/1	0.97	0.62	6.52	56,56,56,56	0
57	MG	BA	3530	1/1	0.94	0.26	6.46	20,20,20,20	0
57	MG	DD	305	1/1	0.88	0.36	6.38	48,48,48,48	0
57	MG	BA	3160	1/1	0.97	0.25	6.33	23,23,23,23	0
57	MG	BA	3067	1/1	0.95	0.25	6.28	26,26,26,26	0
57	MG	DA	3004	1/1	0.96	0.28	6.26	32,32,32,32	0
57	MG	DA	3242	1/1	0.96	0.20	6.21	48,48,48,48	0
57	MG	DA	3127	1/1	0.97	0.35	6.21	40,40,40,40	0
57	MG	BA	3118	1/1	0.94	0.24	6.17	28,28,28,28	0
57	MG	BA	3677	1/1	0.95	0.24	6.10	30,30,30,30	0
57	MG	BA	3396	1/1	0.82	0.24	6.08	20,20,20,20	0
57	MG	DA	3501	1/1	0.93	0.24	6.03	47,47,47,47	0
57	MG	DA	3061	1/1	0.89	0.27	5.85	36,36,36,36	0
57	MG	BA	3212	1/1	0.98	0.29	5.83	24,24,24,24	0
57	MG	BN	3001	1/1	0.96	0.47	5.83	46,46,46,46	0
57	MG	DA	3444	1/1	0.86	0.25	5.78	37,37,37,37	0
57	MG	DA	3410	1/1	0.82	0.23	5.78	37,37,37,37	0
57	MG	AA	3144	1/1	0.94	0.28	5.75	44,44,44,44	0
57	MG	BA	3281	1/1	0.87	0.26	5.70	46,46,46,46	0
57	MG	DA	3448	1/1	0.90	0.25	5.59	36,36,36,36	0
57	MG	AA	3172	1/1	0.85	0.28	5.52	54,54,54,54	0
57	MG	DA	3621	1/1	0.96	0.46	5.49	61,61,61,61	0
57	MG	BA	3114	1/1	0.96	0.24	5.39	41,41,41,41	0
57	MG	BD	311	1/1	0.92	0.36	5.38	60,60,60,60	0
57	MG	DA	3369	1/1	0.85	0.26	5.37	36,36,36,36	0
57	MG	AA	3074	1/1	0.95	0.27	5.36	38,38,38,38	0
57	MG	DA	3162	1/1	0.81	0.44	5.34	58,58,58,58	0
57	MG	DA	3030	1/1	0.97	0.39	5.31	32,32,32,32	0
57	MG	BA	3133	1/1	0.96	0.24	5.28	29,29,29,29	0
57	MG	AA	3030	1/1	0.94	0.27	5.22	41,41,41,41	0
57	MG	DA	3015	1/1	0.98	0.25	5.18	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3192	1/1	0.97	0.23	5.15	31,31,31,31	0
57	MG	DA	3185	1/1	0.94	0.20	5.13	57,57,57,57	0
57	MG	BA	3041	1/1	0.96	0.25	5.10	39,39,39,39	0
57	MG	DA	3538	1/1	0.93	0.23	5.08	77,77,77,77	0
57	MG	AA	3083	1/1	0.98	0.29	5.07	38,38,38,38	0
57	MG	BA	3705	1/1	0.96	0.32	5.04	32,32,32,32	0
57	MG	BA	3423	1/1	0.96	0.25	5.04	26,26,26,26	0
57	MG	DA	3161	1/1	0.89	0.23	5.00	35,35,35,35	0
57	MG	DA	3106	1/1	0.74	0.21	4.91	52,52,52,52	0
57	MG	DA	3174	1/1	0.95	0.19	4.88	38,38,38,38	0
57	MG	DA	3474	1/1	0.97	0.22	4.88	52,52,52,52	0
57	MG	BA	3403	1/1	0.96	0.23	4.78	22,22,22,22	0
57	MG	BR	203	1/1	0.94	0.28	4.76	31,31,31,31	0
57	MG	BQ	3002	1/1	0.97	0.30	4.71	39,39,39,39	0
57	MG	BD	303	1/1	0.97	0.32	4.67	42,42,42,42	0
57	MG	DA	3100	1/1	0.98	0.20	4.62	38,38,38,38	0
57	MG	DA	3552	1/1	0.94	0.23	4.57	43,43,43,43	0
57	MG	DA	3307	1/1	0.80	0.21	4.50	51,51,51,51	0
57	MG	BA	3391	1/1	0.95	0.24	4.50	30,30,30,30	0
57	MG	B7	102	1/1	0.90	0.32	4.47	53,53,53,53	0
57	MG	CA	3097	1/1	0.91	0.22	4.43	43,43,43,43	0
57	MG	CA	3058	1/1	0.83	0.35	4.39	70,70,70,70	0
57	MG	AA	3116	1/1	0.96	0.26	4.38	41,41,41,41	0
57	MG	BA	3152	1/1	0.91	0.25	4.38	45,45,45,45	0
57	MG	BA	3509	1/1	0.91	0.32	4.34	34,34,34,34	0
57	MG	DA	3462	1/1	0.97	0.27	4.33	35,35,35,35	0
57	MG	BA	3310	1/1	0.93	0.21	4.31	43,43,43,43	0
57	MG	DA	3312	1/1	0.87	0.20	4.25	30,30,30,30	0
57	MG	BD	306	1/1	0.91	0.31	4.15	30,30,30,30	0
57	MG	DA	3363	1/1	0.99	0.21	4.15	35,35,35,35	0
57	MG	BF	304	1/1	0.90	0.26	4.10	35,35,35,35	0
57	MG	BA	3436	1/1	0.95	0.22	4.09	21,21,21,21	0
57	MG	DA	3166	1/1	0.95	0.20	4.04	47,47,47,47	0
57	MG	BA	3303	1/1	0.78	0.23	4.04	39,39,39,39	0
57	MG	BA	3706	1/1	0.98	0.25	4.02	27,27,27,27	0
57	MG	DA	3152	1/1	0.96	0.20	4.02	38,38,38,38	0
57	MG	DA	3319	1/1	0.91	0.33	3.95	45,45,45,45	0
57	MG	AA	3090	1/1	0.89	0.20	3.86	70,70,70,70	0
57	MG	DA	3103	1/1	0.90	0.32	3.84	55,55,55,55	0
57	MG	DA	3473	1/1	0.92	0.20	3.83	32,32,32,32	0
57	MG	CA	3070	1/1	0.92	0.24	3.80	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3200	1/1	0.94	0.24	3.80	39,39,39,39	0
57	MG	AA	3204	1/1	0.96	0.23	3.73	64,64,64,64	0
57	MG	BA	3529	1/1	0.97	0.28	3.71	29,29,29,29	0
57	MG	DA	3119	1/1	0.82	0.20	3.65	52,52,52,52	0
57	MG	BA	3532	1/1	0.90	0.24	3.64	39,39,39,39	0
57	MG	CA	3095	1/1	0.90	0.25	3.64	52,52,52,52	0
57	MG	DA	3017	1/1	0.94	0.17	3.62	58,58,58,58	0
57	MG	DA	3230	1/1	0.95	0.22	3.59	46,46,46,46	0
57	MG	DA	3594	1/1	0.97	0.17	3.58	51,51,51,51	0
57	MG	DA	3023	1/1	0.88	0.21	3.57	35,35,35,35	0
57	MG	DA	3466	1/1	0.98	0.24	3.57	41,41,41,41	0
57	MG	BA	3150	1/1	0.97	0.21	3.52	40,40,40,40	0
57	MG	BA	3183	1/1	0.89	0.25	3.44	50,50,50,50	0
57	MG	DA	3348	1/1	0.96	0.20	3.41	33,33,33,33	0
57	MG	DA	3483	1/1	0.96	0.28	3.39	41,41,41,41	0
57	MG	BA	3314	1/1	0.95	0.25	3.35	42,42,42,42	0
57	MG	DF	3004	1/1	0.93	0.27	3.27	56,56,56,56	0
57	MG	DA	3371	1/1	0.92	0.23	3.24	47,47,47,47	0
57	MG	DA	3171	1/1	0.94	0.21	3.17	38,38,38,38	0
57	MG	DA	3387	1/1	0.96	0.18	3.16	29,29,29,29	0
57	MG	DA	3417	1/1	0.91	0.20	3.16	46,46,46,46	0
57	MG	AA	3091	1/1	0.97	0.24	3.13	35,35,35,35	0
57	MG	BA	3253	1/1	0.95	0.22	3.11	28,28,28,28	0
57	MG	BA	3437	1/1	0.92	0.23	3.07	52,52,52,52	0
57	MG	BA	3385	1/1	0.86	0.27	3.06	34,34,34,34	0
57	MG	DA	3183	1/1	0.98	0.21	3.05	31,31,31,31	0
57	MG	BA	3190	1/1	0.98	0.23	3.05	24,24,24,24	0
57	MG	BA	3443	1/1	0.94	0.24	3.03	38,38,38,38	0
57	MG	BA	3366	1/1	0.83	0.22	3.02	38,38,38,38	0
57	MG	DP	202	1/1	0.93	0.28	3.00	48,48,48,48	0
57	MG	BA	3246	1/1	0.96	0.23	2.96	46,46,46,46	0
57	MG	BA	3546	1/1	0.97	0.24	2.96	27,27,27,27	0
57	MG	DA	3020	1/1	0.96	0.19	2.94	32,32,32,32	0
57	MG	DA	3207	1/1	0.97	0.24	2.86	39,39,39,39	0
57	MG	DA	3430	1/1	0.85	0.20	2.86	26,26,26,26	0
57	MG	BA	3026	1/1	0.99	0.25	2.84	36,36,36,36	0
57	MG	DA	3096	1/1	0.97	0.21	2.83	52,52,52,52	0
57	MG	DA	3243	1/1	0.97	0.30	2.79	41,41,41,41	0
57	MG	BA	3193	1/1	0.98	0.20	2.77	30,30,30,30	0
57	MG	BA	3432	1/1	0.97	0.26	2.72	35,35,35,35	0
57	MG	DA	3624	1/1	0.83	0.27	2.66	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3155	1/1	0.90	0.24	2.65	65,65,65,65	0
57	MG	DA	3145	1/1	0.96	0.21	2.65	38,38,38,38	0
57	MG	DA	3453	1/1	0.91	0.22	2.61	44,44,44,44	0
57	MG	BA	3686	1/1	0.96	0.22	2.59	36,36,36,36	0
57	MG	BA	3431	1/1	0.93	0.21	2.56	25,25,25,25	0
57	MG	CA	3074	1/1	0.96	0.23	2.55	51,51,51,51	0
57	MG	DD	303	1/1	0.98	0.24	2.52	42,42,42,42	0
57	MG	BA	3294	1/1	0.94	0.21	2.51	37,37,37,37	0
57	MG	AA	3089	1/1	0.90	0.20	2.46	61,61,61,61	0
57	MG	BA	3508	1/1	0.94	0.19	2.40	52,52,52,52	0
57	MG	DA	3058	1/1	0.94	0.21	2.40	47,47,47,47	0
57	MG	DA	3471	1/1	0.96	0.23	2.38	23,23,23,23	0
57	MG	BD	308	1/1	0.85	0.32	2.36	41,41,41,41	0
57	MG	DA	3475	1/1	0.95	0.19	2.35	35,35,35,35	0
57	MG	BF	307	1/1	0.97	0.24	2.31	25,25,25,25	0
57	MG	DA	3291	1/1	0.87	0.21	2.25	56,56,56,56	0
57	MG	DA	3228	1/1	0.94	0.24	2.19	49,49,49,49	0
57	MG	DA	3059	1/1	0.86	0.16	2.12	60,60,60,60	0
57	MG	DA	3382	1/1	0.98	0.22	2.12	20,20,20,20	0
57	MG	DV	201	1/1	0.96	0.30	2.09	49,49,49,49	0
57	MG	DA	3044	1/1	0.99	0.18	2.08	38,38,38,38	0
57	MG	BA	3148	1/1	0.94	0.20	2.05	44,44,44,44	0
57	MG	CA	3047	1/1	0.98	0.20	2.05	50,50,50,50	0
57	MG	DA	3537	1/1	0.94	0.20	2.02	45,45,45,45	0
57	MG	BA	3545	1/1	0.96	0.24	2.01	34,34,34,34	0
57	MG	BA	3053	1/1	0.97	0.20	2.00	33,33,33,33	0
57	MG	DA	3494	1/1	0.96	0.19	2.00	56,56,56,56	0
57	MG	DA	3014	1/1	0.96	0.19	2.00	45,45,45,45	0
57	MG	BA	3418	1/1	0.97	0.23	1.96	26,26,26,26	0
57	MG	BV	201	1/1	0.98	0.22	1.86	33,33,33,33	0
57	MG	BA	3045	1/1	0.95	0.21	1.85	33,33,33,33	0
57	MG	DA	3427	1/1	0.91	0.20	1.84	26,26,26,26	0
57	MG	DA	3315	1/1	0.97	0.16	1.84	57,57,57,57	0
57	MG	BX	101	1/1	0.94	0.28	1.83	36,36,36,36	0
57	MG	BA	3364	1/1	0.94	0.21	1.82	37,37,37,37	0
57	MG	BA	3347	1/1	0.84	0.22	1.80	32,32,32,32	0
57	MG	DA	3296	1/1	0.97	0.20	1.78	46,46,46,46	0
57	MG	DA	3565	1/1	0.79	0.20	1.72	49,49,49,49	0
57	MG	BA	3510	1/1	0.92	0.24	1.72	20,20,20,20	0
57	MG	CA	3107	1/1	0.77	0.21	1.70	89,89,89,89	0
57	MG	BD	309	1/1	0.97	0.25	1.63	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	B5	101	1/1	0.87	0.21	1.54	30,30,30,30	0
57	MG	AW	101	1/1	0.96	0.24	1.50	24,24,24,24	0
57	MG	AA	3137	1/1	0.98	0.28	1.48	66,66,66,66	0
57	MG	DA	3625	1/1	0.86	0.26	1.45	57,57,57,57	0
57	MG	DA	3098	1/1	0.96	0.19	1.43	32,32,32,32	0
57	MG	BA	3520	1/1	0.96	0.21	1.43	46,46,46,46	0
57	MG	DA	3041	1/1	0.95	0.18	1.34	36,36,36,36	0
57	MG	DA	3514	1/1	0.92	0.20	1.34	34,34,34,34	0
57	MG	DA	3517	1/1	0.91	0.18	1.33	36,36,36,36	0
57	MG	DA	3005	1/1	0.98	0.20	1.32	29,29,29,29	0
57	MG	BA	3609	1/1	0.96	0.18	1.32	47,47,47,47	0
57	MG	BB	3002	1/1	0.97	0.19	1.29	44,44,44,44	0
57	MG	DA	3229	1/1	0.95	0.17	1.25	39,39,39,39	0
57	MG	BA	3189	1/1	0.95	0.19	1.25	33,33,33,33	0
57	MG	BA	3056	1/1	0.95	0.20	1.19	21,21,21,21	0
57	MG	BA	3558	1/1	0.94	0.17	1.13	63,63,63,63	0
57	MG	DA	3549	1/1	0.96	0.20	1.11	47,47,47,47	0
57	MG	BA	3400	1/1	0.95	0.20	1.05	33,33,33,33	0
57	MG	AA	3076	1/1	0.87	0.19	1.01	62,62,62,62	0
57	MG	DA	3032	1/1	0.91	0.18	0.97	34,34,34,34	0
57	MG	BA	3186	1/1	0.97	0.23	0.95	42,42,42,42	0
57	MG	BA	3411	1/1	0.92	0.23	0.93	24,24,24,24	0
57	MG	BA	3162	1/1	0.89	0.20	0.91	39,39,39,39	0
57	MG	DU	3004	1/1	0.92	0.18	0.90	69,69,69,69	0
57	MG	DA	3357	1/1	0.96	0.19	0.89	29,29,29,29	0
57	MG	BD	302	1/1	0.94	0.24	0.88	38,38,38,38	0
57	MG	BA	3043	1/1	0.97	0.17	0.88	44,44,44,44	0
57	MG	CA	3133	1/1	0.82	0.19	0.85	69,69,69,69	0
57	MG	DA	3543	1/1	0.92	0.14	0.85	61,61,61,61	0
57	MG	DA	3489	1/1	0.97	0.15	0.81	38,38,38,38	0
57	MG	DA	3213	1/1	0.93	0.30	0.79	51,51,51,51	0
57	MG	BA	3445	1/1	0.85	0.21	0.78	35,35,35,35	0
57	MG	DA	3511	1/1	0.91	0.17	0.76	40,40,40,40	0
57	MG	BA	3047	1/1	0.89	0.23	0.71	44,44,44,44	0
57	MG	AA	3108	1/1	0.97	0.21	0.67	54,54,54,54	0
57	MG	DA	3347	1/1	0.92	0.19	0.65	32,32,32,32	0
57	MG	CA	3025	1/1	0.66	0.17	0.63	66,66,66,66	0
57	MG	BA	3285	1/1	0.98	0.18	0.61	21,21,21,21	0
57	MG	BA	3407	1/1	0.98	0.19	0.58	29,29,29,29	0
57	MG	BA	3628	1/1	0.93	0.17	0.54	60,60,60,60	0
57	MG	DA	3112	1/1	0.93	0.15	0.54	63,63,63,63	0
57	MG	CA	3076	1/1	0.96	0.20	0.54	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3194	1/1	0.98	0.21	0.51	41,41,41,41	0
57	MG	BA	3408	1/1	0.96	0.21	0.50	42,42,42,42	0
57	MG	DA	3570	1/1	0.98	0.18	0.49	28,28,28,28	0
57	MG	BA	3716	1/1	0.98	0.17	0.49	53,53,53,53	0
57	MG	AA	3021	1/1	0.93	0.16	0.48	58,58,58,58	0
57	MG	DA	3340	1/1	0.98	0.17	0.47	38,38,38,38	0
57	MG	AX	3002	1/1	0.94	0.18	0.43	67,67,67,67	0
57	MG	BR	201	1/1	0.96	0.23	0.42	30,30,30,30	0
57	MG	BA	3154	1/1	0.97	0.20	0.40	36,36,36,36	0
57	MG	DA	3345	1/1	0.88	0.18	0.40	28,28,28,28	0
57	MG	BA	3316	1/1	0.88	0.18	0.39	49,49,49,49	0
57	MG	BA	3571	1/1	0.88	0.20	0.36	24,24,24,24	0
57	MG	CA	3158	1/1	0.76	0.18	0.29	66,66,66,66	0
57	MG	BN	3003	1/1	0.93	0.26	0.29	61,61,61,61	0
57	MG	DA	3582	1/1	0.93	0.16	0.25	24,24,24,24	0
57	MG	DE	304	1/1	0.96	0.15	0.24	47,47,47,47	0
57	MG	BA	3549	1/1	0.85	0.18	0.23	55,55,55,55	0
57	MG	BA	3695	1/1	0.95	0.20	0.20	19,19,19,19	0
57	MG	DA	3499	1/1	0.86	0.14	0.17	47,47,47,47	0
57	MG	BA	3720	1/1	0.95	0.22	0.17	48,48,48,48	0
57	MG	BA	3587	1/1	0.79	0.18	0.16	51,51,51,51	0
57	MG	BA	3051	1/1	0.96	0.18	0.16	36,36,36,36	0
57	MG	DA	3443	1/1	0.94	0.18	0.15	27,27,27,27	0
57	MG	CW	101	1/1	0.86	0.19	0.12	43,43,43,43	0
