



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:01 am GMT

PDB ID : 4V8G  
Title : Crystal structure of RMF bound to the 70S ribosome.  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-11  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28972

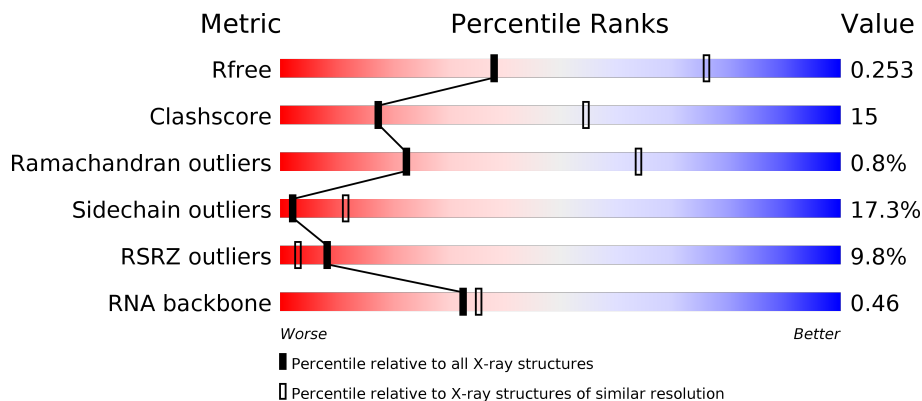
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)
RNA backbone	2435	1007 (3.34-2.66)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	

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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	






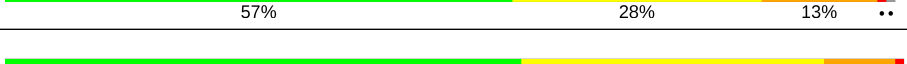
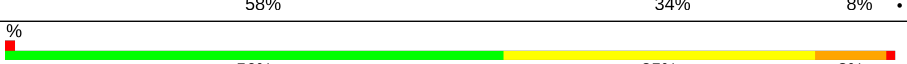
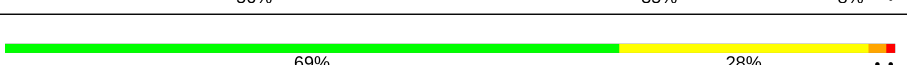
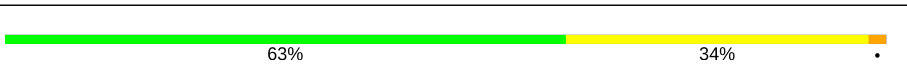


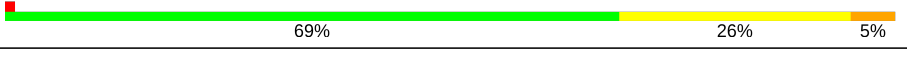

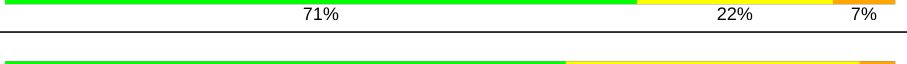


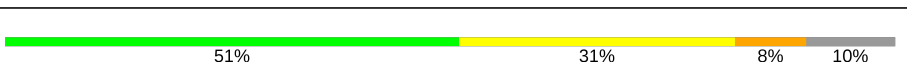








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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	61	
22	CV	61	
23	BA	2915	
23	DA	2915	
24	BB	122	
24	DB	122	
25	BD	276	
25	DD	276	
26	BE	206	
26	DE	206	
27	BF	210	
27	DF	210	

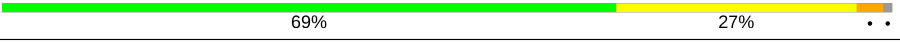















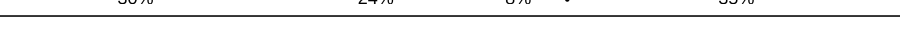
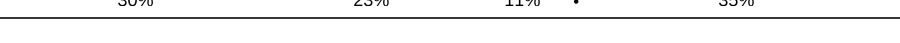
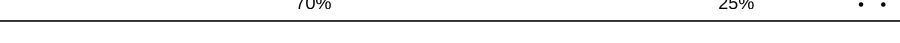

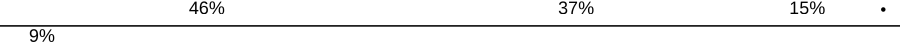
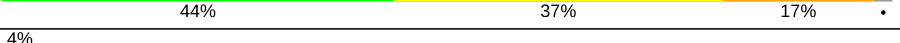



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Mol	Chain	Length	Quality of chain
28	BG	182	
28	DG	182	
29	BH	180	
29	DH	180	
30	BI	148	
30	DI	148	
31	BN	140	
31	DN	140	
32	BO	122	
32	DO	122	
33	BP	150	
33	DP	150	
34	BQ	141	
34	DQ	141	
35	BR	118	
35	DR	118	
36	BS	112	
36	DS	112	
37	BT	146	
37	DT	146	
38	BU	118	
38	DU	118	
39	BV	101	
39	DV	101	
40	BW	113	



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Mol	Chain	Length	Quality of chain
40	DW	113	
41	BX	96	
41	DX	96	
42	BY	110	
42	DY	110	
43	BZ	206	
43	DZ	206	
44	B0	85	
44	D0	85	
45	B1	98	
45	D1	98	
46	B2	72	
46	D2	72	
47	B3	60	
47	D3	60	
48	B4	71	
48	D4	71	
49	B5	60	
49	D5	60	
50	B6	54	
50	D6	54	
51	B7	49	
51	D7	49	
52	B8	65	
52	D8	65	

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Mol	Chain	Length	Quality of chain
53	B9	37	
53	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
54	MG	AA	1604	-	-	-	X
54	MG	AA	1613	-	-	-	X
54	MG	AA	1615	-	-	-	X
54	MG	AA	1621	-	-	-	X
54	MG	AA	1627	-	-	-	X
54	MG	AA	1631	-	-	-	X
54	MG	AA	1640	-	-	-	X
54	MG	AA	1645	-	-	-	X
54	MG	AA	1657	-	-	-	X
54	MG	AA	1659	-	-	-	X
54	MG	AA	1660	-	-	-	X
54	MG	B3	101	-	-	-	X
54	MG	BA	3001	-	-	-	X
54	MG	BA	3003	-	-	-	X
54	MG	BA	3021	-	-	-	X
54	MG	BA	3031	-	-	-	X
54	MG	BA	3033	-	-	-	X
54	MG	BA	3034	-	-	-	X
54	MG	BA	3037	-	-	-	X
54	MG	BA	3039	-	-	-	X
54	MG	BA	3046	-	-	-	X
54	MG	BA	3047	-	-	-	X
54	MG	BA	3053	-	-	-	X
54	MG	BA	3071	-	-	-	X
54	MG	BA	3074	-	-	-	X
54	MG	BA	3078	-	-	-	X
54	MG	BA	3080	-	-	-	X
54	MG	BA	3108	-	-	-	X
54	MG	BA	3109	-	-	-	X
54	MG	BA	3113	-	-	-	X
54	MG	BA	3117	-	-	-	X
54	MG	BA	3119	-	-	-	X
54	MG	BA	3127	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3129	-	-	-	X
54	MG	BA	3133	-	-	-	X
54	MG	BA	3142	-	-	-	X
54	MG	BA	3160	-	-	-	X
54	MG	BA	3161	-	-	-	X
54	MG	BA	3187	-	-	-	X
54	MG	BA	3189	-	-	-	X
54	MG	BA	3197	-	-	-	X
54	MG	BA	3199	-	-	-	X
54	MG	BA	3219	-	-	-	X
54	MG	BA	3228	-	-	-	X
54	MG	BA	3230	-	-	-	X
54	MG	BA	3234	-	-	-	X
54	MG	BA	3236	-	-	-	X
54	MG	BA	3239	-	-	-	X
54	MG	BA	3244	-	-	-	X
54	MG	BA	3253	-	-	-	X
54	MG	BA	3254	-	-	-	X
54	MG	BA	3302	-	-	-	X
54	MG	BA	3307	-	-	-	X
54	MG	BA	3308	-	-	-	X
54	MG	BA	3311	-	-	-	X
54	MG	BA	3330	-	-	-	X
54	MG	BA	3333	-	-	-	X
54	MG	BA	3368	-	-	-	X
54	MG	BA	3387	-	-	-	X
54	MG	BA	3396	-	-	-	X
54	MG	BA	3408	-	-	-	X
54	MG	BA	3423	-	-	-	X
54	MG	BA	3424	-	-	-	X
54	MG	BA	3426	-	-	-	X
54	MG	BA	3427	-	-	-	X
54	MG	BA	3434	-	-	-	X
54	MG	BA	3435	-	-	-	X
54	MG	BA	3441	-	-	-	X
54	MG	BA	3448	-	-	-	X
54	MG	BA	3455	-	-	-	X
54	MG	BA	3461	-	-	-	X
54	MG	BA	3473	-	-	-	X
54	MG	BA	3475	-	-	-	X
54	MG	BA	3489	-	-	-	X
54	MG	BA	3500	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	BA	3504	-	-	-	X
54	MG	BA	3512	-	-	-	X
54	MG	BA	3513	-	-	-	X
54	MG	BA	3517	-	-	-	X
54	MG	BA	3519	-	-	-	X
54	MG	BA	3526	-	-	-	X
54	MG	BA	3551	-	-	-	X
54	MG	BA	3557	-	-	-	X
54	MG	BA	3562	-	-	-	X
54	MG	BB	201	-	-	-	X
54	MG	BB	204	-	-	-	X
54	MG	BB	205	-	-	-	X
54	MG	BD	302	-	-	-	X
54	MG	BE	301	-	-	-	X
54	MG	BQ	202	-	-	-	X
54	MG	BR	201	-	-	-	X
54	MG	CA	1601	-	-	-	X
54	MG	CA	1602	-	-	-	X
54	MG	CA	1612	-	-	-	X
54	MG	CA	1613	-	-	-	X
54	MG	CA	1617	-	-	-	X
54	MG	CA	1618	-	-	-	X
54	MG	CA	1623	-	-	-	X
54	MG	CA	1626	-	-	-	X
54	MG	CA	1628	-	-	-	X
54	MG	CA	1631	-	-	-	X
54	MG	CA	1636	-	-	-	X
54	MG	CA	1638	-	-	-	X
54	MG	CA	1655	-	-	-	X
54	MG	DA	3003	-	-	-	X
54	MG	DA	3006	-	-	-	X
54	MG	DA	3011	-	-	-	X
54	MG	DA	3019	-	-	-	X
54	MG	DA	3020	-	-	-	X
54	MG	DA	3027	-	-	-	X
54	MG	DA	3032	-	-	-	X
54	MG	DA	3040	-	-	-	X
54	MG	DA	3044	-	-	-	X
54	MG	DA	3059	-	-	-	X
54	MG	DA	3062	-	-	-	X
54	MG	DA	3070	-	-	-	X
54	MG	DA	3072	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3073	-	-	-	X
54	MG	DA	3074	-	-	-	X
54	MG	DA	3079	-	-	-	X
54	MG	DA	3084	-	-	-	X
54	MG	DA	3085	-	-	-	X
54	MG	DA	3086	-	-	-	X
54	MG	DA	3092	-	-	-	X
54	MG	DA	3098	-	-	-	X
54	MG	DA	3099	-	-	-	X
54	MG	DA	3115	-	-	-	X
54	MG	DA	3116	-	-	-	X
54	MG	DA	3118	-	-	-	X
54	MG	DA	3120	-	-	-	X
54	MG	DA	3121	-	-	-	X
54	MG	DA	3124	-	-	-	X
54	MG	DA	3128	-	-	-	X
54	MG	DA	3130	-	-	-	X
54	MG	DA	3133	-	-	-	X
54	MG	DA	3138	-	-	-	X
54	MG	DA	3142	-	-	-	X
54	MG	DA	3144	-	-	-	X
54	MG	DA	3146	-	-	-	X
54	MG	DA	3149	-	-	-	X
54	MG	DA	3168	-	-	-	X
54	MG	DA	3169	-	-	-	X
54	MG	DA	3170	-	-	-	X
54	MG	DA	3177	-	-	-	X
54	MG	DA	3185	-	-	-	X
54	MG	DA	3188	-	-	-	X
54	MG	DA	3202	-	-	-	X
54	MG	DA	3204	-	-	-	X
54	MG	DA	3207	-	-	-	X
54	MG	DA	3208	-	-	-	X
54	MG	DA	3217	-	-	-	X
54	MG	DA	3219	-	-	-	X
54	MG	DA	3233	-	-	-	X
54	MG	DA	3236	-	-	-	X
54	MG	DA	3242	-	-	-	X
54	MG	DA	3247	-	-	-	X
54	MG	DA	3267	-	-	-	X
54	MG	DA	3279	-	-	-	X
54	MG	DA	3280	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	DA	3290	-	-	-	X
54	MG	DA	3291	-	-	-	X
54	MG	DA	3297	-	-	-	X
54	MG	DA	3303	-	-	-	X
54	MG	DA	3309	-	-	-	X
54	MG	DA	3324	-	-	-	X
54	MG	DA	3340	-	-	-	X
54	MG	DA	3341	-	-	-	X
54	MG	DA	3349	-	-	-	X
54	MG	DA	3354	-	-	-	X
54	MG	DA	3372	-	-	-	X
54	MG	DA	3374	-	-	-	X
54	MG	DA	3385	-	-	-	X
54	MG	DA	3390	-	-	-	X
54	MG	DA	3394	-	-	-	X
54	MG	DA	3395	-	-	-	X
54	MG	DA	3396	-	-	-	X
54	MG	DA	3410	-	-	-	X
54	MG	DB	201	-	-	-	X
54	MG	DF	301	-	-	-	X
54	MG	DP	201	-	-	-	X

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 283930 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	1505	Total	C	N	O	P	0	0	0
			32353	14399	5995	10454	1505			
1	CA	1501	Total	C	N	O	P	0	0	0
			32270	14362	5983	10424	1501			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	5			
2	CB	229	Total	C	N	O	S	0	0	0
			1775	1132	318	320	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
			1450	906	279	264	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	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
			1526	963	283	274	6			
4	CD	208	Total	C	N	O	S	0	0	0
			1526	963	283	274	6			

- 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
			1105	699	204	198	4			
5	CE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	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
			777	493	137	144	3			
6	CF	100	Total	C	N	O	S	0	0	0
			777	493	137	144	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
			1164	726	224	208	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1164	726	224	208	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			
8	CH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	125	Total	C	N	O	0	0	0
			852	533	163	156			
9	CI	125	Total	C	N	O	0	0	0
			852	533	163	156			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AJ	96	Total	C	N	O	0	0	0
			663	410	132	121			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	CJ	96	Total	C	N	O	0	0	0
			663	410	132	121			

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	114	Total 828	C 516	N 155	O 154	S 3	0	0	0
11	CK	114	Total 828	C 516	N 155	O 154	S 3	0	0	0

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	122	Total 905	C 567	N 178	O 159	S 1	0	0	0
12	CL	122	Total 905	C 567	N 178	O 159	S 1	0	0	0

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			804	497	164	142	1			
13	CM	114	Total	C	N	O	S	0	0	0
			804	497	164	142	1			

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total 478	C 303	N 99	O 72	S 4	0	0	0
14	CN	60	Total 478	C 303	N 99	O 72	S 4	0	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	0	0	0
			724	453	143	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			

- 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
			651	416	123	111	1			
16	CP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	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
			514	329	98	87			
18	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			
19	CS	81	Total	C	N	O	S	0	0	0
			560	351	108	99	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	97	Total	C	N	O	S	0	0	0
			713	438	152	121	2			
20	CT	97	Total	C	N	O	S	0	0	0
			713	438	152	121	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 protein called Ribosome modulation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	53	Total	C	N	O	S	0	0	0
			333	204	66	61	2			
22	CV	53	Total	C	N	O	S	0	0	0
			353	218	67	66	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	56	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	57	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	58	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	59	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	60	HIS	-	EXPRESSION TAG	UNP P0AFW2
AV	61	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	56	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	57	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	58	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	59	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	60	HIS	-	EXPRESSION TAG	UNP P0AFW2
CV	61	HIS	-	EXPRESSION TAG	UNP P0AFW2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BA	2809	Total	C	N	O	P	0	0	0
			60512	26930	11328	19446	2808			
23	DA	2814	Total	C	N	O	P	0	0	0
			60620	26978	11348	19481	2813			

- Molecule 24 is a RNA chain called 5S Ribosomal RNA.

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

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

- Molecule 25 is a protein called 50S Ribosomal Protein L2.

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

- Molecule 26 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			
26	DE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 27 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			
27	DF	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			

- Molecule 28 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			
28	DG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 29 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			
29	DH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 30 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BI	146	Total	C	N	O	S	0	0	0
			1040	669	180	190	1			
30	DI	146	Total	C	N	O	S	0	0	0
			1038	668	180	189	1			

- Molecule 31 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			
31	DN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 32 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			
32	DO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 33 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			
33	DP	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 34 is a protein called 50S Ribosomal Protein L16.

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

- Molecule 35 is a protein called 50S Ribosomal Protein L17.

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

- Molecule 36 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BS	110	Total	C	N	O	S	0	0	0
			865	544	172	149				
36	DS	110	Total	C	N	O	S	0	0	0
			865	544	172	149				

- Molecule 37 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
37	DT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 38 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 39 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BV	100	Total	C	N	O	S	0	0	0
			760	490	136	133	1			
39	DV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 40 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	DW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

- Molecule 41 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
41	DX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

- Molecule 42 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
42	DY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 43 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			
43	DZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 44 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
44	D0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 45 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			
45	D1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 46 is a protein called 50S Ribosomal Protein L29.

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

- Molecule 47 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	B3	59	Total	C	N	O	0	0	0
			458	293	87	78			
47	D3	59	Total	C	N	O	0	0	0
			458	293	87	78			

- Molecule 48 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
48	D4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 49 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
49	D5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 50 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
50	D6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 51 is a protein called 50S Ribosomal Protein L34.

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

- Molecule 52 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
52	D8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 53 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			
53	D9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	618	Total	Mg	0	0
			618	618		
54	CA	69	Total	Mg	0	0
			69	69		
54	DF	2	Total	Mg	0	0
			2	2		
54	B8	3	Total	Mg	0	0
			3	3		
54	BE	6	Total	Mg	0	0
			6	6		
54	B1	1	Total	Mg	0	0
			1	1		
54	BP	1	Total	Mg	0	0
			1	1		
54	D6	1	Total	Mg	0	0
			1	1		
54	B5	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	17	Total 17	Mg 17	0	0
54	D8	1	Total 1	Mg 1	0	0
54	B9	1	Total 1	Mg 1	0	0
54	BF	2	Total 2	Mg 2	0	0
54	B2	2	Total 2	Mg 2	0	0
54	AA	106	Total 106	Mg 106	0	0
54	BQ	3	Total 3	Mg 3	0	0
54	D7	1	Total 1	Mg 1	0	0
54	BU	2	Total 2	Mg 2	0	0
54	AD	1	Total 1	Mg 1	0	0
54	DD	1	Total 1	Mg 1	0	0
54	B3	2	Total 2	Mg 2	0	0
54	BR	2	Total 2	Mg 2	0	0
54	DA	430	Total 430	Mg 430	0	0
54	BV	1	Total 1	Mg 1	0	0
54	DE	1	Total 1	Mg 1	0	0
54	DP	1	Total 1	Mg 1	0	0
54	BD	3	Total 3	Mg 3	0	0
54	B0	2	Total 2	Mg 2	0	0
54	BW	1	Total 1	Mg 1	0	0
54	DB	5	Total 5	Mg 5	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	B5	1	Total 1	Zn 1	0	0
55	B4	1	Total 1	Zn 1	0	0
55	AD	1	Total 1	Zn 1	0	0
55	CD	1	Total 1	Zn 1	0	0
55	B9	1	Total 1	Zn 1	0	0
55	BY	1	Total 1	Zn 1	0	0
55	DY	1	Total 1	Zn 1	0	0
55	D5	1	Total 1	Zn 1	0	0
55	D4	1	Total 1	Zn 1	0	0
55	AN	1	Total 1	Zn 1	0	0
55	CN	1	Total 1	Zn 1	0	0
55	D6	1	Total 1	Zn 1	0	0
55	D9	1	Total 1	Zn 1	0	0
55	B6	1	Total 1	Zn 1	0	0

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	145	Total 145	O 145	0	0
56	AF	1	Total 1	O 1	0	0
56	AK	1	Total 1	O 1	0	0
56	AQ	1	Total 1	O 1	0	0
56	BA	1422	Total 1422	O 1422	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BB	31	Total 31	O 31	0	0
56	BD	10	Total 10	O 10	0	0
56	BE	8	Total 8	O 8	0	0
56	BF	11	Total 11	O 11	0	0
56	BH	2	Total 2	O 2	0	0
56	BN	2	Total 2	O 2	0	0
56	BO	3	Total 3	O 3	0	0
56	BP	6	Total 6	O 6	0	0
56	BQ	2	Total 2	O 2	0	0
56	BR	6	Total 6	O 6	0	0
56	BT	1	Total 1	O 1	0	0
56	BU	2	Total 2	O 2	0	0
56	BV	2	Total 2	O 2	0	0
56	BW	4	Total 4	O 4	0	0
56	BX	2	Total 2	O 2	0	0
56	BY	1	Total 1	O 1	0	0
56	B0	4	Total 4	O 4	0	0
56	B3	1	Total 1	O 1	0	0
56	B4	1	Total 1	O 1	0	0
56	B5	3	Total 3	O 3	0	0
56	B7	3	Total 3	O 3	0	0

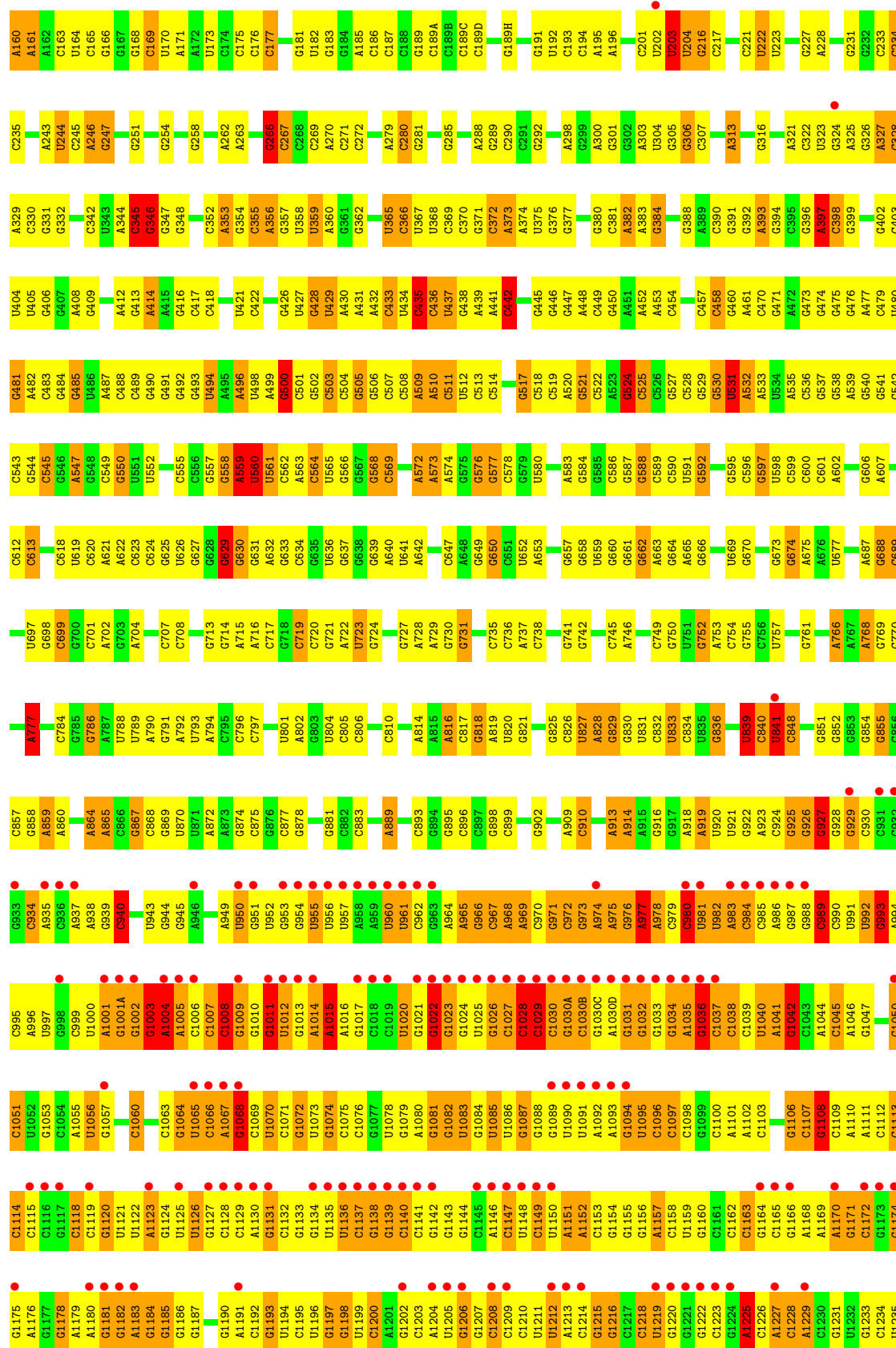
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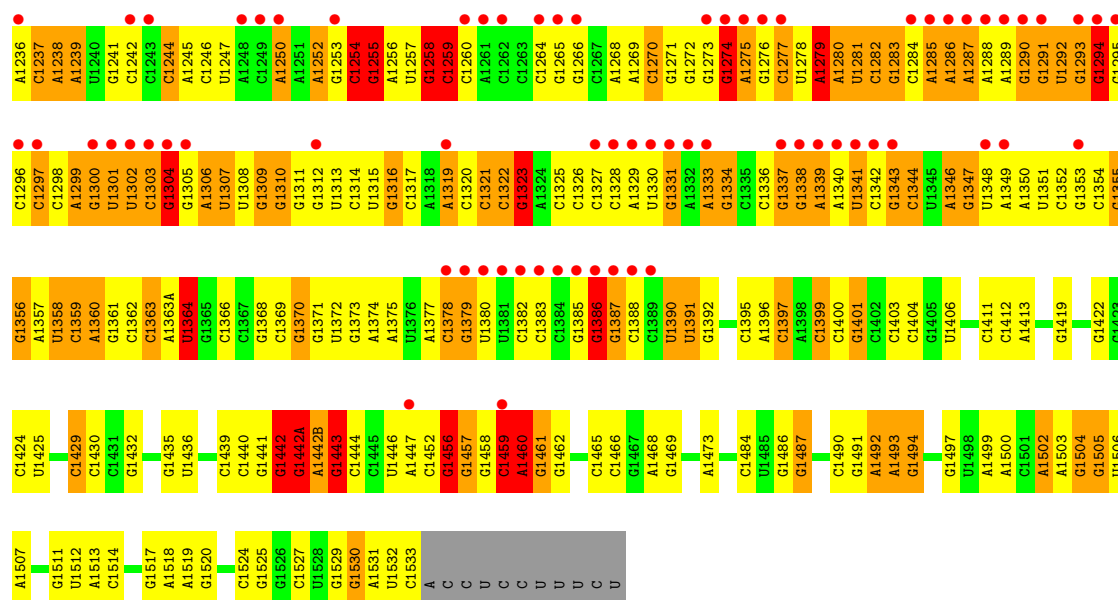
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B8	7	Total 7	O 7	0	0
56	B9	2	Total 2	O 2	0	0
56	CA	119	Total 119	O 119	0	0
56	CD	1	Total 1	O 1	0	0
56	CK	2	Total 2	O 2	0	0
56	CP	1	Total 1	O 1	0	0
56	CT	2	Total 2	O 2	0	0
56	DA	696	Total 696	O 696	0	0
56	DB	9	Total 9	O 9	0	0
56	DD	3	Total 3	O 3	0	0
56	DE	2	Total 2	O 2	0	0
56	DF	5	Total 5	O 5	0	0
56	DP	5	Total 5	O 5	0	0
56	DQ	2	Total 2	O 2	0	0
56	DR	1	Total 1	O 1	0	0
56	DV	1	Total 1	O 1	0	0
56	DX	1	Total 1	O 1	0	0
56	DY	1	Total 1	O 1	0	0
56	D0	1	Total 1	O 1	0	0
56	D1	2	Total 2	O 2	0	0