59	ZN	D5	102	1/1	0.99	0.17	0.10	58,58,58,58	0
57	MG	BA	3247	1/1	0.89	0.18	0.10	37,37,37,37	0
57	MG	BA	3109	1/1	0.82	0.14	0.09	53,53,53,53	0
57	MG	CA	3037	1/1	0.95	0.17	0.09	60,60,60,60	0
57	MG	AA	3094	1/1	0.94	0.19	0.08	54,54,54,54	0
57	MG	DB	3006	1/1	0.97	0.13	0.08	44,44,44,44	0
57	MG	BF	303	1/1	0.98	0.19	0.06	35,35,35,35	0
57	MG	AX	3012	1/1	0.94	0.21	0.03	15,15,15,15	0
57	MG	CK	3001	1/1	0.94	0.18	-0.02	57,57,57,57	0
57	MG	DA	3378	1/1	0.97	0.15	-0.03	33,33,33,33	0
57	MG	DA	3479	1/1	0.95	0.17	-0.06	45,45,45,45	0
57	MG	BA	3274	1/1	0.99	0.17	-0.07	44,44,44,44	0
57	MG	AA	3017	1/1	0.90	0.15	-0.07	63,63,63,63	0
57	MG	AA	3047	1/1	0.85	0.21	-0.07	59,59,59,59	0
57	MG	AA	3011	1/1	0.86	0.16	-0.08	67,67,67,67	0
57	MG	BP	3002	1/1	0.95	0.20	-0.08	32,32,32,32	0
57	MG	DA	3393	1/1	0.97	0.16	-0.08	41,41,41,41	0
57	MG	DA	3364	1/1	0.90	0.17	-0.08	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DE	303	1/1	0.79	0.17	-0.10	49,49,49,49	0
57	MG	BA	3334	1/1	0.85	0.18	-0.14	37,37,37,37	0
57	MG	BA	3350	1/1	0.88	0.16	-0.14	43,43,43,43	0
57	MG	BG	3001	1/1	0.94	0.18	-0.14	44,44,44,44	0
57	MG	BA	3701	1/1	0.96	0.20	-0.14	17,17,17,17	0
57	MG	BA	3572	1/1	0.96	0.20	-0.15	27,27,27,27	0
57	MG	DA	3361	1/1	0.97	0.18	-0.16	32,32,32,32	0
57	MG	DA	3045	1/1	0.94	0.13	-0.16	39,39,39,39	0
57	MG	BA	3097	1/1	0.87	0.20	-0.19	44,44,44,44	0
57	MG	DA	3620	1/1	0.98	0.17	-0.21	47,47,47,47	0
57	MG	CA	3075	1/1	0.91	0.16	-0.22	48,48,48,48	0
59	ZN	B5	102	1/1	0.99	0.16	-0.22	41,41,41,41	0
57	MG	BU	207	1/1	0.99	0.16	-0.23	23,23,23,23	0
57	MG	CA	3104	1/1	0.96	0.16	-0.24	37,37,37,37	0
57	MG	BV	202	1/1	0.98	0.20	-0.26	29,29,29,29	0
57	MG	CA	3105	1/1	0.93	0.17	-0.26	76,76,76,76	0
57	MG	BA	3464	1/1	0.95	0.20	-0.27	26,26,26,26	0
57	MG	BA	3025	1/1	0.97	0.20	-0.27	12,12,12,12	0
57	MG	AA	3183	1/1	0.97	0.19	-0.28	43,43,43,43	0
57	MG	BA	3204	1/1	0.89	0.13	-0.29	61,61,61,61	0
57	MG	BA	3511	1/1	0.92	0.20	-0.29	41,41,41,41	0
57	MG	BA	3421	1/1	0.93	0.18	-0.30	29,29,29,29	0
57	MG	CA	3059	1/1	0.84	0.18	-0.31	60,60,60,60	0
57	MG	BA	3144	1/1	0.86	0.19	-0.33	42,42,42,42	0
57	MG	DA	3617	1/1	0.91	0.18	-0.34	40,40,40,40	0
57	MG	BD	307	1/1	0.97	0.18	-0.35	40,40,40,40	0
57	MG	BA	3469	1/1	0.94	0.18	-0.35	42,42,42,42	0
57	MG	DA	3167	1/1	0.93	0.17	-0.36	26,26,26,26	0
57	MG	AA	3025	1/1	0.93	0.17	-0.36	46,46,46,46	0
57	MG	DA	3029	1/1	0.98	0.16	-0.37	44,44,44,44	0
57	MG	BA	3021	1/1	0.86	0.19	-0.38	35,35,35,35	0
57	MG	BU	203	1/1	0.98	0.18	-0.38	35,35,35,35	0
57	MG	DA	3339	1/1	0.98	0.17	-0.43	23,23,23,23	0
57	MG	DA	3270	1/1	0.94	0.15	-0.44	57,57,57,57	0
57	MG	BF	308	1/1	0.94	0.19	-0.45	46,46,46,46	0
57	MG	AA	3028	1/1	0.88	0.18	-0.46	58,58,58,58	0
57	MG	DA	3268	1/1	0.92	0.12	-0.48	35,35,35,35	0
57	MG	DA	3435	1/1	0.94	0.14	-0.48	59,59,59,59	0
57	MG	AA	3006	1/1	0.93	0.16	-0.49	62,62,62,62	0
57	MG	DA	3154	1/1	0.86	0.16	-0.50	40,40,40,40	0
57	MG	D3	3001	1/1	0.97	0.17	-0.50	54,54,54,54	0
57	MG	B7	101	1/1	0.98	0.18	-0.53	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3615	1/1	0.88	0.13	-0.53	60,60,60,60	0
59	ZN	D4	501	1/1	0.76	0.19	-0.56	154,154,154,154	0
57	MG	DU	3003	1/1	0.97	0.20	-0.57	60,60,60,60	0
57	MG	CA	3146	1/1	0.96	0.15	-0.60	74,74,74,74	0
59	ZN	D6	501	1/1	0.98	0.16	-0.63	64,64,64,64	0
57	MG	BA	3718	1/1	0.98	0.17	-0.63	36,36,36,36	0
57	MG	CA	3038	1/1	0.81	0.14	-0.64	68,68,68,68	0
57	MG	DA	3359	1/1	0.97	0.16	-0.67	42,42,42,42	0
57	MG	DA	3300	1/1	0.95	0.14	-0.68	38,38,38,38	0
57	MG	BA	3380	1/1	0.86	0.16	-0.70	55,55,55,55	0
57	MG	DA	3623	1/1	0.96	0.16	-0.70	31,31,31,31	0
57	MG	CA	3007	1/1	0.84	0.14	-0.70	55,55,55,55	0
57	MG	BA	3497	1/1	0.92	0.19	-0.72	41,41,41,41	0
57	MG	DA	3495	1/1	0.84	0.10	-0.72	48,48,48,48	0
57	MG	BA	3541	1/1	0.96	0.17	-0.72	43,43,43,43	0
57	MG	DF	3003	1/1	0.93	0.17	-0.75	36,36,36,36	0
57	MG	BA	3305	1/1	0.97	0.18	-0.75	45,45,45,45	0
57	MG	DA	3379	1/1	0.92	0.16	-0.75	37,37,37,37	0
57	MG	CA	3115	1/1	0.97	0.14	-0.76	59,59,59,59	0
57	MG	BW	203	1/1	0.92	0.17	-0.79	39,39,39,39	0
57	MG	AA	3007	1/1	0.68	0.20	-0.80	47,47,47,47	0
57	MG	BW	204	1/1	0.98	0.17	-0.83	27,27,27,27	0
57	MG	CA	3044	1/1	0.75	0.14	-0.86	59,59,59,59	0
57	MG	BA	3135	1/1	0.92	0.19	-0.87	48,48,48,48	0
57	MG	AA	3050	1/1	0.93	0.17	-0.88	49,49,49,49	0
57	MG	BA	3492	1/1	0.87	0.18	-0.90	30,30,30,30	0
57	MG	BA	3181	1/1	0.94	0.18	-0.91	49,49,49,49	0
57	MG	AA	3174	1/1	0.95	0.14	-0.93	64,64,64,64	0
57	MG	DA	3031	1/1	0.99	0.14	-0.94	36,36,36,36	0
57	MG	BA	3093	1/1	0.93	0.16	-0.94	23,23,23,23	0
57	MG	BA	3327	1/1	0.93	0.18	-0.94	32,32,32,32	0
57	MG	BF	301	1/1	0.98	0.18	-0.95	30,30,30,30	0
59	ZN	B6	501	1/1	0.99	0.14	-0.96	43,43,43,43	0
57	MG	DA	3349	1/1	0.98	0.16	-0.99	35,35,35,35	0
57	MG	DA	3203	1/1	0.97	0.17	-1.00	46,46,46,46	0
57	MG	BA	3374	1/1	0.91	0.15	-1.01	48,48,48,48	0
57	MG	DA	3583	1/1	0.96	0.14	-1.02	44,44,44,44	0
57	MG	CA	3063	1/1	0.94	0.11	-1.03	59,59,59,59	0
57	MG	BY	201	1/1	0.98	0.16	-1.04	51,51,51,51	0
57	MG	CA	3029	1/1	0.87	0.16	-1.05	48,48,48,48	0
57	MG	AA	3130	1/1	0.94	0.16	-1.05	52,52,52,52	0
57	MG	BA	3410	1/1	0.93	0.19	-1.06	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	D8	101	1/1	0.92	0.15	-1.08	60,60,60,60	0
57	MG	DA	3126	1/1	0.96	0.13	-1.09	39,39,39,39	0
57	MG	BA	3559	1/1	0.92	0.17	-1.10	36,36,36,36	0
57	MG	AA	3103	1/1	0.95	0.15	-1.11	42,42,42,42	0
57	MG	CA	3021	1/1	0.94	0.15	-1.14	46,46,46,46	0
57	MG	BA	3394	1/1	0.96	0.17	-1.14	22,22,22,22	0
57	MG	AE	3002	1/1	0.96	0.15	-1.15	61,61,61,61	0
57	MG	AA	3052	1/1	0.97	0.16	-1.16	53,53,53,53	0
57	MG	CA	3055	1/1	0.83	0.13	-1.16	66,66,66,66	0
57	MG	AA	3004	1/1	0.84	0.17	-1.17	61,61,61,61	0
57	MG	CA	3125	1/1	0.91	0.14	-1.19	64,64,64,64	0
57	MG	DA	3205	1/1	0.87	0.13	-1.19	52,52,52,52	0
57	MG	DA	3467	1/1	0.94	0.15	-1.20	28,28,28,28	0
57	MG	DA	3314	1/1	0.89	0.14	-1.24	56,56,56,56	0
57	MG	BA	3588	1/1	0.99	0.18	-1.25	19,19,19,19	0
57	MG	DA	3414	1/1	0.95	0.15	-1.28	37,37,37,37	0
57	MG	DR	3002	1/1	0.96	0.14	-1.28	51,51,51,51	0
57	MG	CA	3141	1/1	0.96	0.15	-1.29	69,69,69,69	0
57	MG	BA	3426	1/1	0.90	0.18	-1.29	30,30,30,30	0
57	MG	BA	3343	1/1	0.97	0.18	-1.31	18,18,18,18	0
57	MG	CA	3079	1/1	0.97	0.14	-1.34	42,42,42,42	0
57	MG	CA	3043	1/1	0.84	0.13	-1.35	68,68,68,68	0
57	MG	DA	3342	1/1	0.76	0.15	-1.35	49,49,49,49	0
57	MG	AA	3095	1/1	0.98	0.15	-1.38	44,44,44,44	0
57	MG	DA	3021	1/1	0.91	0.13	-1.38	50,50,50,50	0
59	ZN	CN	501	1/1	0.82	0.07	-1.38	101,101,101,101	0
59	ZN	AN	501	1/1	0.95	0.12	-1.38	71,71,71,71	0
57	MG	DA	3510	1/1	0.94	0.13	-1.40	52,52,52,52	0
57	MG	AN	503	1/1	0.95	0.13	-1.42	61,61,61,61	0
57	MG	AA	3170	1/1	0.83	0.15	-1.43	70,70,70,70	0
57	MG	BA	3145	1/1	0.98	0.16	-1.44	41,41,41,41	0
57	MG	DF	3002	1/1	0.94	0.12	-1.44	51,51,51,51	0
57	MG	AN	502	1/1	0.75	0.17	-1.45	61,61,61,61	0
57	MG	BA	3491	1/1	0.96	0.16	-1.45	33,33,33,33	0
57	MG	BA	3352	1/1	0.96	0.14	-1.46	29,29,29,29	0
57	MG	CA	3061	1/1	0.95	0.10	-1.48	87,87,87,87	0
57	MG	CA	3077	1/1	0.97	0.13	-1.48	63,63,63,63	0
57	MG	DD	304	1/1	0.97	0.15	-1.52	40,40,40,40	0
57	MG	BQ	3005	1/1	0.95	0.17	-1.52	39,39,39,39	0
57	MG	AA	3015	1/1	0.94	0.17	-1.55	28,28,28,28	0
57	MG	AA	3003	1/1	0.92	0.10	-1.55	53,53,53,53	0
58	SF4	AD	302	8/8	0.98	0.14	-1.55	59,71,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BU	205	1/1	0.93	0.15	-1.56	32,32,32,32	0
57	MG	DA	3344	1/1	0.92	0.13	-1.61	42,42,42,42	0
57	MG	BA	3128	1/1	0.98	0.16	-1.62	33,33,33,33	0
57	MG	BA	3694	1/1	0.97	0.19	-1.63	11,11,11,11	0
57	MG	AA	3189	1/1	0.95	0.12	-1.63	69,69,69,69	0
59	ZN	DY	501	1/1	0.98	0.10	-1.64	88,88,88,88	0
59	ZN	B9	501	1/1	0.96	0.13	-1.64	59,59,59,59	0
57	MG	DA	3033	1/1	0.97	0.13	-1.64	46,46,46,46	0
57	MG	DF	3001	1/1	0.83	0.12	-1.65	36,36,36,36	0
59	ZN	B4	501	1/1	0.95	0.06	-1.67	94,94,94,94	0
57	MG	BA	3134	1/1	0.93	0.16	-1.70	43,43,43,43	0
57	MG	CA	3045	1/1	0.92	0.15	-1.70	53,53,53,53	0
57	MG	BA	3715	1/1	0.93	0.14	-1.71	33,33,33,33	0
57	MG	BA	3057	1/1	0.98	0.18	-1.71	21,21,21,21	0
57	MG	BA	3566	1/1	0.87	0.17	-1.74	31,31,31,31	0
58	SF4	CD	501	8/8	0.97	0.12	-1.76	59,71,83,91	0
57	MG	CA	3159	1/1	0.94	0.14	-1.76	46,46,46,46	0
57	MG	AA	3018	1/1	0.92	0.14	-1.77	62,62,62,62	0
57	MG	CF	3001	1/1	0.92	0.17	-1.78	51,51,51,51	0
57	MG	BA	3064	1/1	0.93	0.16	-1.79	38,38,38,38	0
57	MG	BA	3024	1/1	0.91	0.15	-1.81	42,42,42,42	0
57	MG	BA	3528	1/1	0.99	0.17	-1.81	37,37,37,37	0
57	MG	BA	3046	1/1	0.95	0.18	-1.81	30,30,30,30	0
57	MG	DA	3513	1/1	0.87	0.11	-1.85	49,49,49,49	0
59	ZN	D9	501	1/1	0.89	0.07	-1.86	75,75,75,75	0
57	MG	DA	3524	1/1	0.91	0.10	-1.86	40,40,40,40	0
57	MG	BA	3276	1/1	0.97	0.16	-1.88	19,19,19,19	0
57	MG	DG	3001	1/1	0.78	0.09	-1.91	49,49,49,49	0
57	MG	DA	3434	1/1	0.94	0.10	-1.94	48,48,48,48	0
57	MG	DA	3432	1/1	0.93	0.12	-1.94	33,33,33,33	0
57	MG	AM	201	1/1	0.92	0.05	-1.96	43,43,43,43	0
57	MG	BA	3286	1/1	0.93	0.15	-1.96	33,33,33,33	0
57	MG	BD	304	1/1	0.98	0.19	-1.97	36,36,36,36	0
57	MG	BA	3452	1/1	0.95	0.18	-1.98	15,15,15,15	0
57	MG	DQ	3001	1/1	0.95	0.08	-1.99	58,58,58,58	0
57	MG	BA	3048	1/1	0.94	0.14	-2.01	44,44,44,44	0
57	MG	DA	3297	1/1	0.83	0.14	-2.04	48,48,48,48	0
57	MG	CA	3094	1/1	0.89	0.09	-2.07	80,80,80,80	0
57	MG	BA	3710	1/1	0.93	0.11	-2.07	21,21,21,21	0
57	MG	BA	3713	1/1	0.94	0.14	-2.08	63,63,63,63	0
57	MG	AA	3119	1/1	0.96	0.13	-2.11	50,50,50,50	0
57	MG	DA	3011	1/1	0.87	0.12	-2.12	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AK	3001	1/1	0.96	0.12	-2.13	55,55,55,55	0
57	MG	DA	3052	1/1	0.96	0.11	-2.14	33,33,33,33	0
57	MG	DA	3221	1/1	0.92	0.13	-2.15	49,49,49,49	0
57	MG	BA	3137	1/1	0.94	0.17	-2.16	57,57,57,57	0
57	MG	BA	3213	1/1	0.93	0.15	-2.16	48,48,48,48	0
57	MG	AA	3001	1/1	0.80	0.13	-2.18	72,72,72,72	0
57	MG	DA	3470	1/1	0.97	0.14	-2.20	34,34,34,34	0
57	MG	DA	3060	1/1	0.94	0.11	-2.23	50,50,50,50	0
57	MG	AA	3157	1/1	0.96	0.13	-2.27	38,38,38,38	0
57	MG	DA	3299	1/1	0.95	0.13	-2.27	32,32,32,32	0
57	MG	BA	3039	1/1	0.96	0.15	-2.35	27,27,27,27	0
57	MG	AA	3008	1/1	0.82	0.11	-2.37	65,65,65,65	0
57	MG	BA	3383	1/1	0.97	0.13	-2.37	37,37,37,37	0
57	MG	CT	3001	1/1	0.92	0.07	-2.40	59,59,59,59	0
57	MG	CA	3052	1/1	0.83	0.09	-2.42	61,61,61,61	0
57	MG	BA	3089	1/1	0.94	0.13	-2.43	30,30,30,30	0
57	MG	DA	3265	1/1	0.91	0.14	-2.43	33,33,33,33	0
57	MG	AA	3140	1/1	0.96	0.12	-2.44	56,56,56,56	0
57	MG	B9	502	1/1	0.91	0.12	-2.48	31,31,31,31	0
57	MG	AA	3104	1/1	0.88	0.15	-2.48	47,47,47,47	0
57	MG	BA	3619	1/1	0.96	0.13	-2.48	54,54,54,54	0
57	MG	AA	3187	1/1	0.96	0.14	-2.49	47,47,47,47	0
57	MG	BA	3023	1/1	0.94	0.16	-2.51	25,25,25,25	0
57	MG	BA	3028	1/1	0.95	0.13	-2.55	31,31,31,31	0
57	MG	DA	3449	1/1	0.91	0.09	-2.56	52,52,52,52	0
57	MG	CA	3039	1/1	0.94	0.10	-2.59	52,52,52,52	0
57	MG	DA	3063	1/1	0.89	0.10	-2.60	40,40,40,40	0
57	MG	BA	3395	1/1	0.95	0.18	-2.63	19,19,19,19	0
57	MG	DA	3223	1/1	0.86	0.11	-2.66	56,56,56,56	0
57	MG	BA	3393	1/1	0.94	0.15	-2.67	30,30,30,30	0
57	MG	DA	3212	1/1	0.92	0.08	-2.67	47,47,47,47	0
57	MG	BA	3077	1/1	0.95	0.12	-2.68	33,33,33,33	0
57	MG	DA	3218	1/1	0.94	0.09	-2.70	36,36,36,36	0
57	MG	AA	3032	1/1	0.92	0.11	-2.70	80,80,80,80	0
57	MG	BA	3302	1/1	0.97	0.17	-2.71	50,50,50,50	0
57	MG	BA	3187	1/1	0.97	0.15	-2.71	35,35,35,35	0
57	MG	DA	3389	1/1	0.91	0.15	-2.73	31,31,31,31	0
57	MG	DB	3003	1/1	0.92	0.06	-2.73	76,76,76,76	0
57	MG	CX	3003	1/1	0.94	0.13	-2.76	53,53,53,53	0
57	MG	DA	3146	1/1	0.89	0.11	-2.77	44,44,44,44	0
57	MG	BA	3037	1/1	0.97	0.17	-2.79	38,38,38,38	0
57	MG	BA	3381	1/1	0.90	0.17	-2.81	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3206	1/1	0.96	0.06	-2.82	62,62,62,62	0
57	MG	BA	3081	1/1	0.96	0.14	-2.83	26,26,26,26	0
59	ZN	BY	202	1/1	0.98	0.12	-2.89	70,70,70,70	0
57	MG	AA	3037	1/1	0.93	0.11	-2.89	48,48,48,48	0
57	MG	BA	3237	1/1	0.92	0.15	-2.91	36,36,36,36	0
57	MG	DA	3498	1/1	0.92	0.08	-2.92	66,66,66,66	0
57	MG	DA	3541	1/1	0.97	0.15	-2.92	40,40,40,40	0
57	MG	B0	103	1/1	0.90	0.12	-2.95	38,38,38,38	0
57	MG	DA	3131	1/1	0.98	0.11	-2.97	34,34,34,34	0
57	MG	DA	3512	1/1	0.97	0.13	-2.97	24,24,24,24	0
57	MG	DA	3007	1/1	0.90	0.08	-2.98	48,48,48,48	0
57	MG	AA	3121	1/1	0.85	0.10	-2.98	66,66,66,66	0
57	MG	BA	3439	1/1	0.95	0.16	-3.00	12,12,12,12	0
57	MG	AA	3026	1/1	0.91	0.08	-3.00	61,61,61,61	0
57	MG	DA	3531	1/1	0.96	0.07	-3.01	40,40,40,40	0
57	MG	BD	305	1/1	0.96	0.16	-3.05	41,41,41,41	0
57	MG	CA	3049	1/1	0.97	0.11	-3.07	42,42,42,42	0
57	MG	CA	3151	1/1	0.93	0.12	-3.08	58,58,58,58	0
57	MG	DA	3332	1/1	0.95	0.11	-3.08	52,52,52,52	0
57	MG	CA	3065	1/1	0.95	0.08	-3.14	60,60,60,60	0
57	MG	BF	306	1/1	0.94	0.08	-3.24	43,43,43,43	0
57	MG	BA	3523	1/1	0.89	0.14	-3.24	31,31,31,31	0
57	MG	DA	3508	1/1	0.90	0.10	-3.25	58,58,58,58	0
57	MG	AA	3061	1/1	0.95	0.10	-3.32	65,65,65,65	0
57	MG	DA	3075	1/1	0.92	0.11	-3.46	40,40,40,40	0
57	MG	DA	3272	1/1	0.97	0.08	-3.47	29,29,29,29	0
57	MG	AA	3164	1/1	0.96	0.12	-3.48	54,54,54,54	0
57	MG	BA	3522	1/1	0.93	0.11	-3.48	34,34,34,34	0
57	MG	BU	201	1/1	0.87	0.11	-3.51	36,36,36,36	0
57	MG	DA	3320	1/1	0.97	0.12	-3.52	19,19,19,19	0
57	MG	DA	3009	1/1	0.98	0.14	-3.55	39,39,39,39	0
57	MG	BA	3084	1/1	0.94	0.14	-3.55	37,37,37,37	0
57	MG	CA	3057	1/1	0.90	0.12	-3.57	48,48,48,48	0
57	MG	AA	3112	1/1	0.95	0.14	-3.57	44,44,44,44	0
57	MG	CA	3024	1/1	0.92	0.07	-3.64	58,58,58,58	0
57	MG	AJ	201	1/1	0.90	0.08	-3.69	67,67,67,67	0
57	MG	DA	3343	1/1	0.92	0.10	-3.75	37,37,37,37	0
57	MG	BA	3206	1/1	0.96	0.13	-3.76	37,37,37,37	0
57	MG	AA	3034	1/1	0.93	0.08	-3.76	47,47,47,47	0
57	MG	B3	3001	1/1	0.96	0.12	-3.78	43,43,43,43	0
57	MG	BB	3004	1/1	0.89	0.11	-3.79	43,43,43,43	0
57	MG	BA	3693	1/1	0.95	0.14	-3.83	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	3145	1/1	0.95	0.10	-3.87	49,49,49,49	0
57	MG	BA	3315	1/1	0.96	0.10	-3.87	42,42,42,42	0
57	MG	BA	3288	1/1	0.96	0.10	-3.89	37,37,37,37	0
57	MG	BA	3399	1/1	0.93	0.15	-3.89	26,26,26,26	0
57	MG	AA	3149	1/1	0.91	0.14	-3.89	48,48,48,48	0
57	MG	CA	3031	1/1	0.84	0.10	-3.91	55,55,55,55	0
57	MG	DA	3480	1/1	0.97	0.11	-3.96	28,28,28,28	0
57	MG	BB	3015	1/1	0.98	0.11	-3.96	42,42,42,42	0
57	MG	DA	3038	1/1	0.91	0.11	-4.00	39,39,39,39	0
57	MG	BA	3337	1/1	0.89	0.15	-4.05	51,51,51,51	0
57	MG	DA	3502	1/1	0.94	0.14	-4.06	51,51,51,51	0
57	MG	DA	3401	1/1	0.96	0.12	-4.12	36,36,36,36	0
57	MG	BA	3040	1/1	0.96	0.14	-4.14	28,28,28,28	0
57	MG	DA	3588	1/1	0.97	0.13	-4.14	21,21,21,21	0
57	MG	CA	3005	1/1	0.82	0.12	-4.17	81,81,81,81	0
57	MG	AX	3004	1/1	0.97	0.12	-4.27	45,45,45,45	0
57	MG	AA	3162	1/1	0.89	0.10	-4.31	40,40,40,40	0
57	MG	BE	3007	1/1	0.99	0.10	-4.37	31,31,31,31	0
57	MG	AA	3096	1/1	0.91	0.06	-4.43	57,57,57,57	0
57	MG	AA	3057	1/1	0.95	0.12	-4.47	38,38,38,38	0
57	MG	BA	3042	1/1	0.97	0.14	-4.49	34,34,34,34	0
57	MG	BV	204	1/1	0.97	0.09	-4.50	36,36,36,36	0
57	MG	DA	3184	1/1	0.95	0.09	-4.51	44,44,44,44	0
57	MG	BB	3007	1/1	0.94	0.10	-4.57	51,51,51,51	0
57	MG	BA	3458	1/1	0.94	0.14	-4.67	40,40,40,40	0
57	MG	BA	3009	1/1	0.97	0.09	-4.68	34,34,34,34	0
57	MG	DA	3164	1/1	0.97	0.08	-4.75	44,44,44,44	0
57	MG	DA	3589	1/1	0.95	0.14	-4.85	52,52,52,52	0
57	MG	AA	3023	1/1	0.96	0.07	-4.90	60,60,60,60	0
57	MG	BE	3004	1/1	0.97	0.12	-4.93	49,49,49,49	0
57	MG	BA	3340	1/1	0.94	0.10	-5.06	59,59,59,59	0
57	MG	BA	3390	1/1	0.96	0.09	-5.07	31,31,31,31	0
57	MG	AA	3066	1/1	0.87	0.09	-5.11	66,66,66,66	0
57	MG	DA	3114	1/1	0.85	0.13	-5.16	51,51,51,51	0
57	MG	BA	3621	1/1	0.93	0.13	-5.17	18,18,18,18	0
57	MG	BA	3284	1/1	0.92	0.12	-5.20	41,41,41,41	0
57	MG	AA	3065	1/1	0.88	0.12	-5.21	48,48,48,48	0
57	MG	BA	3345	1/1	0.95	0.12	-5.26	36,36,36,36	0
57	MG	BA	3172	1/1	0.94	0.17	-5.29	27,27,27,27	0
57	MG	BA	3697	1/1	0.97	0.16	-5.29	23,23,23,23	0
57	MG	BA	3624	1/1	0.97	0.11	-5.35	26,26,26,26	0
57	MG	DA	3121	1/1	0.95	0.12	-5.39	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3593	1/1	0.98	0.11	-5.48	36,36,36,36	0
57	MG	AA	3122	1/1	0.73	0.10	-5.48	52,52,52,52	0
57	MG	DA	3022	1/1	0.99	0.08	-5.62	27,27,27,27	0
57	MG	AA	3022	1/1	0.96	0.07	-5.69	57,57,57,57	0
57	MG	BA	3008	1/1	0.95	0.11	-5.70	22,22,22,22	0
57	MG	BA	3689	1/1	0.87	0.14	-5.73	46,46,46,46	0
57	MG	BA	3589	1/1	0.95	0.13	-5.80	35,35,35,35	0
57	MG	BA	3625	1/1	0.86	0.12	-5.98	46,46,46,46	0
57	MG	BA	3289	1/1	0.95	0.12	-6.09	41,41,41,41	0
57	MG	AA	3153	1/1	0.96	0.09	-6.09	46,46,46,46	0
57	MG	BA	3517	1/1	0.96	0.13	-6.09	20,20,20,20	0
57	MG	BA	3313	1/1	0.93	0.15	-6.26	30,30,30,30	0
57	MG	AA	3152	1/1	0.95	0.09	-6.29	64,64,64,64	0
57	MG	BB	3017	1/1	0.98	0.09	-6.35	28,28,28,28	0
57	MG	BA	3646	1/1	0.96	0.09	-6.36	43,43,43,43	0
57	MG	AA	3036	1/1	0.93	0.11	-6.54	51,51,51,51	0
57	MG	BA	3124	1/1	0.97	0.12	-6.55	31,31,31,31	0
57	MG	BA	3278	1/1	0.94	0.07	-6.63	38,38,38,38	0
57	MG	BA	3565	1/1	0.89	0.10	-6.78	50,50,50,50	0
57	MG	AA	3167	1/1	0.96	0.06	-6.83	65,65,65,65	0
57	MG	BA	3618	1/1	0.85	0.10	-7.53	64,64,64,64	0
57	MG	DA	3012	1/1	0.97	0.08	-7.66	42,42,42,42	0
57	MG	DA	3525	1/1	0.94	0.08	-8.08	40,40,40,40	0
57	MG	DA	3264	1/1	0.92	0.10	-8.18	33,33,33,33	0
57	MG	BA	3554	1/1	0.97	0.08	-8.41	44,44,44,44	0
57	MG	BA	3586	1/1	0.99	0.11	-8.59	33,33,33,33	0
57	MG	B0	102	1/1	0.92	0.13	-8.71	53,53,53,53	0
57	MG	BA	3379	1/1	0.91	0.10	-8.75	69,69,69,69	0
57	MG	DA	3092	1/1	0.96	0.09	-8.91	29,29,29,29	0
57	MG	BA	3420	1/1	0.97	0.11	-9.38	23,23,23,23	0
57	MG	BA	3348	1/1	0.97	0.12	-9.59	17,17,17,17	0
57	MG	BA	3506	1/1	0.96	0.12	-10.04	39,39,39,39	0
57	MG	BA	3501	1/1	0.90	0.07	-11.21	67,67,67,67	0
57	MG	BA	3354	1/1	0.96	0.11	-11.21	31,31,31,31	0
57	MG	BA	3479	1/1	0.99	0.13	-11.32	22,22,22,22	0
57	MG	BA	3038	1/1	0.96	0.06	-11.71	38,38,38,38	0
57	MG	BA	3672	1/1	0.93	0.10	-12.65	28,28,28,28	0
57	MG	BA	3335	1/1	0.94	0.09	-13.85	26,26,26,26	0
57	MG	BA	3341	1/1	0.96	0.06	-19.83	52,52,52,52	0
57	MG	BB	3012	1/1	0.92	0.16	-	33,33,33,33	0
57	MG	CA	3109	1/1	0.90	0.19	-	61,61,61,61	0
57	MG	BF	310	1/1	0.96	0.12	-	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3699	1/1	0.91	0.09	-	33,33,33,33	0
57	MG	DA	3461	1/1	0.88	0.13	-	55,55,55,55	0
57	MG	DA	3219	1/1	0.88	0.22	-	54,54,54,54	0
57	MG	DA	3283	1/1	0.83	0.14	-	40,40,40,40	0
57	MG	BA	3113	1/1	0.71	0.23	-	57,57,57,57	0
57	MG	BA	3142	1/1	0.97	0.20	-	35,35,35,35	0
57	MG	DA	3476	1/1	0.96	0.14	-	49,49,49,49	0
57	MG	AA	3038	1/1	0.96	0.22	-	58,58,58,58	0
57	MG	BA	3032	1/1	0.91	0.23	-	30,30,30,30	0
57	MG	CA	3066	1/1	0.81	0.18	-	69,69,69,69	0
57	MG	DA	3550	1/1	0.72	0.28	-	63,63,63,63	0
57	MG	AA	3068	1/1	0.92	0.12	-	64,64,64,64	0
57	MG	DA	3503	1/1	0.88	0.18	-	51,51,51,51	0
57	MG	AA	3002	1/1	0.95	0.13	-	58,58,58,58	0
57	MG	BA	3499	1/1	0.93	0.22	-	51,51,51,51	0
57	MG	DB	3001	1/1	0.98	0.07	-	50,50,50,50	0
57	MG	CA	3124	1/1	0.87	0.17	-	57,57,57,57	0
57	MG	BA	3696	1/1	0.96	0.11	-	41,41,41,41	0
57	MG	BA	3451	1/1	0.96	0.17	-	59,59,59,59	0
57	MG	CA	3001	1/1	0.86	0.09	-	53,53,53,53	0
57	MG	BA	3688	1/1	0.92	0.33	-	46,46,46,46	0
57	MG	DA	3094	1/1	0.92	0.19	-	38,38,38,38	0
57	MG	DA	3572	1/1	0.91	0.14	-	46,46,46,46	0
57	MG	BN	3002	1/1	0.90	0.25	-	46,46,46,46	0
57	MG	DA	3616	1/1	0.93	0.13	-	28,28,28,28	0
57	MG	BA	3503	1/1	0.98	0.11	-	50,50,50,50	0
57	MG	DA	3156	1/1	0.95	0.16	-	46,46,46,46	0
57	MG	BA	3224	1/1	0.93	0.44	-	48,48,48,48	0
57	MG	BA	3678	1/1	0.94	0.19	-	49,49,49,49	0
57	MG	DA	3601	1/1	0.88	0.11	-	43,43,43,43	0
57	MG	BA	3293	1/1	0.77	0.16	-	43,43,43,43	0
57	MG	DA	3530	1/1	0.92	0.09	-	43,43,43,43	0
57	MG	DA	3198	1/1	0.92	0.08	-	41,41,41,41	0
57	MG	DA	3573	1/1	0.97	0.08	-	49,49,49,49	0
57	MG	BA	3473	1/1	0.97	0.18	-	31,31,31,31	0
57	MG	AA	3100	1/1	0.69	0.17	-	69,69,69,69	0
57	MG	DA	3558	1/1	0.88	0.09	-	45,45,45,45	0
57	MG	CA	3090	1/1	0.93	0.44	-	64,64,64,64	0
57	MG	DA	3108	1/1	0.94	0.15	-	50,50,50,50	0
57	MG	DA	3532	1/1	0.95	0.10	-	43,43,43,43	0
57	MG	BA	3090	1/1	0.94	0.20	-	50,50,50,50	0
57	MG	DA	3250	1/1	0.92	0.16	-	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3172	1/1	0.97	0.09	-	32,32,32,32	0
57	MG	AA	3005	1/1	0.90	0.16	-	66,66,66,66	0
57	MG	BA	3079	1/1	0.82	0.23	-	55,55,55,55	0
57	MG	AX	3006	1/1	0.91	0.27	-	59,59,59,59	0
57	MG	AA	3125	1/1	0.80	0.11	-	60,60,60,60	0
57	MG	BA	3031	1/1	0.90	0.13	-	51,51,51,51	0
57	MG	AA	3045	1/1	0.95	0.12	-	44,44,44,44	0
57	MG	BA	3692	1/1	0.91	0.17	-	64,64,64,64	0
57	MG	AA	3086	1/1	0.91	0.13	-	45,45,45,45	0
57	MG	BA	3474	1/1	0.84	0.17	-	64,64,64,64	0
57	MG	BA	3668	1/1	0.95	0.20	-	39,39,39,39	0
57	MG	BA	3052	1/1	0.85	0.24	-	44,44,44,44	0
57	MG	BA	3599	1/1	0.96	0.19	-	43,43,43,43	0
57	MG	BA	3442	1/1	0.96	0.14	-	51,51,51,51	0
57	MG	DA	3085	1/1	0.95	0.13	-	27,27,27,27	0
57	MG	BA	3304	1/1	0.85	0.26	-	49,49,49,49	0
57	MG	DA	3540	1/1	0.95	0.09	-	43,43,43,43	0
57	MG	CJ	5001	1/1	0.90	0.12	-	51,51,51,51	0
57	MG	BA	3066	1/1	0.86	0.20	-	53,53,53,53	0
57	MG	DY	502	1/1	0.96	0.12	-	56,56,56,56	0
57	MG	DA	3423	1/1	0.98	0.24	-	33,33,33,33	0
57	MG	DA	3008	1/1	0.90	0.22	-	26,26,26,26	0
57	MG	DA	3321	1/1	0.97	0.17	-	40,40,40,40	0
57	MG	CA	3102	1/1	0.89	0.12	-	56,56,56,56	0
57	MG	BA	3085	1/1	0.97	0.15	-	18,18,18,18	0
57	MG	BA	3016	1/1	0.96	0.15	-	35,35,35,35	0
57	MG	BA	3235	1/1	0.87	0.19	-	52,52,52,52	0
57	MG	BA	3132	1/1	0.94	0.18	-	52,52,52,52	0
57	MG	DA	3055	1/1	0.95	0.08	-	35,35,35,35	0
57	MG	BA	3552	1/1	0.93	0.11	-	59,59,59,59	0
57	MG	BA	3355	1/1	0.86	0.12	-	30,30,30,30	0
57	MG	CA	3062	1/1	0.86	0.09	-	73,73,73,73	0
57	MG	DA	3420	1/1	0.96	0.10	-	41,41,41,41	0
57	MG	AA	3084	1/1	0.92	0.14	-	43,43,43,43	0
57	MG	DW	202	1/1	0.90	0.18	-	43,43,43,43	0
57	MG	AA	3175	1/1	0.94	0.32	-	61,61,61,61	0
57	MG	CA	3009	1/1	0.94	0.12	-	44,44,44,44	0
57	MG	DA	3293	1/1	0.88	0.19	-	41,41,41,41	0
57	MG	BA	3369	1/1	0.94	0.16	-	57,57,57,57	0
57	MG	AA	3160	1/1	0.91	0.23	-	58,58,58,58	0