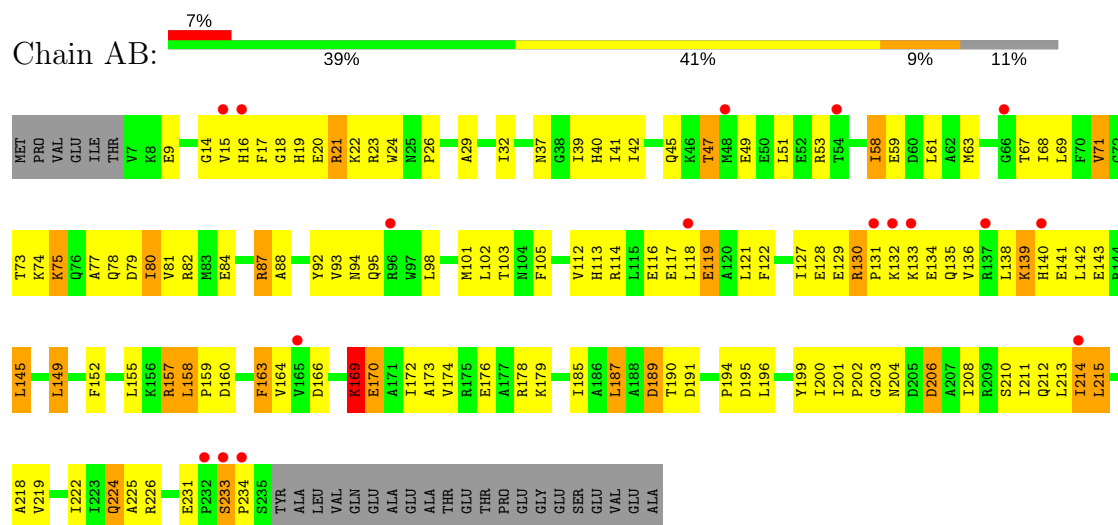




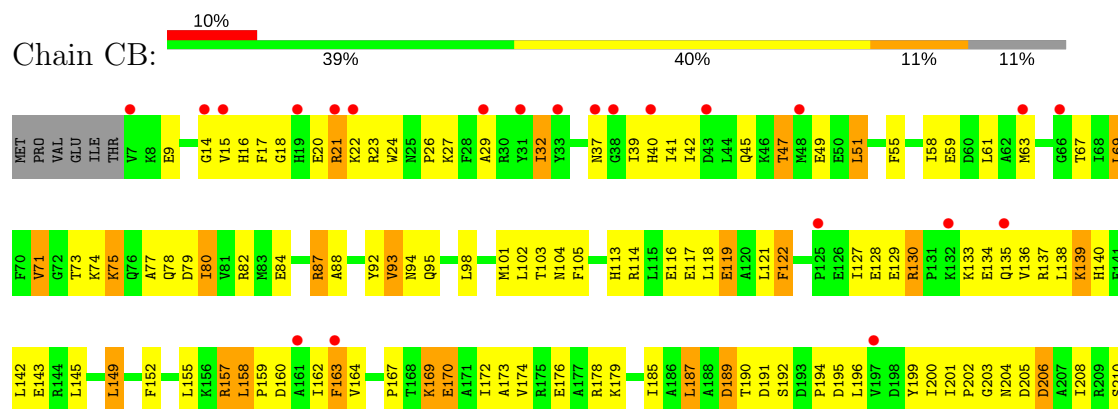


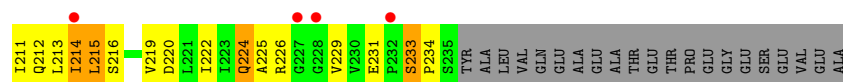


• Molecule 2: 30S Ribosomal Protein S2

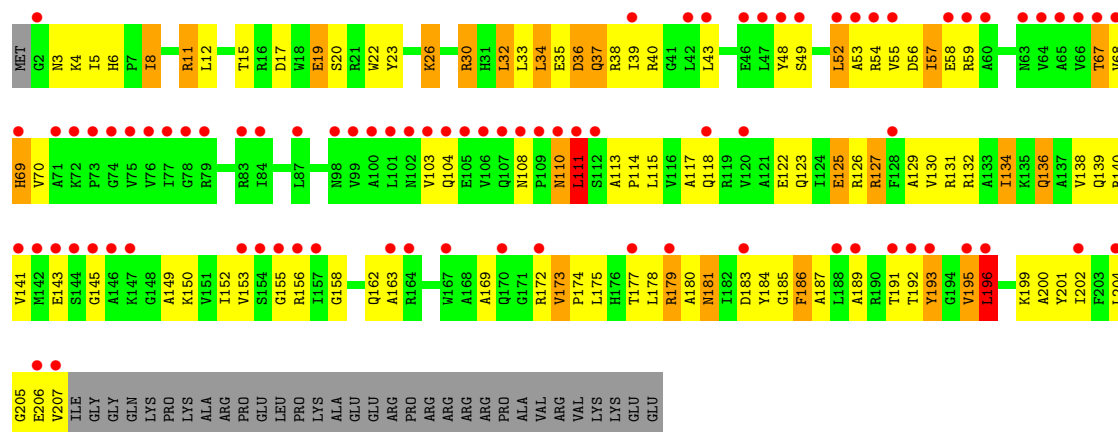


• Molecule 2: 30S Ribosomal Protein S2

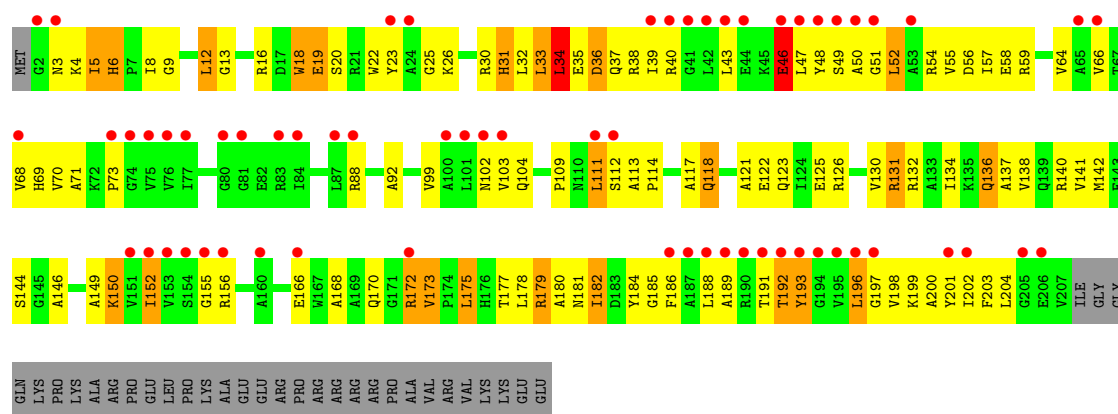
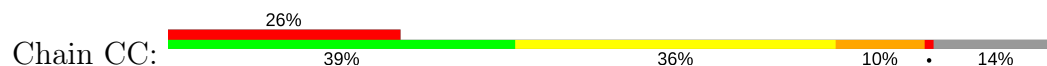




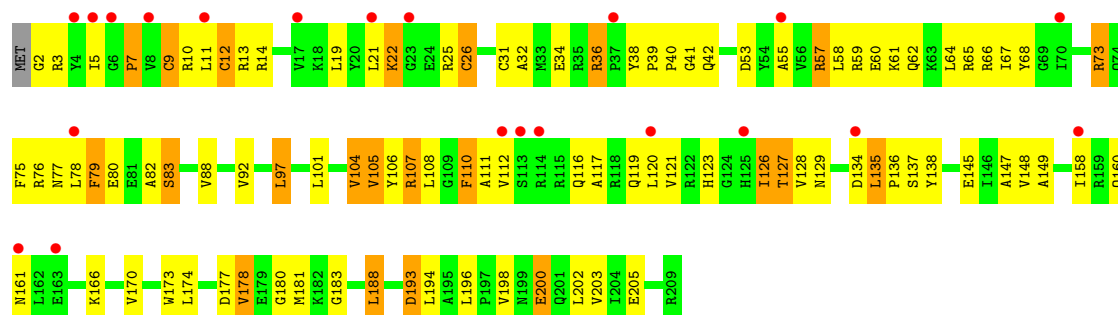
## ● Molecule 3: 30S Ribosomal Protein S3



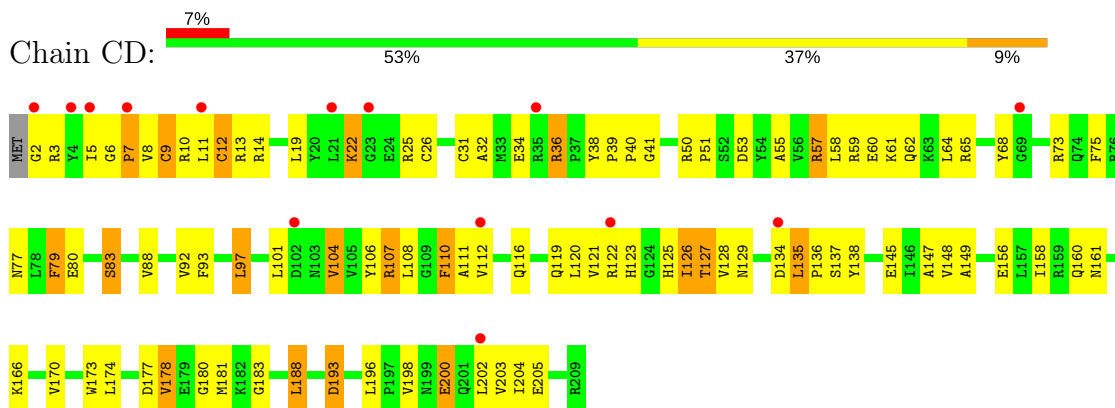
## ● Molecule 3: 30S Ribosomal Protein S3



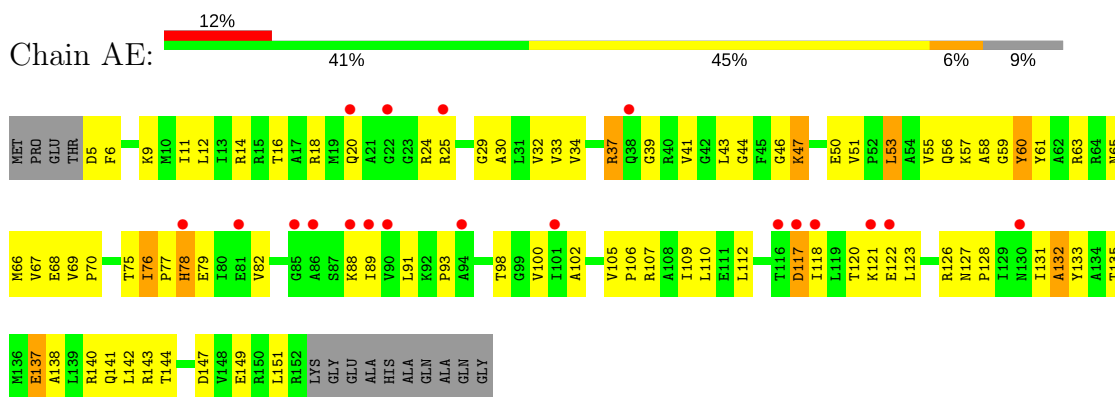
## ● Molecule 4: 30S Ribosomal Protein S4



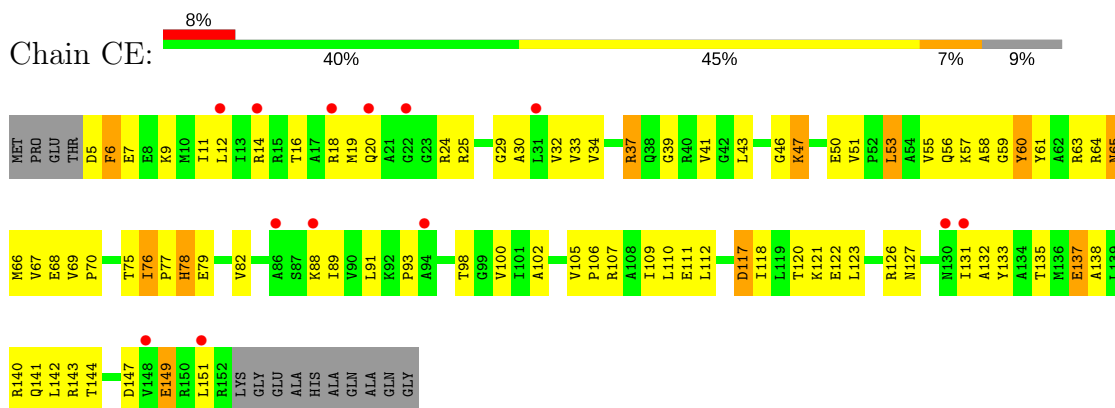
- Molecule 4: 30S Ribosomal Protein S4



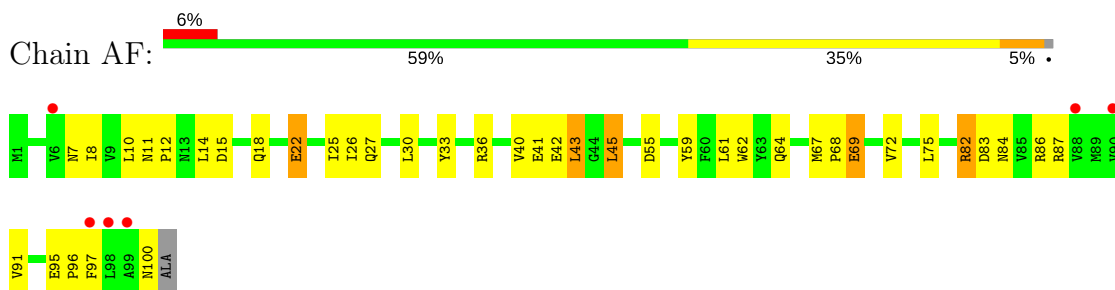
- Molecule 5: 30S Ribosomal Protein S5



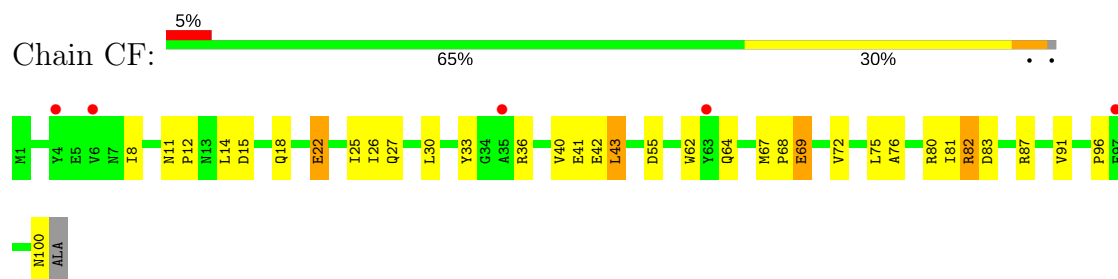
- Molecule 5: 30S Ribosomal Protein S5



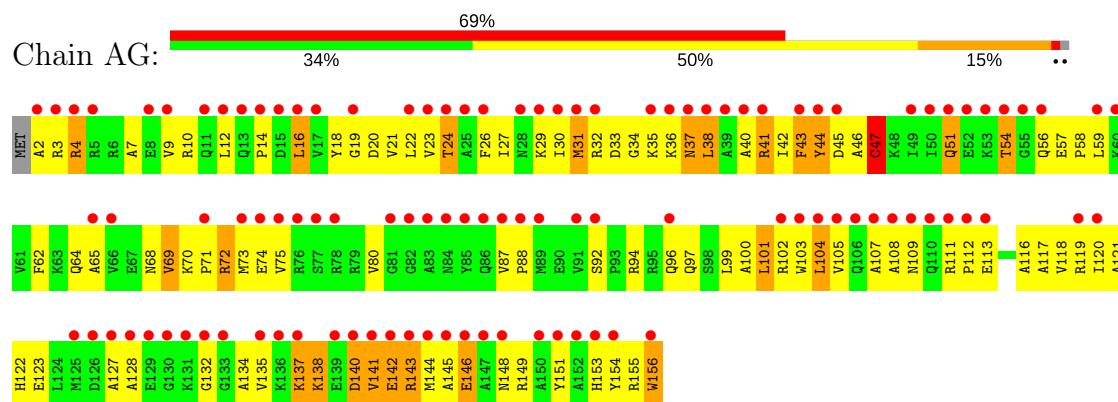
- Molecule 6: 30S Ribosomal Protein S6



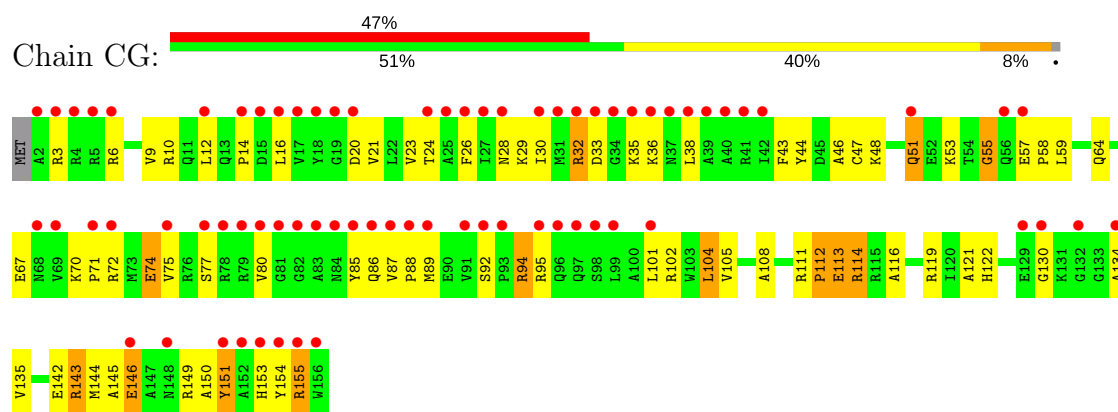
- Molecule 6: 30S Ribosomal Protein S6



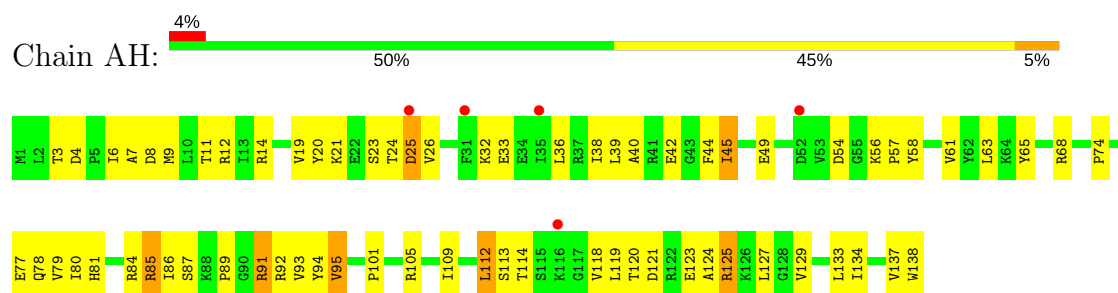
- Molecule 7: 30S Ribosomal Protein S7



- Molecule 7: 30S Ribosomal Protein S7

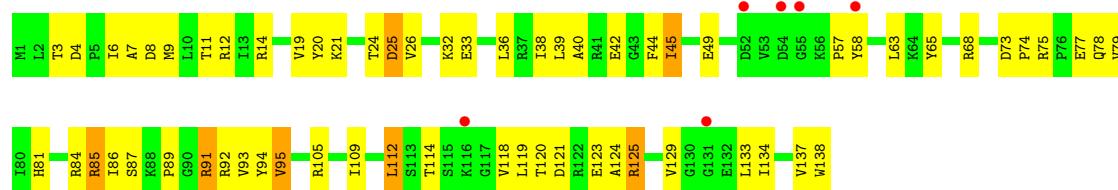


- Molecule 8: 30S Ribosomal Protein S8

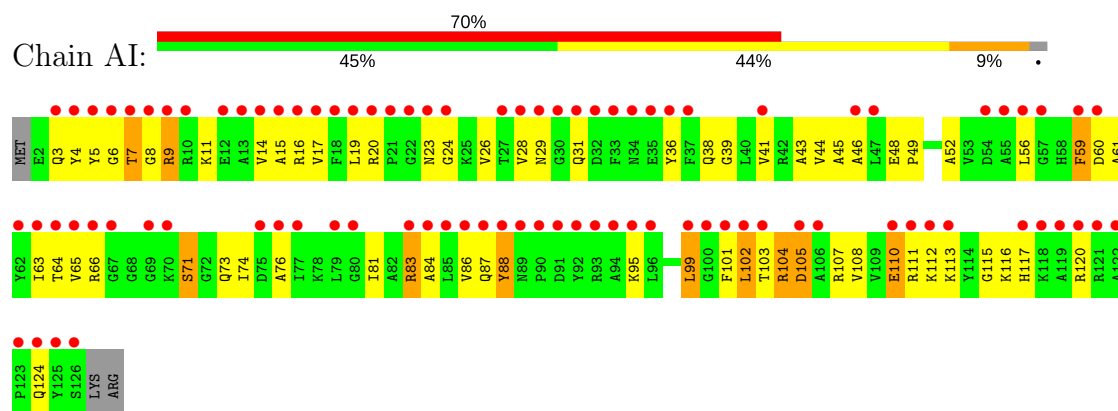


- Molecule 8: 30S Ribosomal Protein S8

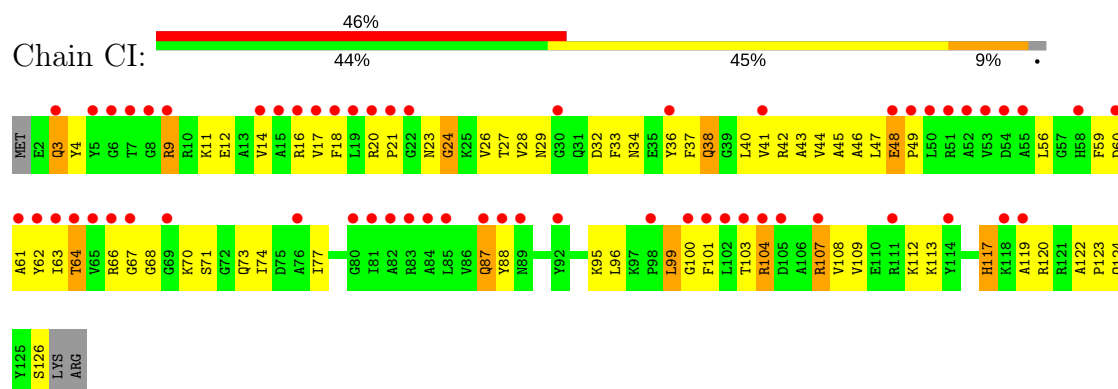




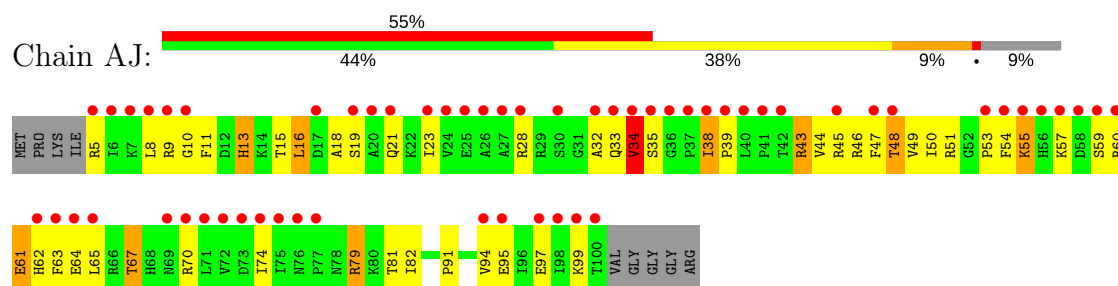
• Molecule 9: 30S Ribosomal Protein S9



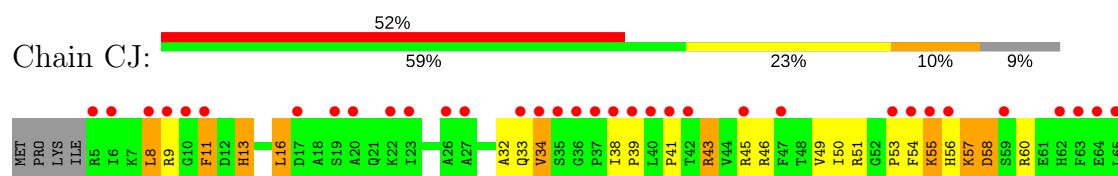
• Molecule 9: 30S Ribosomal Protein S9



• Molecule 10: 30S Ribosomal Protein S10



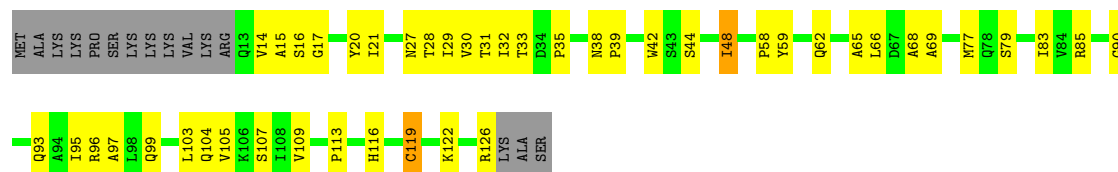
• Molecule 10: 30S Ribosomal Protein S10





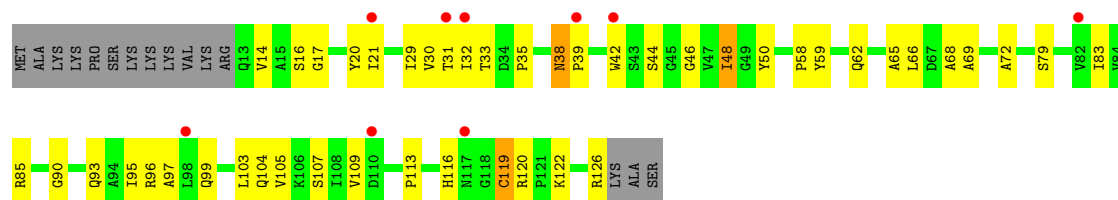
• Molecule 11: 30S Ribosomal Protein S11

Chain AK: 53% 34% 12%



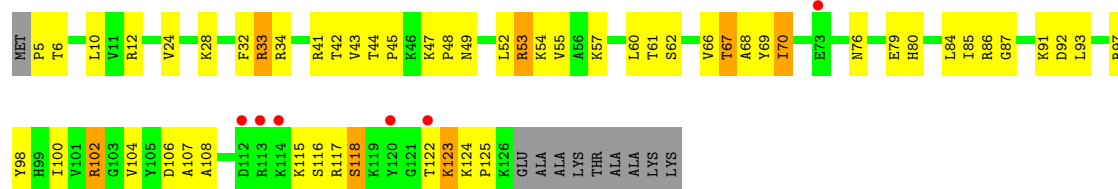
• Molecule 11: 30S Ribosomal Protein S11

Chain CK: 7% 53% 33% 12%



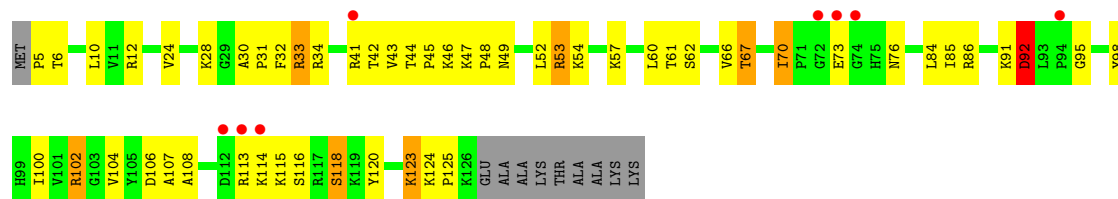
• Molecule 12: 30S Ribosomal Protein S12

Chain AL: 5% 50% 37% 5% 8%



• Molecule 12: 30S Ribosomal Protein S12

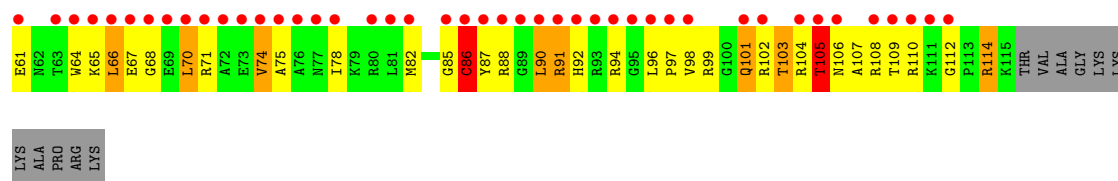
Chain CL: 6% 52% 35% 5% 8%



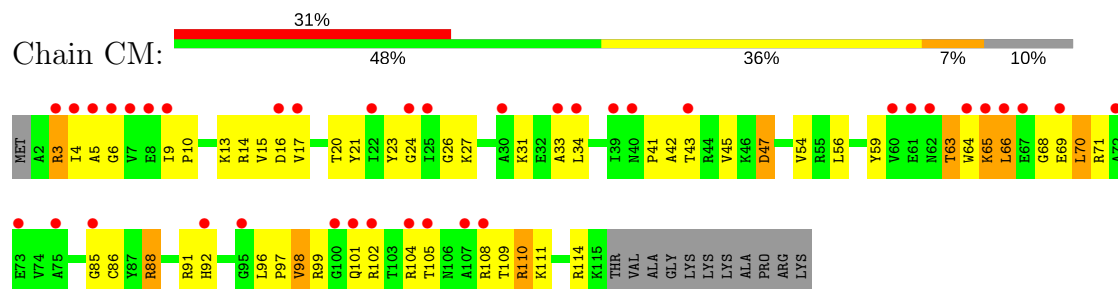
• Molecule 13: 30S Ribosomal Protein S13

Chain AM: 71% 40% 39% 10% 10%

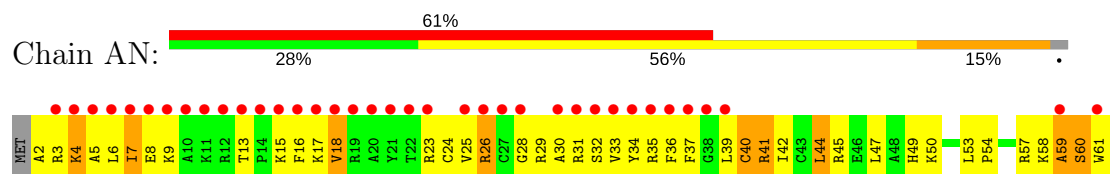




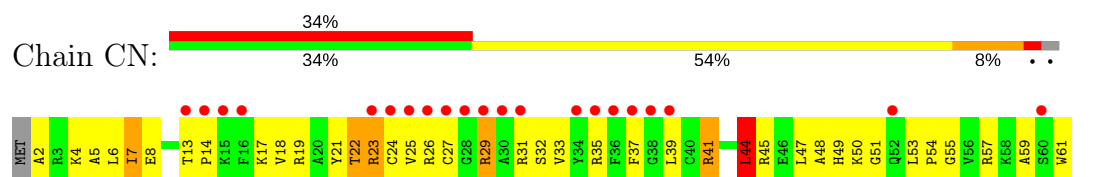
• Molecule 13: 30S Ribosomal Protein S13



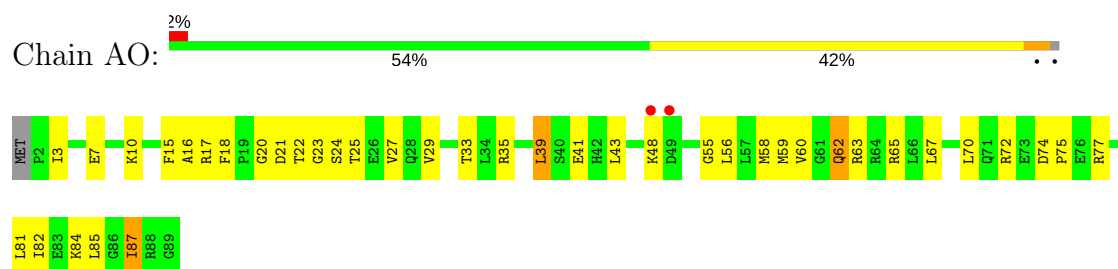
• Molecule 14: 30S Ribosomal Protein S14