57	MG	CA	3022	1/1	0.88	0.28	-	55,55,55,55	0
57	MG	D5	101	1/1	0.94	0.20	-	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3522	1/1	0.91	0.17	-	41,41,41,41	0
57	MG	DA	3627	1/1	0.90	0.23	-	56,56,56,56	0
57	MG	AA	3195	1/1	0.92	0.10	-	58,58,58,58	0
57	MG	DA	3515	1/1	0.90	0.17	-	53,53,53,53	0
57	MG	AA	3101	1/1	0.96	0.19	-	53,53,53,53	0
57	MG	DA	3358	1/1	0.94	0.53	-	45,45,45,45	0
57	MG	BA	3071	1/1	0.94	0.20	-	48,48,48,48	0
57	MG	DA	3497	1/1	0.91	0.17	-	61,61,61,61	0
57	MG	AA	3088	1/1	0.96	0.22	-	40,40,40,40	0
57	MG	AA	3062	1/1	0.87	0.23	-	57,57,57,57	0
57	MG	DA	3439	1/1	0.83	0.17	-	44,44,44,44	0
57	MG	BA	3562	1/1	0.96	0.16	-	47,47,47,47	0
57	MG	BA	3657	1/1	0.96	0.12	-	55,55,55,55	0
57	MG	DA	3093	1/1	0.91	0.13	-	45,45,45,45	0
57	MG	DA	3240	1/1	0.98	0.24	-	36,36,36,36	0
57	MG	DA	3053	1/1	0.95	0.22	-	50,50,50,50	0
60	K	AX	3001	1/1	0.94	0.10	-	39,39,39,39	0
57	MG	DA	3091	1/1	0.91	0.22	-	37,37,37,37	0
57	MG	BA	3372	1/1	0.89	0.08	-	58,58,58,58	0
57	MG	BA	3579	1/1	0.81	0.32	-	44,44,44,44	0
57	MG	BA	3120	1/1	0.92	0.36	-	52,52,52,52	0
57	MG	DA	3079	1/1	0.95	0.14	-	41,41,41,41	0
57	MG	BA	3112	1/1	0.85	0.28	-	58,58,58,58	0
57	MG	BA	3389	1/1	0.94	0.11	-	57,57,57,57	0
57	MG	AF	3001	1/1	0.73	0.20	-	58,58,58,58	0
57	MG	AA	3178	1/1	0.96	0.18	-	67,67,67,67	0
57	MG	DA	3395	1/1	0.99	0.11	-	31,31,31,31	0
57	MG	BA	3171	1/1	0.95	0.36	-	44,44,44,44	0
57	MG	DA	3220	1/1	0.93	0.20	-	54,54,54,54	0
57	MG	CA	3157	1/1	0.94	0.09	-	61,61,61,61	0
57	MG	BA	3168	1/1	0.93	0.19	-	32,32,32,32	0
57	MG	BA	3658	1/1	0.92	0.22	-	16,16,16,16	0
57	MG	AA	3161	1/1	0.96	0.20	-	28,28,28,28	0
57	MG	BA	3671	1/1	0.93	0.15	-	55,55,55,55	0
57	MG	CA	3018	1/1	0.92	0.13	-	47,47,47,47	0
57	MG	DA	3237	1/1	0.97	0.31	-	41,41,41,41	0
57	MG	BU	202	1/1	0.95	0.10	-	45,45,45,45	0
57	MG	BA	3115	1/1	0.92	0.48	-	49,49,49,49	0
57	MG	CA	3056	1/1	0.75	0.12	-	56,56,56,56	0
57	MG	CA	3106	1/1	0.88	0.14	-	65,65,65,65	0
57	MG	BA	3332	1/1	0.97	0.22	-	29,29,29,29	0
57	MG	AA	3141	1/1	0.85	0.11	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3357	1/1	0.93	0.20	-	31,31,31,31	0
57	MG	BA	3301	1/1	0.93	0.23	-	43,43,43,43	0
57	MG	DA	3122	1/1	0.88	0.13	-	58,58,58,58	0
57	MG	BA	3556	1/1	0.91	0.16	-	52,52,52,52	0
57	MG	BA	3367	1/1	0.94	0.06	-	42,42,42,42	0
57	MG	BA	3091	1/1	0.85	0.19	-	56,56,56,56	0
57	MG	DA	3308	1/1	0.89	0.14	-	52,52,52,52	0
57	MG	AX	3003	1/1	0.86	0.33	-	66,66,66,66	0
57	MG	BA	3365	1/1	0.96	0.14	-	40,40,40,40	0
57	MG	DA	3089	1/1	0.93	0.19	-	36,36,36,36	0
57	MG	DA	3551	1/1	0.95	0.11	-	57,57,57,57	0
57	MG	DA	3134	1/1	0.81	0.16	-	59,59,59,59	0
57	MG	DA	3067	1/1	0.90	0.13	-	54,54,54,54	0
57	MG	CA	3117	1/1	0.91	0.14	-	100,100,100,100	0
57	MG	BE	3003	1/1	0.95	0.16	-	25,25,25,25	0
57	MG	BA	3402	1/1	0.97	0.22	-	39,39,39,39	0
57	MG	DA	3478	1/1	0.95	0.17	-	57,57,57,57	0
57	MG	DA	3280	1/1	0.90	0.19	-	49,49,49,49	0
57	MG	AA	3190	1/1	0.78	0.12	-	75,75,75,75	0
57	MG	BA	3531	1/1	0.96	0.28	-	20,20,20,20	0
57	MG	DA	3071	1/1	0.98	0.15	-	42,42,42,42	0
57	MG	BB	3003	1/1	0.98	0.17	-	40,40,40,40	0
57	MG	AA	3196	1/1	0.95	0.12	-	60,60,60,60	0
57	MG	DA	3187	1/1	0.87	0.23	-	39,39,39,39	0
57	MG	DA	3190	1/1	0.95	0.26	-	52,52,52,52	0
57	MG	BO	5001	1/1	0.94	0.14	-	49,49,49,49	0
57	MG	DA	3101	1/1	0.97	0.28	-	45,45,45,45	0
57	MG	DA	3608	1/1	0.82	0.15	-	61,61,61,61	0
57	MG	BA	3096	1/1	0.95	0.18	-	39,39,39,39	0
57	MG	AA	3138	1/1	0.97	0.20	-	40,40,40,40	0
57	MG	DA	3302	1/1	0.97	0.18	-	30,30,30,30	0
57	MG	AA	3013	1/1	0.97	0.12	-	53,53,53,53	0
57	MG	BA	3070	1/1	0.88	0.20	-	44,44,44,44	0
57	MG	DA	3303	1/1	0.79	0.18	-	57,57,57,57	0
57	MG	DA	3090	1/1	0.84	0.16	-	52,52,52,52	0
57	MG	DA	3472	1/1	0.95	0.20	-	24,24,24,24	0
57	MG	DA	3051	1/1	0.94	0.09	-	54,54,54,54	0
57	MG	DA	3115	1/1	0.93	0.13	-	58,58,58,58	0
57	MG	DA	3590	1/1	0.93	0.10	-	58,58,58,58	0
57	MG	BA	3666	1/1	0.93	0.17	-	79,79,79,79	0
57	MG	DA	3459	1/1	0.94	0.43	-	40,40,40,40	0
57	MG	DA	3507	1/1	0.97	0.24	-	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3093	1/1	0.95	0.20	-	56,56,56,56	0
57	MG	DD	301	1/1	0.97	0.22	-	31,31,31,31	0
57	MG	BA	3262	1/1	0.92	0.27	-	38,38,38,38	0
57	MG	BA	3147	1/1	0.99	0.23	-	34,34,34,34	0
57	MG	DA	3460	1/1	0.94	0.07	-	57,57,57,57	0
57	MG	BA	3551	1/1	0.96	0.24	-	17,17,17,17	0
57	MG	BA	3502	1/1	0.50	0.23	-	57,57,57,57	0
57	MG	BA	3163	1/1	0.97	0.26	-	43,43,43,43	0
57	MG	DA	3386	1/1	0.99	0.21	-	39,39,39,39	0
57	MG	DA	3377	1/1	0.94	0.17	-	31,31,31,31	0
57	MG	CA	3100	1/1	0.96	0.20	-	48,48,48,48	0
57	MG	BA	3447	1/1	0.89	0.12	-	44,44,44,44	0
57	MG	BA	3197	1/1	0.97	0.19	-	32,32,32,32	0
57	MG	DV	202	1/1	0.63	0.76	-	75,75,75,75	0
57	MG	CA	3072	1/1	0.95	0.28	-	38,38,38,38	0
57	MG	BA	3690	1/1	0.98	0.17	-	49,49,49,49	0
57	MG	DA	3226	1/1	0.88	0.18	-	54,54,54,54	0
57	MG	BA	3075	1/1	0.92	0.35	-	45,45,45,45	0
57	MG	DA	3043	1/1	0.86	0.15	-	44,44,44,44	0
57	MG	BA	3222	1/1	0.93	0.20	-	52,52,52,52	0
57	MG	BA	3614	1/1	0.94	0.12	-	64,64,64,64	0
57	MG	BA	3017	1/1	0.92	0.23	-	48,48,48,48	0
57	MG	BA	3409	1/1	0.93	0.27	-	27,27,27,27	0
57	MG	DA	3026	1/1	0.96	0.14	-	41,41,41,41	0
57	MG	DA	3372	1/1	0.96	0.10	-	49,49,49,49	0
57	MG	DA	3247	1/1	0.97	0.11	-	43,43,43,43	0
57	MG	BA	3441	1/1	0.98	0.13	-	56,56,56,56	0
57	MG	DA	3241	1/1	0.96	0.18	-	40,40,40,40	0
57	MG	AA	3072	1/1	0.91	0.08	-	65,65,65,65	0
57	MG	BA	3636	1/1	0.88	0.29	-	45,45,45,45	0
57	MG	AA	3173	1/1	0.90	0.21	-	53,53,53,53	0
57	MG	DA	3442	1/1	0.94	0.23	-	34,34,34,34	0
57	MG	DA	3301	1/1	0.97	0.11	-	54,54,54,54	0
57	MG	DA	3346	1/1	0.92	0.12	-	39,39,39,39	0
57	MG	DA	3398	1/1	0.97	0.13	-	37,37,37,37	0
57	MG	BA	3515	1/1	0.87	0.17	-	44,44,44,44	0
57	MG	DA	3561	1/1	0.94	0.13	-	51,51,51,51	0
57	MG	CA	3003	1/1	0.85	0.13	-	74,74,74,74	0
57	MG	AA	3201	1/1	0.96	0.10	-	68,68,68,68	0
57	MG	DA	3422	1/1	0.92	0.26	-	40,40,40,40	0
57	MG	BA	3058	1/1	0.94	0.20	-	24,24,24,24	0
57	MG	DA	3102	1/1	0.74	0.14	-	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	3118	1/1	0.94	0.17	-	69,69,69,69	0
57	MG	BA	3687	1/1	0.98	0.12	-	30,30,30,30	0
57	MG	BA	3223	1/1	0.89	0.15	-	38,38,38,38	0
57	MG	DA	3385	1/1	0.97	0.09	-	47,47,47,47	0
57	MG	AX	3008	1/1	0.81	0.11	-	58,58,58,58	0
57	MG	AA	3180	1/1	0.87	0.21	-	61,61,61,61	0
57	MG	BA	3368	1/1	0.96	0.32	-	26,26,26,26	0
57	MG	BA	3430	1/1	0.94	0.13	-	54,54,54,54	0
57	MG	DA	3504	1/1	0.95	0.17	-	46,46,46,46	0
57	MG	BA	3564	1/1	0.93	0.19	-	44,44,44,44	0
57	MG	AA	3056	1/1	0.84	0.31	-	66,66,66,66	0
57	MG	BA	3485	1/1	0.97	0.11	-	40,40,40,40	0
57	MG	BA	3230	1/1	0.92	0.35	-	45,45,45,45	0
57	MG	DA	3235	1/1	0.97	0.36	-	48,48,48,48	0
57	MG	BA	3104	1/1	0.87	0.20	-	54,54,54,54	0
57	MG	BF	309	1/1	0.71	0.41	-	61,61,61,61	0
57	MG	DN	5001	1/1	0.98	0.06	-	53,53,53,53	0
57	MG	BA	3270	1/1	0.97	0.41	-	47,47,47,47	0
57	MG	DA	3137	1/1	0.87	0.28	-	48,48,48,48	0
57	MG	DB	3009	1/1	0.91	0.21	-	55,55,55,55	0
57	MG	BA	3563	1/1	0.94	0.10	-	38,38,38,38	0
57	MG	DA	3298	1/1	0.99	0.11	-	35,35,35,35	0
57	MG	BA	3141	1/1	0.97	0.21	-	38,38,38,38	0
57	MG	DA	3189	1/1	0.86	0.19	-	57,57,57,57	0
57	MG	BA	3567	1/1	0.94	0.21	-	55,55,55,55	0
57	MG	DA	3019	1/1	0.91	0.18	-	54,54,54,54	0
57	MG	CA	3127	1/1	0.86	0.33	-	76,76,76,76	0
57	MG	DA	3433	1/1	0.98	0.23	-	27,27,27,27	0
57	MG	DA	3585	1/1	0.97	0.27	-	45,45,45,45	0
57	MG	DA	3110	1/1	0.85	0.10	-	60,60,60,60	0
57	MG	DA	3509	1/1	0.87	0.24	-	42,42,42,42	0
57	MG	DA	3481	1/1	0.95	0.12	-	69,69,69,69	0
57	MG	DA	3353	1/1	0.88	0.11	-	42,42,42,42	0
57	MG	DA	3282	1/1	0.94	0.19	-	36,36,36,36	0
57	MG	BA	3033	1/1	0.89	0.16	-	39,39,39,39	0
57	MG	BA	3548	1/1	0.87	0.18	-	54,54,54,54	0
57	MG	DR	3001	1/1	0.94	1.11	-	66,66,66,66	0
57	MG	DA	3217	1/1	0.83	0.35	-	50,50,50,50	0
57	MG	CA	3015	1/1	0.81	0.11	-	61,61,61,61	0
57	MG	BA	3194	1/1	0.97	0.21	-	42,42,42,42	0
57	MG	BA	3015	1/1	0.92	0.15	-	50,50,50,50	0
57	MG	BA	3598	1/1	0.91	0.22	-	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3494	1/1	0.85	0.22	-	30,30,30,30	0
57	MG	DA	3487	1/1	0.97	0.09	-	44,44,44,44	0
57	MG	BA	3700	1/1	0.83	0.20	-	69,69,69,69	0
57	MG	DA	3607	1/1	0.92	0.18	-	73,73,73,73	0
57	MG	BA	3414	1/1	0.97	0.24	-	59,59,59,59	0
57	MG	CA	3048	1/1	0.89	0.18	-	48,48,48,48	0
57	MG	DA	3253	1/1	0.96	0.23	-	34,34,34,34	0
57	MG	CA	3023	1/1	0.83	0.10	-	88,88,88,88	0
57	MG	AA	3019	1/1	0.93	0.12	-	52,52,52,52	0
57	MG	BP	3003	1/1	0.96	0.14	-	42,42,42,42	0
57	MG	BA	3099	1/1	0.92	0.32	-	36,36,36,36	0
57	MG	BA	3568	1/1	0.96	0.25	-	43,43,43,43	0
57	MG	DA	3148	1/1	0.84	0.20	-	45,45,45,45	0
57	MG	DA	3491	1/1	0.85	0.17	-	43,43,43,43	0
57	MG	BA	3638	1/1	0.95	0.09	-	41,41,41,41	0
57	MG	CA	3138	1/1	0.95	0.15	-	66,66,66,66	0
57	MG	DA	3606	1/1	0.97	0.19	-	54,54,54,54	0
57	MG	AA	3051	1/1	0.84	0.27	-	51,51,51,51	0
57	MG	DA	3028	1/1	0.90	0.15	-	52,52,52,52	0
57	MG	DA	3081	1/1	0.91	0.30	-	45,45,45,45	0
57	MG	BA	3641	1/1	0.93	0.18	-	33,33,33,33	0
57	MG	DA	3328	1/1	0.78	0.15	-	66,66,66,66	0
57	MG	BA	3184	1/1	0.96	0.26	-	42,42,42,42	0
57	MG	CA	3010	1/1	0.92	0.20	-	56,56,56,56	0
57	MG	BA	3110	1/1	0.98	0.18	-	40,40,40,40	0
57	MG	AA	3053	1/1	0.89	0.16	-	54,54,54,54	0
57	MG	AA	3193	1/1	0.89	0.31	-	77,77,77,77	0
57	MG	DA	3199	1/1	0.94	0.07	-	41,41,41,41	0
57	MG	AA	3115	1/1	0.93	0.33	-	38,38,38,38	0
57	MG	DA	3404	1/1	0.95	0.08	-	48,48,48,48	0
57	MG	BA	3526	1/1	0.90	0.16	-	48,48,48,48	0
57	MG	DA	3176	1/1	0.97	0.15	-	42,42,42,42	0
57	MG	CA	3050	1/1	0.87	0.12	-	56,56,56,56	0
57	MG	BA	3082	1/1	0.95	0.16	-	57,57,57,57	0
57	MG	BA	3539	1/1	0.95	0.22	-	18,18,18,18	0
57	MG	DA	3322	1/1	0.90	0.18	-	51,51,51,51	0
57	MG	BZ	3001	1/1	0.81	0.27	-	56,56,56,56	0
57	MG	DA	3451	1/1	0.99	0.21	-	39,39,39,39	0
57	MG	DA	3138	1/1	0.89	0.21	-	39,39,39,39	0
57	MG	DA	3383	1/1	0.92	0.13	-	45,45,45,45	0
57	MG	DA	3362	1/1	0.89	0.27	-	48,48,48,48	0
57	MG	BA	3504	1/1	0.97	0.24	-	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3339	1/1	0.96	0.40	-	52,52,52,52	0
57	MG	BA	3382	1/1	0.96	0.19	-	31,31,31,31	0
57	MG	BA	3220	1/1	0.96	0.23	-	54,54,54,54	0
57	MG	DA	3276	1/1	0.80	0.17	-	56,56,56,56	0
57	MG	AA	3171	1/1	0.92	0.16	-	45,45,45,45	0
57	MG	BA	3121	1/1	0.97	0.24	-	48,48,48,48	0
57	MG	BA	3216	1/1	0.79	0.17	-	35,35,35,35	0
57	MG	DA	3168	1/1	0.98	0.32	-	50,50,50,50	0
57	MG	BA	3123	1/1	0.92	0.12	-	56,56,56,56	0
57	MG	DA	3109	1/1	0.92	0.17	-	45,45,45,45	0
57	MG	DA	3144	1/1	0.94	0.08	-	48,48,48,48	0
57	MG	BE	3005	1/1	0.96	0.16	-	15,15,15,15	0
57	MG	BA	3478	1/1	0.96	0.15	-	22,22,22,22	0
57	MG	BA	3378	1/1	0.93	0.18	-	45,45,45,45	0
57	MG	BA	3088	1/1	0.89	0.41	-	59,59,59,59	0
57	MG	DA	3445	1/1	0.97	0.09	-	59,59,59,59	0
57	MG	CA	3012	1/1	0.85	0.34	-	45,45,45,45	0
57	MG	DA	3034	1/1	0.90	0.26	-	46,46,46,46	0
57	MG	DA	3169	1/1	0.98	0.20	-	45,45,45,45	0
57	MG	AA	3124	1/1	0.90	0.21	-	58,58,58,58	0
60	K	CX	3001	1/1	0.96	0.08	-	54,54,54,54	0