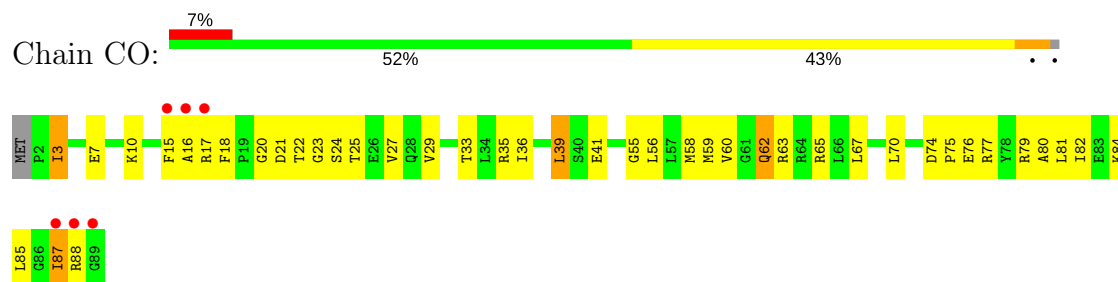
• Molecule 14: 30S Ribosomal Protein S14



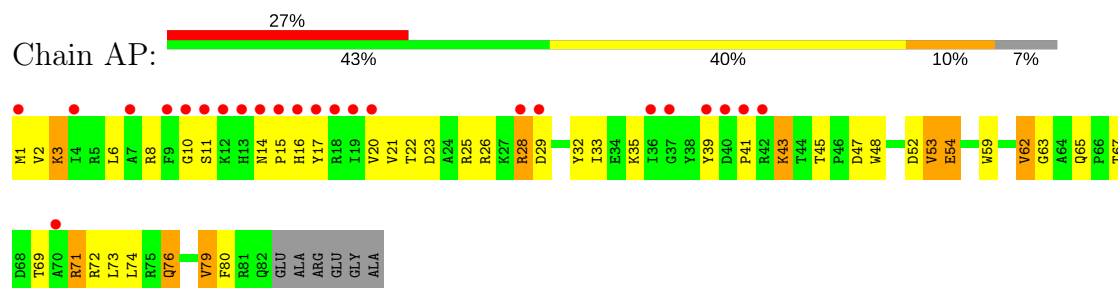
• Molecule 15: 30S Ribosomal Protein S15



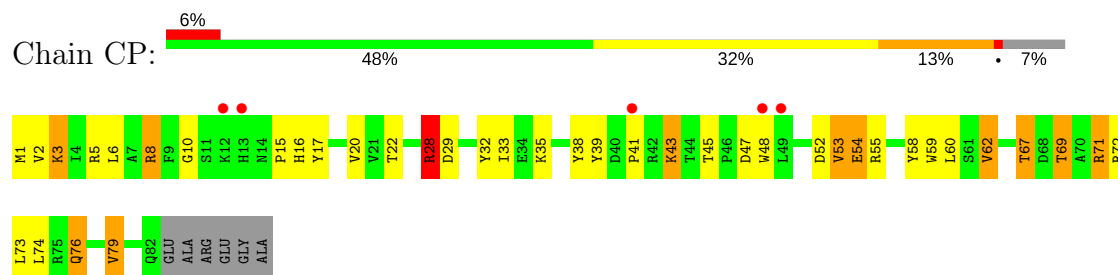
• Molecule 15: 30S Ribosomal Protein S15



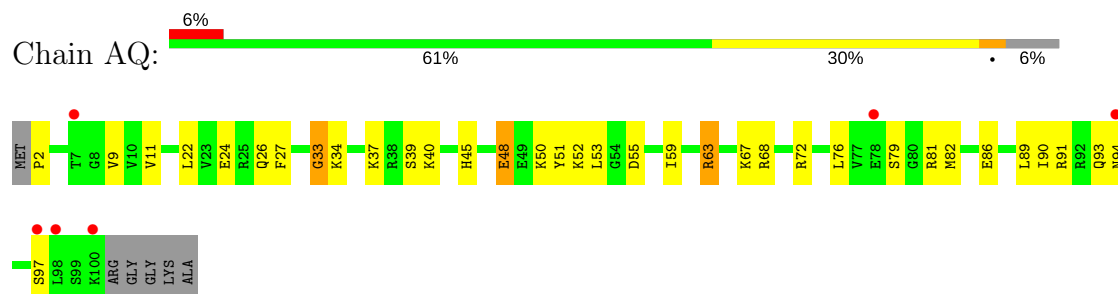
- Molecule 16: 30S Ribosomal Protein S16



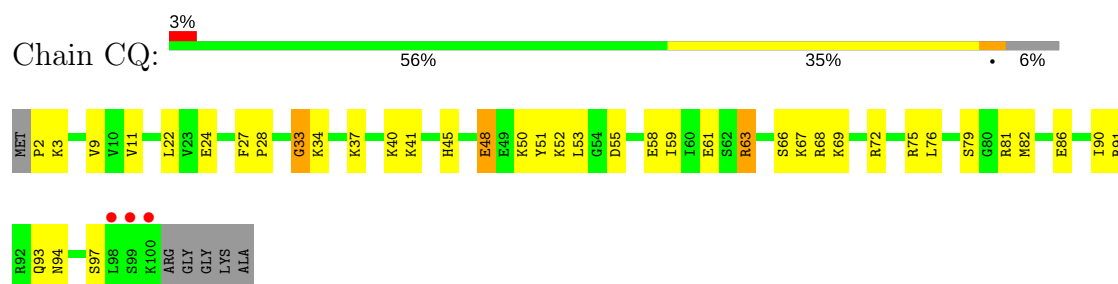
- Molecule 16: 30S Ribosomal Protein S16



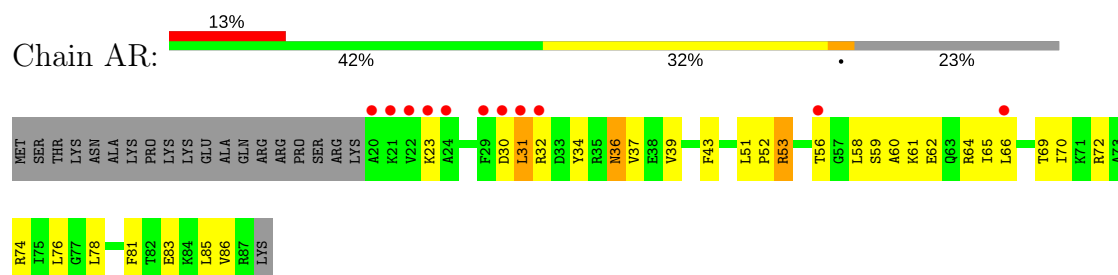
- Molecule 17: 30S Ribosomal Protein S17



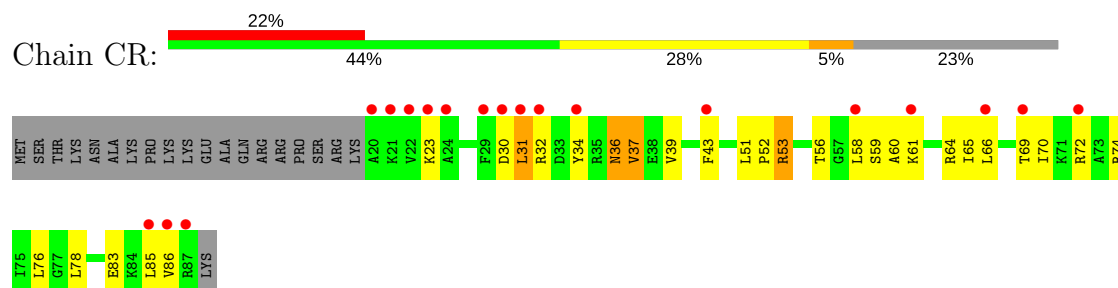
- Molecule 17: 30S Ribosomal Protein S17



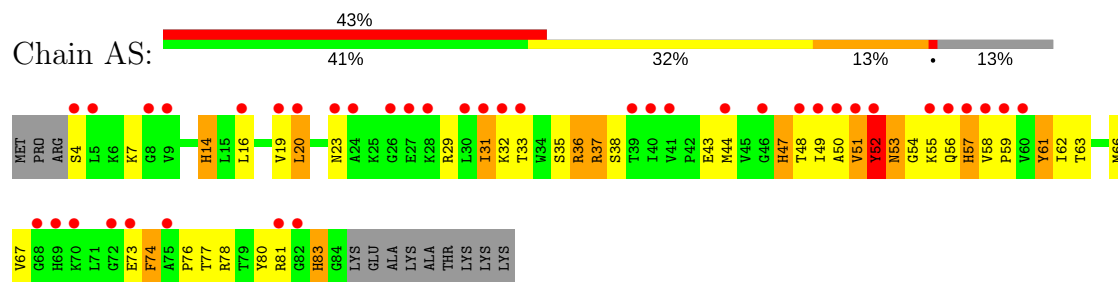
- Molecule 18: 30S Ribosomal Protein S18



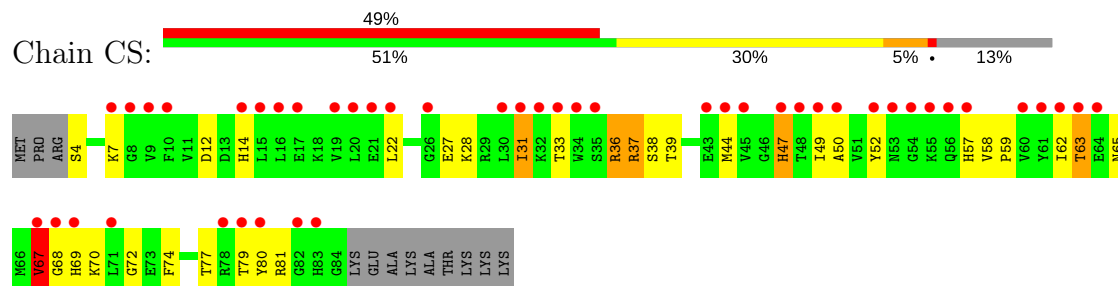
- Molecule 18: 30S Ribosomal Protein S18



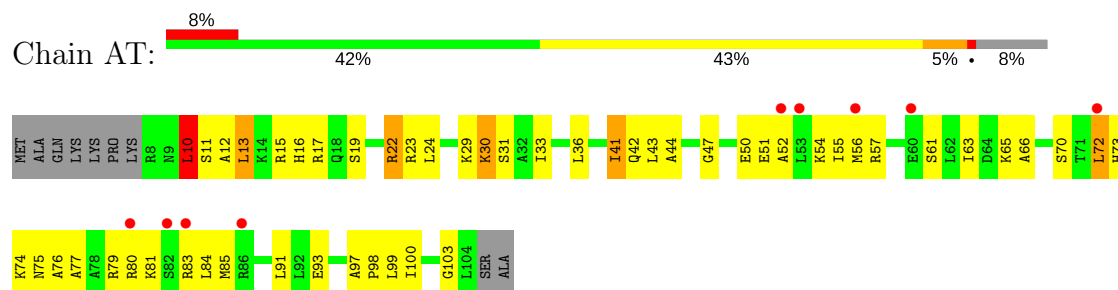
- Molecule 19: 30S Ribosomal Protein S19



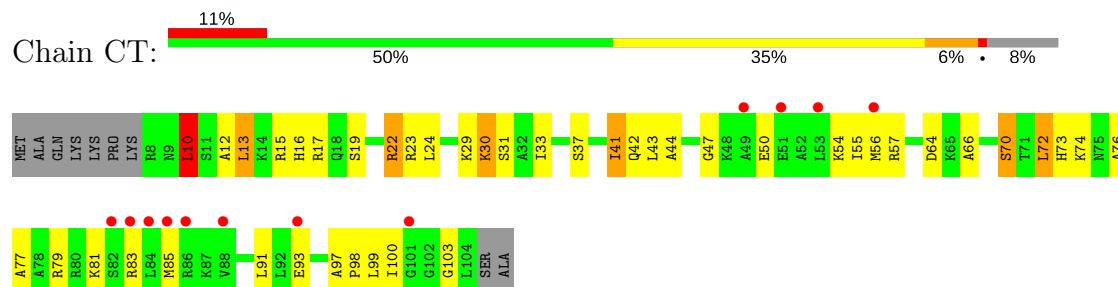
- Molecule 19: 30S Ribosomal Protein S19



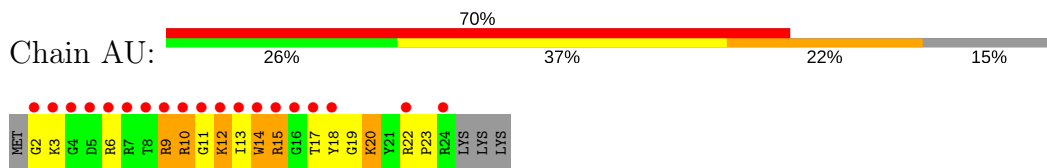
- Molecule 20: 30S Ribosomal Protein S20



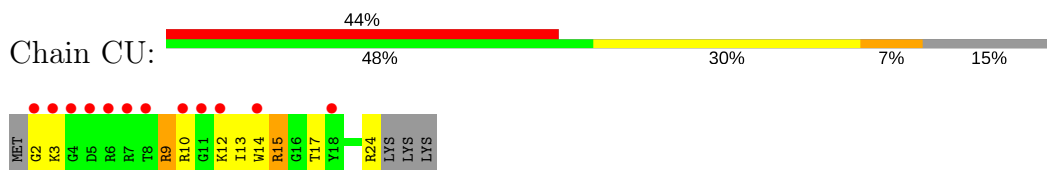
- Molecule 20: 30S Ribosomal Protein S20



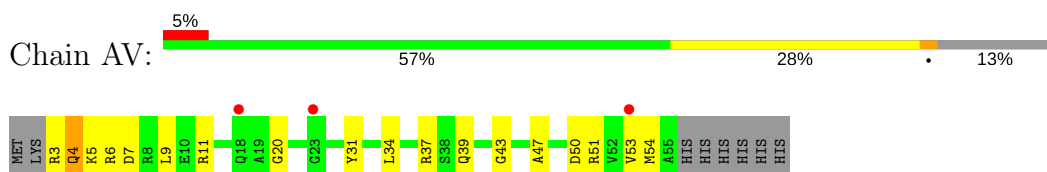
## ● Molecule 21: 30S Ribosomal Protein THX



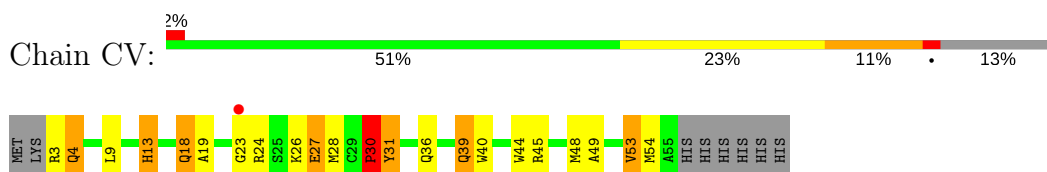
## ● Molecule 21: 30S Ribosomal Protein THX



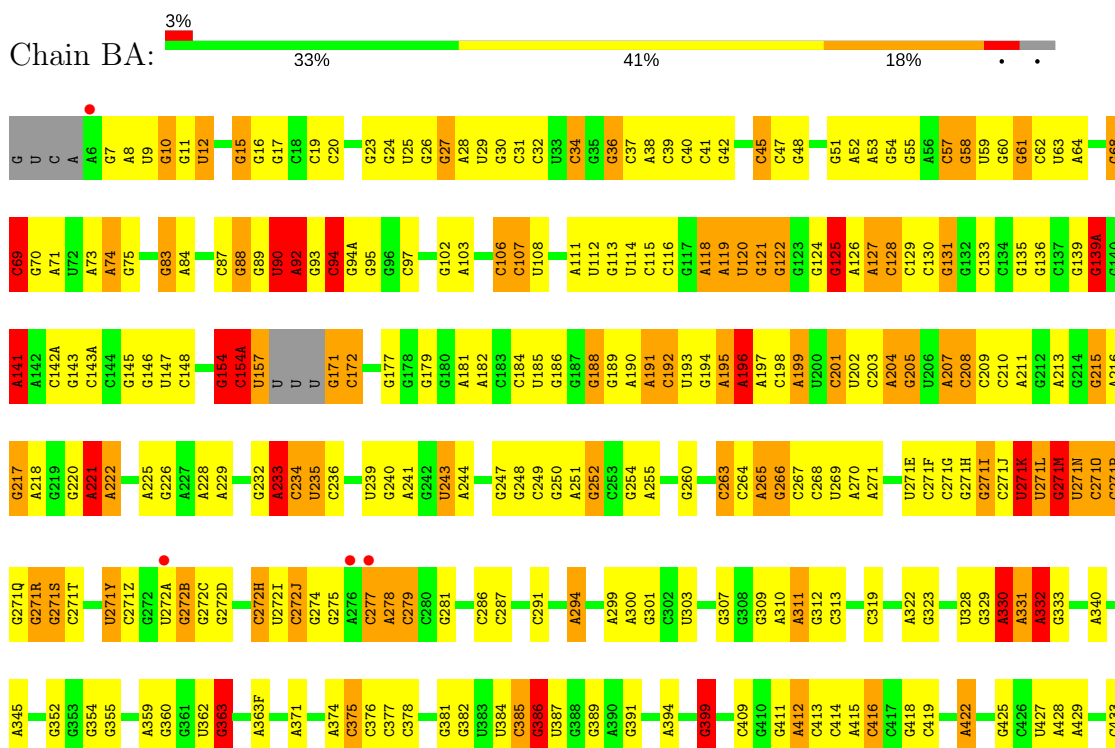
## ● Molecule 22: Ribosome modulation factor



## ● Molecule 22: Ribosome modulation factor



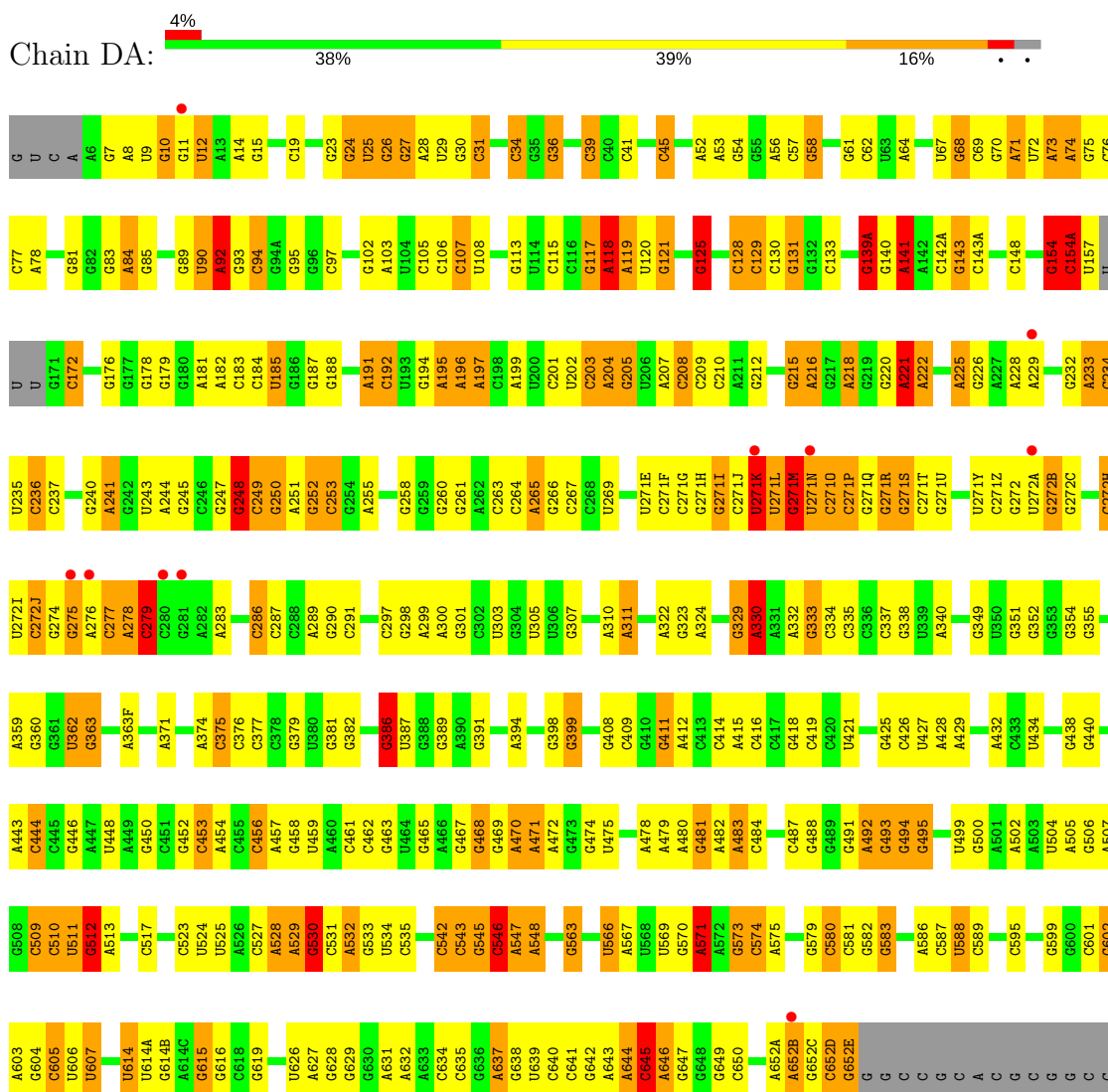
## ● Molecule 23: 23S Ribosomal RNA



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C1450A	G1380	U1165	G1239	A	C1038	A973	C902	G830	G646	C887	C646	C580	G508	C436
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G1459	G1382	G1311	A1241	C	C1040	G975	C904	G832	G648	A689	G648	G582	C510	A443
A1460	C1383	U1312	G1242	U	G1041	G975A	U905	U833	G649	G690	G650	G583	U511	C444
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C1467	G1385	A	G1244	A	C1043	G977	U907	A835	G651	C892	G651	C587	A513	G446
U1471	U1392	U	G1245	C	G1044	G978	A910	G836	G652	C893	G652	U588	A514	A447
A1472	A1393	U	A1246	C	A1045	G979	A911	C937	A652A	U694	A652A	C589	A515	U448
A1477	A1394	U	A1247	U	A1046	A980	C914	U839	G652C	C698	G652C	C590	G517	C450
A1479	A1395	U	G1248	G	G1047	A981	C915	G844	G652E	G700	G652E	C591	G518	C451
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G2578	G1633	G1708	U1799	A1891	C2044	G2104	G2164	G2238	A2305	G2367	A2439	G2505	G2578
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- Molecule 23: 23S Ribosomal RNA

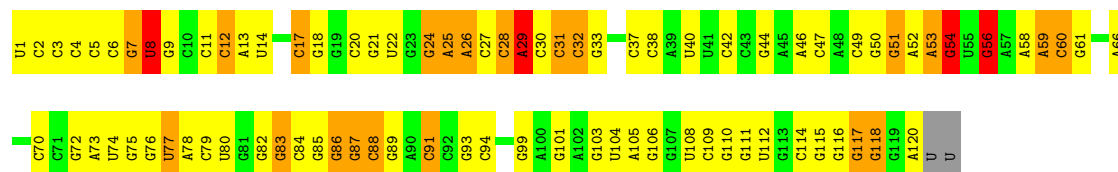
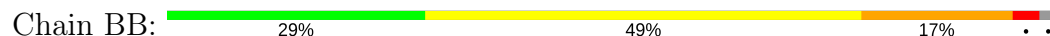




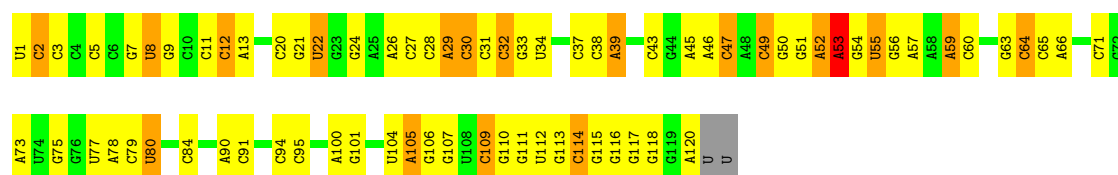
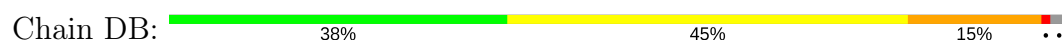
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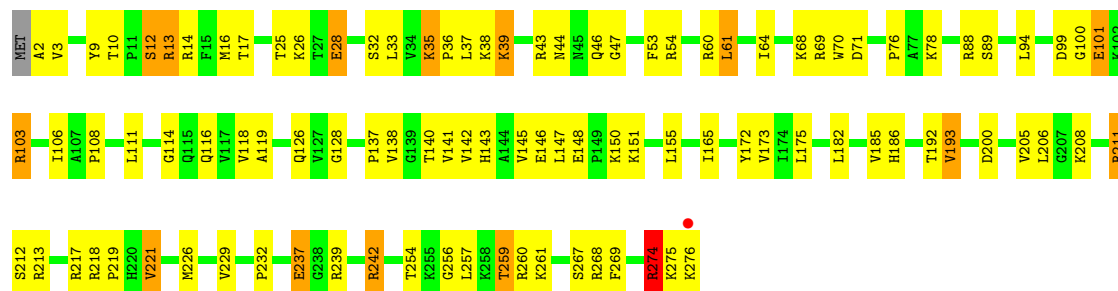
• Molecule 24: 5S Ribosomal RNA



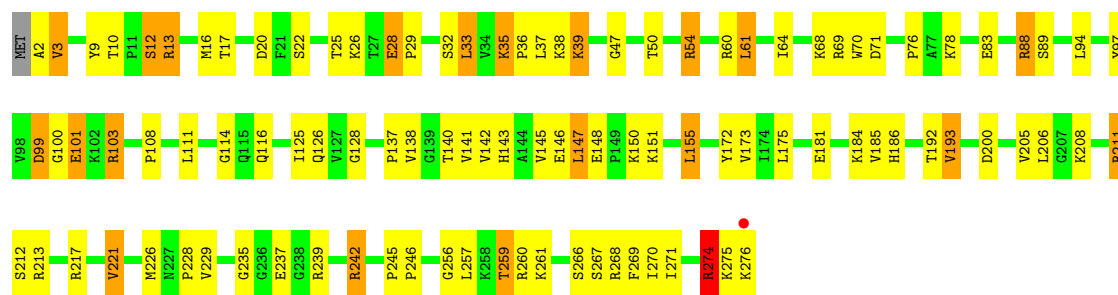
• Molecule 24: 5S Ribosomal RNA



• Molecule 25: 50S Ribosomal Protein L2

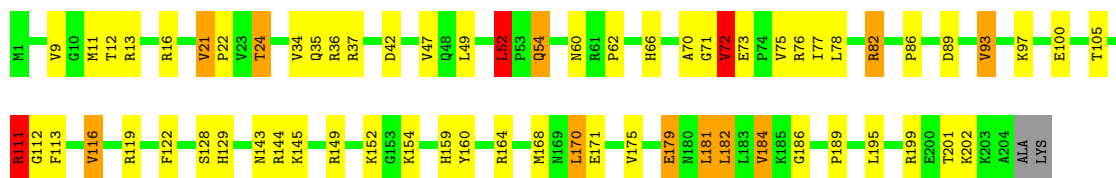


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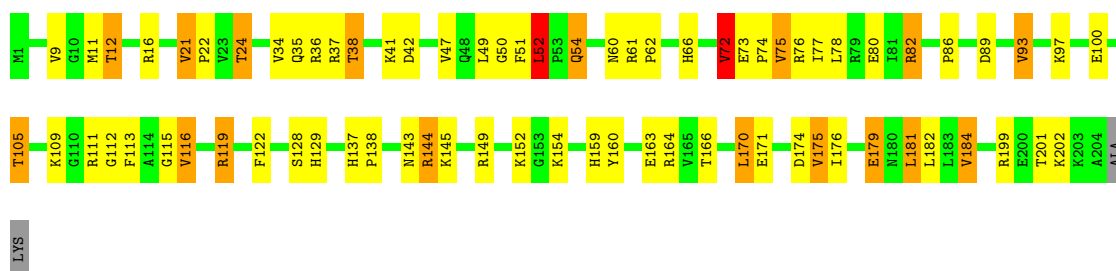
• Molecule 26: 50S Ribosomal Protein L3

Chain BE:  67% 25% 5% ..



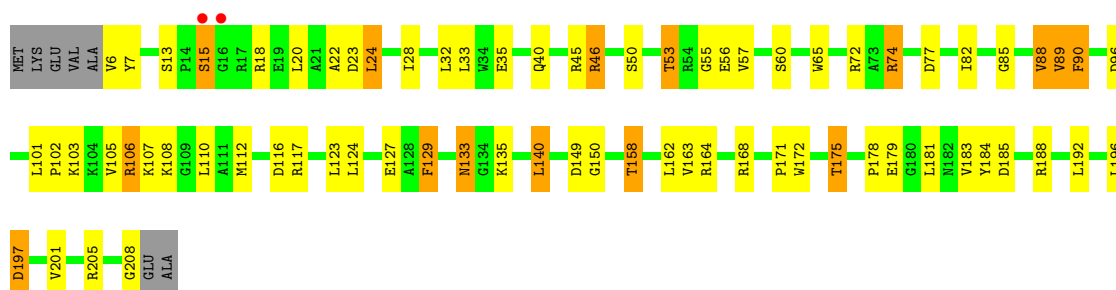
• Molecule 26: 50S Ribosomal Protein L3

Chain DE:  63% 27% 8% ..