57	MG	DA	3317	1/1	0.92	0.24	-	42,42,42,42	0
57	MG	AA	3148	1/1	0.97	0.16	-	61,61,61,61	0
57	MG	DA	3356	1/1	0.88	0.22	-	53,53,53,53	0
57	MG	BA	3535	1/1	0.91	0.25	-	29,29,29,29	0
57	MG	CA	3004	1/1	0.67	0.23	-	70,70,70,70	0
57	MG	DA	3367	1/1	0.85	0.15	-	24,24,24,24	0
57	MG	AA	3067	1/1	0.94	0.13	-	47,47,47,47	0
57	MG	BA	3584	1/1	0.91	0.10	-	59,59,59,59	0
57	MG	BA	3061	1/1	0.90	0.10	-	58,58,58,58	0
57	MG	DA	3013	1/1	0.85	0.15	-	43,43,43,43	0
57	MG	BA	3375	1/1	0.95	0.26	-	46,46,46,46	0
57	MG	AA	3073	1/1	0.89	0.12	-	59,59,59,59	0
57	MG	BA	3149	1/1	0.91	0.19	-	40,40,40,40	0
57	MG	DA	3539	1/1	0.90	0.26	-	52,52,52,52	0
57	MG	DA	3571	1/1	0.93	0.18	-	54,54,54,54	0
57	MG	BA	3373	1/1	0.95	0.24	-	46,46,46,46	0
57	MG	DA	3437	1/1	0.94	0.17	-	48,48,48,48	0
57	MG	B2	3001	1/1	0.95	0.11	-	43,43,43,43	0
57	MG	BA	3419	1/1	0.90	0.24	-	58,58,58,58	0
57	MG	BA	3550	1/1	0.96	0.15	-	60,60,60,60	0
57	MG	BA	3662	1/1	0.98	0.25	-	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3438	1/1	0.96	0.13	-	42,42,42,42	0
57	MG	BA	3165	1/1	0.95	0.22	-	34,34,34,34	0
57	MG	DA	3496	1/1	0.87	0.19	-	63,63,63,63	0
57	MG	BA	3440	1/1	0.97	0.23	-	40,40,40,40	0
57	MG	BA	3146	1/1	0.89	0.20	-	47,47,47,47	0
57	MG	BA	3252	1/1	0.98	0.22	-	30,30,30,30	0
57	MG	CA	3020	1/1	0.92	0.06	-	51,51,51,51	0
57	MG	DA	3463	1/1	0.96	0.08	-	54,54,54,54	0
57	MG	BA	3637	1/1	0.99	0.15	-	40,40,40,40	0
57	MG	DA	3254	1/1	0.94	0.27	-	42,42,42,42	0
57	MG	BA	3719	1/1	0.88	0.09	-	53,53,53,53	0
57	MG	BA	3682	1/1	0.94	0.19	-	30,30,30,30	0
57	MG	BA	3065	1/1	0.93	0.27	-	43,43,43,43	0
57	MG	BA	3322	1/1	0.90	0.18	-	40,40,40,40	0
57	MG	BA	3453	1/1	0.90	0.11	-	47,47,47,47	0
57	MG	DA	3516	1/1	0.96	0.07	-	43,43,43,43	0
57	MG	AA	3082	1/1	0.96	0.15	-	55,55,55,55	0
57	MG	DW	201	1/1	0.62	0.20	-	70,70,70,70	0
57	MG	BA	3585	1/1	0.93	0.15	-	45,45,45,45	0
57	MG	BA	3459	1/1	0.94	0.28	-	44,44,44,44	0
57	MG	AA	3176	1/1	0.92	0.09	-	43,43,43,43	0
57	MG	BA	3468	1/1	0.96	0.14	-	42,42,42,42	0
57	MG	BA	3512	1/1	0.97	0.10	-	32,32,32,32	0
57	MG	DA	3027	1/1	0.76	0.18	-	42,42,42,42	0
57	MG	BA	3078	1/1	0.87	0.20	-	55,55,55,55	0
57	MG	BA	3003	1/1	0.72	0.16	-	44,44,44,44	0
57	MG	BA	3577	1/1	0.89	0.24	-	35,35,35,35	0
57	MG	DA	3529	1/1	0.95	0.12	-	43,43,43,43	0
57	MG	DA	3178	1/1	0.91	0.21	-	39,39,39,39	0
57	MG	DA	3535	1/1	0.94	0.22	-	21,21,21,21	0
57	MG	CA	3148	1/1	0.64	0.17	-	81,81,81,81	0
57	MG	CA	3082	1/1	0.78	0.14	-	71,71,71,71	0
57	MG	DA	3132	1/1	0.82	0.14	-	53,53,53,53	0
57	MG	DA	3450	1/1	0.92	0.17	-	34,34,34,34	0
57	MG	DA	3113	1/1	0.92	0.24	-	42,42,42,42	0
57	MG	CA	3064	1/1	0.90	0.16	-	64,64,64,64	0
57	MG	BA	3083	1/1	0.94	0.18	-	33,33,33,33	0
57	MG	DA	3153	1/1	0.92	0.15	-	34,34,34,34	0
57	MG	DA	3227	1/1	0.94	0.13	-	57,57,57,57	0
57	MG	BA	3256	1/1	0.99	0.10	-	36,36,36,36	0
57	MG	DA	3155	1/1	0.92	0.21	-	34,34,34,34	0
57	MG	DA	3049	1/1	0.94	0.15	-	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3127	1/1	0.82	0.27	-	73,73,73,73	0
57	MG	DA	3506	1/1	0.94	0.21	-	38,38,38,38	0
57	MG	CA	3144	1/1	0.97	0.23	-	58,58,58,58	0
57	MG	BQ	3004	1/1	0.95	0.26	-	35,35,35,35	0
57	MG	BA	3455	1/1	0.92	0.17	-	44,44,44,44	0
57	MG	BA	3629	1/1	0.94	0.19	-	37,37,37,37	0
57	MG	DA	3306	1/1	0.94	0.12	-	31,31,31,31	0
57	MG	AA	3079	1/1	0.94	0.06	-	62,62,62,62	0
57	MG	DA	3587	1/1	0.87	0.20	-	35,35,35,35	0
57	MG	BA	3318	1/1	0.94	0.18	-	39,39,39,39	0
57	MG	BA	3537	1/1	0.94	0.18	-	35,35,35,35	0
57	MG	CA	3040	1/1	0.79	0.26	-	67,67,67,67	0
57	MG	DA	3003	1/1	0.81	0.19	-	56,56,56,56	0
57	MG	BA	3312	1/1	0.95	0.16	-	44,44,44,44	0
57	MG	DA	3311	1/1	0.86	0.18	-	42,42,42,42	0
57	MG	DA	3618	1/1	0.97	0.16	-	46,46,46,46	0
57	MG	AA	3151	1/1	0.86	0.16	-	72,72,72,72	0
57	MG	DA	3505	1/1	0.97	0.07	-	41,41,41,41	0
57	MG	DA	3324	1/1	0.96	0.26	-	42,42,42,42	0
57	MG	DA	3469	1/1	0.98	0.31	-	41,41,41,41	0
57	MG	BA	3282	1/1	0.94	0.10	-	44,44,44,44	0
57	MG	DA	3072	1/1	0.85	0.37	-	46,46,46,46	0
57	MG	BA	3174	1/1	0.91	0.16	-	44,44,44,44	0
57	MG	BA	3062	1/1	0.75	0.26	-	52,52,52,52	0
57	MG	CA	3002	1/1	0.96	0.20	-	66,66,66,66	0
57	MG	DA	3070	1/1	0.85	0.22	-	35,35,35,35	0
57	MG	BA	3416	1/1	0.86	0.14	-	73,73,73,73	0
57	MG	BA	3320	1/1	0.93	0.12	-	56,56,56,56	0
57	MG	DA	3547	1/1	0.84	0.25	-	68,68,68,68	0
57	MG	DA	3163	1/1	0.95	0.27	-	43,43,43,43	0
57	MG	BA	3547	1/1	0.93	0.18	-	33,33,33,33	0
57	MG	BA	3035	1/1	0.94	0.21	-	28,28,28,28	0
57	MG	AA	3179	1/1	0.97	0.12	-	56,56,56,56	0
57	MG	AA	3035	1/1	0.96	0.39	-	52,52,52,52	0
57	MG	AA	3064	1/1	0.68	0.14	-	65,65,65,65	0
57	MG	DA	3130	1/1	0.74	0.23	-	55,55,55,55	0
57	MG	DA	3209	1/1	0.94	0.17	-	53,53,53,53	0
57	MG	DA	3215	1/1	0.97	0.18	-	35,35,35,35	0
57	MG	DA	3200	1/1	0.93	0.18	-	38,38,38,38	0
57	MG	AA	3197	1/1	0.93	0.14	-	50,50,50,50	0
57	MG	DA	3289	1/1	0.98	0.25	-	50,50,50,50	0
57	MG	BA	3607	1/1	0.96	0.19	-	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3622	1/1	0.91	1.07	-	58,58,58,58	0
57	MG	DA	3281	1/1	0.89	0.13	-	37,37,37,37	0
57	MG	BA	3505	1/1	0.93	0.20	-	16,16,16,16	0
57	MG	DA	3574	1/1	0.88	0.14	-	59,59,59,59	0
57	MG	BA	3360	1/1	0.87	0.16	-	60,60,60,60	0
57	MG	BA	3703	1/1	0.94	0.09	-	47,47,47,47	0
57	MG	BA	3192	1/1	0.97	0.10	-	35,35,35,35	0
57	MG	BA	3346	1/1	0.98	0.23	-	29,29,29,29	0
57	MG	DA	3603	1/1	0.93	0.14	-	40,40,40,40	0
57	MG	BA	3242	1/1	0.88	0.22	-	45,45,45,45	0
57	MG	AA	3041	1/1	0.67	0.19	-	62,62,62,62	0
57	MG	AA	3128	1/1	0.93	0.23	-	53,53,53,53	0
57	MG	BA	3191	1/1	0.97	0.09	-	22,22,22,22	0
57	MG	BA	3643	1/1	0.98	0.15	-	47,47,47,47	0
57	MG	DA	3088	1/1	0.87	0.20	-	41,41,41,41	0
57	MG	BA	3632	1/1	0.90	0.10	-	43,43,43,43	0
57	MG	BA	3049	1/1	0.93	0.25	-	53,53,53,53	0
57	MG	BA	3645	1/1	0.98	0.14	-	43,43,43,43	0
57	MG	DA	3553	1/1	0.36	0.40	-	75,75,75,75	0
57	MG	AA	3177	1/1	0.97	0.15	-	66,66,66,66	0
57	MG	AA	3111	1/1	0.79	0.13	-	70,70,70,70	0
57	MG	BA	3456	1/1	0.97	0.13	-	44,44,44,44	0
57	MG	AA	3120	1/1	0.95	0.13	-	53,53,53,53	0
57	MG	BA	3006	1/1	0.93	0.14	-	38,38,38,38	0
57	MG	BA	3685	1/1	0.98	0.18	-	40,40,40,40	0
57	MG	BA	3542	1/1	0.88	0.12	-	40,40,40,40	0
57	MG	BA	3074	1/1	0.94	0.12	-	43,43,43,43	0
57	MG	AA	3078	1/1	0.97	0.17	-	66,66,66,66	0
57	MG	CA	3013	1/1	0.91	0.17	-	45,45,45,45	0
57	MG	BA	3007	1/1	0.96	0.13	-	39,39,39,39	0
57	MG	BB	3020	1/1	0.81	0.16	-	55,55,55,55	0
57	MG	AA	3063	1/1	0.16	0.12	-	89,89,89,89	0
57	MG	DA	3400	1/1	0.96	0.13	-	33,33,33,33	0
57	MG	DA	3316	1/1	0.97	0.17	-	39,39,39,39	0
57	MG	DA	3010	1/1	0.95	0.12	-	51,51,51,51	0
57	MG	BA	3180	1/1	0.83	0.27	-	32,32,32,32	0
57	MG	BA	3392	1/1	0.94	0.18	-	27,27,27,27	0
57	MG	BA	3069	1/1	0.95	0.21	-	48,48,48,48	0
57	MG	DA	3087	1/1	0.82	0.14	-	65,65,65,65	0
57	MG	DE	301	1/1	0.90	0.10	-	52,52,52,52	0
57	MG	AA	3166	1/1	0.61	0.20	-	70,70,70,70	0
57	MG	DA	3464	1/1	0.98	0.15	-	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3298	1/1	0.87	0.25	-	50,50,50,50	0
57	MG	BA	3376	1/1	0.99	0.21	-	21,21,21,21	0
57	MG	DA	3160	1/1	0.57	0.11	-	65,65,65,65	0
57	MG	BA	3358	1/1	0.97	0.09	-	35,35,35,35	0
57	MG	DA	3352	1/1	0.95	0.24	-	25,25,25,25	0
57	MG	DA	3191	1/1	0.84	0.08	-	54,54,54,54	0
57	MG	BA	3044	1/1	0.94	0.07	-	40,40,40,40	0
57	MG	CA	3147	1/1	0.90	0.12	-	56,56,56,56	0
57	MG	BA	3477	1/1	0.98	0.14	-	19,19,19,19	0
57	MG	BA	3207	1/1	0.92	0.16	-	55,55,55,55	0
57	MG	DA	3368	1/1	0.84	0.09	-	58,58,58,58	0
57	MG	DA	3006	1/1	0.95	0.14	-	40,40,40,40	0
57	MG	BA	3633	1/1	0.95	0.14	-	54,54,54,54	0
57	MG	AX	3011	1/1	0.92	0.37	-	73,73,73,73	0
57	MG	BA	3211	1/1	0.95	0.16	-	50,50,50,50	0
57	MG	BA	3261	1/1	0.80	0.19	-	52,52,52,52	0
57	MG	CA	3143	1/1	0.96	0.12	-	59,59,59,59	0
57	MG	BA	3338	1/1	0.95	0.08	-	50,50,50,50	0
57	MG	BA	3691	1/1	0.87	0.32	-	54,54,54,54	0
57	MG	BA	3151	1/1	0.95	0.13	-	42,42,42,42	0
57	MG	CA	3129	1/1	0.90	0.22	-	83,83,83,83	0
57	MG	BB	3009	1/1	0.91	0.18	-	63,63,63,63	0
57	MG	DA	3409	1/1	0.94	0.08	-	70,70,70,70	0
57	MG	DA	3083	1/1	0.85	0.24	-	30,30,30,30	0
57	MG	BA	3225	1/1	0.95	0.12	-	45,45,45,45	0
57	MG	BA	3258	1/1	0.83	0.22	-	35,35,35,35	0
57	MG	DA	3278	1/1	0.93	0.07	-	38,38,38,38	0
57	MG	BA	3654	1/1	0.97	0.19	-	42,42,42,42	0
57	MG	AA	3039	1/1	0.90	0.28	-	62,62,62,62	0
57	MG	DA	3076	1/1	0.93	0.34	-	53,53,53,53	0
57	MG	BA	3424	1/1	0.93	0.21	-	29,29,29,29	0
57	MG	AA	3169	1/1	0.99	0.13	-	48,48,48,48	0
57	MG	DA	3025	1/1	0.96	0.18	-	35,35,35,35	0
57	MG	CA	3120	1/1	0.85	0.27	-	72,72,72,72	0
57	MG	BA	3518	1/1	0.96	0.22	-	48,48,48,48	0
57	MG	BA	3030	1/1	0.98	0.12	-	44,44,44,44	0
57	MG	BA	3604	1/1	0.79	0.10	-	62,62,62,62	0
57	MG	BA	3544	1/1	0.94	0.17	-	52,52,52,52	0
57	MG	CA	3060	1/1	0.87	0.16	-	78,78,78,78	0
57	MG	BA	3415	1/1	0.92	0.23	-	61,61,61,61	0
57	MG	DA	3521	1/1	0.92	0.09	-	57,57,57,57	0
57	MG	B1	101	1/1	0.94	0.42	-	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3231	1/1	0.97	0.28	-	33,33,33,33	0
57	MG	AA	3070	1/1	0.91	0.24	-	43,43,43,43	0
57	MG	BA	3202	1/1	0.95	0.17	-	42,42,42,42	0
57	MG	CA	3152	1/1	0.88	0.15	-	66,66,66,66	0
57	MG	BA	3156	1/1	0.93	0.12	-	43,43,43,43	0
57	MG	BB	3011	1/1	0.95	0.12	-	40,40,40,40	0
57	MG	DA	3194	1/1	0.92	0.28	-	43,43,43,43	0
57	MG	BA	3072	1/1	0.94	0.12	-	32,32,32,32	0
57	MG	BA	3635	1/1	0.92	0.11	-	59,59,59,59	0
57	MG	BA	3170	1/1	0.96	0.18	-	41,41,41,41	0
57	MG	BA	3103	1/1	0.86	0.50	-	62,62,62,62	0
57	MG	BA	3576	1/1	0.95	0.26	-	29,29,29,29	0
57	MG	BA	3428	1/1	0.97	0.17	-	54,54,54,54	0
57	MG	BA	3218	1/1	0.91	0.59	-	52,52,52,52	0
57	MG	DA	3545	1/1	0.80	0.18	-	70,70,70,70	0
57	MG	DA	3180	1/1	0.95	0.30	-	41,41,41,41	0
57	MG	DA	3150	1/1	0.98	0.36	-	41,41,41,41	0
57	MG	DA	3325	1/1	0.95	0.12	-	43,43,43,43	0
57	MG	AA	3012	1/1	0.95	0.23	-	61,61,61,61	0
57	MG	BA	3076	1/1	0.97	0.24	-	34,34,34,34	0
57	MG	DA	3310	1/1	0.98	0.16	-	43,43,43,43	0
57	MG	DA	3458	1/1	0.87	0.08	-	44,44,44,44	0
57	MG	DU	3002	1/1	0.94	0.42	-	67,67,67,67	0
57	MG	BA	3601	1/1	0.89	0.18	-	69,69,69,69	0
57	MG	BA	3178	1/1	0.84	0.24	-	52,52,52,52	0
57	MG	BA	3470	1/1	0.78	0.13	-	69,69,69,69	0
57	MG	BA	3143	1/1	0.88	0.18	-	41,41,41,41	0
57	MG	DO	5001	1/1	0.89	0.16	-	53,53,53,53	0
57	MG	DA	3391	1/1	0.94	0.21	-	39,39,39,39	0
57	MG	DA	3129	1/1	0.91	0.13	-	41,41,41,41	0
57	MG	BA	3513	1/1	0.93	0.12	-	55,55,55,55	0
57	MG	BA	3251	1/1	0.94	0.27	-	48,48,48,48	0
57	MG	BA	3597	1/1	0.92	0.29	-	56,56,56,56	0
57	MG	BA	3106	1/1	0.97	0.25	-	24,24,24,24	0
57	MG	BA	3493	1/1	0.97	0.13	-	39,39,39,39	0
57	MG	B0	101	1/1	0.94	0.11	-	33,33,33,33	0
57	MG	BA	3417	1/1	0.94	0.17	-	49,49,49,49	0
57	MG	BA	3311	1/1	0.97	0.07	-	42,42,42,42	0
57	MG	DA	3596	1/1	0.88	0.25	-	71,71,71,71	0
57	MG	CA	3046	1/1	0.95	0.18	-	53,53,53,53	0
57	MG	BA	3140	1/1	0.99	0.20	-	26,26,26,26	0
57	MG	AA	3146	1/1	0.79	0.12	-	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	3149	1/1	0.86	0.10	-	49,49,49,49	0
57	MG	CA	3081	1/1	0.86	0.13	-	67,67,67,67	0
57	MG	CA	3085	1/1	0.78	0.32	-	71,71,71,71	0