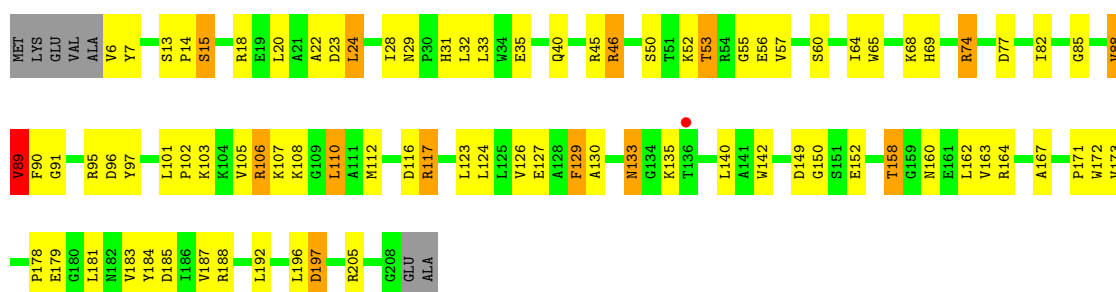
• Molecule 27: 50S Ribosomal Protein L4

Chain BF:  62% 28% 7% .



• Molecule 27: 50S Ribosomal Protein L4

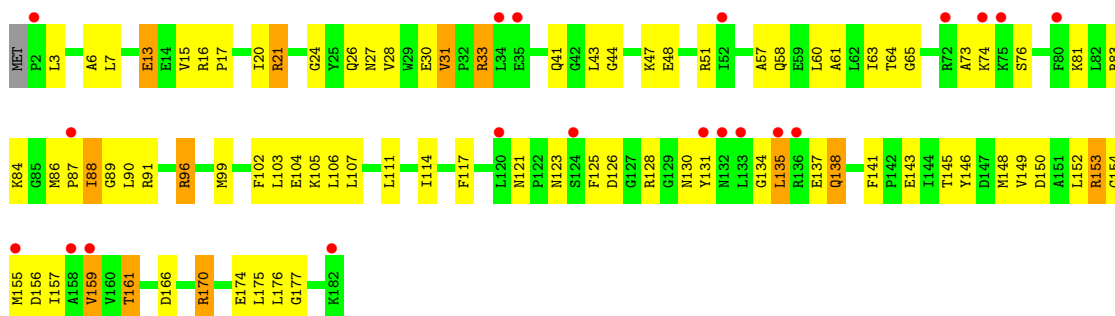
Chain DF:  56% 34% 6% .



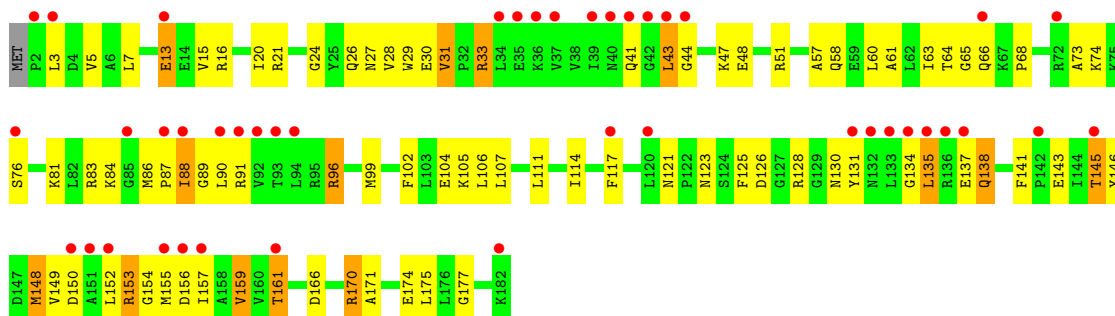
• Molecule 28: 50S Ribosomal Protein L5

Chain BG:  53% 40% 7% .

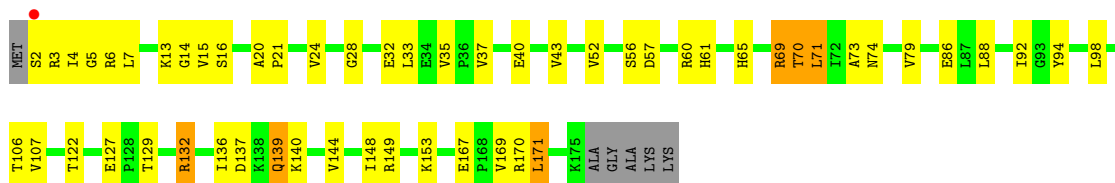




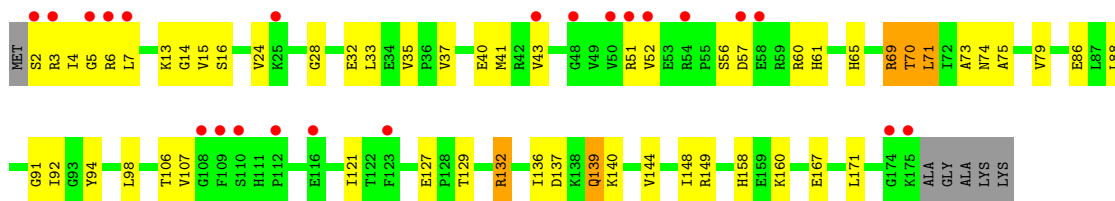
• Molecule 28: 50S Ribosomal Protein L5



• Molecule 29: 50S Ribosomal Protein L6



• Molecule 29: 50S Ribosomal Protein L6

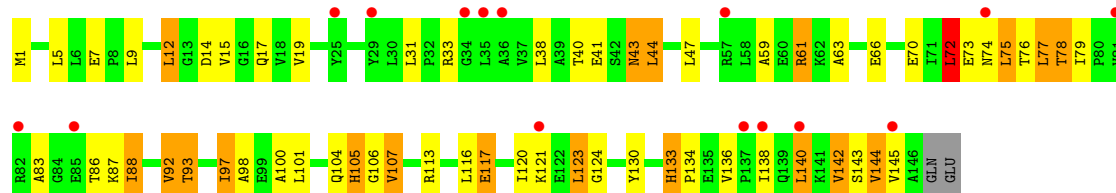


• Molecule 30: 50S Ribosomal Protein L9

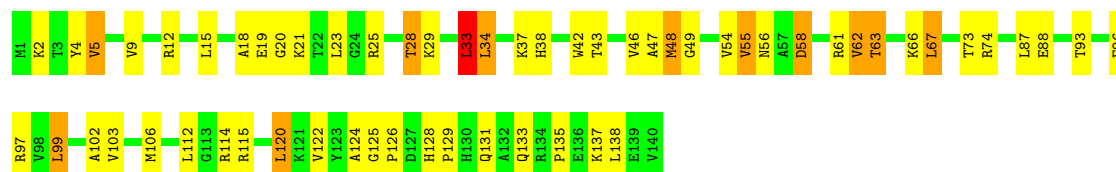




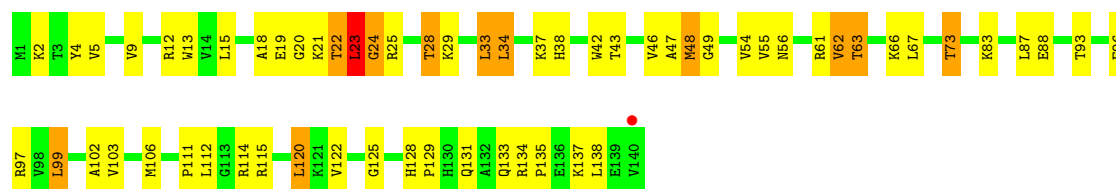
• Molecule 30: 50S Ribosomal Protein L9



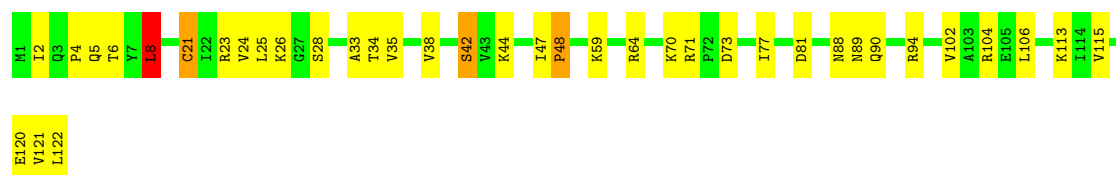
• Molecule 31: 50S Ribosomal Protein L13



• Molecule 31: 50S Ribosomal Protein L13



• Molecule 32: 50S Ribosomal Protein L14



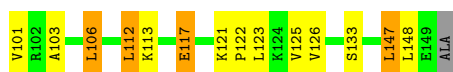
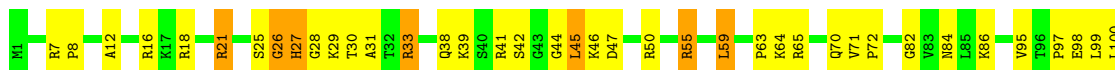
• Molecule 32: 50S Ribosomal Protein L14





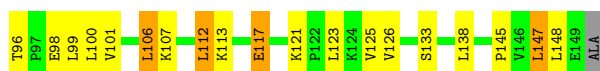
• Molecule 33: 50S Ribosomal Protein L15

Chain BP: 64% 28% 7%



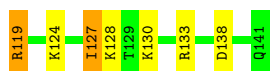
• Molecule 33: 50S Ribosomal Protein L15

Chain DP: 2% 64% 30% 5%



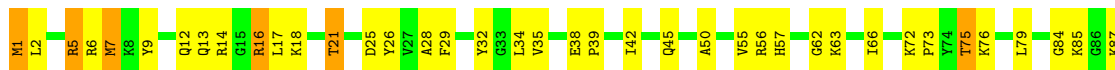
• Molecule 34: 50S Ribosomal Protein L16

Chain BQ: 69% 26% 5%



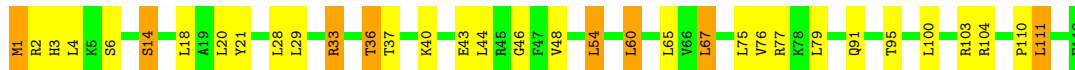
• Molecule 34: 50S Ribosomal Protein L16

Chain DQ: 58% 35% 6%



• Molecule 35: 50S Ribosomal Protein L17

Chain BR: 71% 22% 7%



• Molecule 35: 50S Ribosomal Protein L17

- Molecule 36: 50S Ribosomal Protein L18

- Molecule 36: 50S Ribosomal Protein L18

- Molecule 37: 50S Ribosomal Protein L19

- Molecule 37: 50S Ribosomal Protein L19

- Molecule 38: 50S Ribosomal Protein L20

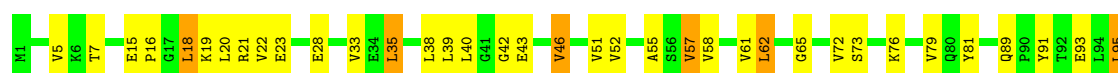




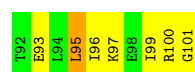
• Molecule 38: 50S Ribosomal Protein L20



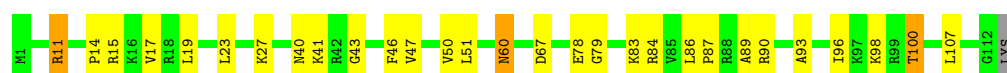
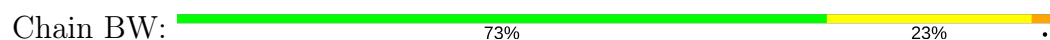
• Molecule 39: 50S Ribosomal Protein L21



• Molecule 39: 50S Ribosomal Protein L21



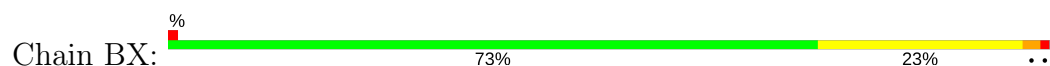
• Molecule 40: 50S Ribosomal Protein L22

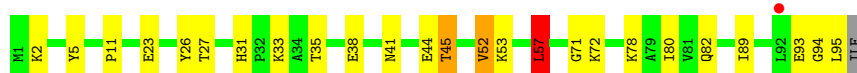


• Molecule 40: 50S Ribosomal Protein L22



• Molecule 41: 50S Ribosomal Protein L23





• Molecule 41: 50S Ribosomal Protein L23

Chain DX: 72% 25% ...



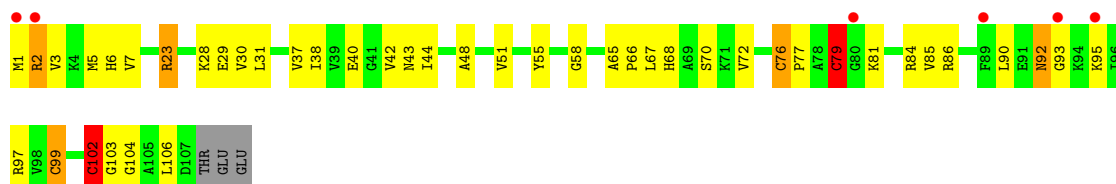
• Molecule 42: 50S Ribosomal Protein L24

Chain BY: 2% 54% 39% 5% .



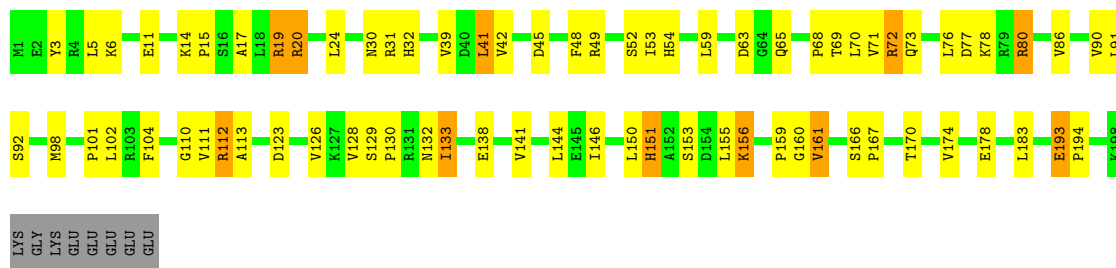
• Molecule 42: 50S Ribosomal Protein L24

Chain DY: 5% 57% 34% 5% . .



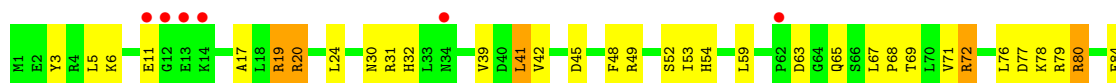
• Molecule 43: 50S Ribosomal Protein L25

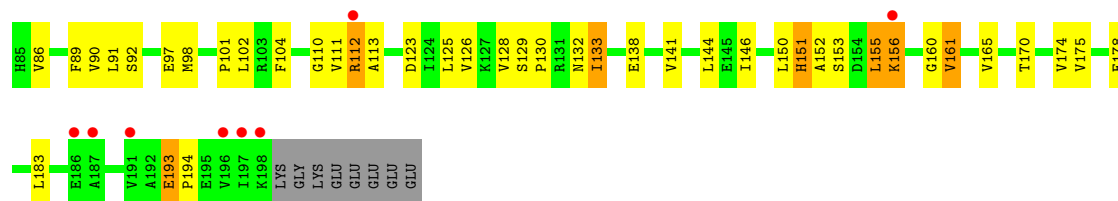
Chain BZ: 60% 31% 5% .



• Molecule 43: 50S Ribosomal Protein L25

Chain DZ: 7% 59% 31% 6% .





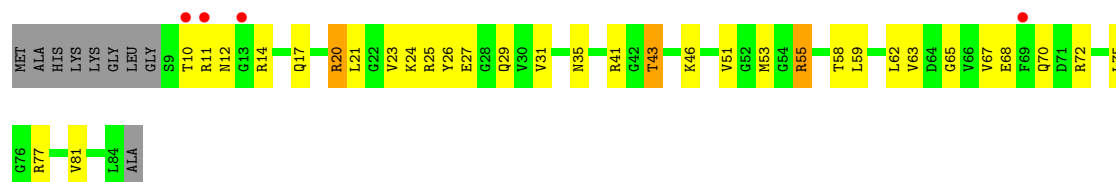
• Molecule 44: 50S Ribosomal Protein L27

Chain B0: 60% 26% 11%



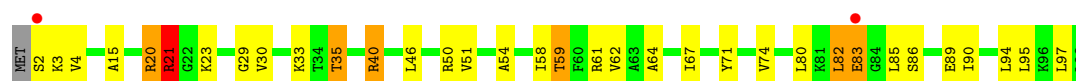
• Molecule 44: 50S Ribosomal Protein L27

Chain D0: 5% 51% 35% 11%



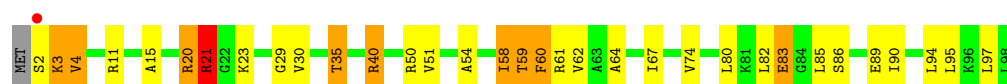
• Molecule 45: 50S Ribosomal Protein L28

Chain B1: 2% 64% 28% 6% ..



• Molecule 45: 50S Ribosomal Protein L28

Chain D1: % 65% 23% 9% ..



• Molecule 46: 50S Ribosomal Protein L29

Chain B2: 57% 38% ..



• Molecule 46: 50S Ribosomal Protein L29

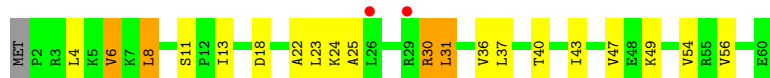
Chain D2: 4% 54% 39% ..




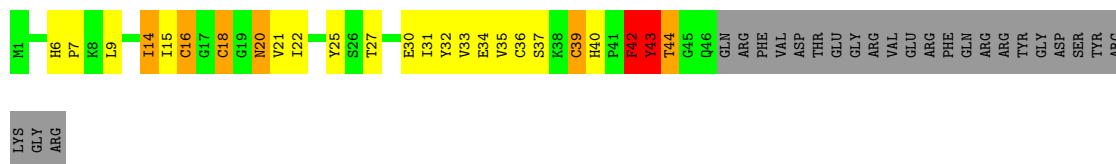
## • Molecule 47: 50S Ribosomal Protein L30

Chain B3:  72% 22% 5% .

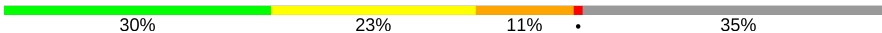
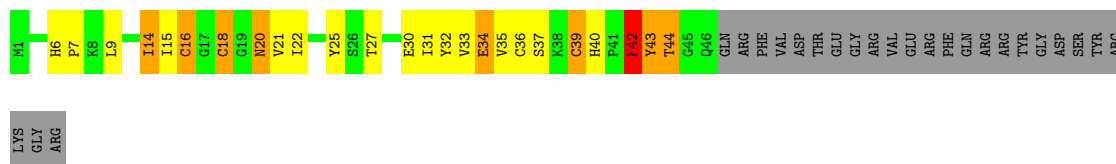
## • Molecule 47: 50S Ribosomal Protein L30

Chain D3:  3% 65% 27% 7% .

## • Molecule 48: 50S Ribosomal Protein L31

Chain B4:  30% 24% 8% 35%

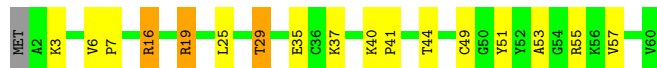
## • Molecule 48: 50S Ribosomal Protein L31

Chain D4:  30% 23% 11% 35%

## • Molecule 49: 50S Ribosomal Protein L32

Chain B5:  70% 25% . .

## • Molecule 49: 50S Ribosomal Protein L32

Chain D5:  70% 23% 5% .

## • Molecule 50: 50S Ribosomal Protein L33

Chain B6:  4% 46% 37% 15% .



• Molecule 50: 50S Ribosomal Protein L33



• Molecule 51: 50S Ribosomal Protein L34



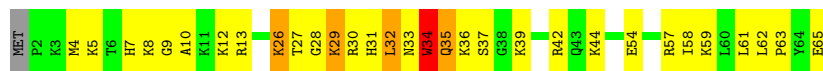
• Molecule 51: 50S Ribosomal Protein L34



• Molecule 52: 50S Ribosomal Protein L35



• Molecule 52: 50S Ribosomal Protein L35



• Molecule 53: 50S Ribosomal Protein L36



• Molecule 53: 50S Ribosomal Protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.24Å 451.44Å 621.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.00 49.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.75-3.00) 98.0 (49.75-3.00)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.218 , 0.254 0.218 , 0.253	Depositor DCC
$R_{free}$ test set	57194 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	68.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	283930	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	0.99	24/36215 (0.1%)	1.43	546/56522 (1.0%)
1	CA	0.91	21/36123 (0.1%)	1.38	452/56379 (0.8%)
2	AB	0.59	0/1809	0.73	1/2450 (0.0%)
2	CB	0.61	0/1809	0.73	1/2450 (0.0%)
3	AC	0.72	0/1474	0.82	2/2003 (0.1%)
3	CC	0.68	0/1474	0.79	2/2003 (0.1%)
4	AD	0.69	3/1556 (0.2%)	0.76	2/2113 (0.1%)
4	CD	0.64	2/1556 (0.1%)	0.74	2/2113 (0.1%)
5	AE	0.58	0/1121	0.79	0/1517
5	CE	0.58	0/1121	0.78	1/1517 (0.1%)
6	AF	0.55	0/790	0.71	0/1077
6	CF	0.54	0/790	0.70	0/1077
7	AG	0.83	0/1183	0.89	1/1599 (0.1%)
7	CG	0.72	0/1183	0.77	0/1599
8	AH	0.51	0/1065	0.67	0/1445
8	CH	0.50	0/1065	0.67	0/1445
9	AI	0.84	0/867	0.84	0/1180
9	CI	0.74	0/867	0.84	1/1180 (0.1%)
10	AJ	0.78	0/676	0.86	0/924
10	CJ	0.75	0/676	0.88	2/924 (0.2%)
11	AK	0.51	0/843	0.71	0/1144
11	CK	0.53	0/843	0.69	0/1144
12	AL	0.56	0/921	0.74	0/1247
12	CL	0.54	0/921	0.73	0/1247
13	AM	0.92	0/814	0.92	2/1107 (0.2%)
13	CM	0.72	0/814	0.83	0/1107
14	AN	0.79	0/487	0.93	0/649
14	CN	0.66	0/487	0.71	1/649 (0.2%)
15	AO	0.52	0/735	0.72	0/981
15	CO	0.52	0/735	0.72	0/981
16	AP	0.56	0/667	0.82	0/905
16	CP	0.54	0/667	0.84	1/905 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.56	0/836	0.72	0/1117
17	CQ	0.57	0/836	0.72	0/1117
18	AR	0.54	0/519	0.79	0/699
18	CR	0.56	0/519	0.79	0/699
19	AS	0.92	0/574	0.92	0/781
19	CS	0.69	0/574	0.81	0/781
20	AT	0.54	0/715	0.78	0/947
20	CT	0.52	0/715	0.77	0/947
21	AU	0.78	0/203	0.77	0/266
21	CU	0.73	0/203	0.68	0/266
22	AV	0.63	0/339	0.75	0/464
22	CV	0.65	0/360	0.85	1/492 (0.2%)
23	BA	1.60	727/67771 (1.1%)	1.72	2179/105789 (2.1%)
23	DA	1.16	149/67893 (0.2%)	1.60	1664/105982 (1.6%)
24	BB	1.11	3/2878 (0.1%)	1.57	62/4490 (1.4%)
24	DB	0.97	4/2878 (0.1%)	1.46	37/4490 (0.8%)
25	BD	0.88	3/2186 (0.1%)	0.96	0/2944
25	DD	0.80	2/2186 (0.1%)	0.91	1/2944 (0.0%)
26	BE	0.89	0/1588	0.96	3/2145 (0.1%)
26	DE	0.75	0/1588	0.92	0/2145
27	BF	0.88	1/1615 (0.1%)	0.86	0/2188
27	DF	0.70	0/1615	0.90	2/2188 (0.1%)
28	BG	0.53	0/1393	0.71	0/1892
28	DG	0.59	0/1393	0.71	0/1892
29	BH	0.68	0/1343	0.80	3/1820 (0.2%)
29	DH	0.60	0/1343	0.77	2/1820 (0.1%)
30	BI	0.64	0/1055	0.83	0/1445
30	DI	0.65	0/1053	0.84	1/1442 (0.1%)
31	BN	0.86	0/1139	0.87	2/1538 (0.1%)
31	DN	0.65	0/1139	0.87	1/1538 (0.1%)
32	BO	0.79	1/933 (0.1%)	0.86	1/1257 (0.1%)
32	DO	0.70	0/933	0.86	1/1257 (0.1%)
33	BP	0.80	0/1148	0.93	1/1529 (0.1%)
33	DP	0.67	0/1148	0.93	2/1529 (0.1%)
34	BQ	0.79	0/1143	0.89	0/1527
34	DQ	0.70	0/1143	0.86	0/1527
35	BR	0.82	0/982	0.94	2/1312 (0.2%)
35	DR	0.74	0/982	0.93	2/1312 (0.2%)
36	BS	0.65	0/875	0.88	0/1168
36	DS	0.66	0/875	0.84	0/1168
37	BT	0.74	0/1077	0.87	0/1444
37	DT	0.66	0/1077	0.85	0/1444
38	BU	1.02	0/977	0.89	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DU	0.79	0/977	0.88	0/1301
39	BV	0.89	0/771	0.84	0/1037
39	DV	0.70	0/782	0.84	1/1049 (0.1%)
40	BW	1.04	0/891	0.99	2/1197 (0.2%)
40	DW	0.87	0/891	0.91	0/1197
41	BX	0.87	0/756	0.88	1/1016 (0.1%)
41	DX	0.78	0/756	0.84	1/1016 (0.1%)
42	BY	0.81	0/798	0.88	0/1073
42	DY	0.72	1/798 (0.1%)	0.87	1/1073 (0.1%)
43	BZ	0.62	0/1555	0.82	1/2118 (0.0%)
43	DZ	0.63	0/1555	0.80	1/2118 (0.0%)
44	B0	0.83	0/602	0.86	0/804
44	D0	0.73	0/602	0.81	0/804
45	B1	0.80	0/752	1.00	3/1003 (0.3%)
45	D1	0.77	0/752	0.99	2/1003 (0.2%)
46	B2	0.81	0/590	0.82	0/781
46	D2	0.71	0/590	0.83	0/781
47	B3	0.79	0/463	0.86	1/623 (0.2%)
47	D3	0.64	0/463	0.82	0/623
48	B4	0.64	0/358	0.82	1/487 (0.2%)
48	D4	0.70	0/358	0.82	1/487 (0.2%)
49	B5	1.01	0/469	0.99	1/634 (0.2%)
49	D5	0.75	0/469	0.95	1/634 (0.2%)
50	B6	0.84	1/456 (0.2%)	0.86	0/609
50	D6	0.92	2/456 (0.4%)	0.89	2/609 (0.3%)
51	B7	1.07	0/426	1.16	2/561 (0.4%)
51	D7	0.92	0/426	1.00	0/561
52	B8	0.88	0/516	1.00	2/679 (0.3%)
52	D8	0.73	1/516 (0.2%)	0.92	1/679 (0.1%)
53	B9	0.85	0/300	0.91	0/395
53	D9	0.68	0/300	0.83	0/395
All	All	1.12	945/304490 (0.3%)	1.42	5009/455973 (1.1%)

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	3
2	CB	0	3
3	AC	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	CC	0	2
5	CE	0	1
7	AG	0	4
7	CG	0	1
9	AI	0	2
9	CI	0	1
10	AJ	0	3
12	AL	0	1
12	CL	0	1
13	AM	0	3
13	CM	0	1
14	AN	0	3
17	AQ	0	1
17	CQ	0	1
19	AS	0	1
20	AT	0	2
20	CT	0	1
22	CV	0	3
25	BD	0	1
25	DD	0	1
26	BE	0	2
26	DE	0	1
27	BF	0	2
27	DF	0	3
28	BG	0	1
28	DG	0	1
30	BI	0	1
30	DI	0	1
31	BN	0	1
31	DN	0	2
32	BO	0	1
32	DO	0	1
33	BP	0	4
33	DP	0	2
36	BS	0	2
36	DS	0	1
37	BT	0	1
37	DT	0	1
41	BX	0	1
41	DX	0	1
42	BY	0	1
42	DY	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	BZ	0	1
45	B1	0	1
45	D1	0	1
48	B4	0	3
48	D4	0	2
52	D8	0	2
All	All	0	83

The worst 5 of 945 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1459	C	N1-C2	17.17	1.57	1.40
1	AA	1459	C	N1-C2	16.97	1.57	1.40
1	AA	1442(A)	G	N9-C4	16.14	1.50	1.38
1	CA	1442(A)	G	N9-C4	15.91	1.50	1.38
23	DA	528	A	N9-C4	-14.88	1.28	1.37

The worst 5 of 5009 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1442(A)	G	N3-C4-C5	-27.29	114.95	128.60
1	CA	1459	C	N3-C2-O2	-27.00	103.00	121.90
1	AA	1442(A)	G	N3-C4-C5	-26.82	115.19	128.60
1	CA	1459	C	C6-N1-C2	-26.34	109.77	120.30
1	AA	1459	C	N3-C2-O2	-25.91	103.77	121.90

There are no chirality outliers.

5 of 83 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	128	GLU	Peptide
2	AB	14	GLY	Peptide
2	AB	71	VAL	Peptide
3	AC	186	PHE	Peptide
7	AG	19	GLY	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	32353	0	16329	1267	0
1	CA	32270	0	16287	987	1
2	AB	1775	0	1743	99	0
2	CB	1775	0	1743	93	0
3	AC	1450	0	1314	80	0
3	CC	1450	0	1314	99	0
4	AD	1526	0	1417	79	0
4	CD	1526	0	1415	91	0
5	AE	1105	0	1130	55	0
5	CE	1105	0	1130	60	0
6	AF	777	0	737	26	0
6	CF	777	0	737	24	0
7	AG	1164	0	1106	100	0
7	CG	1164	0	1106	54	0
8	AH	1045	0	1033	52	0
8	CH	1045	0	1033	52	0
9	AI	852	0	742	69	0
9	CI	852	0	742	62	0
10	AJ	663	0	558	56	0
10	CJ	663	0	558	30	0
11	AK	828	0	822	28	0
11	CK	828	0	822	31	0
12	AL	905	0	916	44	0
12	CL	905	0	916	44	0
13	AM	804	0	752	62	0
13	CM	804	0	752	48	0
14	AN	478	0	497	50	0
14	CN	478	0	497	35	0
15	AO	724	0	749	25	0
15	CO	724	0	749	29	0
16	AP	651	0	638	33	0
16	CP	651	0	638	35	0
17	AQ	823	0	891	16	0
17	CQ	823	0	891	18	0
18	AR	514	0	530	24	0
18	CR	514	0	530	24	0
19	AS	560	0	466	41	0
19	CS	560	0	466	23	0
20	AT	713	0	766	36	0
20	CT	713	0	766	30	0
21	AU	199	0	208	26	0
21	CU	199	0	208	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AV	333	0	235	14	0
22	CV	353	0	266	13	0
23	BA	60512	0	30492	877	0
23	DA	60620	0	30560	944	0
24	BB	2573	0	1304	45	0
24	DB	2573	0	1304	52	0
25	BD	2136	0	2218	67	0
25	DD	2136	0	2218	68	0
26	BE	1555	0	1607	39	0
26	DE	1555	0	1607	52	0
27	BF	1580	0	1621	51	0
27	DF	1580	0	1621	65	0
28	BG	1368	0	1324	51	0
28	DG	1368	0	1324	56	0
29	BH	1317	0	1376	30	0
29	DH	1317	0	1376	31	0
30	BI	1040	0	1045	55	1
30	DI	1038	0	1040	38	0
31	BN	1112	0	1180	37	0
31	DN	1112	0	1180	37	0
32	BO	923	0	981	24	0
32	DO	923	0	981	29	0
33	BP	1131	0	1201	38	0
33	DP	1131	0	1201	39	0
34	BQ	1122	0	1179	33	0
34	DQ	1122	0	1179	45	0
35	BR	968	0	1033	22	0
35	DR	968	0	1033	29	0
36	BS	865	0	905	46	0
36	DS	865	0	905	52	0
37	BT	1063	0	1103	41	0
37	DT	1063	0	1103	40	0
38	BU	959	0	1019	24	0
38	DU	959	0	1019	29	0
39	BV	760	0	816	20	0
39	DV	771	0	830	24	0
40	BW	881	0	935	17	0
40	DW	881	0	935	21	0
41	BX	742	0	799	17	0
41	DX	742	0	799	18	0
42	BY	785	0	828	31	0
42	DY	785	0	828	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BZ	1522	0	1511	49	0
43	DZ	1522	0	1511	52	0
44	B0	594	0	604	23	0
44	D0	594	0	604	31	0
45	B1	745	0	804	31	0
45	D1	745	0	804	31	0
46	B2	588	0	643	19	0
46	D2	588	0	643	24	0
47	B3	458	0	503	9	0
47	D3	458	0	503	13	0
48	B4	349	0	336	20	0
48	D4	349	0	336	20	0
49	B5	455	0	472	14	0
49	D5	455	0	472	17	0
50	B6	449	0	462	19	0
50	D6	449	0	462	18	0
51	B7	418	0	467	11	0
51	D7	418	0	467	15	0
52	B8	509	0	565	23	0
52	D8	509	0	565	28	0
53	B9	297	0	316	8	0
53	D9	297	0	316	10	0
54	AA	106	0	0	0	0
54	AD	1	0	0	0	0
54	B0	2	0	0	0	0
54	B1	1	0	0	0	0
54	B2	2	0	0	0	0
54	B3	2	0	0	0	0
54	B5	2	0	0	0	0
54	B8	3	0	0	0	0
54	B9	1	0	0	0	0
54	BA	618	0	0	0	0
54	BB	17	0	0	0	0
54	BD	3	0	0	0	0
54	BE	6	0	0	0	0
54	BF	2	0	0	0	0
54	BP	1	0	0	0	0
54	BQ	3	0	0	0	0
54	BR	2	0	0	0	0
54	BU	2	0	0	0	0
54	BV	1	0	0	0	0
54	BW	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	CA	69	0	0	0	0
54	D6	1	0	0	0	0
54	D7	1	0	0	0	0
54	D8	1	0	0	0	0
54	DA	430	0	0	0	0
54	DB	5	0	0	0	0
54	DD	1	0	0	0	0
54	DE	1	0	0	0	0
54	DF	2	0	0	0	0
54	DP	1	0	0	0	0
55	AD	1	0	0	0	0
55	AN	1	0	0	0	0
55	B4	1	0	0	0	0
55	B5	1	0	0	0	0
55	B6	1	0	0	0	0
55	B9	1	0	0	0	0
55	BY	1	0	0	0	0
55	CD	1	0	0	0	0
55	CN	1	0	0	0	0
55	D4	1	0	0	0	0
55	D5	1	0	0	0	0
55	D6	1	0	0	0	0
55	D9	1	0	0	0	0
55	DY	1	0	0	0	0
56	AA	145	0	0	23	0
56	AF	1	0	0	0	0
56	AK	1	0	0	0	0
56	AQ	1	0	0	0	0
56	B0	4	0	0	0	0
56	B3	1	0	0	0	0
56	B4	1	0	0	0	0
56	B5	3	0	0	1	0
56	B7	3	0	0	0	0
56	B8	7	0	0	0	0
56	B9	2	0	0	1	0
56	BA	1422	0	0	86	0
56	BB	31	0	0	1	0
56	BD	10	0	0	4	0
56	BE	8	0	0	0	0
56	BF	11	0	0	0	0
56	BH	2	0	0	0	0
56	BN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BO	3	0	0	0	0
56	BP	6	0	0	0	0
56	BQ	2	0	0	0	0
56	BR	6	0	0	0	0
56	BT	1	0	0	0	0
56	BU	2	0	0	0	0
56	BV	2	0	0	0	0
56	BW	4	0	0	0	0
56	BX	2	0	0	0	0
56	BY	1	0	0	0	0
56	CA	119	0	0	13	0
56	CD	1	0	0	0	0
56	CK	2	0	0	0	0
56	CP	1	0	0	0	0
56	CT	2	0	0	0	0
56	D0	1	0	0	0	0
56	D1	2	0	0	0	0
56	DA	696	0	0	56	0
56	DB	9	0	0	0	0
56	DD	3	0	0	0	0
56	DE	2	0	0	0	0
56	DF	5	0	0	0	0
56	DP	5	0	0	0	0
56	DQ	2	0	0	0	0
56	DR	1	0	0	0	0
56	DV	1	0	0	0	0
56	DX	1	0	0	0	0
56	DY	1	0	0	0	0
All	All	283930	0	186520	7011	1

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 15.

The worst 5 of 7011 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:AA:1303:C:N4	1:AA:1334:G:H1	1.41	1.17
23:BA:2296:U:O4	23:BA:2335:A:N6	1.76	1.15
23:DA:2296:U:O4	23:DA:2335:A:N6	1.79	1.15
1:AA:1003:G:H1	1:AA:1037:C:N4	1.46	1.14
1:AA:559:A:H4'	1:AA:560:U:H3'	1.35	1.07

All (1) 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)
30:BI:91:SER:OG	1:CA:368:U:OP1[3_654]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	227/256 (89%)	188 (83%)	37 (16%)	2 (1%)	20	62
2	CB	227/256 (89%)	192 (85%)	33 (14%)	2 (1%)	20	62
3	AC	204/239 (85%)	179 (88%)	25 (12%)	0	100	100
3	CC	204/239 (85%)	177 (87%)	27 (13%)	0	100	100
4	AD	206/209 (99%)	179 (87%)	25 (12%)	2 (1%)	18	59
4	CD	206/209 (99%)	180 (87%)	24 (12%)	2 (1%)	18	59
5	AE	146/162 (90%)	125 (86%)	20 (14%)	1 (1%)	25	67
5	CE	146/162 (90%)	126 (86%)	20 (14%)	0	100	100
6	AF	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
6	CF	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
7	AG	153/156 (98%)	132 (86%)	19 (12%)	2 (1%)	14	51
7	CG	153/156 (98%)	128 (84%)	23 (15%)	2 (1%)	14	51
8	AH	136/138 (99%)	122 (90%)	14 (10%)	0	100	100
8	CH	136/138 (99%)	125 (92%)	11 (8%)	0	100	100
9	AI	123/128 (96%)	106 (86%)	15 (12%)	2 (2%)	11	46
9	CI	123/128 (96%)	109 (89%)	12 (10%)	2 (2%)	11	46
10	AJ	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	8	38
10	CJ	94/105 (90%)	74 (79%)	18 (19%)	2 (2%)	8	38
11	AK	112/129 (87%)	100 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CK	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
12	AL	120/132 (91%)	109 (91%)	10 (8%)	1 (1%)	22	64
12	CL	120/132 (91%)	107 (89%)	11 (9%)	2 (2%)	11	44
13	AM	112/126 (89%)	82 (73%)	27 (24%)	3 (3%)	6	30
13	CM	112/126 (89%)	84 (75%)	27 (24%)	1 (1%)	20	62
14	AN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	14
14	CN	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	11	44
15	AO	86/89 (97%)	71 (83%)	15 (17%)	0	100	100
15	CO	86/89 (97%)	72 (84%)	14 (16%)	0	100	100
16	AP	80/88 (91%)	69 (86%)	9 (11%)	2 (2%)	6	32
16	CP	80/88 (91%)	71 (89%)	7 (9%)	2 (2%)	6	32
17	AQ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
17	CQ	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
18	AR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
18	CR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
19	AS	79/93 (85%)	62 (78%)	16 (20%)	1 (1%)	14	51
19	CS	79/93 (85%)	60 (76%)	16 (20%)	3 (4%)	4	21
20	AT	95/106 (90%)	82 (86%)	10 (10%)	3 (3%)	5	26
20	CT	95/106 (90%)	81 (85%)	11 (12%)	3 (3%)	5	26
21	AU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
21	CU	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
22	AV	51/61 (84%)	42 (82%)	9 (18%)	0	100	100
22	CV	51/61 (84%)	34 (67%)	14 (28%)	3 (6%)	2	11
25	BD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	38	78
25	DD	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	38	78
26	BE	202/206 (98%)	188 (93%)	12 (6%)	2 (1%)	18	59
26	DE	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	18	59
27	BF	201/210 (96%)	187 (93%)	13 (6%)	1 (0%)	32	74
27	DF	201/210 (96%)	188 (94%)	12 (6%)	1 (0%)	32	74
28	BG	179/182 (98%)	151 (84%)	28 (16%)	0	100	100
28	DG	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	28	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BH	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	15	53
29	DH	172/180 (96%)	158 (92%)	12 (7%)	2 (1%)	15	53
30	BI	144/148 (97%)	114 (79%)	27 (19%)	3 (2%)	8	38
30	DI	144/148 (97%)	113 (78%)	29 (20%)	2 (1%)	13	49
31	BN	138/140 (99%)	128 (93%)	6 (4%)	4 (3%)	5	28
31	DN	138/140 (99%)	126 (91%)	7 (5%)	5 (4%)	4	22
32	BO	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
32	DO	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
33	BP	147/150 (98%)	134 (91%)	12 (8%)	1 (1%)	25	67
33	DP	147/150 (98%)	134 (91%)	13 (9%)	0	100	100
34	BQ	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
34	DQ	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
35	BR	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
35	DR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
36	BS	108/112 (96%)	96 (89%)	11 (10%)	1 (1%)	20	62
36	DS	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	20	62
37	BT	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
37	DT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
38	BU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
38	DU	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
39	BV	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
39	DV	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
40	BW	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
40	DW	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
41	BX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
41	DX	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
42	BY	105/110 (96%)	94 (90%)	9 (9%)	2 (2%)	9	41
42	DY	105/110 (96%)	95 (90%)	8 (8%)	2 (2%)	9	41
43	BZ	196/206 (95%)	178 (91%)	15 (8%)	3 (2%)	12	48
43	DZ	196/206 (95%)	177 (90%)	16 (8%)	3 (2%)	12	48
44	B0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	D0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	B1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
45	D1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	17	56
46	B2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
46	D2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
47	B3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
47	D3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
48	B4	44/71 (62%)	37 (84%)	7 (16%)	0	100	100
48	D4	44/71 (62%)	38 (86%)	6 (14%)	0	100	100
49	B5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
49	D5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
50	B6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
50	D6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
51	B7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	8	36
51	D7	46/49 (94%)	45 (98%)	0	1 (2%)	8	36
52	B8	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	11	46
52	D8	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	5	26
53	B9	34/37 (92%)	34 (100%)	0	0	100	100
53	D9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	11473/12250 (94%)	10289 (90%)	1089 (10%)	95 (1%)	22	64

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	AM	91	ARG
33	BP	27	HIS
12	CL	92	ASP
31	DN	23	LEU
31	DN	24	GLY

### 5.3.2 Protein sidechains [i](#)

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	177/220 (80%)	135 (76%)	42 (24%)	1	4
2	CB	177/220 (80%)	135 (76%)	42 (24%)	1	4
3	AC	114/188 (61%)	74 (65%)	40 (35%)	0	1
3	CC	114/188 (61%)	78 (68%)	36 (32%)	0	1
4	AD	141/181 (78%)	113 (80%)	28 (20%)	1	8
4	CD	141/181 (78%)	114 (81%)	27 (19%)	2	9
5	AE	108/123 (88%)	84 (78%)	24 (22%)	1	5
5	CE	108/123 (88%)	84 (78%)	24 (22%)	1	5
6	AF	76/90 (84%)	68 (90%)	8 (10%)	8	30
6	CF	76/90 (84%)	69 (91%)	7 (9%)	11	38
7	AG	103/127 (81%)	68 (66%)	35 (34%)	0	1
7	CG	103/127 (81%)	77 (75%)	26 (25%)	0	3
8	AH	103/119 (87%)	83 (81%)	20 (19%)	1	9
8	CH	103/119 (87%)	84 (82%)	19 (18%)	2	10
9	AI	62/99 (63%)	49 (79%)	13 (21%)	1	6
9	CI	62/99 (63%)	48 (77%)	14 (23%)	1	5
10	AJ	53/92 (58%)	41 (77%)	12 (23%)	1	5
10	CJ	53/92 (58%)	39 (74%)	14 (26%)	0	3
11	AK	81/99 (82%)	70 (86%)	11 (14%)	4	19
11	CK	81/99 (82%)	70 (86%)	11 (14%)	4	19
12	AL	91/109 (84%)	80 (88%)	11 (12%)	6	24
12	CL	91/109 (84%)	79 (87%)	12 (13%)	5	20
13	AM	64/101 (63%)	45 (70%)	19 (30%)	0	2
13	CM	64/101 (63%)	49 (77%)	15 (23%)	1	4
14	AN	46/50 (92%)	37 (80%)	9 (20%)	1	8
14	CN	46/50 (92%)	33 (72%)	13 (28%)	0	2
15	AO	77/80 (96%)	70 (91%)	7 (9%)	11	39
15	CO	77/80 (96%)	71 (92%)	6 (8%)	15	47
16	AP	63/74 (85%)	47 (75%)	16 (25%)	0	3
16	CP	63/74 (85%)	47 (75%)	16 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AQ	94/97 (97%)	80 (85%)	14 (15%)	3	16
17	CQ	94/97 (97%)	80 (85%)	14 (15%)	3	16
18	AR	49/77 (64%)	43 (88%)	6 (12%)	6	24
18	CR	49/77 (64%)	42 (86%)	7 (14%)	4	18
19	AS	43/80 (54%)	24 (56%)	19 (44%)	0	0
19	CS	43/80 (54%)	32 (74%)	11 (26%)	0	3
20	AT	65/82 (79%)	56 (86%)	9 (14%)	4	19
20	CT	65/82 (79%)	55 (85%)	10 (15%)	3	15
21	AU	18/22 (82%)	11 (61%)	7 (39%)	0	0
21	CU	18/22 (82%)	13 (72%)	5 (28%)	0	2
22	AV	16/50 (32%)	13 (81%)	3 (19%)	2	10
22	CV	21/50 (42%)	14 (67%)	7 (33%)	0	1
25	BD	215/218 (99%)	181 (84%)	34 (16%)	3	14
25	DD	215/218 (99%)	180 (84%)	35 (16%)	3	13
26	BE	163/166 (98%)	138 (85%)	25 (15%)	3	15
26	DE	163/166 (98%)	135 (83%)	28 (17%)	2	12
27	BF	159/166 (96%)	133 (84%)	26 (16%)	2	13
27	DF	159/166 (96%)	133 (84%)	26 (16%)	2	13
28	BG	128/156 (82%)	106 (83%)	22 (17%)	2	12
28	DG	128/156 (82%)	106 (83%)	22 (17%)	2	12
29	BH	141/148 (95%)	127 (90%)	14 (10%)	9	34
29	DH	141/148 (95%)	127 (90%)	14 (10%)	9	34
30	BI	99/124 (80%)	75 (76%)	24 (24%)	1	4
30	DI	98/124 (79%)	67 (68%)	31 (32%)	0	1
31	BN	117/119 (98%)	92 (79%)	25 (21%)	1	6
31	DN	117/119 (98%)	93 (80%)	24 (20%)	1	7
32	BO	98/100 (98%)	90 (92%)	8 (8%)	13	44
32	DO	98/100 (98%)	90 (92%)	8 (8%)	13	44
33	BP	114/116 (98%)	98 (86%)	16 (14%)	4	18
33	DP	114/116 (98%)	100 (88%)	14 (12%)	5	24
34	BQ	111/111 (100%)	95 (86%)	16 (14%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DQ	111/111 (100%)	96 (86%)	15 (14%)	4	19
35	BR	101/101 (100%)	82 (81%)	19 (19%)	2	10
35	DR	101/101 (100%)	83 (82%)	18 (18%)	2	11
36	BS	84/88 (96%)	69 (82%)	15 (18%)	2	11
36	DS	84/88 (96%)	72 (86%)	12 (14%)	4	18
37	BT	110/127 (87%)	95 (86%)	15 (14%)	4	19
37	DT	110/127 (87%)	92 (84%)	18 (16%)	2	13
38	BU	93/94 (99%)	84 (90%)	9 (10%)	9	35
38	DU	93/94 (99%)	84 (90%)	9 (10%)	9	35
39	BV	79/82 (96%)	62 (78%)	17 (22%)	1	6
39	DV	80/82 (98%)	64 (80%)	16 (20%)	1	8
40	BW	89/92 (97%)	78 (88%)	11 (12%)	5	23
40	DW	89/92 (97%)	76 (85%)	13 (15%)	3	17
41	BX	75/78 (96%)	70 (93%)	5 (7%)	19	54
41	DX	75/78 (96%)	70 (93%)	5 (7%)	19	54
42	BY	80/91 (88%)	66 (82%)	14 (18%)	2	11
42	DY	80/91 (88%)	63 (79%)	17 (21%)	1	6
43	BZ	159/179 (89%)	141 (89%)	18 (11%)	7	27
43	DZ	159/179 (89%)	141 (89%)	18 (11%)	7	27
44	B0	59/67 (88%)	54 (92%)	5 (8%)	12	43
44	D0	59/67 (88%)	54 (92%)	5 (8%)	12	43
45	B1	78/83 (94%)	67 (86%)	11 (14%)	4	18
45	D1	78/83 (94%)	67 (86%)	11 (14%)	4	18
46	B2	65/67 (97%)	59 (91%)	6 (9%)	11	38
46	D2	65/67 (97%)	58 (89%)	7 (11%)	7	29
47	B3	49/52 (94%)	43 (88%)	6 (12%)	6	24
47	D3	49/52 (94%)	42 (86%)	7 (14%)	4	18
48	B4	39/63 (62%)	29 (74%)	10 (26%)	0	3
48	D4	39/63 (62%)	29 (74%)	10 (26%)	0	3
49	B5	50/52 (96%)	45 (90%)	5 (10%)	9	33
49	D5	50/52 (96%)	45 (90%)	5 (10%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B6	50/52 (96%)	39 (78%)	11 (22%)	1	5
50	D6	50/52 (96%)	37 (74%)	13 (26%)	0	3
51	B7	41/42 (98%)	32 (78%)	9 (22%)	1	5
51	D7	41/42 (98%)	34 (83%)	7 (17%)	2	12
52	B8	52/55 (94%)	43 (83%)	9 (17%)	2	12
52	D8	52/55 (94%)	43 (83%)	9 (17%)	2	12
53	B9	32/34 (94%)	29 (91%)	3 (9%)	10	37
53	D9	32/34 (94%)	29 (91%)	3 (9%)	10	37
All	All	8753/10166 (86%)	7236 (83%)	1517 (17%)	2	12

5 of 1517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	B0	20	ARG
4	CD	97	LEU
41	DX	45	THR
46	B2	53	LEU
2	CB	58	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
9	CI	38	GLN
15	CO	37	ASN
42	DY	6	HIS
9	CI	73	GLN
10	CJ	33	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	425 (28%)	0
1	CA	1499/1522 (98%)	383 (25%)	0
23	BA	2801/2915 (96%)	556 (19%)	0
23	DA	2807/2915 (96%)	552 (19%)	0
24	BB	119/122 (97%)	21 (17%)	0
24	DB	119/122 (97%)	21 (17%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	8848/9118 (97%)	1958 (22%)	0

5 of 1958 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	10	A
1	AA	22	G

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1302 ligands modelled in this entry, 1302 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1505/1522 (98%)	1.08	302 (20%) 1 1	52, 116, 177, 188	0
1	CA	1501/1522 (98%)	0.62	215 (14%) 3 1	53, 112, 168, 181	0
2	AB	229/256 (89%)	0.32	17 (7%) 15 6	114, 135, 150, 160	0
2	CB	229/256 (89%)	0.61	26 (11%) 6 2	113, 135, 150, 160	0
3	AC	206/239 (86%)	1.84	83 (40%) 0 0	122, 148, 164, 172	0
3	CC	206/239 (86%)	1.48	62 (30%) 1 0	119, 140, 153, 162	0
4	AD	208/209 (99%)	0.40	21 (10%) 8 3	100, 116, 133, 143	0
4	CD	208/209 (99%)	0.19	14 (6%) 19 7	95, 111, 129, 142	0
5	AE	148/162 (91%)	0.43	19 (12%) 4 2	85, 109, 124, 129	0
5	CE	148/162 (91%)	0.42	13 (8%) 11 4	87, 108, 124, 132	0
6	AF	100/101 (99%)	-0.08	6 (6%) 23 9	88, 102, 122, 136	0
6	CF	100/101 (99%)	0.08	5 (5%) 30 12	93, 107, 123, 135	0
7	AG	155/156 (99%)	3.54	107 (69%) 0 0	134, 156, 166, 168	0
7	CG	155/156 (99%)	2.14	73 (47%) 0 0	118, 144, 151, 158	0
8	AH	138/138 (100%)	0.07	5 (3%) 43 18	93, 111, 121, 131	0
8	CH	138/138 (100%)	0.14	6 (4%) 36 15	89, 110, 120, 133	0
9	AI	125/128 (97%)	3.97	89 (71%) 0 0	131, 157, 170, 176	0
9	CI	125/128 (97%)	2.56	59 (47%) 0 0	129, 151, 161, 173	0
10	AJ	96/105 (91%)	3.60	58 (60%) 0 0	137, 155, 171, 176	0
10	CJ	96/105 (91%)	2.67	55 (57%) 0 0	130, 149, 161, 169	0
11	AK	114/129 (88%)	0.10	0 100 100	74, 109, 123, 127	0
11	CK	114/129 (88%)	0.36	9 (7%) 13 5	79, 109, 122, 124	0
12	AL	122/132 (92%)	0.16	6 (4%) 30 12	72, 95, 111, 120	0
12	CL	122/132 (92%)	0.28	8 (6%) 19 7	72, 92, 106, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	114/126 (90%)	4.49	90 (78%) 0 0	147, 160, 171, 177	0
13	CM	114/126 (90%)	1.97	39 (34%) 0 0	124, 145, 155, 158	0
14	AN	60/61 (98%)	3.85	37 (61%) 0 0	134, 160, 169, 174	0
14	CN	60/61 (98%)	1.86	21 (35%) 0 0	136, 146, 152, 155	0
15	AO	88/89 (98%)	0.01	2 (2%) 61 31	78, 103, 120, 131	0
15	CO	88/89 (98%)	0.06	6 (6%) 18 7	79, 102, 122, 129	0
16	AP	82/88 (93%)	1.26	24 (29%) 1 0	98, 112, 132, 138	0
16	CP	82/88 (93%)	0.52	5 (6%) 22 8	89, 105, 123, 132	0
17	AQ	99/105 (94%)	0.36	6 (6%) 22 8	86, 99, 113, 118	0
17	CQ	99/105 (94%)	0.01	3 (3%) 51 23	84, 98, 113, 117	0
18	AR	68/88 (77%)	0.67	11 (16%) 2 1	93, 104, 138, 141	0
18	CR	68/88 (77%)	1.11	19 (27%) 1 0	95, 107, 138, 143	0
19	AS	81/93 (87%)	2.93	40 (49%) 0 0	131, 164, 174, 179	0
19	CS	81/93 (87%)	2.62	46 (56%) 0 0	125, 146, 153, 155	0
20	AT	97/106 (91%)	0.51	9 (9%) 9 3	90, 106, 127, 131	0
20	CT	97/106 (91%)	0.66	12 (12%) 4 2	84, 103, 125, 132	0
21	AU	23/27 (85%)	6.67	19 (82%) 0 0	147, 161, 169, 174	0
21	CU	23/27 (85%)	2.44	12 (52%) 0 0	130, 145, 153, 154	0
22	AV	53/61 (86%)	0.14	3 (5%) 24 9	93, 105, 121, 143	0
22	CV	53/61 (86%)	-0.40	1 (1%) 67 37	90, 115, 141, 151	0
23	BA	2809/2915 (96%)	0.03	82 (2%) 52 24	31, 50, 134, 186	0
23	DA	2814/2915 (96%)	-0.13	109 (3%) 40 16	34, 56, 138, 189	0
24	BB	120/122 (98%)	-0.36	0 100 100	46, 72, 94, 119	0
24	DB	120/122 (98%)	-0.24	0 100 100	63, 90, 111, 129	0
25	BD	275/276 (99%)	-0.32	1 (0%) 92 77	34, 52, 69, 117	0
25	DD	275/276 (99%)	-0.42	1 (0%) 92 77	36, 55, 72, 119	0
26	BE	204/206 (99%)	-0.20	0 100 100	32, 55, 78, 95	0
26	DE	204/206 (99%)	-0.33	0 100 100	35, 61, 84, 101	0
27	BF	203/210 (96%)	-0.28	2 (0%) 82 58	30, 60, 92, 136	0
27	DF	203/210 (96%)	-0.26	1 (0%) 90 74	34, 67, 96, 136	0
28	BG	181/182 (99%)	0.42	20 (11%) 6 2	80, 120, 143, 152	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DG	181/182 (99%)	1.14	43 (23%) 1 0	92, 126, 146, 156	0
29	BH	174/180 (96%)	-0.19	1 (0%) 89 71	58, 79, 97, 110	0
29	DH	174/180 (96%)	0.43	22 (12%) 4 2	70, 92, 107, 122	0
30	BI	146/148 (98%)	-0.14	1 (0%) 87 67	57, 90, 108, 120	0
30	DI	146/148 (98%)	0.48	15 (10%) 7 3	60, 108, 127, 131	0
31	BN	140/140 (100%)	-0.34	0 100 100	39, 55, 83, 98	0
31	DN	140/140 (100%)	-0.56	1 (0%) 87 67	45, 63, 89, 101	0
32	BO	122/122 (100%)	-0.26	0 100 100	43, 58, 79, 85	0
32	DO	122/122 (100%)	-0.44	0 100 100	46, 62, 82, 86	0
33	BP	149/150 (99%)	0.02	0 100 100	34, 63, 98, 109	0
33	DP	149/150 (99%)	-0.23	3 (2%) 65 36	38, 70, 102, 111	0
34	BQ	141/141 (100%)	-0.17	1 (0%) 87 67	43, 61, 77, 91	0
34	DQ	141/141 (100%)	-0.21	0 100 100	47, 67, 85, 94	0
35	BR	118/118 (100%)	-0.27	0 100 100	38, 50, 70, 78	0
35	DR	118/118 (100%)	-0.35	0 100 100	42, 55, 73, 82	0
36	BS	110/112 (98%)	0.05	0 100 100	58, 75, 93, 101	0
36	DS	110/112 (98%)	0.10	3 (2%) 55 26	64, 82, 99, 110	0
37	BT	131/146 (89%)	-0.27	0 100 100	51, 63, 98, 117	0
37	DT	131/146 (89%)	-0.39	1 (0%) 86 64	55, 67, 101, 118	0
38	BU	116/118 (98%)	-0.19	1 (0%) 84 61	35, 48, 69, 81	0
38	DU	116/118 (98%)	-0.14	2 (1%) 70 42	40, 56, 76, 86	0
39	BV	100/101 (99%)	-0.28	0 100 100	34, 62, 81, 91	0
39	DV	101/101 (100%)	-0.07	0 100 100	40, 72, 90, 98	0
40	BW	112/113 (99%)	-0.42	0 100 100	36, 43, 64, 102	0
40	DW	112/113 (99%)	-0.60	0 100 100	40, 48, 69, 95	0
41	BX	95/96 (98%)	-0.18	1 (1%) 80 55	41, 51, 74, 98	0
41	DX	95/96 (98%)	-0.47	0 100 100	47, 56, 80, 102	0
42	BY	107/110 (97%)	-0.23	2 (1%) 67 37	52, 64, 89, 107	0
42	DY	107/110 (97%)	0.13	6 (5%) 25 10	59, 72, 96, 116	0
43	BZ	198/206 (96%)	-0.17	0 100 100	65, 85, 111, 126	0
43	DZ	198/206 (96%)	0.19	14 (7%) 17 6	73, 92, 115, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	B0	76/85 (89%)	-0.32	0 100 100	48, 55, 71, 87	0
44	D0	76/85 (89%)	0.26	4 (5%) 27 11	53, 61, 76, 90	0
45	B1	97/98 (98%)	-0.17	2 (2%) 64 34	37, 57, 89, 103	0
45	D1	97/98 (98%)	-0.24	1 (1%) 82 58	41, 61, 91, 108	0
46	B2	70/72 (97%)	-0.15	0 100 100	50, 66, 84, 103	0
46	D2	70/72 (97%)	0.05	3 (4%) 36 15	55, 71, 88, 112	0
47	B3	59/60 (98%)	-0.32	0 100 100	43, 57, 85, 101	0
47	D3	59/60 (98%)	0.21	2 (3%) 46 20	49, 64, 92, 112	0
48	B4	46/71 (64%)	-0.58	0 100 100	106, 141, 151, 154	0
48	D4	46/71 (64%)	0.04	0 100 100	113, 141, 152, 163	0
49	B5	59/60 (98%)	-0.37	0 100 100	33, 51, 68, 89	0
49	D5	59/60 (98%)	-0.39	0 100 100	37, 55, 73, 95	0
50	B6	53/54 (98%)	0.26	2 (3%) 41 17	53, 61, 75, 78	0
50	D6	53/54 (98%)	0.53	5 (9%) 9 3	56, 65, 79, 82	0
51	B7	48/49 (97%)	0.05	2 (4%) 37 15	32, 37, 61, 78	0
51	D7	48/49 (97%)	-0.13	0 100 100	36, 40, 64, 83	0
52	B8	64/65 (98%)	-0.10	0 100 100	42, 49, 58, 70	0
52	D8	64/65 (98%)	-0.44	0 100 100	46, 53, 62, 72	0
53	B9	36/37 (97%)	0.09	0 100 100	49, 59, 72, 83	0
53	D9	36/37 (97%)	0.58	3 (8%) 12 4	58, 68, 81, 91	0
All	All	20542/21368 (96%)	0.35	2020 (9%) 8 3	30, 80, 160, 189	0