57	MG	DA	3149	1/1	0.94	0.19	-	42,42,42,42	0
57	MG	CA	3111	1/1	0.93	0.07	-	65,65,65,65	0
57	MG	DA	3486	1/1	0.94	0.16	-	37,37,37,37	0
57	MG	BA	3610	1/1	0.85	0.19	-	60,60,60,60	0
57	MG	BA	3300	1/1	0.92	0.12	-	55,55,55,55	0
57	MG	DA	3097	1/1	0.93	0.16	-	50,50,50,50	0
57	MG	AA	3202	1/1	0.93	0.06	-	60,60,60,60	0
57	MG	DA	3262	1/1	0.93	0.08	-	39,39,39,39	0
57	MG	CA	3068	1/1	0.93	0.12	-	53,53,53,53	0
57	MG	CA	3067	1/1	0.84	0.14	-	45,45,45,45	0
57	MG	BA	3467	1/1	0.80	0.24	-	51,51,51,51	0
57	MG	B8	101	1/1	0.95	0.15	-	34,34,34,34	0
57	MG	DA	3104	1/1	0.92	0.19	-	47,47,47,47	0
57	MG	DA	3604	1/1	0.96	0.28	-	61,61,61,61	0
57	MG	DQ	3002	1/1	0.96	0.15	-	45,45,45,45	0
57	MG	DA	3195	1/1	0.97	0.26	-	42,42,42,42	0
57	MG	AA	3199	1/1	0.92	0.17	-	58,58,58,58	0
57	MG	CA	3155	1/1	0.87	0.16	-	66,66,66,66	0
57	MG	BA	3291	1/1	0.87	0.18	-	44,44,44,44	0
57	MG	BA	3177	1/1	0.84	0.20	-	39,39,39,39	0
57	MG	BA	3356	1/1	0.97	0.11	-	36,36,36,36	0
57	MG	BA	3331	1/1	0.82	0.26	-	39,39,39,39	0
57	MG	AA	3077	1/1	0.96	0.27	-	52,52,52,52	0
57	MG	BA	3126	1/1	0.94	0.28	-	34,34,34,34	0
57	MG	CA	3028	1/1	0.96	0.31	-	57,57,57,57	0
57	MG	BA	3102	1/1	0.97	0.26	-	43,43,43,43	0
57	MG	DA	3064	1/1	0.89	0.31	-	52,52,52,52	0
57	MG	DD	302	1/1	0.93	0.14	-	50,50,50,50	0
57	MG	BA	3581	1/1	0.90	0.08	-	55,55,55,55	0
57	MG	BA	3005	1/1	0.86	0.19	-	44,44,44,44	0
57	MG	CA	3096	1/1	0.83	0.18	-	51,51,51,51	0
57	MG	DA	3107	1/1	0.92	0.17	-	39,39,39,39	0
57	MG	DA	3335	1/1	0.98	0.13	-	48,48,48,48	0
57	MG	DA	3054	1/1	0.81	0.17	-	40,40,40,40	0
57	MG	DA	3567	1/1	0.97	0.09	-	49,49,49,49	0
57	MG	CA	3026	1/1	0.87	0.13	-	59,59,59,59	0
57	MG	AA	3139	1/1	0.97	0.13	-	51,51,51,51	0
57	MG	DA	3419	1/1	0.93	0.20	-	37,37,37,37	0
57	MG	BA	3444	1/1	0.96	0.23	-	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3215	1/1	0.93	0.10	-	53,53,53,53	0
57	MG	BA	3595	1/1	0.89	0.21	-	52,52,52,52	0
57	MG	AA	3054	1/1	0.71	0.16	-	62,62,62,62	0
57	MG	DA	3397	1/1	0.96	0.08	-	46,46,46,46	0
57	MG	BA	3060	1/1	0.87	0.22	-	59,59,59,59	0
57	MG	B0	104	1/1	0.98	0.10	-	49,49,49,49	0
57	MG	BA	3457	1/1	0.98	0.11	-	41,41,41,41	0
57	MG	AA	3133	1/1	0.94	0.16	-	59,59,59,59	0
57	MG	DA	3518	1/1	0.98	0.08	-	42,42,42,42	0
57	MG	BA	3351	1/1	0.82	0.11	-	62,62,62,62	0
57	MG	DA	3286	1/1	0.94	0.25	-	45,45,45,45	0
57	MG	AA	3131	1/1	0.93	0.20	-	56,56,56,56	0
57	MG	DA	3252	1/1	0.83	0.12	-	63,63,63,63	0
57	MG	BA	3287	1/1	0.85	0.27	-	42,42,42,42	0
57	MG	DA	3105	1/1	0.83	0.21	-	37,37,37,37	0
57	MG	BA	3466	1/1	0.89	0.25	-	57,57,57,57	0
57	MG	AA	3059	1/1	0.92	0.30	-	61,61,61,61	0
57	MG	DA	3527	1/1	0.91	0.26	-	52,52,52,52	0
57	MG	BA	3608	1/1	0.81	0.09	-	50,50,50,50	0
57	MG	CA	3101	1/1	0.97	0.14	-	41,41,41,41	0
57	MG	DA	3338	1/1	0.93	0.11	-	36,36,36,36	0
57	MG	DA	3018	1/1	0.91	0.33	-	51,51,51,51	0
57	MG	DA	3165	1/1	0.95	0.14	-	54,54,54,54	0
57	MG	CA	3080	1/1	0.97	0.16	-	61,61,61,61	0
57	MG	BA	3650	1/1	0.90	0.10	-	49,49,49,49	0
57	MG	BA	3631	1/1	0.95	0.12	-	53,53,53,53	0
57	MG	D8	102	1/1	0.89	0.25	-	63,63,63,63	0
57	MG	CA	3006	1/1	0.96	0.12	-	43,43,43,43	0
57	MG	CA	3086	1/1	0.94	0.14	-	56,56,56,56	0
57	MG	BA	3616	1/1	0.91	0.17	-	32,32,32,32	0
57	MG	AA	3110	1/1	0.95	0.19	-	52,52,52,52	0
57	MG	BA	3155	1/1	0.92	0.20	-	44,44,44,44	0
57	MG	BA	3233	1/1	0.68	0.31	-	55,55,55,55	0
57	MG	BA	3538	1/1	0.95	0.17	-	25,25,25,25	0
57	MG	BA	3507	1/1	0.84	0.18	-	48,48,48,48	0
57	MG	BA	3173	1/1	0.91	0.27	-	28,28,28,28	0
57	MG	BA	3199	1/1	0.81	0.26	-	60,60,60,60	0
57	MG	CA	3154	1/1	0.86	0.14	-	68,68,68,68	0
57	MG	DA	3519	1/1	0.67	0.17	-	60,60,60,60	0
57	MG	DA	3259	1/1	0.87	0.14	-	39,39,39,39	0
57	MG	AA	3106	1/1	0.93	0.07	-	53,53,53,53	0
57	MG	CA	3122	1/1	0.91	0.09	-	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DB	3010	1/1	0.92	0.19	-	55,55,55,55	0
57	MG	AA	3060	1/1	0.94	0.38	-	49,49,49,49	0
57	MG	BA	3108	1/1	0.93	0.15	-	36,36,36,36	0
57	MG	DA	3374	1/1	0.76	0.15	-	42,42,42,42	0
57	MG	DA	3493	1/1	0.95	0.10	-	53,53,53,53	0
57	MG	AA	3075	1/1	0.96	0.14	-	57,57,57,57	0
57	MG	DA	3069	1/1	0.63	0.49	-	59,59,59,59	0
57	MG	DA	3457	1/1	0.78	0.22	-	45,45,45,45	0
57	MG	DA	3605	1/1	0.88	0.08	-	64,64,64,64	0
57	MG	BA	3669	1/1	0.90	0.19	-	34,34,34,34	0
57	MG	BF	302	1/1	0.92	0.18	-	59,59,59,59	0
57	MG	DA	3412	1/1	0.86	0.09	-	60,60,60,60	0
57	MG	CA	3131	1/1	0.94	0.14	-	57,57,57,57	0
57	MG	BA	3319	1/1	0.96	0.15	-	37,37,37,37	0
57	MG	BB	3010	1/1	0.98	0.10	-	28,28,28,28	0
57	MG	DA	3179	1/1	0.98	0.24	-	50,50,50,50	0
57	MG	BA	3446	1/1	0.94	0.09	-	49,49,49,49	0
57	MG	BA	3377	1/1	0.93	0.25	-	58,58,58,58	0
57	MG	DA	3520	1/1	0.80	0.20	-	51,51,51,51	0
57	MG	BA	3068	1/1	0.92	0.15	-	46,46,46,46	0
57	MG	CA	3035	1/1	0.84	0.28	-	63,63,63,63	0
57	MG	BA	3521	1/1	0.93	0.28	-	32,32,32,32	0
57	MG	BA	3209	1/1	0.97	0.23	-	32,32,32,32	0
57	MG	DA	3542	1/1	0.96	0.10	-	44,44,44,44	0
57	MG	BA	3482	1/1	0.87	0.13	-	56,56,56,56	0
57	MG	AA	3203	1/1	0.94	0.10	-	42,42,42,42	0
57	MG	CA	3112	1/1	0.95	0.10	-	31,31,31,31	0
57	MG	BA	3119	1/1	0.94	0.24	-	41,41,41,41	0
57	MG	BA	3268	1/1	0.93	0.16	-	45,45,45,45	0
57	MG	BA	3594	1/1	0.95	0.11	-	34,34,34,34	0
57	MG	BA	3317	1/1	0.92	0.14	-	49,49,49,49	0
57	MG	BA	3136	1/1	0.84	0.21	-	56,56,56,56	0
57	MG	DA	3528	1/1	0.93	0.12	-	60,60,60,60	0
57	MG	AA	3043	1/1	0.81	0.27	-	59,59,59,59	0
57	MG	AA	3154	1/1	0.90	0.19	-	46,46,46,46	0
57	MG	BA	3613	1/1	0.91	0.09	-	74,74,74,74	0
57	MG	BA	3434	1/1	0.93	0.21	-	27,27,27,27	0
57	MG	BA	3296	1/1	0.96	0.24	-	31,31,31,31	0
57	MG	BA	3059	1/1	0.94	0.29	-	50,50,50,50	0
57	MG	BB	3005	1/1	0.90	0.17	-	42,42,42,42	0
57	MG	BA	3203	1/1	0.89	0.23	-	56,56,56,56	0
57	MG	DA	3429	1/1	0.96	0.15	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3606	1/1	0.96	0.18	-	39,39,39,39	0
57	MG	BA	3116	1/1	0.94	0.28	-	54,54,54,54	0
57	MG	DA	3197	1/1	0.85	0.15	-	35,35,35,35	0
57	MG	CA	3137	1/1	0.81	0.17	-	81,81,81,81	0
57	MG	DA	3073	1/1	0.98	0.31	-	49,49,49,49	0
57	MG	AA	3107	1/1	0.94	0.14	-	50,50,50,50	0
57	MG	AA	3042	1/1	0.78	0.17	-	52,52,52,52	0
57	MG	BA	3325	1/1	0.95	0.12	-	38,38,38,38	0
57	MG	DA	3577	1/1	0.85	0.18	-	25,25,25,25	0
57	MG	BA	3387	1/1	0.94	0.16	-	29,29,29,29	0
57	MG	BA	3622	1/1	0.95	0.13	-	24,24,24,24	0
57	MG	BA	3681	1/1	0.96	0.22	-	42,42,42,42	0
57	MG	DA	3157	1/1	0.95	0.18	-	44,44,44,44	0
57	MG	DA	3181	1/1	0.97	0.21	-	36,36,36,36	0
57	MG	BA	3159	1/1	0.95	0.26	-	43,43,43,43	0
57	MG	DA	3233	1/1	0.97	0.28	-	41,41,41,41	0
57	MG	DA	3275	1/1	0.95	0.18	-	36,36,36,36	0
57	MG	DA	3261	1/1	0.96	0.23	-	38,38,38,38	0
57	MG	BA	3195	1/1	0.96	0.28	-	46,46,46,46	0
57	MG	DA	3288	1/1	0.91	0.24	-	32,32,32,32	0
57	MG	BV	203	1/1	0.97	0.10	-	31,31,31,31	0
57	MG	BA	3425	1/1	0.87	0.20	-	28,28,28,28	0
57	MG	DA	3355	1/1	0.95	0.20	-	48,48,48,48	0
57	MG	CA	3032	1/1	0.87	0.42	-	58,58,58,58	0
57	MG	BA	3580	1/1	0.98	0.27	-	13,13,13,13	0
57	MG	CA	3030	1/1	0.82	0.09	-	75,75,75,75	0
57	MG	DA	3597	1/1	0.88	0.09	-	42,42,42,42	0
57	MG	BA	3574	1/1	0.90	0.12	-	41,41,41,41	0
57	MG	DA	3490	1/1	0.93	0.10	-	62,62,62,62	0
57	MG	DQ	3003	1/1	0.90	0.28	-	59,59,59,59	0
57	MG	DA	3208	1/1	0.95	0.13	-	50,50,50,50	0
57	MG	DA	3188	1/1	0.94	0.21	-	48,48,48,48	0
57	MG	DA	3331	1/1	0.93	0.26	-	54,54,54,54	0
57	MG	BA	3164	1/1	0.87	0.27	-	44,44,44,44	0
57	MG	BA	3232	1/1	0.90	0.18	-	31,31,31,31	0
57	MG	BA	3540	1/1	0.94	0.20	-	24,24,24,24	0
57	MG	AA	3010	1/1	0.95	0.05	-	54,54,54,54	0
57	MG	DA	3599	1/1	0.99	0.23	-	36,36,36,36	0
57	MG	BA	3433	1/1	0.93	0.12	-	32,32,32,32	0
57	MG	DA	3566	1/1	0.86	0.08	-	40,40,40,40	0
57	MG	DD	307	1/1	0.81	0.12	-	50,50,50,50	0
57	MG	BA	3264	1/1	0.96	0.09	-	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3292	1/1	0.89	0.12	-	29,29,29,29	0
57	MG	DA	3354	1/1	0.99	0.26	-	25,25,25,25	0
57	MG	BA	3361	1/1	0.90	0.08	-	38,38,38,38	0
57	MG	BA	3342	1/1	0.92	0.20	-	38,38,38,38	0
57	MG	AA	3147	1/1	0.94	0.06	-	51,51,51,51	0
57	MG	DA	3613	1/1	0.91	0.37	-	45,45,45,45	0
57	MG	DA	3256	1/1	0.89	0.12	-	52,52,52,52	0
57	MG	BW	201	1/1	0.92	0.18	-	48,48,48,48	0
57	MG	DA	3211	1/1	0.95	0.15	-	43,43,43,43	0
57	MG	BA	3702	1/1	0.92	0.12	-	41,41,41,41	0
57	MG	DA	3610	1/1	0.89	0.16	-	42,42,42,42	0
57	MG	DA	3556	1/1	0.97	0.14	-	49,49,49,49	0
57	MG	DA	3612	1/1	0.95	0.11	-	64,64,64,64	0
57	MG	DA	3384	1/1	0.93	0.09	-	41,41,41,41	0
57	MG	BA	3406	1/1	0.85	0.22	-	24,24,24,24	0
57	MG	AA	3186	1/1	0.97	0.10	-	43,43,43,43	0
57	MG	AA	3081	1/1	0.98	0.09	-	44,44,44,44	0
57	MG	BA	3386	1/1	0.98	0.25	-	30,30,30,30	0
57	MG	BA	3087	1/1	0.94	0.21	-	44,44,44,44	0
57	MG	BA	3336	1/1	0.93	0.10	-	47,47,47,47	0
57	MG	BA	3704	1/1	0.92	0.13	-	31,31,31,31	0
57	MG	BA	3263	1/1	0.86	0.30	-	50,50,50,50	0
57	MG	BA	3205	1/1	0.93	0.12	-	52,52,52,52	0
57	MG	DA	3580	1/1	0.73	0.11	-	47,47,47,47	0
57	MG	BA	3363	1/1	0.96	0.21	-	31,31,31,31	0
57	MG	DA	3084	1/1	0.95	0.17	-	42,42,42,42	0
57	MG	CA	3114	1/1	0.85	0.24	-	96,96,96,96	0
57	MG	DA	3402	1/1	0.88	0.15	-	47,47,47,47	0
57	MG	BA	3228	1/1	0.93	0.28	-	33,33,33,33	0
57	MG	BA	3094	1/1	0.85	0.15	-	46,46,46,46	0
57	MG	DA	3484	1/1	0.91	0.10	-	41,41,41,41	0
57	MG	BA	3011	1/1	0.89	0.18	-	32,32,32,32	0
57	MG	BA	3272	1/1	0.98	0.21	-	38,38,38,38	0
57	MG	BA	3018	1/1	0.91	0.21	-	58,58,58,58	0
57	MG	BA	3012	1/1	0.95	0.16	-	38,38,38,38	0
57	MG	DA	3232	1/1	0.96	0.07	-	48,48,48,48	0
57	MG	DA	3586	1/1	0.95	0.13	-	21,21,21,21	0
57	MG	AA	3033	1/1	0.90	0.19	-	43,43,43,43	0
57	MG	CA	3139	1/1	0.87	0.09	-	82,82,82,82	0
57	MG	BA	3660	1/1	0.93	0.11	-	62,62,62,62	0
57	MG	DA	3062	1/1	0.92	0.24	-	49,49,49,49	0
57	MG	DA	3388	1/1	0.93	0.22	-	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3655	1/1	0.99	0.09	-	68,68,68,68	0
57	MG	DA	3294	1/1	0.96	0.17	-	18,18,18,18	0
57	MG	CA	3132	1/1	0.95	0.13	-	51,51,51,51	0
57	MG	BA	3349	1/1	0.89	0.19	-	55,55,55,55	0
57	MG	BA	3620	1/1	0.98	0.13	-	35,35,35,35	0
57	MG	BA	3182	1/1	0.86	0.18	-	36,36,36,36	0
57	MG	BA	3266	1/1	0.92	0.21	-	53,53,53,53	0
57	MG	BA	3483	1/1	0.94	0.14	-	36,36,36,36	0
57	MG	DA	3196	1/1	0.91	0.23	-	46,46,46,46	0
57	MG	AA	3163	1/1	0.87	0.17	-	70,70,70,70	0
57	MG	AA	3136	1/1	0.97	0.15	-	43,43,43,43	0
57	MG	BA	3575	1/1	0.94	0.17	-	30,30,30,30	0
57	MG	BA	3524	1/1	0.93	0.12	-	39,39,39,39	0
57	MG	AA	3048	1/1	0.93	0.19	-	42,42,42,42	0
57	MG	CA	3033	1/1	0.83	0.15	-	67,67,67,67	0
57	MG	BA	3275	1/1	0.99	0.10	-	38,38,38,38	0
57	MG	DA	3086	1/1	0.96	0.08	-	41,41,41,41	0
57	MG	CA	3121	1/1	0.97	0.20	-	51,51,51,51	0
57	MG	BA	3117	1/1	0.98	0.17	-	24,24,24,24	0
57	MG	AA	3198	1/1	0.74	0.12	-	66,66,66,66	0
57	MG	DA	3263	1/1	0.91	0.13	-	47,47,47,47	0
57	MG	BA	3157	1/1	0.94	0.12	-	42,42,42,42	0
57	MG	DA	3066	1/1	0.89	0.10	-	55,55,55,55	0
57	MG	BA	3472	1/1	0.94	0.10	-	39,39,39,39	0
57	MG	CA	3083	1/1	0.91	0.27	-	71,71,71,71	0
57	MG	AA	3184	1/1	0.97	0.11	-	56,56,56,56	0
57	MG	DA	3202	1/1	0.95	0.48	-	41,41,41,41	0