The worst 5 of 2020 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AM	43	THR	23.6
14	AN	13	THR	22.9
9	CI	7	THR	17.5
10	AJ	72	VAL	16.9
21	AU	11	GLY	15.4

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
54	MG	DA	3118	1/1	0.98	0.43	68.26	44,44,44,44	0
54	MG	DA	3177	1/1	0.85	0.84	66.13	59,59,59,59	0
54	MG	DA	3121	1/1	0.84	0.65	65.54	53,53,53,53	0
54	MG	DA	3086	1/1	0.94	0.63	62.53	54,54,54,54	0
54	MG	AA	1657	1/1	0.92	0.53	37.94	81,81,81,81	0
54	MG	AA	1645	1/1	0.95	0.86	37.70	77,77,77,77	0
54	MG	DA	3138	1/1	0.91	0.74	34.31	60,60,60,60	0
54	MG	AA	1660	1/1	0.92	0.96	33.47	91,91,91,91	0
54	MG	DA	3120	1/1	0.88	0.71	32.36	52,52,52,52	0
54	MG	AA	1621	1/1	0.93	0.98	31.33	80,80,80,80	0
54	MG	CA	1631	1/1	0.71	0.99	27.33	88,88,88,88	0
54	MG	DA	3207	1/1	0.93	0.42	26.72	53,53,53,53	0
54	MG	CA	1601	1/1	0.95	0.37	26.41	50,50,50,50	0
54	MG	BA	3078	1/1	0.90	0.35	25.83	38,38,38,38	0
54	MG	BA	3080	1/1	0.98	0.51	25.25	42,42,42,42	0
54	MG	DA	3074	1/1	0.96	0.50	23.59	38,38,38,38	0
54	MG	BA	3308	1/1	0.86	0.54	22.99	51,51,51,51	0
54	MG	CA	1613	1/1	0.87	1.04	22.47	71,71,71,71	0
54	MG	DA	3185	1/1	0.95	0.45	22.43	47,47,47,47	0
54	MG	CA	1617	1/1	0.93	0.89	21.17	70,70,70,70	0
54	MG	BA	3001	1/1	0.89	0.43	20.80	56,56,56,56	0
54	MG	DA	3242	1/1	0.90	0.55	20.14	38,38,38,38	0
54	MG	BA	3160	1/1	0.89	0.38	19.50	46,46,46,46	0
54	MG	BA	3455	1/1	0.97	0.34	18.93	42,42,42,42	0
54	MG	DA	3144	1/1	0.95	0.30	18.55	42,42,42,42	0
54	MG	BA	3396	1/1	0.81	0.43	16.96	23,23,23,23	0
54	MG	BE	301	1/1	0.88	0.53	16.74	43,43,43,43	0
54	MG	DA	3208	1/1	0.90	0.43	15.95	52,52,52,52	0
54	MG	AA	1615	1/1	0.90	0.37	14.92	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DP	201	1/1	0.79	0.78	14.55	58,58,58,58	0
54	MG	BA	3033	1/1	0.96	0.36	14.36	40,40,40,40	0
54	MG	BR	201	1/1	0.83	0.60	14.30	58,58,58,58	0
54	MG	DA	3279	1/1	0.98	0.33	14.24	40,40,40,40	0
54	MG	BA	3244	1/1	0.88	0.46	14.03	45,45,45,45	0
54	MG	DA	3385	1/1	0.97	0.36	14.03	49,49,49,49	0
54	MG	BA	3113	1/1	0.94	0.40	13.94	35,35,35,35	0
54	MG	BA	3557	1/1	0.98	0.49	13.88	42,42,42,42	0
54	MG	DA	3003	1/1	0.92	0.35	13.77	35,35,35,35	0
54	MG	DA	3027	1/1	0.93	0.42	13.63	51,51,51,51	0
54	MG	DA	3099	1/1	0.93	0.26	13.38	40,40,40,40	0
54	MG	BA	3473	1/1	0.95	0.44	13.27	59,59,59,59	0
54	MG	DA	3236	1/1	0.98	0.54	13.21	44,44,44,44	0
54	MG	DA	3372	1/1	0.94	0.33	13.12	40,40,40,40	0
54	MG	BA	3129	1/1	0.95	0.40	12.75	49,49,49,49	0
54	MG	BA	3234	1/1	0.98	0.33	12.68	34,34,34,34	0
54	MG	BA	3333	1/1	0.94	0.30	12.56	36,36,36,36	0
54	MG	DA	3116	1/1	0.96	0.39	12.03	46,46,46,46	0
54	MG	DA	3204	1/1	0.97	0.30	11.72	37,37,37,37	0
54	MG	CA	1618	1/1	0.93	0.37	11.70	75,75,75,75	0
54	MG	DA	3146	1/1	0.92	0.44	11.27	35,35,35,35	0
54	MG	DA	3070	1/1	0.92	0.33	11.26	53,53,53,53	0
54	MG	BA	3034	1/1	0.77	0.29	11.24	46,46,46,46	0
54	MG	BA	3031	1/1	0.85	0.39	11.10	41,41,41,41	0
54	MG	DA	3309	1/1	0.97	0.47	11.10	48,48,48,48	0
54	MG	BQ	202	1/1	0.92	0.36	10.82	53,53,53,53	0
54	MG	AA	1627	1/1	0.76	0.50	10.60	70,70,70,70	0
54	MG	BA	3003	1/1	0.90	0.34	10.55	29,29,29,29	0
54	MG	DA	3133	1/1	0.85	0.39	10.52	78,78,78,78	0
54	MG	DA	3124	1/1	0.96	0.46	10.34	35,35,35,35	0
54	MG	BA	3161	1/1	0.89	0.34	10.28	54,54,54,54	0
54	MG	AA	1659	1/1	0.84	0.44	10.20	62,62,62,62	0
54	MG	BA	3046	1/1	0.90	0.28	9.73	49,49,49,49	0
54	MG	DA	3142	1/1	0.91	0.24	9.52	46,46,46,46	0
54	MG	BA	3368	1/1	0.99	0.30	9.43	34,34,34,34	0
54	MG	BA	3228	1/1	0.97	0.38	9.25	26,26,26,26	0
54	MG	DA	3394	1/1	0.94	0.33	9.09	56,56,56,56	0
54	MG	DA	3085	1/1	0.93	0.45	8.97	51,51,51,51	0
54	MG	BA	3197	1/1	0.90	0.31	8.94	62,62,62,62	0
54	MG	DA	3247	1/1	0.94	0.37	8.90	52,52,52,52	0
54	MG	CA	1636	1/1	0.69	0.42	8.87	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3475	1/1	0.89	0.22	8.78	53,53,53,53	0
54	MG	BA	3074	1/1	0.90	0.38	8.38	55,55,55,55	0
54	MG	BA	3519	1/1	0.82	0.33	8.36	90,90,90,90	0
54	MG	CA	1612	1/1	0.59	0.42	8.26	84,84,84,84	0
54	MG	BA	3562	1/1	0.82	0.33	8.25	43,43,43,43	0
54	MG	BA	3109	1/1	0.94	0.25	8.19	57,57,57,57	0
54	MG	BA	3408	1/1	0.97	0.32	8.12	34,34,34,34	0
54	MG	BA	3142	1/1	0.83	0.53	7.99	53,53,53,53	0
54	MG	DA	3006	1/1	0.86	0.28	7.89	44,44,44,44	0
54	MG	DA	3149	1/1	0.98	0.38	7.86	36,36,36,36	0
54	MG	DA	3098	1/1	0.66	0.29	7.77	62,62,62,62	0
54	MG	DA	3168	1/1	0.94	0.29	7.06	42,42,42,42	0
54	MG	DA	3032	1/1	0.96	0.30	7.06	43,43,43,43	0
54	MG	CA	1602	1/1	0.94	0.58	6.96	82,82,82,82	0
54	MG	CA	1638	1/1	0.61	0.37	6.91	71,71,71,71	0
54	MG	DA	3115	1/1	0.95	0.41	6.88	39,39,39,39	0
54	MG	BA	3330	1/1	0.88	0.28	6.56	36,36,36,36	0
54	MG	BA	3053	1/1	0.89	0.34	6.43	53,53,53,53	0
54	MG	CA	1628	1/1	0.94	0.27	6.42	55,55,55,55	0
54	MG	DA	3280	1/1	0.98	0.26	6.25	40,40,40,40	0
54	MG	DA	3340	1/1	0.95	0.38	6.23	44,44,44,44	0
54	MG	BA	3526	1/1	0.93	0.29	6.14	28,28,28,28	0
54	MG	BA	3187	1/1	0.91	0.27	6.05	30,30,30,30	0
54	MG	DA	3062	1/1	0.81	0.22	6.02	65,65,65,65	0
54	MG	BA	3117	1/1	0.93	0.26	6.01	31,31,31,31	0
54	MG	B3	101	1/1	0.90	0.43	5.99	60,60,60,60	0
54	MG	DB	201	1/1	0.86	0.28	5.91	75,75,75,75	0
54	MG	DA	3374	1/1	0.90	0.26	5.85	44,44,44,44	0
54	MG	BA	3219	1/1	0.91	0.32	5.78	62,62,62,62	0
54	MG	AA	1640	1/1	0.94	0.50	5.74	80,80,80,80	0
54	MG	BA	3512	1/1	0.96	0.33	5.62	45,45,45,45	0
54	MG	DA	3291	1/1	0.82	0.33	5.56	43,43,43,43	0
54	MG	BA	3021	1/1	0.96	0.27	5.56	33,33,33,33	0
54	MG	DA	3219	1/1	0.90	0.30	5.54	38,38,38,38	0
54	MG	DA	3073	1/1	0.88	0.21	5.47	54,54,54,54	0
54	MG	DA	3349	1/1	0.89	0.29	5.45	54,54,54,54	0
54	MG	BA	3435	1/1	0.92	0.28	5.42	36,36,36,36	0
54	MG	DA	3233	1/1	0.95	0.32	5.34	43,43,43,43	0
54	MG	BA	3189	1/1	0.94	0.28	5.04	46,46,46,46	0
54	MG	BA	3047	1/1	0.97	0.28	4.89	50,50,50,50	0
54	MG	BA	3448	1/1	0.89	0.26	4.88	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3504	1/1	0.99	0.39	4.74	28,28,28,28	0
54	MG	DA	3170	1/1	0.95	0.25	4.62	52,52,52,52	0
54	MG	DA	3059	1/1	0.93	0.26	4.59	55,55,55,55	0
54	MG	DA	3092	1/1	0.95	0.23	4.58	63,63,63,63	0
54	MG	BA	3199	1/1	0.95	0.23	4.57	31,31,31,31	0
54	MG	DA	3040	1/1	0.84	0.31	4.56	50,50,50,50	0
54	MG	BA	3434	1/1	0.95	0.38	4.53	36,36,36,36	0
54	MG	BA	3239	1/1	0.91	0.26	4.51	38,38,38,38	0
54	MG	BA	3517	1/1	0.84	0.26	4.29	51,51,51,51	0
54	MG	BA	3230	1/1	0.95	0.38	4.28	50,50,50,50	0
54	MG	DA	3396	1/1	0.88	0.24	4.24	37,37,37,37	0
54	MG	BA	3551	1/1	0.95	0.26	4.23	40,40,40,40	0
54	MG	DA	3341	1/1	0.89	0.24	4.18	39,39,39,39	0
54	MG	BA	3108	1/1	0.94	0.26	4.08	56,56,56,56	0
54	MG	BA	3441	1/1	0.97	0.25	4.06	35,35,35,35	0
54	MG	BA	3427	1/1	0.96	0.22	4.06	32,32,32,32	0
54	MG	DA	3395	1/1	0.95	0.26	4.04	37,37,37,37	0
54	MG	DA	3084	1/1	0.82	0.30	4.02	62,62,62,62	0
54	MG	BA	3311	1/1	0.95	0.27	3.89	60,60,60,60	0
54	MG	BA	3039	1/1	0.83	0.30	3.84	44,44,44,44	0
54	MG	CA	1623	1/1	0.81	0.88	3.82	73,73,73,73	0
54	MG	DA	3130	1/1	0.81	0.24	3.78	59,59,59,59	0
54	MG	BA	3133	1/1	0.95	0.30	3.71	31,31,31,31	0
54	MG	DA	3020	1/1	0.97	0.20	3.61	39,39,39,39	0
54	MG	BA	3302	1/1	0.94	0.28	3.58	45,45,45,45	0
54	MG	BA	3254	1/1	0.90	0.20	3.54	67,67,67,67	0
54	MG	AA	1613	1/1	0.91	0.25	3.54	74,74,74,74	0
54	MG	BB	205	1/1	0.98	0.29	3.48	57,57,57,57	0
54	MG	BA	3253	1/1	0.96	0.23	3.48	38,38,38,38	0
54	MG	DA	3354	1/1	0.93	0.27	3.45	41,41,41,41	0
54	MG	BB	201	1/1	0.95	0.22	3.45	61,61,61,61	0
54	MG	DA	3044	1/1	0.89	0.22	3.42	51,51,51,51	0
54	MG	BA	3071	1/1	0.92	0.20	3.42	49,49,49,49	0
54	MG	DA	3072	1/1	0.92	0.35	3.34	50,50,50,50	0
54	MG	DA	3188	1/1	0.95	0.23	3.23	54,54,54,54	0
54	MG	BA	3500	1/1	0.86	0.21	3.19	33,33,33,33	0
54	MG	DA	3267	1/1	0.97	0.19	3.18	59,59,59,59	0
54	MG	CA	1626	1/1	0.92	0.26	3.13	86,86,86,86	0
54	MG	DA	3169	1/1	0.97	0.25	3.10	39,39,39,39	0
54	MG	DA	3019	1/1	0.92	0.20	3.10	41,41,41,41	0
54	MG	CA	1655	1/1	0.89	0.28	3.05	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3387	1/1	0.95	0.25	3.03	33,33,33,33	0
54	MG	AA	1604	1/1	0.55	0.32	3.02	81,81,81,81	0
54	MG	DA	3217	1/1	0.78	0.26	2.98	69,69,69,69	0
54	MG	DA	3324	1/1	0.92	0.20	2.90	64,64,64,64	0
54	MG	DA	3290	1/1	0.95	0.24	2.81	42,42,42,42	0
54	MG	BA	3037	1/1	0.89	0.22	2.81	52,52,52,52	0
54	MG	DA	3297	1/1	0.82	0.22	2.81	66,66,66,66	0
54	MG	BA	3424	1/1	0.99	0.23	2.79	32,32,32,32	0
54	MG	DA	3128	1/1	0.80	0.29	2.67	72,72,72,72	0
54	MG	BA	3513	1/1	0.80	0.21	2.57	66,66,66,66	0
54	MG	BA	3426	1/1	0.96	0.22	2.56	28,28,28,28	0
54	MG	DA	3011	1/1	0.85	0.22	2.55	46,46,46,46	0
54	MG	BA	3127	1/1	0.92	0.23	2.54	51,51,51,51	0
54	MG	DF	301	1/1	0.97	0.37	2.53	58,58,58,58	0
54	MG	BA	3119	1/1	0.95	0.21	2.48	39,39,39,39	0
54	MG	DA	3410	1/1	0.82	0.18	2.44	72,72,72,72	0
54	MG	BA	3461	1/1	0.98	0.23	2.39	38,38,38,38	0
54	MG	DA	3390	1/1	0.83	0.17	2.37	69,69,69,69	0
54	MG	DA	3303	1/1	0.94	0.19	2.29	37,37,37,37	0
54	MG	BA	3423	1/1	0.97	0.22	2.28	30,30,30,30	0
54	MG	DA	3079	1/1	0.91	0.20	2.24	60,60,60,60	0
54	MG	BA	3236	1/1	0.95	0.21	2.23	50,50,50,50	0
54	MG	DA	3202	1/1	0.98	0.22	2.21	37,37,37,37	0
54	MG	BA	3489	1/1	0.89	0.20	2.15	38,38,38,38	0
54	MG	BA	3307	1/1	0.98	0.20	2.03	29,29,29,29	0
54	MG	BB	204	1/1	0.82	0.20	2.02	67,67,67,67	0
54	MG	BD	302	1/1	0.98	0.28	2.00	38,38,38,38	0
54	MG	DA	3302	1/1	0.94	0.26	2.00	36,36,36,36	0
54	MG	DA	3325	1/1	0.97	0.26	1.96	36,36,36,36	0
54	MG	BA	3180	1/1	0.89	0.25	1.94	51,51,51,51	0
54	MG	CA	1632	1/1	0.95	0.28	1.89	65,65,65,65	0
54	MG	DA	3304	1/1	0.96	0.18	1.84	38,38,38,38	0
54	MG	BA	3178	1/1	0.81	0.18	1.81	58,58,58,58	0
54	MG	BB	213	1/1	0.84	0.21	1.77	69,69,69,69	0
54	MG	DA	3402	1/1	0.95	0.22	1.76	59,59,59,59	0
54	MG	BA	3407	1/1	0.92	0.22	1.75	35,35,35,35	0
54	MG	DA	3342	1/1	0.80	0.24	1.73	41,41,41,41	0
54	MG	DA	3028	1/1	0.92	0.20	1.71	53,53,53,53	0
54	MG	DA	3406	1/1	0.85	0.25	1.69	35,35,35,35	0
54	MG	DA	3135	1/1	0.92	0.26	1.68	44,44,44,44	0
54	MG	DA	3066	1/1	0.88	0.18	1.62	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3428	1/1	0.93	0.24	1.62	35,35,35,35	0
54	MG	BA	3390	1/1	0.98	0.21	1.58	29,29,29,29	0
54	MG	BA	3417	1/1	0.95	0.21	1.45	37,37,37,37	0
54	MG	DA	3353	1/1	0.94	0.20	1.38	40,40,40,40	0
54	MG	BA	3351	1/1	0.54	0.24	1.38	57,57,57,57	0
54	MG	AA	1605	1/1	0.78	0.29	1.36	74,74,74,74	0
54	MG	BA	3222	1/1	0.95	0.19	1.36	51,51,51,51	0
54	MG	BA	3422	1/1	0.87	0.23	1.31	27,27,27,27	0
54	MG	CA	1653	1/1	0.68	0.24	1.28	83,83,83,83	0
54	MG	CA	1607	1/1	0.92	0.25	1.26	72,72,72,72	0
54	MG	BA	3367	1/1	0.97	0.21	1.26	33,33,33,33	0
54	MG	BA	3107	1/1	0.87	0.13	1.15	49,49,49,49	0
54	MG	BA	3030	1/1	0.88	0.25	1.14	37,37,37,37	0
54	MG	BA	3451	1/1	0.98	0.23	1.13	34,34,34,34	0
54	MG	DA	3095	1/1	0.82	0.21	1.07	71,71,71,71	0
54	MG	BA	3007	1/1	0.94	0.22	1.00	36,36,36,36	0
54	MG	B9	102	1/1	0.95	0.31	0.98	45,45,45,45	0
54	MG	B8	102	1/1	0.85	0.33	0.93	61,61,61,61	0
54	MG	BA	3057	1/1	0.95	0.20	0.91	46,46,46,46	0
54	MG	BA	3131	1/1	0.96	0.19	0.86	44,44,44,44	0
54	MG	BA	3193	1/1	0.93	0.19	0.75	50,50,50,50	0
54	MG	DA	3226	1/1	0.93	0.22	0.74	53,53,53,53	0
54	MG	DA	3012	1/1	0.76	0.21	0.71	60,60,60,60	0
54	MG	BA	3465	1/1	0.89	0.20	0.69	38,38,38,38	0
54	MG	DA	3064	1/1	0.90	0.17	0.67	53,53,53,53	0
54	MG	DA	3222	1/1	0.94	0.26	0.61	47,47,47,47	0
54	MG	DA	3004	1/1	0.99	0.14	0.49	59,59,59,59	0
54	MG	BA	3412	1/1	0.88	0.21	0.46	41,41,41,41	0
54	MG	BA	3048	1/1	0.96	0.20	0.46	42,42,42,42	0
54	MG	DA	3370	1/1	0.94	0.19	0.45	51,51,51,51	0
54	MG	AA	1674	1/1	0.93	0.20	0.41	73,73,73,73	0
54	MG	DA	3408	1/1	0.86	0.15	0.36	65,65,65,65	0
54	MG	BB	215	1/1	0.73	0.18	0.28	77,77,77,77	0
54	MG	DA	3356	1/1	0.97	0.20	0.26	42,42,42,42	0
54	MG	AA	1631	1/1	0.91	0.41	0.25	64,64,64,64	0
54	MG	BA	3345	1/1	0.95	0.16	0.23	45,45,45,45	0
54	MG	AA	1703	1/1	0.91	0.20	0.23	89,89,89,89	0
54	MG	DA	3405	1/1	0.94	0.17	0.23	70,70,70,70	0
54	MG	DA	3240	1/1	0.92	0.21	0.19	67,67,67,67	0
54	MG	DA	3041	1/1	0.87	0.19	0.17	49,49,49,49	0
54	MG	BA	3410	1/1	0.94	0.20	0.14	34,34,34,34	0
54	MG	DA	3292	1/1	0.93	0.18	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3432	1/1	0.96	0.18	0.06	31,31,31,31	0
55	ZN	CD	301	1/1	0.90	0.32	0.06	96,96,96,96	0
54	MG	BA	3164	1/1	0.96	0.17	0.03	39,39,39,39	0
54	MG	BA	3221	1/1	0.97	0.17	-0.04	51,51,51,51	0
54	MG	BA	3456	1/1	0.79	0.13	-0.07	89,89,89,89	0
54	MG	BA	3094	1/1	0.94	0.17	-0.07	41,41,41,41	0
54	MG	DA	3018	1/1	0.92	0.16	-0.08	42,42,42,42	0
54	MG	AD	302	1/1	0.92	0.17	-0.10	120,120,120,120	0
54	MG	DA	3427	1/1	0.96	0.16	-0.14	40,40,40,40	0
54	MG	BA	3157	1/1	0.88	0.15	-0.30	46,46,46,46	0
54	MG	DA	3013	1/1	0.94	0.15	-0.30	41,41,41,41	0
54	MG	BA	3553	1/1	0.73	0.18	-0.35	70,70,70,70	0
54	MG	BB	202	1/1	0.83	0.14	-0.38	46,46,46,46	0
55	ZN	BY	201	1/1	0.95	0.13	-0.39	74,74,74,74	0
54	MG	BA	3232	1/1	0.91	0.14	-0.40	54,54,54,54	0
54	MG	BE	304	1/1	0.91	0.17	-0.47	32,32,32,32	0
54	MG	AA	1694	1/1	0.85	0.19	-0.53	110,110,110,110	0
55	ZN	AD	301	1/1	0.93	0.24	-0.54	107,107,107,107	0
54	MG	DA	3412	1/1	0.93	0.16	-0.55	45,45,45,45	0
54	MG	BA	3429	1/1	0.95	0.17	-0.63	29,29,29,29	0
54	MG	DD	301	1/1	0.97	0.15	-0.66	40,40,40,40	0
54	MG	AA	1636	1/1	0.94	0.18	-0.70	86,86,86,86	0
54	MG	DA	3269	1/1	0.91	0.15	-0.70	54,54,54,54	0
54	MG	BA	3438	1/1	0.96	0.17	-0.72	38,38,38,38	0
54	MG	BA	3149	1/1	0.95	0.14	-0.72	49,49,49,49	0
54	MG	DA	3278	1/1	0.62	0.16	-0.75	46,46,46,46	0
54	MG	CA	1644	1/1	0.98	0.15	-0.83	74,74,74,74	0
55	ZN	B5	103	1/1	0.99	0.14	-0.83	58,58,58,58	0
54	MG	BA	3552	1/1	0.97	0.18	-0.85	38,38,38,38	0
54	MG	BA	3416	1/1	0.95	0.17	-0.89	46,46,46,46	0
54	MG	DA	3014	1/1	0.88	0.10	-0.92	52,52,52,52	0
55	ZN	DY	201	1/1	0.84	0.09	-0.99	128,128,128,128	0
54	MG	DA	3322	1/1	0.96	0.15	-1.02	35,35,35,35	0
54	MG	DA	3285	1/1	0.98	0.13	-1.04	52,52,52,52	0
54	MG	BA	3406	1/1	0.97	0.18	-1.05	40,40,40,40	0
55	ZN	B6	101	1/1	0.99	0.12	-1.14	54,54,54,54	0
54	MG	DA	3094	1/1	0.97	0.12	-1.14	39,39,39,39	0
55	ZN	D5	101	1/1	0.98	0.07	-1.18	65,65,65,65	0
54	MG	BA	3603	1/1	0.98	0.19	-1.19	30,30,30,30	0
54	MG	BA	3029	1/1	0.87	0.15	-1.23	83,83,83,83	0
54	MG	BA	3238	1/1	0.97	0.16	-1.23	32,32,32,32	0
54	MG	CA	1641	1/1	0.90	0.19	-1.24	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3389	1/1	0.95	0.14	-1.26	58,58,58,58	0
54	MG	AA	1697	1/1	0.69	0.16	-1.31	75,75,75,75	0
55	ZN	AN	101	1/1	0.36	0.14	-1.33	213,213,213,213	0
54	MG	BA	3314	1/1	0.58	0.16	-1.34	71,71,71,71	0
54	MG	DA	3376	1/1	0.87	0.13	-1.36	43,43,43,43	0
54	MG	BA	3320	1/1	0.77	0.15	-1.37	57,57,57,57	0
54	MG	DA	3360	1/1	0.49	0.13	-1.40	63,63,63,63	0
54	MG	BA	3304	1/1	0.95	0.17	-1.43	27,27,27,27	0
54	MG	BA	3515	1/1	0.94	0.12	-1.48	46,46,46,46	0
55	ZN	CN	101	1/1	0.65	0.17	-1.49	188,188,188,188	0
54	MG	BA	3511	1/1	0.90	0.16	-1.53	33,33,33,33	0
54	MG	CA	1666	1/1	0.89	0.09	-1.57	131,131,131,131	0
54	MG	BA	3386	1/1	0.78	0.12	-1.60	77,77,77,77	0
54	MG	BA	3570	1/1	0.98	0.17	-1.63	36,36,36,36	0
54	MG	BA	3006	1/1	0.88	0.17	-1.66	44,44,44,44	0
55	ZN	D6	101	1/1	0.96	0.10	-1.67	86,86,86,86	0
54	MG	BA	3397	1/1	0.93	0.18	-1.68	31,31,31,31	0
55	ZN	D4	101	1/1	0.83	0.05	-1.71	176,176,176,176	0
54	MG	BA	3023	1/1	0.84	0.12	-1.74	52,52,52,52	0
54	MG	BA	3309	1/1	0.97	0.16	-1.78	38,38,38,38	0
54	MG	DA	3296	1/1	0.91	0.12	-1.80	50,50,50,50	0
54	MG	DA	3355	1/1	0.83	0.11	-1.83	37,37,37,37	0
54	MG	DA	3306	1/1	0.85	0.11	-1.84	88,88,88,88	0
54	MG	BA	3357	1/1	0.90	0.15	-1.86	47,47,47,47	0
54	MG	BA	3156	1/1	0.94	0.15	-1.87	57,57,57,57	0
55	ZN	D9	101	1/1	0.97	0.05	-1.95	87,87,87,87	0
54	MG	DA	3329	1/1	0.86	0.12	-1.97	47,47,47,47	0
54	MG	BA	3355	1/1	0.94	0.16	-1.99	54,54,54,54	0
54	MG	DA	3058	1/1	0.81	0.11	-2.00	51,51,51,51	0
54	MG	BA	3105	1/1	0.87	0.12	-2.01	40,40,40,40	0
54	MG	DA	3375	1/1	0.92	0.14	-2.02	50,50,50,50	0
55	ZN	B9	101	1/1	0.98	0.13	-2.04	69,69,69,69	0
54	MG	DA	3276	1/1	0.97	0.12	-2.09	51,51,51,51	0
55	ZN	B4	101	1/1	0.65	0.06	-2.10	200,200,200,200	0
54	MG	DA	3183	1/1	0.94	0.13	-2.13	50,50,50,50	0
54	MG	BA	3378	1/1	0.98	0.12	-2.13	38,38,38,38	0
54	MG	BA	3485	1/1	0.95	0.14	-2.15	60,60,60,60	0
54	MG	AA	1664	1/1	0.93	0.15	-2.19	85,85,85,85	0
54	MG	DA	3274	1/1	0.96	0.10	-2.20	35,35,35,35	0
54	MG	DA	3299	1/1	0.80	0.14	-2.22	54,54,54,54	0
54	MG	DA	3333	1/1	0.96	0.06	-2.26	53,53,53,53	0
54	MG	DA	3377	1/1	0.96	0.10	-2.37	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3312	1/1	0.92	0.09	-2.45	67,67,67,67	0
54	MG	DA	3288	1/1	0.97	0.12	-2.46	37,37,37,37	0
54	MG	DA	3315	1/1	0.88	0.13	-2.47	59,59,59,59	0
54	MG	BA	3402	1/1	0.92	0.08	-2.49	47,47,47,47	0
54	MG	BA	3528	1/1	0.96	0.12	-2.54	43,43,43,43	0
54	MG	BA	3331	1/1	0.98	0.16	-2.57	51,51,51,51	0
54	MG	CA	1643	1/1	0.74	0.06	-2.60	109,109,109,109	0
54	MG	DA	3363	1/1	0.73	0.10	-2.65	72,72,72,72	0
54	MG	BA	3479	1/1	0.93	0.17	-2.66	35,35,35,35	0
54	MG	BA	3038	1/1	0.96	0.10	-2.70	36,36,36,36	0
54	MG	DA	3352	1/1	0.99	0.10	-2.79	61,61,61,61	0
54	MG	AA	1693	1/1	0.92	0.10	-2.82	78,78,78,78	0