57	MG	BA	3309	1/1	0.99	0.10	-	31,31,31,31	0
57	MG	BA	3388	1/1	0.89	0.15	-	31,31,31,31	0
57	MG	DA	3136	1/1	0.96	0.18	-	62,62,62,62	0
57	MG	DA	3562	1/1	0.89	0.09	-	58,58,58,58	0
57	MG	DA	3313	1/1	0.95	0.04	-	51,51,51,51	0
57	MG	CA	3016	1/1	0.93	0.05	-	52,52,52,52	0
57	MG	DA	3047	1/1	0.88	0.19	-	44,44,44,44	0
57	MG	CA	3110	1/1	0.90	0.19	-	56,56,56,56	0
57	MG	BA	3098	1/1	0.93	0.58	-	50,50,50,50	0
57	MG	BA	3674	1/1	0.56	0.19	-	59,59,59,59	0
57	MG	BB	3019	1/1	0.91	0.15	-	62,62,62,62	0
57	MG	BA	3527	1/1	0.87	0.17	-	37,37,37,37	0
57	MG	BA	3656	1/1	0.91	0.15	-	57,57,57,57	0
57	MG	DA	3323	1/1	0.95	0.11	-	39,39,39,39	0
57	MG	BA	3661	1/1	0.94	0.19	-	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3591	1/1	0.93	0.10	-	42,42,42,42	0
57	MG	BA	3248	1/1	0.96	0.24	-	32,32,32,32	0
57	MG	AX	3005	1/1	0.93	0.32	-	57,57,57,57	0
57	MG	BA	3371	1/1	0.90	0.16	-	53,53,53,53	0
57	MG	DA	3554	1/1	0.84	0.18	-	46,46,46,46	0
57	MG	BA	3626	1/1	0.94	0.22	-	48,48,48,48	0
57	MG	DA	3095	1/1	0.90	0.25	-	45,45,45,45	0
57	MG	AA	3029	1/1	0.97	0.07	-	42,42,42,42	0
57	MG	BA	3489	1/1	0.96	0.22	-	36,36,36,36	0
57	MG	DB	3008	1/1	0.75	0.10	-	59,59,59,59	0
57	MG	BA	3647	1/1	0.96	0.12	-	41,41,41,41	0
57	MG	BA	3002	1/1	0.82	0.14	-	45,45,45,45	0
57	MG	BA	3238	1/1	0.90	0.26	-	26,26,26,26	0
57	MG	AA	3097	1/1	0.83	0.16	-	45,45,45,45	0
57	MG	BA	3561	1/1	0.94	0.18	-	37,37,37,37	0
57	MG	BA	3100	1/1	0.94	0.20	-	40,40,40,40	0
57	MG	BA	3449	1/1	0.95	0.15	-	31,31,31,31	0
57	MG	DA	3546	1/1	0.83	0.14	-	41,41,41,41	0
57	MG	BA	3073	1/1	0.94	0.29	-	39,39,39,39	0
57	MG	AV	3001	1/1	0.92	0.20	-	59,59,59,59	0
57	MG	BA	3169	1/1	0.96	0.15	-	40,40,40,40	0
57	MG	DA	3002	1/1	0.94	0.31	-	44,44,44,44	0
57	MG	DA	3186	1/1	0.95	0.08	-	33,33,33,33	0
57	MG	DA	3285	1/1	0.92	0.12	-	50,50,50,50	0
57	MG	DA	3488	1/1	0.92	0.14	-	47,47,47,47	0
57	MG	BA	3013	1/1	0.95	0.28	-	36,36,36,36	0
57	MG	BA	3398	1/1	0.94	0.25	-	36,36,36,36	0
57	MG	BA	3328	1/1	0.80	0.09	-	55,55,55,55	0
57	MG	BA	3095	1/1	0.97	0.23	-	29,29,29,29	0
57	MG	BA	3022	1/1	0.92	0.23	-	47,47,47,47	0
57	MG	BA	3673	1/1	0.93	0.11	-	55,55,55,55	0
57	MG	AA	3182	1/1	0.98	0.15	-	40,40,40,40	0
57	MG	DA	3050	1/1	0.98	0.14	-	48,48,48,48	0
57	MG	BA	3210	1/1	0.91	0.15	-	42,42,42,42	0
57	MG	DA	3128	1/1	0.95	0.20	-	45,45,45,45	0
57	MG	DA	3477	1/1	0.96	0.10	-	37,37,37,37	0
57	MG	AA	3165	1/1	0.97	0.24	-	47,47,47,47	0
57	MG	BA	3055	1/1	0.93	0.20	-	43,43,43,43	0
57	MG	BA	3630	1/1	0.95	0.13	-	72,72,72,72	0
57	MG	DA	3436	1/1	0.81	0.12	-	61,61,61,61	0
57	MG	DA	3304	1/1	0.81	0.14	-	44,44,44,44	0
57	MG	DA	3143	1/1	0.90	0.22	-	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3205	1/1	0.86	0.26	-	48,48,48,48	0
57	MG	DA	3077	1/1	0.88	0.19	-	58,58,58,58	0
57	MG	DA	3204	1/1	0.88	0.19	-	39,39,39,39	0
57	MG	BA	3138	1/1	0.93	0.26	-	57,57,57,57	0
57	MG	BA	3496	1/1	0.98	0.29	-	33,33,33,33	0
57	MG	AA	3049	1/1	0.95	0.19	-	43,43,43,43	0
57	MG	CA	3019	1/1	0.83	0.13	-	57,57,57,57	0
57	MG	DA	3249	1/1	0.96	0.19	-	48,48,48,48	0
57	MG	BA	3486	1/1	0.95	0.16	-	32,32,32,32	0
57	MG	BA	3569	1/1	0.97	0.24	-	46,46,46,46	0
57	MG	BA	3344	1/1	0.92	0.19	-	48,48,48,48	0
57	MG	BA	3249	1/1	0.93	0.22	-	44,44,44,44	0
57	MG	AA	3156	1/1	0.87	0.15	-	86,86,86,86	0
57	MG	DA	3037	1/1	0.87	0.16	-	41,41,41,41	0
57	MG	AA	3027	1/1	0.91	0.18	-	55,55,55,55	0
57	MG	DA	3600	1/1	0.87	0.10	-	45,45,45,45	0
57	MG	AA	3181	1/1	0.80	0.07	-	82,82,82,82	0
57	MG	DA	3182	1/1	0.92	0.39	-	52,52,52,52	0
57	MG	DA	3593	1/1	0.93	0.20	-	49,49,49,49	0
57	MG	BA	3665	1/1	0.89	0.14	-	50,50,50,50	0
57	MG	DB	3004	1/1	0.97	0.11	-	38,38,38,38	0
57	MG	BA	3676	1/1	0.97	0.18	-	44,44,44,44	0
57	MG	BA	3623	1/1	0.86	0.14	-	42,42,42,42	0
57	MG	BA	3308	1/1	0.93	0.15	-	14,14,14,14	0
57	MG	BA	3321	1/1	0.97	0.16	-	31,31,31,31	0
57	MG	BA	3605	1/1	0.93	0.25	-	44,44,44,44	0
57	MG	BA	3269	1/1	0.98	0.24	-	30,30,30,30	0
57	MG	BA	3603	1/1	0.72	0.18	-	42,42,42,42	0
57	MG	BA	3644	1/1	0.94	0.19	-	48,48,48,48	0
57	MG	BA	3050	1/1	0.95	0.10	-	44,44,44,44	0
57	MG	BA	3711	1/1	0.94	0.19	-	46,46,46,46	0
57	MG	AA	3009	1/1	0.97	0.09	-	40,40,40,40	0
57	MG	AA	3109	1/1	0.75	0.26	-	75,75,75,75	0
57	MG	BA	3717	1/1	0.93	0.44	-	40,40,40,40	0
57	MG	DA	3318	1/1	0.93	0.19	-	39,39,39,39	0
57	MG	DA	3327	1/1	0.91	0.12	-	49,49,49,49	0
57	MG	BP	3004	1/1	0.96	0.11	-	41,41,41,41	0
57	MG	DA	3111	1/1	0.77	0.25	-	54,54,54,54	0
57	MG	CA	3011	1/1	0.96	0.28	-	39,39,39,39	0
57	MG	BF	305	1/1	0.88	0.15	-	33,33,33,33	0
57	MG	BA	3254	1/1	0.96	0.20	-	30,30,30,30	0
57	MG	DA	3222	1/1	0.96	0.22	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3234	1/1	0.89	0.43	-	39,39,39,39	0
57	MG	BA	3297	1/1	0.93	0.22	-	36,36,36,36	0
57	MG	CA	3123	1/1	0.98	0.09	-	53,53,53,53	0
57	MG	DA	3536	1/1	0.96	0.15	-	48,48,48,48	0
57	MG	DA	3560	1/1	0.98	0.20	-	48,48,48,48	0
57	MG	BA	3240	1/1	0.94	0.33	-	52,52,52,52	0
57	MG	CA	3108	1/1	0.97	0.15	-	51,51,51,51	0
57	MG	DA	3548	1/1	0.66	0.15	-	58,58,58,58	0
57	MG	BA	3592	1/1	0.99	0.18	-	14,14,14,14	0
57	MG	DA	3416	1/1	0.97	0.09	-	46,46,46,46	0
57	MG	BA	3560	1/1	0.95	0.16	-	54,54,54,54	0
57	MG	DA	3446	1/1	0.82	0.23	-	37,37,37,37	0
57	MG	BA	3034	1/1	0.96	0.11	-	21,21,21,21	0
57	MG	DA	3239	1/1	0.98	0.31	-	51,51,51,51	0
57	MG	BA	3292	1/1	0.96	0.17	-	26,26,26,26	0
57	MG	CA	3014	1/1	0.94	0.12	-	58,58,58,58	0
57	MG	DA	3260	1/1	0.74	0.20	-	43,43,43,43	0
57	MG	AA	3016	1/1	0.91	0.14	-	52,52,52,52	0
57	MG	CA	3073	1/1	0.98	0.09	-	57,57,57,57	0
57	MG	DA	3117	1/1	0.88	0.12	-	40,40,40,40	0
57	MG	DA	3309	1/1	0.96	0.12	-	34,34,34,34	0
57	MG	BA	3219	1/1	0.97	0.42	-	42,42,42,42	0
57	MG	DA	3396	1/1	0.95	0.11	-	43,43,43,43	0
57	MG	DA	3024	1/1	0.98	0.09	-	29,29,29,29	0
57	MG	DA	3557	1/1	0.90	0.07	-	54,54,54,54	0
57	MG	DA	3159	1/1	0.93	0.14	-	32,32,32,32	0
57	MG	AX	3010	1/1	0.88	0.15	-	61,61,61,61	0
57	MG	BA	3495	1/1	0.95	0.22	-	47,47,47,47	0
57	MG	BA	3127	1/1	0.96	0.24	-	41,41,41,41	0
57	MG	BA	3010	1/1	0.97	0.20	-	45,45,45,45	0
57	MG	BA	3329	1/1	0.94	0.12	-	21,21,21,21	0
57	MG	BA	3684	1/1	0.92	0.10	-	47,47,47,47	0
57	MG	BA	3231	1/1	0.89	0.21	-	42,42,42,42	0
57	MG	AA	3159	1/1	0.95	0.14	-	31,31,31,31	0
57	MG	BA	3480	1/1	0.95	0.27	-	50,50,50,50	0
57	MG	CA	3087	1/1	0.98	0.14	-	50,50,50,50	0
57	MG	BA	3167	1/1	0.99	0.23	-	51,51,51,51	0
57	MG	AA	3105	1/1	0.82	0.26	-	59,59,59,59	0
57	MG	BA	3450	1/1	0.93	0.07	-	45,45,45,45	0
57	MG	CA	3134	1/1	0.94	0.18	-	72,72,72,72	0
57	MG	AA	3080	1/1	0.78	0.16	-	82,82,82,82	0
57	MG	DA	3425	1/1	0.85	0.12	-	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3198	1/1	0.95	0.19	-	45,45,45,45	0
57	MG	BA	3708	1/1	0.94	0.16	-	38,38,38,38	0
57	MG	BA	3427	1/1	0.98	0.16	-	23,23,23,23	0
57	MG	DA	3078	1/1	0.97	0.04	-	49,49,49,49	0
57	MG	CA	3042	1/1	0.80	0.16	-	68,68,68,68	0
57	MG	DA	3370	1/1	0.87	0.11	-	72,72,72,72	0
57	MG	AA	3040	1/1	0.75	0.21	-	67,67,67,67	0
57	MG	DA	3615	1/1	0.88	0.15	-	36,36,36,36	0
57	MG	BA	3362	1/1	0.97	0.13	-	43,43,43,43	0
57	MG	BA	3583	1/1	0.88	0.10	-	54,54,54,54	0
57	MG	BA	3413	1/1	0.85	0.09	-	50,50,50,50	0
57	MG	BA	3648	1/1	0.95	0.13	-	50,50,50,50	0
57	MG	CA	3103	1/1	0.95	0.16	-	71,71,71,71	0
57	MG	BA	3475	1/1	0.97	0.10	-	31,31,31,31	0
57	MG	DA	3564	1/1	0.88	0.17	-	48,48,48,48	0
57	MG	BB	3014	1/1	0.95	0.08	-	41,41,41,41	0
57	MG	BA	3019	1/1	0.94	0.15	-	30,30,30,30	0
57	MG	BA	3307	1/1	0.96	0.26	-	31,31,31,31	0
57	MG	BB	3013	1/1	0.98	0.18	-	43,43,43,43	0
57	MG	BA	3129	1/1	0.88	0.13	-	30,30,30,30	0
57	MG	CA	3071	1/1	0.95	0.40	-	49,49,49,49	0
57	MG	DA	3290	1/1	0.95	0.14	-	43,43,43,43	0
57	MG	CA	3113	1/1	0.80	0.17	-	75,75,75,75	0
57	MG	DA	3578	1/1	0.76	0.23	-	63,63,63,63	0
57	MG	DA	3016	1/1	0.97	0.13	-	34,34,34,34	0
57	MG	BA	3578	1/1	0.95	0.14	-	43,43,43,43	0
57	MG	AA	3143	1/1	0.88	0.15	-	32,32,32,32	0
57	MG	DA	3629	1/1	0.97	0.22	-	40,40,40,40	0
57	MG	AX	3009	1/1	0.96	0.13	-	50,50,50,50	0
57	MG	DA	3365	1/1	0.96	0.08	-	54,54,54,54	0
57	MG	AA	3114	1/1	0.74	0.31	-	57,57,57,57	0
57	MG	AA	3192	1/1	0.92	0.12	-	72,72,72,72	0
57	MG	DA	3403	1/1	0.96	0.13	-	31,31,31,31	0
57	MG	BN	3005	1/1	0.97	0.22	-	31,31,31,31	0
57	MG	CA	3034	1/1	0.93	0.27	-	49,49,49,49	0
57	MG	DA	3399	1/1	0.99	0.13	-	26,26,26,26	0
57	MG	AA	3188	1/1	0.89	0.10	-	62,62,62,62	0
57	MG	DA	3523	1/1	0.97	0.15	-	45,45,45,45	0
57	MG	DA	3452	1/1	0.88	0.19	-	40,40,40,40	0
57	MG	BB	3001	1/1	0.90	0.16	-	44,44,44,44	0
57	MG	BA	3516	1/1	0.93	0.14	-	32,32,32,32	0
57	MG	BG	3002	1/1	0.86	0.12	-	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	3119	1/1	0.90	0.09	-	74,74,74,74	0
57	MG	DA	3366	1/1	0.86	0.16	-	40,40,40,40	0
57	MG	BA	3236	1/1	0.96	0.15	-	39,39,39,39	0
57	MG	DA	3584	1/1	0.98	0.14	-	63,63,63,63	0
57	MG	CA	3142	1/1	0.87	0.20	-	55,55,55,55	0
57	MG	DA	3201	1/1	0.90	0.27	-	42,42,42,42	0
57	MG	BA	3712	1/1	0.90	0.11	-	30,30,30,30	0
57	MG	BA	3404	1/1	0.91	0.22	-	30,30,30,30	0
57	MG	DA	3375	1/1	0.90	0.23	-	30,30,30,30	0
57	MG	DA	3465	1/1	0.96	0.14	-	45,45,45,45	0
57	MG	BA	3208	1/1	0.95	0.10	-	33,33,33,33	0
57	MG	BA	3175	1/1	0.82	0.18	-	55,55,55,55	0
57	MG	BA	3330	1/1	0.99	0.17	-	14,14,14,14	0
57	MG	BA	3536	1/1	0.97	0.11	-	42,42,42,42	0
57	MG	BA	3465	1/1	0.90	0.17	-	44,44,44,44	0
57	MG	BA	3500	1/1	0.91	0.10	-	54,54,54,54	0
57	MG	DA	3333	1/1	0.97	0.12	-	41,41,41,41	0
57	MG	DA	3394	1/1	0.91	0.11	-	48,48,48,48	0
57	MG	BA	3166	1/1	0.83	0.26	-	45,45,45,45	0
57	MG	DA	3224	1/1	0.83	0.29	-	60,60,60,60	0
57	MG	BA	3063	1/1	0.88	0.14	-	39,39,39,39	0
57	MG	DA	3279	1/1	0.96	0.32	-	50,50,50,50	0
57	MG	CA	3084	1/1	0.86	0.15	-	58,58,58,58	0
57	MG	DA	3334	1/1	0.96	0.13	-	31,31,31,31	0
57	MG	DA	3056	1/1	0.89	0.08	-	35,35,35,35	0
57	MG	BA	3611	1/1	0.83	0.12	-	61,61,61,61	0
57	MG	BA	3229	1/1	0.89	0.51	-	52,52,52,52	0
57	MG	BA	3642	1/1	0.93	0.18	-	50,50,50,50	0
57	MG	BA	3476	1/1	0.92	0.14	-	37,37,37,37	0
57	MG	BA	3487	1/1	0.80	0.11	-	70,70,70,70	0
57	MG	BA	3460	1/1	0.93	0.14	-	43,43,43,43	0
57	MG	AA	3118	1/1	0.95	0.17	-	50,50,50,50	0
57	MG	AD	301	1/1	0.95	0.10	-	47,47,47,47	0
57	MG	BA	3454	1/1	0.92	0.15	-	45,45,45,45	0
57	MG	DA	3147	1/1	0.91	0.18	-	42,42,42,42	0
57	MG	AA	3102	1/1	0.96	0.29	-	52,52,52,52	0
57	MG	BA	3359	1/1	0.96	0.14	-	56,56,56,56	0
57	MG	BA	3573	1/1	0.96	0.15	-	29,29,29,29	0
57	MG	CA	3008	1/1	0.72	0.13	-	67,67,67,67	0
57	MG	DA	3336	1/1	0.98	0.21	-	38,38,38,38	0
57	MG	BA	3683	1/1	0.88	0.27	-	44,44,44,44	0
57	MG	DA	3626	1/1	0.89	0.22	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3652	1/1	0.96	0.19	-	65,65,65,65	0
57	MG	DA	3418	1/1	0.94	0.21	-	41,41,41,41	0
57	MG	CA	3069	1/1	0.91	0.33	-	56,56,56,56	0
57	MG	DA	3035	1/1	0.92	0.19	-	45,45,45,45	0
57	MG	BA	3188	1/1	0.96	0.19	-	48,48,48,48	0
57	MG	DA	3048	1/1	0.93	0.16	-	53,53,53,53	0
57	MG	BA	3370	1/1	0.98	0.21	-	32,32,32,32	0
57	MG	AA	3126	1/1	0.76	0.17	-	52,52,52,52	0