54	MG	BA	3576	1/1	0.97	0.12	-2.82	41,41,41,41	0
54	MG	BA	3022	1/1	0.89	0.09	-2.85	57,57,57,57	0
54	MG	AA	1691	1/1	0.79	0.10	-2.86	58,58,58,58	0
54	MG	BE	306	1/1	0.93	0.09	-2.89	56,56,56,56	0
54	MG	CA	1654	1/1	0.98	0.11	-2.93	95,95,95,95	0
54	MG	BA	3491	1/1	0.94	0.14	-2.95	65,65,65,65	0
54	MG	DA	3104	1/1	0.88	0.11	-2.95	57,57,57,57	0
54	MG	AA	1704	1/1	0.93	0.11	-3.03	90,90,90,90	0
54	MG	BA	3025	1/1	0.96	0.11	-3.03	52,52,52,52	0
54	MG	CA	1627	1/1	0.88	0.13	-3.08	79,79,79,79	0
54	MG	DA	3418	1/1	0.99	0.07	-3.27	39,39,39,39	0
54	MG	BA	3421	1/1	0.97	0.14	-3.39	36,36,36,36	0
54	MG	AA	1617	1/1	0.93	0.11	-3.48	82,82,82,82	0
54	MG	BA	3484	1/1	0.98	0.12	-3.48	40,40,40,40	0
54	MG	DA	3281	1/1	0.99	0.09	-3.52	36,36,36,36	0
54	MG	BA	3505	1/1	0.92	0.07	-3.55	76,76,76,76	0
54	MG	BA	3596	1/1	0.98	0.13	-3.57	46,46,46,46	0
54	MG	BA	3404	1/1	0.94	0.11	-3.59	46,46,46,46	0
54	MG	DA	3270	1/1	0.98	0.11	-3.60	34,34,34,34	0
54	MG	BA	3398	1/1	0.97	0.17	-3.66	36,36,36,36	0
54	MG	DA	3010	1/1	0.96	0.15	-3.77	43,43,43,43	0
54	MG	BA	3403	1/1	0.98	0.13	-3.94	44,44,44,44	0
54	MG	BA	3605	1/1	0.98	0.12	-3.98	30,30,30,30	0
54	MG	DA	3382	1/1	0.92	0.10	-4.02	53,53,53,53	0
54	MG	BA	3327	1/1	0.86	0.17	-4.10	34,34,34,34	0
54	MG	BA	3560	1/1	0.99	0.12	-4.19	29,29,29,29	0
54	MG	BA	3295	1/1	0.91	0.11	-4.20	44,44,44,44	0
54	MG	BA	3321	1/1	0.96	0.11	-4.39	65,65,65,65	0
54	MG	BA	3602	1/1	0.98	0.09	-4.64	24,24,24,24	0
54	MG	AA	1689	1/1	0.98	0.09	-4.77	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3385	1/1	0.97	0.10	-4.85	73,73,73,73	0
54	MG	BA	3409	1/1	0.97	0.18	-5.21	26,26,26,26	0
54	MG	CA	1652	1/1	0.98	0.10	-5.49	65,65,65,65	0
54	MG	BA	3019	1/1	0.94	0.11	-5.67	39,39,39,39	0
54	MG	BA	3177	1/1	0.98	0.10	-6.08	45,45,45,45	0
54	MG	BA	3597	1/1	0.99	0.09	-6.29	26,26,26,26	0
54	MG	BA	3532	1/1	0.89	0.09	-6.31	35,35,35,35	0
54	MG	BA	3376	1/1	0.95	0.11	-6.52	55,55,55,55	0
54	MG	BA	3379	1/1	0.96	0.06	-7.04	56,56,56,56	0
54	MG	BA	3516	1/1	0.97	0.14	-7.27	39,39,39,39	0
54	MG	BA	3020	1/1	0.97	0.10	-7.42	34,34,34,34	0
54	MG	BA	3601	1/1	0.98	0.06	-7.58	33,33,33,33	0
54	MG	BA	3540	1/1	0.98	0.06	-9.15	61,61,61,61	0
54	MG	BA	3312	1/1	0.96	0.09	-10.41	50,50,50,50	0
54	MG	BA	3354	1/1	0.96	0.06	-11.60	49,49,49,49	0
54	MG	BA	3494	1/1	0.94	0.46	-	44,44,44,44	0
54	MG	BA	3174	1/1	0.77	0.40	-	71,71,71,71	0
54	MG	BA	3618	1/1	0.77	0.18	-	85,85,85,85	0
54	MG	AA	1649	1/1	0.93	0.20	-	66,66,66,66	0
54	MG	AA	1658	1/1	0.94	0.16	-	60,60,60,60	0
54	MG	BA	3118	1/1	0.79	0.88	-	57,57,57,57	0
54	MG	BA	3181	1/1	0.91	0.21	-	48,48,48,48	0
54	MG	BA	3425	1/1	0.87	0.14	-	37,37,37,37	0
54	MG	DA	3286	1/1	0.92	0.16	-	50,50,50,50	0
54	MG	DA	3150	1/1	0.96	0.38	-	41,41,41,41	0
54	MG	BA	3229	1/1	0.96	0.36	-	51,51,51,51	0
54	MG	DA	3225	1/1	0.94	0.26	-	64,64,64,64	0
54	MG	AA	1648	1/1	0.94	0.19	-	62,62,62,62	0
54	MG	DA	3249	1/1	0.95	0.37	-	67,67,67,67	0
54	MG	DA	3415	1/1	0.89	0.10	-	89,89,89,89	0
54	MG	DA	3126	1/1	0.81	0.12	-	80,80,80,80	0
54	MG	BA	3581	1/1	0.83	0.14	-	47,47,47,47	0
54	MG	CA	1630	1/1	0.92	0.47	-	72,72,72,72	0
54	MG	DA	3065	1/1	0.92	0.19	-	58,58,58,58	0
54	MG	BA	3049	1/1	0.94	0.19	-	54,54,54,54	0
54	MG	BA	3530	1/1	0.89	0.11	-	84,84,84,84	0
54	MG	BA	3436	1/1	0.89	0.32	-	38,38,38,38	0
54	MG	DA	3428	1/1	0.94	0.12	-	81,81,81,81	0
54	MG	BA	3617	1/1	0.76	0.15	-	93,93,93,93	0
54	MG	DA	3198	1/1	0.91	0.17	-	55,55,55,55	0
54	MG	BA	3477	1/1	0.98	0.08	-	45,45,45,45	0
54	MG	BA	3604	1/1	0.97	0.07	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3187	1/1	0.91	0.66	-	47,47,47,47	0
54	MG	AA	1675	1/1	0.67	0.40	-	73,73,73,73	0
54	MG	BA	3082	1/1	0.84	0.28	-	71,71,71,71	0
54	MG	BA	3430	1/1	0.98	0.22	-	30,30,30,30	0
54	MG	AA	1638	1/1	0.79	0.24	-	78,78,78,78	0
54	MG	BE	302	1/1	0.89	0.21	-	52,52,52,52	0
54	MG	BA	3076	1/1	0.77	0.13	-	70,70,70,70	0
54	MG	BA	3115	1/1	0.96	0.36	-	43,43,43,43	0
54	MG	DA	3419	1/1	0.98	0.08	-	50,50,50,50	0
54	MG	BA	3286	1/1	0.92	0.24	-	52,52,52,52	0
54	MG	BA	3482	1/1	0.98	0.18	-	58,58,58,58	0
54	MG	DA	3337	1/1	0.94	0.10	-	42,42,42,42	0
54	MG	BA	3442	1/1	0.97	0.15	-	31,31,31,31	0
54	MG	AA	1671	1/1	0.86	0.25	-	89,89,89,89	0
54	MG	DA	3265	1/1	0.95	0.21	-	39,39,39,39	0
54	MG	BA	3527	1/1	0.90	0.15	-	51,51,51,51	0
54	MG	BA	3050	1/1	0.89	0.23	-	46,46,46,46	0
54	MG	BA	3507	1/1	0.97	0.15	-	53,53,53,53	0
54	MG	DA	3068	1/1	0.95	0.23	-	48,48,48,48	0
54	MG	DA	3210	1/1	0.71	0.28	-	60,60,60,60	0
54	MG	AA	1678	1/1	0.74	0.45	-	75,75,75,75	0
54	MG	BA	3549	1/1	0.89	0.12	-	68,68,68,68	0
54	MG	BA	3279	1/1	0.92	0.17	-	54,54,54,54	0
54	MG	DA	3250	1/1	0.93	0.43	-	41,41,41,41	0
54	MG	DA	3266	1/1	0.95	0.09	-	58,58,58,58	0
54	MG	DA	3230	1/1	0.95	0.17	-	67,67,67,67	0
54	MG	BA	3388	1/1	0.88	0.17	-	54,54,54,54	0
54	MG	DA	3232	1/1	0.87	0.36	-	46,46,46,46	0
54	MG	BA	3064	1/1	0.88	0.27	-	45,45,45,45	0
54	MG	BA	3319	1/1	0.95	0.06	-	68,68,68,68	0
54	MG	AA	1667	1/1	0.80	0.28	-	63,63,63,63	0
54	MG	BA	3443	1/1	0.99	0.26	-	41,41,41,41	0
54	MG	DA	3272	1/1	0.96	0.18	-	47,47,47,47	0
54	MG	BA	3089	1/1	0.92	0.40	-	46,46,46,46	0
54	MG	CA	1667	1/1	0.87	0.14	-	64,64,64,64	0
54	MG	BA	3216	1/1	0.79	0.23	-	52,52,52,52	0
54	MG	BA	3125	1/1	0.94	0.23	-	50,50,50,50	0
54	MG	DA	3195	1/1	0.87	0.84	-	75,75,75,75	0
54	MG	CA	1605	1/1	0.83	0.32	-	74,74,74,74	0
54	MG	BE	303	1/1	0.96	0.14	-	54,54,54,54	0
54	MG	BA	3251	1/1	0.78	0.34	-	63,63,63,63	0
54	MG	DA	3026	1/1	0.85	0.16	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3109	1/1	0.78	0.26	-	70,70,70,70	0
54	MG	BA	3263	1/1	0.96	0.62	-	41,41,41,41	0
54	MG	BA	3220	1/1	0.76	0.24	-	79,79,79,79	0
54	MG	BA	3194	1/1	0.73	0.22	-	79,79,79,79	0
54	MG	CA	1621	1/1	0.83	0.26	-	64,64,64,64	0
54	MG	AA	1626	1/1	0.96	0.52	-	67,67,67,67	0
54	MG	DA	3031	1/1	0.95	0.45	-	43,43,43,43	0
54	MG	BA	3171	1/1	0.84	0.24	-	67,67,67,67	0
54	MG	BA	3574	1/1	0.98	0.06	-	41,41,41,41	0
54	MG	DA	3254	1/1	0.80	0.39	-	43,43,43,43	0
54	MG	BA	3287	1/1	0.95	0.45	-	65,65,65,65	0
54	MG	BA	3591	1/1	0.97	0.13	-	56,56,56,56	0
54	MG	DA	3139	1/1	0.88	0.49	-	65,65,65,65	0
54	MG	BA	3248	1/1	0.98	0.19	-	50,50,50,50	0
54	MG	BA	3168	1/1	0.95	0.39	-	52,52,52,52	0
54	MG	AA	1628	1/1	0.69	0.28	-	84,84,84,84	0
54	MG	DA	3075	1/1	0.68	0.45	-	71,71,71,71	0
54	MG	BA	3296	1/1	0.98	0.08	-	48,48,48,48	0
54	MG	DA	3244	1/1	0.89	0.46	-	35,35,35,35	0
54	MG	BA	3214	1/1	0.94	0.56	-	34,34,34,34	0
54	MG	DA	3206	1/1	0.65	0.18	-	75,75,75,75	0
54	MG	DA	3330	1/1	0.92	0.25	-	44,44,44,44	0
54	MG	BA	3203	1/1	0.94	0.31	-	69,69,69,69	0
54	MG	DA	3211	1/1	0.82	0.26	-	53,53,53,53	0
54	MG	DA	3411	1/1	0.90	0.15	-	90,90,90,90	0
54	MG	BA	3073	1/1	0.90	0.11	-	67,67,67,67	0
54	MG	DA	3100	1/1	0.95	0.32	-	61,61,61,61	0
54	MG	BA	3488	1/1	0.97	0.15	-	34,34,34,34	0
54	MG	AA	1629	1/1	0.93	0.15	-	63,63,63,63	0
54	MG	BA	3462	1/1	0.97	0.12	-	25,25,25,25	0
54	MG	DA	3143	1/1	0.67	0.55	-	62,62,62,62	0
54	MG	DA	3156	1/1	0.96	0.26	-	52,52,52,52	0
54	MG	BA	3061	1/1	0.90	0.51	-	64,64,64,64	0
54	MG	AA	1688	1/1	0.83	0.21	-	111,111,111,111	0
54	MG	DA	3253	1/1	0.96	0.30	-	42,42,42,42	0
54	MG	DA	3386	1/1	0.90	0.11	-	63,63,63,63	0
54	MG	BA	3610	1/1	0.95	0.06	-	56,56,56,56	0
54	MG	BA	3042	1/1	0.95	0.50	-	47,47,47,47	0
54	MG	DA	3316	1/1	0.88	0.12	-	75,75,75,75	0
54	MG	BA	3072	1/1	0.89	0.28	-	59,59,59,59	0
54	MG	BA	3508	1/1	0.95	0.12	-	40,40,40,40	0
54	MG	DA	3228	1/1	0.95	0.54	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3176	1/1	0.94	0.33	-	61,61,61,61	0
54	MG	BA	3347	1/1	0.91	0.22	-	55,55,55,55	0
54	MG	DA	3193	1/1	0.93	0.33	-	63,63,63,63	0
54	MG	BA	3155	1/1	0.90	0.36	-	64,64,64,64	0
54	MG	BA	3233	1/1	0.95	0.13	-	59,59,59,59	0
54	MG	DA	3379	1/1	0.65	0.09	-	94,94,94,94	0
54	MG	BA	3375	1/1	0.81	0.33	-	46,46,46,46	0
54	MG	AA	1652	1/1	0.72	0.66	-	82,82,82,82	0
54	MG	BA	3558	1/1	0.75	0.17	-	61,61,61,61	0
54	MG	DA	3141	1/1	0.81	0.53	-	74,74,74,74	0
54	MG	DA	3351	1/1	0.96	0.15	-	78,78,78,78	0
54	MG	DA	3399	1/1	0.94	0.41	-	60,60,60,60	0
54	MG	BA	3015	1/1	0.92	0.37	-	42,42,42,42	0
54	MG	BA	3176	1/1	0.87	0.50	-	69,69,69,69	0
54	MG	BF	301	1/1	0.91	0.39	-	56,56,56,56	0
54	MG	BA	3260	1/1	0.94	0.61	-	50,50,50,50	0
54	MG	BB	212	1/1	0.93	0.06	-	68,68,68,68	0
54	MG	BA	3054	1/1	0.94	0.15	-	52,52,52,52	0
54	MG	DA	3103	1/1	0.74	0.30	-	71,71,71,71	0
54	MG	DA	3346	1/1	0.66	0.10	-	89,89,89,89	0
54	MG	BB	214	1/1	0.83	0.17	-	67,67,67,67	0
54	MG	DA	3339	1/1	0.91	0.11	-	48,48,48,48	0
54	MG	DA	3275	1/1	0.96	0.12	-	48,48,48,48	0
54	MG	DA	3361	1/1	0.96	0.06	-	67,67,67,67	0
54	MG	BA	3358	1/1	0.90	0.07	-	64,64,64,64	0
54	MG	AA	1663	1/1	0.77	0.43	-	70,70,70,70	0
54	MG	DA	3049	1/1	0.89	0.30	-	58,58,58,58	0
54	MG	AA	1607	1/1	0.93	0.40	-	69,69,69,69	0
54	MG	BA	3135	1/1	0.80	0.45	-	54,54,54,54	0
54	MG	DA	3338	1/1	0.95	0.19	-	50,50,50,50	0
54	MG	BA	3469	1/1	0.77	0.25	-	77,77,77,77	0
54	MG	DA	3320	1/1	0.97	0.13	-	57,57,57,57	0
54	MG	BA	3269	1/1	0.88	0.26	-	54,54,54,54	0
54	MG	BA	3027	1/1	0.92	0.15	-	56,56,56,56	0
54	MG	DA	3310	1/1	0.76	0.29	-	56,56,56,56	0
54	MG	BA	3564	1/1	0.96	0.28	-	36,36,36,36	0
54	MG	BA	3011	1/1	0.81	0.58	-	50,50,50,50	0
54	MG	BA	3146	1/1	0.93	0.50	-	52,52,52,52	0
54	MG	BA	3166	1/1	0.82	0.48	-	58,58,58,58	0
54	MG	DA	3091	1/1	0.68	0.16	-	70,70,70,70	0
54	MG	BA	3144	1/1	0.89	0.36	-	54,54,54,54	0
54	MG	DA	3093	1/1	0.87	0.72	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3171	1/1	0.97	0.31	-	53,53,53,53	0
54	MG	BA	3440	1/1	0.97	0.09	-	63,63,63,63	0
54	MG	DA	3251	1/1	0.95	0.48	-	39,39,39,39	0
54	MG	AA	1683	1/1	0.82	0.30	-	139,139,139,139	0
54	MG	BA	3506	1/1	0.97	0.16	-	61,61,61,61	0
54	MG	DA	3234	1/1	0.95	0.48	-	56,56,56,56	0
54	MG	DA	3220	1/1	0.98	0.25	-	48,48,48,48	0
54	MG	DA	3023	1/1	0.82	0.49	-	61,61,61,61	0
54	MG	BA	3184	1/1	0.76	0.20	-	66,66,66,66	0
54	MG	AA	1687	1/1	0.73	0.14	-	70,70,70,70	0
54	MG	BA	3018	1/1	0.92	0.11	-	72,72,72,72	0
54	MG	DA	3148	1/1	0.93	0.41	-	70,70,70,70	0
54	MG	DA	3414	1/1	0.97	0.12	-	68,68,68,68	0
54	MG	DA	3307	1/1	0.98	0.22	-	39,39,39,39	0
54	MG	BA	3359	1/1	0.94	0.13	-	49,49,49,49	0
54	MG	BA	3352	1/1	0.97	0.09	-	53,53,53,53	0
54	MG	BA	3547	1/1	0.94	0.24	-	31,31,31,31	0
54	MG	BP	201	1/1	0.91	0.28	-	43,43,43,43	0
54	MG	BA	3062	1/1	0.84	0.08	-	69,69,69,69	0
54	MG	DA	3298	1/1	0.87	0.14	-	71,71,71,71	0
54	MG	BA	3413	1/1	0.95	0.28	-	31,31,31,31	0
54	MG	BA	3593	1/1	0.69	0.10	-	70,70,70,70	0
54	MG	DA	3182	1/1	0.88	0.28	-	59,59,59,59	0
54	MG	BA	3463	1/1	0.88	0.20	-	36,36,36,36	0
54	MG	BA	3316	1/1	0.90	0.32	-	34,34,34,34	0
54	MG	BA	3150	1/1	0.90	0.22	-	61,61,61,61	0
54	MG	DA	3218	1/1	0.96	0.71	-	53,53,53,53	0
54	MG	BA	3147	1/1	0.82	0.30	-	57,57,57,57	0
54	MG	CA	1657	1/1	0.91	0.23	-	86,86,86,86	0
54	MG	BA	3567	1/1	0.82	0.09	-	62,62,62,62	0
54	MG	CA	1619	1/1	0.61	0.45	-	69,69,69,69	0
54	MG	AA	1706	1/1	0.89	0.08	-	100,100,100,100	0
54	MG	DA	3293	1/1	0.91	0.29	-	50,50,50,50	0
54	MG	BA	3224	1/1	0.79	0.31	-	61,61,61,61	0
54	MG	DA	3404	1/1	0.99	0.06	-	53,53,53,53	0
54	MG	BA	3495	1/1	0.85	0.19	-	70,70,70,70	0
54	MG	CA	1651	1/1	0.95	0.17	-	61,61,61,61	0
54	MG	DA	3321	1/1	0.95	0.21	-	53,53,53,53	0
54	MG	BA	3101	1/1	0.91	0.28	-	51,51,51,51	0
54	MG	AA	1620	1/1	0.77	0.92	-	77,77,77,77	0
54	MG	DA	3332	1/1	0.98	0.05	-	62,62,62,62	0
54	MG	DA	3359	1/1	0.93	0.37	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3041	1/1	0.91	0.12	-	56,56,56,56	0
54	MG	BA	3539	1/1	0.97	0.06	-	61,61,61,61	0
54	MG	BA	3335	1/1	0.89	0.15	-	55,55,55,55	0
54	MG	BA	3453	1/1	0.94	0.17	-	74,74,74,74	0
54	MG	BA	3188	1/1	0.93	0.28	-	43,43,43,43	0
54	MG	DA	3255	1/1	0.97	0.37	-	63,63,63,63	0
54	MG	BA	3502	1/1	0.97	0.17	-	41,41,41,41	0
54	MG	DA	3161	1/1	0.87	0.47	-	55,55,55,55	0
54	MG	BA	3608	1/1	0.60	0.12	-	87,87,87,87	0
54	MG	BA	3490	1/1	0.96	0.27	-	53,53,53,53	0
54	MG	CA	1610	1/1	0.84	0.43	-	80,80,80,80	0
54	MG	DA	3362	1/1	0.85	0.11	-	63,63,63,63	0
54	MG	DA	3166	1/1	0.96	0.22	-	55,55,55,55	0
54	MG	BA	3079	1/1	0.81	0.27	-	68,68,68,68	0
54	MG	DA	3239	1/1	0.89	0.28	-	39,39,39,39	0
54	MG	BA	3349	1/1	0.96	0.13	-	39,39,39,39	0
54	MG	BA	3616	1/1	0.90	0.08	-	82,82,82,82	0
54	MG	BA	3400	1/1	0.94	0.19	-	34,34,34,34	0
54	MG	DA	3201	1/1	0.93	0.36	-	69,69,69,69	0
54	MG	BA	3235	1/1	0.94	0.12	-	45,45,45,45	0
54	MG	AA	1637	1/1	0.75	0.33	-	82,82,82,82	0
54	MG	BA	3058	1/1	0.96	0.10	-	56,56,56,56	0
54	MG	DA	3042	1/1	0.92	0.58	-	46,46,46,46	0
54	MG	DA	3191	1/1	0.95	0.26	-	50,50,50,50	0
54	MG	BA	3008	1/1	0.96	0.28	-	32,32,32,32	0
54	MG	DA	3106	1/1	0.81	0.33	-	56,56,56,56	0
54	MG	DA	3063	1/1	0.85	0.19	-	54,54,54,54	0
54	MG	BA	3369	1/1	0.91	0.31	-	74,74,74,74	0
54	MG	BA	3459	1/1	0.40	0.14	-	130,130,130,130	0
54	MG	DA	3089	1/1	0.75	0.38	-	82,82,82,82	0
54	MG	DA	3153	1/1	0.95	0.47	-	38,38,38,38	0
54	MG	BA	3538	1/1	0.84	0.13	-	70,70,70,70	0
54	MG	BA	3128	1/1	0.94	0.20	-	53,53,53,53	0
54	MG	D7	101	1/1	0.91	0.30	-	52,52,52,52	0
54	MG	BA	3250	1/1	0.90	0.23	-	47,47,47,47	0
54	MG	BA	3541	1/1	0.96	0.30	-	54,54,54,54	0
54	MG	BA	3542	1/1	0.92	0.23	-	60,60,60,60	0
54	MG	DA	3308	1/1	0.97	0.42	-	49,49,49,49	0
54	MG	AA	1665	1/1	0.54	0.53	-	86,86,86,86	0
54	MG	BE	305	1/1	0.97	0.22	-	32,32,32,32	0
54	MG	DA	3102	1/1	0.71	0.47	-	79,79,79,79	0
54	MG	BA	3365	1/1	0.84	0.10	-	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1646	1/1	0.86	0.38	-	73,73,73,73	0
54	MG	AA	1611	1/1	0.84	0.30	-	69,69,69,69	0
54	MG	BA	3582	1/1	0.96	0.12	-	54,54,54,54	0
54	MG	CA	1606	1/1	0.80	0.62	-	81,81,81,81	0
54	MG	DA	3105	1/1	0.92	0.55	-	33,33,33,33	0
54	MG	BA	3545	1/1	0.80	0.18	-	79,79,79,79	0
54	MG	DA	3212	1/1	0.94	0.26	-	38,38,38,38	0
54	MG	BA	3381	1/1	0.98	0.08	-	49,49,49,49	0
54	MG	DA	3077	1/1	0.79	0.21	-	66,66,66,66	0
54	MG	DA	3241	1/1	0.96	0.25	-	63,63,63,63	0
54	MG	DA	3384	1/1	0.93	0.21	-	57,57,57,57	0
54	MG	BA	3481	1/1	0.93	0.10	-	76,76,76,76	0
54	MG	DA	3287	1/1	0.97	0.07	-	46,46,46,46	0
54	MG	CA	1629	1/1	0.87	0.23	-	72,72,72,72	0
54	MG	DA	3257	1/1	0.92	0.61	-	59,59,59,59	0
54	MG	BA	3586	1/1	0.94	0.09	-	58,58,58,58	0
54	MG	AA	1601	1/1	0.91	0.29	-	68,68,68,68	0
54	MG	BA	3100	1/1	0.84	0.33	-	72,72,72,72	0
54	MG	CA	1603	1/1	0.94	0.28	-	73,73,73,73	0
54	MG	BA	3518	1/1	0.97	0.36	-	59,59,59,59	0
54	MG	BA	3566	1/1	0.95	0.21	-	40,40,40,40	0
54	MG	DA	3034	1/1	0.90	0.27	-	74,74,74,74	0
54	MG	BA	3318	1/1	0.92	0.23	-	73,73,73,73	0
54	MG	BA	3373	1/1	0.95	0.09	-	55,55,55,55	0
54	MG	DA	3345	1/1	0.86	0.27	-	100,100,100,100	0
54	MG	DA	3175	1/1	0.81	0.27	-	69,69,69,69	0
54	MG	BA	3140	1/1	0.88	0.46	-	59,59,59,59	0
54	MG	BA	3114	1/1	0.89	0.25	-	43,43,43,43	0
54	MG	BA	3124	1/1	0.90	0.23	-	68,68,68,68	0
54	MG	DA	3248	1/1	0.94	0.55	-	44,44,44,44	0
54	MG	DA	3200	1/1	0.81	0.19	-	67,67,67,67	0
54	MG	BA	3225	1/1	0.81	0.34	-	61,61,61,61	0
54	MG	DA	3331	1/1	0.95	0.17	-	69,69,69,69	0
54	MG	BA	3380	1/1	0.97	0.07	-	50,50,50,50	0
54	MG	AA	1680	1/1	0.92	0.17	-	83,83,83,83	0
54	MG	AA	1692	1/1	0.83	0.53	-	113,113,113,113	0
54	MG	BA	3299	1/1	0.98	0.22	-	38,38,38,38	0
54	MG	DA	3367	1/1	0.91	0.14	-	68,68,68,68	0
54	MG	BA	3278	1/1	0.96	0.25	-	43,43,43,43	0
54	MG	BB	203	1/1	0.94	0.19	-	80,80,80,80	0
54	MG	BA	3584	1/1	0.86	0.14	-	68,68,68,68	0
54	MG	DA	3318	1/1	0.93	0.08	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	AA	1606	1/1	0.84	0.90	-	74,74,74,74	0
54	MG	BA	3294	1/1	0.93	0.20	-	37,37,37,37	0
54	MG	DA	3422	1/1	0.95	0.10	-	75,75,75,75	0
54	MG	DA	3192	1/1	0.77	0.19	-	66,66,66,66	0
54	MG	DA	3009	1/1	0.94	0.26	-	54,54,54,54	0
54	MG	DA	3347	1/1	0.92	0.07	-	76,76,76,76	0
54	MG	BA	3353	1/1	0.95	0.13	-	28,28,28,28	0
54	MG	DA	3025	1/1	0.97	0.18	-	57,57,57,57	0
54	MG	DA	3157	1/1	0.92	0.33	-	69,69,69,69	0
54	MG	AA	1641	1/1	0.81	0.65	-	93,93,93,93	0
54	MG	BD	301	1/1	0.90	0.20	-	41,41,41,41	0
54	MG	DA	3184	1/1	0.94	0.44	-	39,39,39,39	0
54	MG	DA	3216	1/1	0.91	0.19	-	53,53,53,53	0
54	MG	AA	1612	1/1	0.86	0.36	-	76,76,76,76	0
54	MG	BA	3247	1/1	0.89	0.25	-	53,53,53,53	0
54	MG	BA	3313	1/1	0.98	0.12	-	42,42,42,42	0
54	MG	DA	3173	1/1	0.92	0.40	-	49,49,49,49	0
54	MG	BA	3391	1/1	0.96	0.28	-	38,38,38,38	0
54	MG	BA	3218	1/1	0.93	0.37	-	54,54,54,54	0
54	MG	BA	3589	1/1	0.92	0.06	-	70,70,70,70	0
54	MG	DA	3016	1/1	0.95	0.11	-	41,41,41,41	0
54	MG	D6	102	1/1	0.92	0.50	-	64,64,64,64	0
54	MG	BA	3266	1/1	0.93	0.77	-	48,48,48,48	0
54	MG	BA	3401	1/1	0.96	0.17	-	45,45,45,45	0
54	MG	BA	3341	1/1	0.88	0.08	-	69,69,69,69	0
54	MG	BA	3521	1/1	0.92	0.19	-	41,41,41,41	0
54	MG	BA	3383	1/1	0.95	0.17	-	71,71,71,71	0
54	MG	DA	3229	1/1	0.92	0.37	-	55,55,55,55	0
54	MG	BA	3024	1/1	0.87	0.29	-	48,48,48,48	0
54	MG	DA	3005	1/1	0.94	0.19	-	64,64,64,64	0
54	MG	AA	1685	1/1	0.95	0.11	-	77,77,77,77	0
54	MG	BA	3561	1/1	0.94	0.27	-	49,49,49,49	0
54	MG	BA	3342	1/1	0.94	0.08	-	57,57,57,57	0