57	MG	DA	3415	1/1	0.92	0.36	-	55,55,55,55	0
57	MG	BA	3679	1/1	0.94	0.15	-	38,38,38,38	0
57	MG	DA	3140	1/1	0.98	0.25	-	38,38,38,38	0
57	MG	CA	3053	1/1	0.91	0.17	-	59,59,59,59	0
57	MG	BA	3265	1/1	0.98	0.14	-	30,30,30,30	0
57	MG	DA	3534	1/1	0.97	0.12	-	30,30,30,30	0
57	MG	BA	3092	1/1	0.91	0.14	-	32,32,32,32	0
57	MG	DA	3455	1/1	0.88	0.35	-	34,34,34,34	0
57	MG	BA	3217	1/1	0.90	0.36	-	57,57,57,57	0
57	MG	DA	3065	1/1	0.96	0.14	-	38,38,38,38	0
57	MG	BA	3617	1/1	0.97	0.13	-	59,59,59,59	0
57	MG	DA	3592	1/1	0.89	0.14	-	62,62,62,62	0
57	MG	AA	3020	1/1	0.93	0.18	-	62,62,62,62	0
57	MG	DA	3485	1/1	0.94	0.20	-	41,41,41,41	0
57	MG	AA	3099	1/1	0.94	0.11	-	59,59,59,59	0
57	MG	DA	3563	1/1	0.91	0.15	-	55,55,55,55	0
57	MG	CA	3036	1/1	0.91	0.10	-	47,47,47,47	0
57	MG	DA	3206	1/1	0.98	0.22	-	37,37,37,37	0
57	MG	BA	3525	1/1	0.89	0.18	-	49,49,49,49	0
57	MG	CA	3027	1/1	0.88	0.08	-	62,62,62,62	0
57	MG	BA	3429	1/1	0.89	0.13	-	37,37,37,37	0
57	MG	DA	3575	1/1	0.89	0.21	-	19,19,19,19	0
57	MG	AA	3145	1/1	0.78	0.23	-	71,71,71,71	0
57	MG	BB	3016	1/1	0.98	0.06	-	39,39,39,39	0
57	MG	BA	3659	1/1	0.97	0.22	-	47,47,47,47	0
57	MG	AS	101	1/1	0.88	0.09	-	55,55,55,55	0
57	MG	BA	3570	1/1	0.81	0.12	-	48,48,48,48	0
57	MG	BA	3273	1/1	0.93	0.17	-	30,30,30,30	0
57	MG	DA	3555	1/1	0.82	0.15	-	70,70,70,70	0
57	MG	CA	3089	1/1	0.96	0.12	-	65,65,65,65	0
57	MG	DA	3569	1/1	0.91	0.15	-	42,42,42,42	0
57	MG	BA	3639	1/1	0.73	0.15	-	46,46,46,46	0
57	MG	AA	3129	1/1	0.98	0.15	-	37,37,37,37	0
57	MG	CA	3160	1/1	0.94	0.38	-	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3290	1/1	0.98	0.14	-	43,43,43,43	0
57	MG	BA	3020	1/1	0.83	0.30	-	55,55,55,55	0
57	MG	CX	3002	1/1	0.73	0.35	-	75,75,75,75	0
57	MG	AA	3071	1/1	0.97	0.39	-	41,41,41,41	0
57	MG	BA	3107	1/1	0.93	0.28	-	49,49,49,49	0
57	MG	DA	3057	1/1	0.96	0.25	-	22,22,22,22	0
57	MG	AA	3031	1/1	0.92	0.10	-	41,41,41,41	0
57	MG	AA	3168	1/1	0.89	0.09	-	56,56,56,56	0
57	MG	DA	3193	1/1	0.83	0.21	-	43,43,43,43	0
57	MG	BA	3243	1/1	0.87	0.24	-	46,46,46,46	0
57	MG	AA	3158	1/1	0.92	0.09	-	72,72,72,72	0
57	MG	DA	3214	1/1	0.93	0.13	-	43,43,43,43	0
57	MG	B3	3002	1/1	0.97	0.17	-	58,58,58,58	0
57	MG	BA	3306	1/1	0.72	0.20	-	32,32,32,32	0
57	MG	DA	3266	1/1	0.85	0.14	-	45,45,45,45	0
57	MG	DB	3002	1/1	0.86	0.07	-	75,75,75,75	0
57	MG	DA	3544	1/1	0.94	0.08	-	59,59,59,59	0
57	MG	AA	3085	1/1	0.73	0.15	-	69,69,69,69	0
57	MG	DA	3337	1/1	0.84	0.22	-	46,46,46,46	0
57	MG	BA	3295	1/1	0.86	0.14	-	56,56,56,56	0
57	MG	DA	3142	1/1	0.93	0.23	-	50,50,50,50	0
57	MG	B7	103	1/1	0.85	0.21	-	51,51,51,51	0
57	MG	DA	3125	1/1	0.92	0.11	-	48,48,48,48	0
57	MG	AA	3092	1/1	0.94	0.15	-	36,36,36,36	0
57	MG	AA	3014	1/1	0.90	0.14	-	73,73,73,73	0
57	MG	CA	3091	1/1	0.93	0.20	-	75,75,75,75	0
57	MG	BA	3555	1/1	0.93	0.08	-	62,62,62,62	0
57	MG	BA	3130	1/1	0.83	0.39	-	39,39,39,39	0
57	MG	DA	3380	1/1	0.90	0.13	-	65,65,65,65	0
57	MG	DA	3246	1/1	0.92	0.30	-	57,57,57,57	0
57	MG	BA	3438	1/1	0.96	0.16	-	19,19,19,19	0
57	MG	AA	3134	1/1	0.86	0.15	-	59,59,59,59	0
57	MG	BA	3627	1/1	0.97	0.09	-	28,28,28,28	0
57	MG	BA	3670	1/1	0.98	0.11	-	25,25,25,25	0
57	MG	DA	3120	1/1	0.87	0.26	-	55,55,55,55	0
57	MG	DA	3151	1/1	0.96	0.20	-	48,48,48,48	0
57	MG	DA	3390	1/1	0.70	0.17	-	54,54,54,54	0
57	MG	DA	3360	1/1	0.93	0.11	-	54,54,54,54	0
57	MG	DA	3244	1/1	0.86	0.22	-	43,43,43,43	0
57	MG	BA	3640	1/1	0.96	0.15	-	53,53,53,53	0
57	MG	DA	3411	1/1	0.93	0.10	-	51,51,51,51	0
57	MG	DB	3007	1/1	0.98	0.09	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	3092	1/1	0.83	0.16	-	76,76,76,76	0
57	MG	DA	3595	1/1	0.89	0.14	-	65,65,65,65	0
57	MG	DA	3526	1/1	0.96	0.10	-	41,41,41,41	0
57	MG	BA	3299	1/1	0.85	0.20	-	27,27,27,27	0
57	MG	BA	3422	1/1	0.80	0.15	-	39,39,39,39	0
57	MG	BA	3600	1/1	0.96	0.25	-	59,59,59,59	0
57	MG	BA	3435	1/1	0.96	0.24	-	31,31,31,31	0
57	MG	BA	3582	1/1	0.95	0.16	-	23,23,23,23	0
57	MG	DA	3124	1/1	0.97	0.26	-	30,30,30,30	0
57	MG	BA	3260	1/1	0.94	0.26	-	45,45,45,45	0
57	MG	DA	3074	1/1	0.94	0.18	-	38,38,38,38	0
57	MG	DA	3305	1/1	0.88	0.07	-	48,48,48,48	0
57	MG	AA	3150	1/1	0.89	0.09	-	65,65,65,65	0
57	MG	BB	3018	1/1	0.92	0.09	-	43,43,43,43	0
57	MG	BA	3553	1/1	0.98	0.19	-	41,41,41,41	0
57	MG	CA	3041	1/1	0.84	0.10	-	62,62,62,62	0
57	MG	BA	3179	1/1	0.93	0.20	-	49,49,49,49	0
57	MG	BA	3239	1/1	0.99	0.17	-	42,42,42,42	0
57	MG	BA	3014	1/1	0.98	0.13	-	46,46,46,46	0
57	MG	DA	3135	1/1	0.65	0.18	-	61,61,61,61	0
57	MG	DA	3581	1/1	0.93	0.17	-	53,53,53,53	0
57	MG	BA	3675	1/1	0.92	0.19	-	41,41,41,41	0
57	MG	DA	3118	1/1	0.94	0.09	-	46,46,46,46	0
57	MG	CE	3001	1/1	0.81	0.19	-	80,80,80,80	0
57	MG	BA	3519	1/1	0.89	0.16	-	26,26,26,26	0
57	MG	DA	3408	1/1	0.94	0.10	-	44,44,44,44	0
57	MG	DA	3123	1/1	0.97	0.16	-	45,45,45,45	0
57	MG	CA	3098	1/1	0.88	0.07	-	76,76,76,76	0
57	MG	AA	3132	1/1	0.96	0.20	-	67,67,67,67	0
57	MG	DA	3611	1/1	0.91	0.17	-	58,58,58,58	0
57	MG	DA	3468	1/1	0.96	0.26	-	64,64,64,64	0
57	MG	DA	3133	1/1	0.91	0.14	-	52,52,52,52	0
57	MG	DA	3225	1/1	0.93	0.14	-	42,42,42,42	0
57	MG	DA	3454	1/1	0.97	0.27	-	28,28,28,28	0
57	MG	DA	3082	1/1	0.93	0.17	-	47,47,47,47	0
57	MG	BA	3001	1/1	0.91	0.20	-	48,48,48,48	0
57	MG	BE	3006	1/1	0.90	0.34	-	72,72,72,72	0
57	MG	DA	3576	1/1	0.91	0.27	-	46,46,46,46	0
57	MG	CA	3128	1/1	0.93	0.12	-	43,43,43,43	0
57	MG	BA	3255	1/1	0.98	0.06	-	37,37,37,37	0
57	MG	DA	3036	1/1	0.87	0.14	-	48,48,48,48	0
57	MG	AA	3117	1/1	0.96	0.12	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3139	1/1	0.86	0.20	-	49,49,49,49	0
57	MG	DA	3598	1/1	0.90	0.11	-	48,48,48,48	0
57	MG	BA	3612	1/1	0.95	0.23	-	58,58,58,58	0
57	MG	BW	205	1/1	0.98	0.14	-	30,30,30,30	0
57	MG	BA	3488	1/1	0.97	0.05	-	34,34,34,34	0
57	MG	BB	3008	1/1	0.92	0.11	-	60,60,60,60	0
57	MG	DA	3492	1/1	0.91	0.10	-	45,45,45,45	0
57	MG	BA	3653	1/1	0.98	0.21	-	51,51,51,51	0
57	MG	BA	3176	1/1	0.92	0.23	-	35,35,35,35	0
57	MG	BA	3326	1/1	0.85	0.15	-	40,40,40,40	0
57	MG	DA	3080	1/1	0.96	0.10	-	64,64,64,64	0
57	MG	DA	3568	1/1	0.85	0.14	-	45,45,45,45	0
57	MG	DA	3287	1/1	0.89	0.29	-	58,58,58,58	0
57	MG	DA	3482	1/1	0.99	0.25	-	31,31,31,31	0
57	MG	CA	3153	1/1	0.96	0.15	-	57,57,57,57	0
57	MG	BA	3214	1/1	0.90	0.22	-	48,48,48,48	0
57	MG	BA	3139	1/1	0.90	0.32	-	45,45,45,45	0
57	MG	BA	3250	1/1	0.93	0.15	-	47,47,47,47	0
57	MG	BA	3280	1/1	0.98	0.17	-	46,46,46,46	0
57	MG	B5	103	1/1	0.96	0.08	-	50,50,50,50	0
57	MG	BA	3634	1/1	0.95	0.23	-	58,58,58,58	0
57	MG	BA	3397	1/1	0.92	0.11	-	33,33,33,33	0
57	MG	DA	3248	1/1	0.89	0.20	-	59,59,59,59	0
57	MG	CA	3130	1/1	0.85	0.16	-	88,88,88,88	0
57	MG	CA	3150	1/1	0.95	0.11	-	66,66,66,66	0
57	MG	BA	3029	1/1	0.86	0.19	-	53,53,53,53	0
57	MG	BA	3201	1/1	0.94	0.17	-	44,44,44,44	0
57	MG	BA	3080	1/1	0.94	0.20	-	51,51,51,51	0
57	MG	AA	3185	1/1	0.91	0.15	-	50,50,50,50	0
57	MG	CA	3099	1/1	0.88	0.22	-	50,50,50,50	0
57	MG	BA	3353	1/1	0.94	0.08	-	46,46,46,46	0
57	MG	DA	3591	1/1	0.88	0.10	-	69,69,69,69	0
57	MG	BA	3596	1/1	0.98	0.14	-	56,56,56,56	0
57	MG	DP	201	1/1	0.95	0.25	-	61,61,61,61	0
57	MG	AA	3142	1/1	0.95	0.29	-	53,53,53,53	0
57	MG	BA	3481	1/1	0.97	0.23	-	35,35,35,35	0
57	MG	BA	3333	1/1	0.89	0.10	-	58,58,58,58	0
57	MG	AA	3098	1/1	0.90	0.14	-	42,42,42,42	0
57	MG	BR	202	1/1	0.90	0.18	-	49,49,49,49	0
57	MG	BA	3714	1/1	0.95	0.10	-	42,42,42,42	0
57	MG	AA	3191	1/1	0.95	0.21	-	56,56,56,56	0
57	MG	CA	3093	1/1	0.93	0.16	-	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
57	MG	CA	3135	1/1	0.84	0.10	-	85,85,85,85	0
57	MG	DA	3424	1/1	0.95	0.08	-	56,56,56,56	0
57	MG	DA	3500	1/1	0.96	0.15	-	32,32,32,32	0
57	MG	BB	3006	1/1	0.95	0.19	-	42,42,42,42	0
57	MG	BA	3471	1/1	0.94	0.10	-	42,42,42,42	0
57	MG	BA	3664	1/1	0.93	0.14	-	66,66,66,66	0
57	MG	AA	3058	1/1	0.86	0.21	-	48,48,48,48	0
57	MG	DA	3392	1/1	0.98	0.23	-	40,40,40,40	0
57	MG	BA	3324	1/1	0.92	0.20	-	61,61,61,61	0
57	MG	AA	3123	1/1	0.86	0.10	-	59,59,59,59	0
57	MG	CA	3051	1/1	0.93	0.30	-	57,57,57,57	0
57	MG	BA	3196	1/1	0.97	0.27	-	51,51,51,51	0
57	MG	AA	3087	1/1	0.86	0.13	-	57,57,57,57	0
57	MG	DA	3413	1/1	0.93	0.29	-	30,30,30,30	0
57	MG	AA	3135	1/1	0.94	0.07	-	52,52,52,52	0
57	MG	BA	3649	1/1	0.95	0.14	-	65,65,65,65	0
57	MG	DA	3175	1/1	0.96	0.24	-	42,42,42,42	0
57	MG	AA	3207	1/1	0.95	0.10	-	57,57,57,57	0
57	MG	DA	3326	1/1	0.91	0.09	-	40,40,40,40	0
57	MG	BA	3221	1/1	0.83	0.25	-	59,59,59,59	0
57	MG	DA	3269	1/1	0.98	0.16	-	40,40,40,40	0
57	MG	BA	3279	1/1	0.92	0.21	-	48,48,48,48	0
57	MG	DA	3158	1/1	0.78	0.13	-	52,52,52,52	0
57	MG	BA	3153	1/1	0.87	0.12	-	53,53,53,53	0
57	MG	DA	3273	1/1	0.96	0.21	-	41,41,41,41	0
57	MG	BA	3122	1/1	0.92	0.22	-	39,39,39,39	0
57	MG	BA	3590	1/1	0.91	0.24	-	62,62,62,62	0
57	MG	DA	3431	1/1	0.92	0.15	-	56,56,56,56	0
57	MG	DA	3447	1/1	0.95	0.14	-	48,48,48,48	0
57	MG	DA	3245	1/1	0.96	0.12	-	46,46,46,46	0
57	MG	BA	3227	1/1	0.97	0.19	-	39,39,39,39	0
57	MG	BA	3557	1/1	0.93	0.17	-	35,35,35,35	0
57	MG	BA	3004	1/1	0.98	0.18	-	26,26,26,26	0
57	MG	AA	3200	1/1	0.94	0.10	-	58,58,58,58	0
57	MG	BA	3086	1/1	0.98	0.22	-	15,15,15,15	0
57	MG	AE	3001	1/1	0.93	0.37	-	85,85,85,85	0
57	MG	BA	3462	1/1	0.95	0.23	-	51,51,51,51	0
57	MG	DA	3099	1/1	0.92	0.15	-	40,40,40,40	0
57	MG	AD	303	1/1	0.89	0.20	-	60,60,60,60	0
57	MG	BA	3543	1/1	0.84	0.11	-	69,69,69,69	0
57	MG	AA	3044	1/1	0.94	0.14	-	46,46,46,46	0
57	MG	CA	3136	1/1	0.92	0.11	-	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3241	1/1	0.91	0.33	-	53,53,53,53	0
57	MG	DA	3330	1/1	0.95	0.18	-	49,49,49,49	0
57	MG	CA	3078	1/1	0.90	0.18	-	63,63,63,63	0
57	MG	BA	3667	1/1	0.94	0.18	-	31,31,31,31	0
57	MG	DA	3046	1/1	0.87	0.33	-	50,50,50,50	0
57	MG	CA	3140	1/1	0.90	0.07	-	48,48,48,48	0
57	MG	BA	3484	1/1	0.96	0.08	-	50,50,50,50	0
57	MG	DA	3236	1/1	0.94	0.10	-	45,45,45,45	0
57	MG	BA	3161	1/1	0.96	0.21	-	54,54,54,54	0
57	MG	DA	3406	1/1	0.82	0.15	-	62,62,62,62	0
57	MG	BA	3323	1/1	0.94	0.10	-	59,59,59,59	0
57	MG	DA	3284	1/1	0.86	0.20	-	51,51,51,51	0
57	MG	DA	3405	1/1	0.96	0.08	-	45,45,45,45	0
57	MG	DA	3295	1/1	0.96	0.08	-	58,58,58,58	0
57	MG	DA	3381	1/1	0.93	0.22	-	55,55,55,55	0
57	MG	BA	3158	1/1	0.79	0.28	-	48,48,48,48	0
57	MG	DA	3341	1/1	0.94	0.14	-	32,32,32,32	0
57	MG	DA	3407	1/1	0.76	0.16	-	67,67,67,67	0
57	MG	DA	3421	1/1	0.87	0.07	-	31,31,31,31	0
57	MG	CA	3088	1/1	0.88	0.11	-	61,61,61,61	0
57	MG	AA	3069	1/1	0.82	0.11	-	75,75,75,75	0
57	MG	AA	3046	1/1	0.91	0.18	-	72,72,72,72	0
57	MG	BA	3463	1/1	0.94	0.12	-	43,43,43,43	0
57	MG	DA	3271	1/1	0.92	0.22	-	47,47,47,47	0
57	MG	DA	3068	1/1	0.90	0.17	-	48,48,48,48	0
57	MG	BA	3448	1/1	0.94	0.08	-	42,42,42,42	0
57	MG	BA	3680	1/1	0.86	0.13	-	46,46,46,46	0
57	MG	DA	3428	1/1	0.90	0.19	-	46,46,46,46	0
57	MG	DA	3329	1/1	0.99	0.25	-	54,54,54,54	0
57	MG	CA	3156	1/1	0.98	0.05	-	57,57,57,57	0
57	MG	DA	3040	1/1	0.92	0.43	-	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.