54	MG	DA	3057	1/1	0.90	0.14	-	67,67,67,67	0
54	MG	CA	1661	1/1	0.78	0.27	-	100,100,100,100	0
54	MG	DA	3069	1/1	0.82	0.48	-	61,61,61,61	0
54	MG	BA	3476	1/1	0.98	0.23	-	44,44,44,44	0
54	MG	BA	3026	1/1	0.90	0.18	-	68,68,68,68	0
54	MG	DA	3295	1/1	0.92	0.17	-	42,42,42,42	0
54	MG	BA	3524	1/1	0.87	0.17	-	77,77,77,77	0
54	MG	DA	3235	1/1	0.96	0.33	-	36,36,36,36	0
54	MG	BA	3270	1/1	0.77	0.32	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3206	1/1	0.84	0.13	-	68,68,68,68	0
54	MG	CA	1669	1/1	0.83	0.10	-	117,117,117,117	0
54	MG	DA	3189	1/1	0.81	0.80	-	66,66,66,66	0
54	MG	DA	3051	1/1	0.94	0.15	-	43,43,43,43	0
54	MG	DA	3227	1/1	0.90	0.39	-	65,65,65,65	0
54	MG	BA	3487	1/1	0.67	0.22	-	94,94,94,94	0
54	MG	AA	1634	1/1	0.91	0.77	-	95,95,95,95	0
54	MG	BA	3578	1/1	0.98	0.20	-	60,60,60,60	0
54	MG	DA	3311	1/1	0.85	0.07	-	65,65,65,65	0
54	MG	DA	3403	1/1	0.88	0.18	-	49,49,49,49	0
54	MG	BA	3464	1/1	0.82	0.32	-	41,41,41,41	0
54	MG	AA	1677	1/1	0.90	0.89	-	81,81,81,81	0
54	MG	DA	3158	1/1	0.91	0.43	-	72,72,72,72	0
54	MG	DA	3081	1/1	0.86	0.23	-	52,52,52,52	0
54	MG	BA	3165	1/1	0.93	0.13	-	56,56,56,56	0
54	MG	B5	102	1/1	0.99	0.08	-	42,42,42,42	0
54	MG	DA	3147	1/1	0.95	0.68	-	78,78,78,78	0
54	MG	BA	3085	1/1	0.92	0.30	-	63,63,63,63	0
54	MG	BA	3356	1/1	0.90	0.28	-	59,59,59,59	0
54	MG	BV	201	1/1	0.80	0.36	-	74,74,74,74	0
54	MG	AA	1603	1/1	0.91	0.11	-	68,68,68,68	0
54	MG	DA	3401	1/1	0.91	0.07	-	85,85,85,85	0
54	MG	BA	3179	1/1	0.95	0.44	-	48,48,48,48	0
54	MG	BA	3446	1/1	0.94	0.10	-	40,40,40,40	0
54	MG	BA	3102	1/1	0.90	0.25	-	59,59,59,59	0
54	MG	BA	3568	1/1	0.96	0.14	-	60,60,60,60	0
54	MG	BA	3298	1/1	0.92	0.11	-	53,53,53,53	0
54	MG	BA	3533	1/1	0.90	0.19	-	48,48,48,48	0
54	MG	AA	1633	1/1	0.89	0.52	-	72,72,72,72	0
54	MG	BA	3445	1/1	0.93	0.09	-	56,56,56,56	0
54	MG	AA	1672	1/1	0.95	0.66	-	82,82,82,82	0
54	MG	DA	3024	1/1	0.88	0.40	-	49,49,49,49	0
54	MG	DA	3335	1/1	0.94	0.25	-	72,72,72,72	0
54	MG	BA	3273	1/1	0.89	0.22	-	66,66,66,66	0
54	MG	AA	1643	1/1	0.77	0.85	-	96,96,96,96	0
54	MG	BA	3418	1/1	0.93	0.09	-	54,54,54,54	0
54	MG	BA	3035	1/1	0.96	0.24	-	45,45,45,45	0
54	MG	DA	3039	1/1	0.97	0.28	-	41,41,41,41	0
54	MG	BA	3343	1/1	0.87	0.06	-	91,91,91,91	0
54	MG	DA	3423	1/1	0.83	0.14	-	79,79,79,79	0
54	MG	BA	3306	1/1	0.94	0.16	-	51,51,51,51	0
54	MG	DA	3271	1/1	0.94	0.10	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3119	1/1	0.92	0.60	-	57,57,57,57	0
54	MG	BB	210	1/1	0.86	0.14	-	67,67,67,67	0
54	MG	BA	3537	1/1	0.93	0.17	-	38,38,38,38	0
54	MG	DA	3131	1/1	0.95	0.28	-	39,39,39,39	0
54	MG	BA	3563	1/1	0.94	0.11	-	67,67,67,67	0
54	MG	DA	3256	1/1	0.82	0.58	-	59,59,59,59	0
54	MG	DA	3426	1/1	0.98	0.10	-	94,94,94,94	0
54	MG	DA	3137	1/1	0.96	0.57	-	64,64,64,64	0
54	MG	BA	3291	1/1	0.95	0.13	-	59,59,59,59	0
54	MG	BA	3588	1/1	0.93	0.25	-	86,86,86,86	0
54	MG	BA	3523	1/1	0.95	0.06	-	79,79,79,79	0
54	MG	BW	201	1/1	0.93	0.17	-	51,51,51,51	0
54	MG	BA	3120	1/1	0.88	0.31	-	42,42,42,42	0
54	MG	BA	3339	1/1	0.83	0.08	-	91,91,91,91	0
54	MG	DA	3164	1/1	0.96	0.23	-	46,46,46,46	0
54	MG	DA	3368	1/1	0.94	0.17	-	78,78,78,78	0
54	MG	BF	302	1/1	0.93	0.21	-	62,62,62,62	0
54	MG	BA	3284	1/1	0.95	0.13	-	40,40,40,40	0
54	MG	AA	1681	1/1	0.92	0.12	-	65,65,65,65	0
54	MG	DA	3348	1/1	0.93	0.12	-	85,85,85,85	0
54	MG	CA	1634	1/1	0.86	0.35	-	101,101,101,101	0
54	MG	BA	3529	1/1	0.78	0.29	-	86,86,86,86	0
54	MG	AA	1644	1/1	0.95	0.34	-	74,74,74,74	0
54	MG	BA	3077	1/1	0.88	0.59	-	43,43,43,43	0
54	MG	DA	3140	1/1	0.93	0.54	-	70,70,70,70	0
54	MG	DA	3260	1/1	0.91	0.50	-	44,44,44,44	0
54	MG	BA	3261	1/1	0.96	0.29	-	59,59,59,59	0
54	MG	CA	1620	1/1	0.96	0.32	-	57,57,57,57	0
54	MG	AA	1610	1/1	0.96	0.29	-	75,75,75,75	0
54	MG	BA	3450	1/1	0.87	0.13	-	71,71,71,71	0
54	MG	BA	3364	1/1	0.96	0.12	-	46,46,46,46	0
54	MG	AA	1661	1/1	0.73	0.80	-	77,77,77,77	0
54	MG	DA	3223	1/1	0.80	0.09	-	104,104,104,104	0
54	MG	BA	3103	1/1	0.91	0.47	-	67,67,67,67	0
54	MG	BA	3075	1/1	0.96	0.30	-	53,53,53,53	0
54	MG	DA	3172	1/1	0.82	0.27	-	50,50,50,50	0
54	MG	BA	3172	1/1	0.93	0.22	-	71,71,71,71	0
54	MG	DA	3179	1/1	0.94	0.27	-	62,62,62,62	0
54	MG	BA	3614	1/1	0.74	0.31	-	94,94,94,94	0
54	MG	BA	3569	1/1	0.81	0.27	-	68,68,68,68	0
54	MG	BA	3496	1/1	0.81	0.10	-	79,79,79,79	0
54	MG	AA	1656	1/1	0.59	0.83	-	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3315	1/1	0.72	0.17	-	84,84,84,84	0
54	MG	BA	3577	1/1	0.94	0.23	-	58,58,58,58	0
54	MG	DA	3424	1/1	0.86	0.14	-	130,130,130,130	0
54	MG	CA	1656	1/1	0.70	0.12	-	97,97,97,97	0
54	MG	BA	3536	1/1	0.85	0.09	-	82,82,82,82	0
54	MG	BA	3310	1/1	0.99	0.21	-	44,44,44,44	0
54	MG	BA	3257	1/1	0.69	0.40	-	64,64,64,64	0
54	MG	BA	3612	1/1	0.78	0.12	-	100,100,100,100	0
54	MG	DA	3357	1/1	0.82	0.14	-	53,53,53,53	0
54	MG	BA	3186	1/1	0.91	0.40	-	64,64,64,64	0
54	MG	BA	3478	1/1	0.90	0.16	-	92,92,92,92	0
54	MG	DA	3381	1/1	0.89	0.09	-	79,79,79,79	0
54	MG	DA	3336	1/1	0.79	0.16	-	87,87,87,87	0
54	MG	BA	3088	1/1	0.93	0.35	-	46,46,46,46	0
54	MG	BA	3452	1/1	0.95	0.11	-	62,62,62,62	0
54	MG	BA	3466	1/1	0.98	0.07	-	67,67,67,67	0
54	MG	DA	3082	1/1	0.76	0.40	-	51,51,51,51	0
54	MG	BA	3449	1/1	0.89	0.18	-	49,49,49,49	0
54	MG	AA	1632	1/1	0.85	0.52	-	93,93,93,93	0
54	MG	DA	3076	1/1	0.96	0.17	-	70,70,70,70	0
54	MG	DA	3180	1/1	0.93	0.24	-	78,78,78,78	0
54	MG	BB	217	1/1	0.99	0.25	-	42,42,42,42	0
54	MG	BA	3531	1/1	0.93	0.15	-	49,49,49,49	0
54	MG	BA	3503	1/1	0.72	0.22	-	68,68,68,68	0
54	MG	BA	3362	1/1	0.89	0.11	-	73,73,73,73	0
54	MG	DA	3197	1/1	0.88	0.65	-	66,66,66,66	0
54	MG	BA	3272	1/1	0.90	0.07	-	65,65,65,65	0
54	MG	BA	3599	1/1	0.97	0.09	-	50,50,50,50	0
54	MG	BA	3324	1/1	0.96	0.10	-	82,82,82,82	0
54	MG	BA	3012	1/1	0.94	0.20	-	34,34,34,34	0
54	MG	AA	1698	1/1	0.91	0.44	-	68,68,68,68	0
54	MG	DA	3021	1/1	0.93	0.24	-	53,53,53,53	0
54	MG	BA	3213	1/1	0.89	0.37	-	64,64,64,64	0
54	MG	AA	1650	1/1	0.88	0.27	-	70,70,70,70	0
54	MG	BA	3325	1/1	0.89	0.11	-	47,47,47,47	0
54	MG	DA	3022	1/1	0.97	0.36	-	52,52,52,52	0
54	MG	BA	3116	1/1	0.88	0.37	-	56,56,56,56	0
54	MG	DA	3300	1/1	0.98	0.20	-	62,62,62,62	0
54	MG	BA	3600	1/1	0.99	0.20	-	31,31,31,31	0
54	MG	DA	3107	1/1	0.77	0.20	-	47,47,47,47	0
54	MG	BA	3439	1/1	0.87	0.18	-	53,53,53,53	0
54	MG	BA	3190	1/1	0.96	0.31	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3585	1/1	0.94	0.24	-	54,54,54,54	0
54	MG	BA	3092	1/1	0.92	0.41	-	55,55,55,55	0
54	MG	AA	1690	1/1	0.93	0.12	-	59,59,59,59	0
54	MG	BA	3096	1/1	0.93	0.53	-	63,63,63,63	0
54	MG	BA	3415	1/1	0.88	0.12	-	49,49,49,49	0
54	MG	DA	3289	1/1	0.95	0.20	-	52,52,52,52	0
54	MG	AA	1679	1/1	0.84	0.35	-	64,64,64,64	0
54	MG	DA	3008	1/1	0.85	0.22	-	48,48,48,48	0
54	MG	BA	3550	1/1	0.98	0.28	-	37,37,37,37	0
54	MG	BA	3099	1/1	0.94	0.28	-	52,52,52,52	0
54	MG	DA	3258	1/1	0.92	0.10	-	56,56,56,56	0
54	MG	BA	3419	1/1	0.97	0.25	-	35,35,35,35	0
54	MG	DA	3430	1/1	0.97	0.05	-	72,72,72,72	0
54	MG	BA	3162	1/1	0.96	0.48	-	62,62,62,62	0
54	MG	BA	3182	1/1	0.95	0.09	-	69,69,69,69	0
54	MG	BA	3534	1/1	0.67	0.27	-	76,76,76,76	0
54	MG	AA	1701	1/1	0.93	0.12	-	96,96,96,96	0
54	MG	BA	3154	1/1	0.90	0.15	-	49,49,49,49	0
54	MG	BA	3609	1/1	0.98	0.18	-	51,51,51,51	0
54	MG	DA	3037	1/1	0.77	0.45	-	49,49,49,49	0
54	MG	BA	3433	1/1	0.94	0.14	-	35,35,35,35	0
54	MG	BA	3068	1/1	0.86	0.18	-	70,70,70,70	0
54	MG	BA	3374	1/1	0.57	0.14	-	75,75,75,75	0
54	MG	AA	1639	1/1	0.87	0.20	-	74,74,74,74	0
54	MG	B5	101	1/1	0.91	0.29	-	51,51,51,51	0
54	MG	BA	3384	1/1	0.80	0.11	-	62,62,62,62	0
54	MG	DB	203	1/1	0.93	0.48	-	61,61,61,61	0
54	MG	DA	3045	1/1	0.94	0.36	-	72,72,72,72	0
54	MG	DA	3391	1/1	0.83	0.14	-	67,67,67,67	0
54	MG	BA	3264	1/1	0.87	0.61	-	38,38,38,38	0
54	MG	BA	3158	1/1	0.89	0.35	-	51,51,51,51	0
54	MG	BA	3444	1/1	0.90	0.06	-	61,61,61,61	0
54	MG	BA	3431	1/1	0.98	0.25	-	34,34,34,34	0
54	MG	DA	3050	1/1	0.69	0.16	-	90,90,90,90	0
54	MG	DA	3096	1/1	0.93	0.41	-	46,46,46,46	0
54	MG	BA	3571	1/1	0.92	0.14	-	76,76,76,76	0
54	MG	BA	3056	1/1	0.95	0.40	-	48,48,48,48	0
54	MG	BA	3065	1/1	0.94	0.13	-	47,47,47,47	0
54	MG	BA	3252	1/1	0.95	0.24	-	44,44,44,44	0
54	MG	DA	3152	1/1	0.93	0.46	-	58,58,58,58	0
54	MG	DA	3048	1/1	0.75	0.47	-	53,53,53,53	0
54	MG	DA	3111	1/1	0.87	0.46	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3097	1/1	0.87	0.72	-	64,64,64,64	0
54	MG	DA	3056	1/1	0.87	0.44	-	61,61,61,61	0
54	MG	BA	3138	1/1	0.90	0.19	-	54,54,54,54	0
54	MG	BA	3322	1/1	0.95	0.13	-	45,45,45,45	0
54	MG	BA	3467	1/1	0.92	0.13	-	73,73,73,73	0
54	MG	DA	3035	1/1	0.82	0.64	-	68,68,68,68	0
54	MG	BA	3126	1/1	0.95	0.40	-	57,57,57,57	0
54	MG	DA	3387	1/1	0.81	0.09	-	71,71,71,71	0
54	MG	AA	1642	1/1	0.94	0.16	-	64,64,64,64	0
54	MG	BA	3215	1/1	0.96	0.14	-	61,61,61,61	0
54	MG	BA	3377	1/1	0.93	0.12	-	69,69,69,69	0
54	MG	DA	3194	1/1	0.93	0.54	-	77,77,77,77	0
54	MG	CA	1665	1/1	0.85	0.14	-	76,76,76,76	0
54	MG	DA	3167	1/1	0.94	0.10	-	59,59,59,59	0
54	MG	BA	3196	1/1	0.80	0.79	-	80,80,80,80	0
54	MG	DA	3407	1/1	0.94	0.25	-	59,59,59,59	0
54	MG	AA	1668	1/1	0.98	0.12	-	83,83,83,83	0
54	MG	BA	3005	1/1	0.95	0.14	-	42,42,42,42	0
54	MG	DA	3136	1/1	0.96	0.52	-	42,42,42,42	0
54	MG	BA	3573	1/1	0.96	0.09	-	55,55,55,55	0
54	MG	DA	3108	1/1	0.83	0.18	-	80,80,80,80	0
54	MG	BA	3044	1/1	0.92	0.16	-	49,49,49,49	0
54	MG	BA	3098	1/1	0.91	0.39	-	54,54,54,54	0
54	MG	B2	102	1/1	0.92	0.25	-	60,60,60,60	0
54	MG	BA	3212	1/1	0.95	0.15	-	47,47,47,47	0
54	MG	BA	3093	1/1	0.81	0.18	-	81,81,81,81	0
54	MG	BA	3492	1/1	0.88	0.15	-	78,78,78,78	0
54	MG	AA	1676	1/1	0.81	0.62	-	84,84,84,84	0
54	MG	BA	3595	1/1	0.89	0.09	-	82,82,82,82	0
54	MG	BA	3066	1/1	0.87	0.11	-	43,43,43,43	0
54	MG	CA	1642	1/1	0.96	0.08	-	87,87,87,87	0
54	MG	DA	3165	1/1	0.94	0.17	-	58,58,58,58	0
54	MG	DA	3047	1/1	0.60	0.44	-	65,65,65,65	0
54	MG	DA	3323	1/1	0.96	0.20	-	36,36,36,36	0
54	MG	BA	3414	1/1	0.89	0.28	-	26,26,26,26	0
54	MG	BA	3361	1/1	0.91	0.20	-	53,53,53,53	0
54	MG	BA	3470	1/1	0.97	0.23	-	35,35,35,35	0
54	MG	BA	3145	1/1	0.26	0.48	-	78,78,78,78	0
54	MG	DA	3429	1/1	0.95	0.16	-	44,44,44,44	0
54	MG	DA	3417	1/1	0.86	0.26	-	81,81,81,81	0
54	MG	BA	3167	1/1	0.82	0.35	-	68,68,68,68	0
54	MG	BU	201	1/1	0.81	0.40	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3364	1/1	0.93	0.12	-	67,67,67,67	0
54	MG	BA	3231	1/1	0.92	0.41	-	45,45,45,45	0
54	MG	BA	3134	1/1	0.95	0.45	-	44,44,44,44	0
54	MG	BB	206	1/1	0.93	0.15	-	62,62,62,62	0
54	MG	DA	3088	1/1	0.96	0.26	-	65,65,65,65	0
54	MG	CA	1604	1/1	0.95	0.19	-	110,110,110,110	0
54	MG	CA	1668	1/1	0.65	0.22	-	105,105,105,105	0
54	MG	DA	3215	1/1	0.92	0.23	-	58,58,58,58	0
54	MG	DA	3294	1/1	0.93	0.16	-	52,52,52,52	0
54	MG	BA	3382	1/1	0.94	0.08	-	58,58,58,58	0
54	MG	BA	3055	1/1	0.84	0.32	-	58,58,58,58	0
54	MG	CA	1660	1/1	0.81	0.15	-	106,106,106,106	0
54	MG	BA	3275	1/1	0.94	0.18	-	41,41,41,41	0
54	MG	DA	3159	1/1	0.92	0.61	-	59,59,59,59	0
54	MG	BA	3143	1/1	0.94	0.40	-	45,45,45,45	0
54	MG	BA	3211	1/1	0.95	0.19	-	53,53,53,53	0
54	MG	BA	3163	1/1	0.97	0.43	-	42,42,42,42	0
54	MG	BA	3245	1/1	0.99	0.12	-	36,36,36,36	0
54	MG	BA	3265	1/1	0.94	0.39	-	30,30,30,30	0
54	MG	DA	3145	1/1	0.97	0.44	-	47,47,47,47	0
54	MG	BA	3613	1/1	0.80	0.12	-	109,109,109,109	0
54	MG	AA	1608	1/1	0.80	0.15	-	90,90,90,90	0
54	MG	BA	3185	1/1	0.91	0.23	-	44,44,44,44	0
54	MG	BA	3002	1/1	0.86	0.19	-	98,98,98,98	0
54	MG	BA	3087	1/1	0.89	0.25	-	56,56,56,56	0
54	MG	BA	3063	1/1	0.83	0.21	-	84,84,84,84	0
54	MG	B2	101	1/1	0.83	0.26	-	75,75,75,75	0
54	MG	BA	3338	1/1	0.91	0.15	-	30,30,30,30	0
54	MG	BA	3317	1/1	0.97	0.09	-	51,51,51,51	0
54	MG	CA	1659	1/1	0.90	0.21	-	60,60,60,60	0
54	MG	CA	1662	1/1	0.88	0.18	-	95,95,95,95	0
54	MG	BA	3293	1/1	0.97	0.21	-	29,29,29,29	0
54	MG	BB	207	1/1	0.67	0.60	-	69,69,69,69	0
54	MG	BA	3280	1/1	0.39	0.44	-	89,89,89,89	0
54	MG	BA	3032	1/1	0.86	0.21	-	67,67,67,67	0
54	MG	DA	3129	1/1	0.84	0.35	-	78,78,78,78	0
54	MG	BA	3242	1/1	0.80	0.40	-	66,66,66,66	0
54	MG	BA	3598	1/1	0.95	0.13	-	39,39,39,39	0
54	MG	DA	3273	1/1	0.98	0.11	-	37,37,37,37	0
54	MG	BA	3285	1/1	0.89	0.55	-	59,59,59,59	0
54	MG	BA	3514	1/1	0.71	0.19	-	97,97,97,97	0
54	MG	DA	3190	1/1	0.74	0.34	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3213	1/1	0.90	0.13	-	64,64,64,64	0
54	MG	DA	3263	1/1	0.97	0.08	-	70,70,70,70	0
54	MG	BA	3204	1/1	0.90	0.18	-	47,47,47,47	0
54	MG	BA	3004	1/1	0.90	0.22	-	41,41,41,41	0
54	MG	BA	3346	1/1	0.96	0.07	-	45,45,45,45	0
54	MG	DA	3080	1/1	0.83	1.04	-	73,73,73,73	0
54	MG	DA	3110	1/1	0.98	0.08	-	46,46,46,46	0
54	MG	BA	3393	1/1	0.99	0.19	-	38,38,38,38	0
54	MG	BA	3255	1/1	0.94	0.58	-	65,65,65,65	0
54	MG	CA	1645	1/1	0.92	0.30	-	63,63,63,63	0
54	MG	BA	3336	1/1	0.95	0.12	-	46,46,46,46	0
54	MG	BA	3136	1/1	0.80	0.24	-	73,73,73,73	0
54	MG	BD	303	1/1	0.95	0.35	-	58,58,58,58	0
54	MG	CA	1608	1/1	0.70	0.44	-	67,67,67,67	0
54	MG	DA	3392	1/1	0.98	0.09	-	56,56,56,56	0
54	MG	DA	3261	1/1	0.91	0.42	-	56,56,56,56	0
54	MG	BA	3399	1/1	0.92	0.23	-	41,41,41,41	0
54	MG	BA	3084	1/1	0.95	0.17	-	56,56,56,56	0
54	MG	BA	3535	1/1	0.84	0.24	-	70,70,70,70	0
54	MG	DA	3378	1/1	0.90	0.14	-	98,98,98,98	0
54	MG	CA	1649	1/1	0.89	0.16	-	92,92,92,92	0
54	MG	BA	3198	1/1	0.95	0.25	-	29,29,29,29	0
54	MG	DE	301	1/1	0.94	0.51	-	37,37,37,37	0
54	MG	DA	3155	1/1	0.79	0.28	-	57,57,57,57	0
54	MG	AA	1635	1/1	0.94	0.21	-	71,71,71,71	0
54	MG	AA	1662	1/1	0.94	0.22	-	83,83,83,83	0
54	MG	BA	3297	1/1	0.83	0.17	-	35,35,35,35	0
54	MG	BA	3013	1/1	0.87	0.60	-	103,103,103,103	0
54	MG	DA	3343	1/1	0.94	0.17	-	35,35,35,35	0
54	MG	BU	202	1/1	0.92	0.53	-	62,62,62,62	0
54	MG	CA	1611	1/1	0.91	0.18	-	64,64,64,64	0
54	MG	DA	3224	1/1	0.89	0.34	-	80,80,80,80	0
54	MG	CA	1622	1/1	0.90	0.32	-	74,74,74,74	0
54	MG	BA	3340	1/1	0.78	0.21	-	65,65,65,65	0
54	MG	BA	3036	1/1	0.89	0.41	-	49,49,49,49	0
54	MG	BA	3615	1/1	0.93	0.06	-	91,91,91,91	0
54	MG	DA	3358	1/1	0.92	0.15	-	68,68,68,68	0
54	MG	DA	3400	1/1	0.69	0.33	-	95,95,95,95	0
54	MG	BA	3110	1/1	0.97	0.37	-	23,23,23,23	0
54	MG	DA	3371	1/1	0.93	0.19	-	50,50,50,50	0
54	MG	BA	3217	1/1	0.71	0.39	-	51,51,51,51	0
54	MG	CA	1625	1/1	0.86	0.36	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3389	1/1	0.92	0.20	-	33,33,33,33	0
54	MG	BA	3192	1/1	0.96	0.33	-	43,43,43,43	0
54	MG	BA	3363	1/1	0.73	0.26	-	74,74,74,74	0
54	MG	DA	3060	1/1	0.91	0.21	-	60,60,60,60	0
54	MG	BA	3195	1/1	0.68	0.31	-	84,84,84,84	0
54	MG	DA	3151	1/1	0.94	0.37	-	58,58,58,58	0
54	MG	BR	202	1/1	0.94	0.38	-	49,49,49,49	0
54	MG	BA	3282	1/1	0.94	0.28	-	43,43,43,43	0
54	MG	DA	3221	1/1	0.85	0.48	-	69,69,69,69	0
54	MG	BA	3592	1/1	0.91	0.08	-	51,51,51,51	0
54	MG	BA	3290	1/1	0.95	0.37	-	47,47,47,47	0
54	MG	AA	1614	1/1	0.98	0.23	-	62,62,62,62	0
54	MG	DA	3380	1/1	0.78	0.10	-	91,91,91,91	0
54	MG	BB	216	1/1	0.98	0.33	-	46,46,46,46	0
54	MG	BA	3223	1/1	0.95	0.18	-	57,57,57,57	0
54	MG	DA	3231	1/1	0.91	0.48	-	54,54,54,54	0
54	MG	BA	3337	1/1	0.89	0.24	-	33,33,33,33	0
54	MG	DA	3413	1/1	0.95	0.17	-	37,37,37,37	0
54	MG	DA	3090	1/1	0.94	0.24	-	53,53,53,53	0
54	MG	DA	3326	1/1	0.83	0.10	-	95,95,95,95	0
54	MG	DA	3314	1/1	0.91	0.23	-	54,54,54,54	0
54	MG	AA	1616	1/1	0.72	0.45	-	79,79,79,79	0
54	MG	D8	101	1/1	0.89	0.61	-	49,49,49,49	0
54	MG	BA	3141	1/1	0.90	0.27	-	65,65,65,65	0
54	MG	CA	1650	1/1	0.92	0.20	-	100,100,100,100	0
54	MG	BA	3510	1/1	0.94	0.17	-	33,33,33,33	0
54	MG	BA	3246	1/1	0.98	0.21	-	49,49,49,49	0
54	MG	AA	1651	1/1	0.89	0.85	-	69,69,69,69	0
54	MG	BA	3606	1/1	0.95	0.11	-	29,29,29,29	0
54	MG	BA	3183	1/1	0.46	0.28	-	76,76,76,76	0
54	MG	BA	3458	1/1	0.72	0.19	-	45,45,45,45	0
54	MG	BA	3328	1/1	0.95	0.20	-	27,27,27,27	0
54	MG	BQ	203	1/1	0.96	0.23	-	44,44,44,44	0
54	MG	DA	3038	1/1	0.95	0.33	-	39,39,39,39	0
54	MG	BA	3572	1/1	0.70	0.13	-	49,49,49,49	0
54	MG	DB	202	1/1	0.74	1.21	-	86,86,86,86	0
54	MG	AA	1630	1/1	0.64	0.51	-	76,76,76,76	0
54	MG	BB	209	1/1	0.84	0.17	-	79,79,79,79	0
54	MG	BA	3277	1/1	0.87	0.20	-	66,66,66,66	0
54	MG	BA	3360	1/1	0.86	0.17	-	53,53,53,53	0
54	MG	BA	3543	1/1	0.94	0.19	-	59,59,59,59	0
54	MG	BA	3069	1/1	0.92	0.51	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3015	1/1	0.82	0.39	-	71,71,71,71	0
54	MG	DA	3083	1/1	0.89	0.34	-	55,55,55,55	0
54	MG	DA	3262	1/1	0.91	0.16	-	46,46,46,46	0
54	MG	BA	3051	1/1	0.91	0.15	-	52,52,52,52	0
54	MG	DA	3117	1/1	0.96	0.34	-	34,34,34,34	0
54	MG	AA	1696	1/1	0.81	0.18	-	74,74,74,74	0
54	MG	DA	3071	1/1	0.84	0.34	-	60,60,60,60	0
54	MG	DA	3101	1/1	0.93	0.20	-	62,62,62,62	0
54	MG	BA	3009	1/1	0.83	0.23	-	59,59,59,59	0
54	MG	DA	3317	1/1	0.78	0.18	-	94,94,94,94	0
54	MG	BA	3202	1/1	0.98	0.53	-	65,65,65,65	0
54	MG	DA	3369	1/1	0.92	0.17	-	57,57,57,57	0
54	MG	BA	3344	1/1	0.82	0.10	-	52,52,52,52	0
54	MG	BA	3590	1/1	0.86	0.16	-	82,82,82,82	0
54	MG	BA	3205	1/1	0.65	0.41	-	61,61,61,61	0
54	MG	DA	3252	1/1	0.81	0.36	-	41,41,41,41	0
54	MG	BA	3191	1/1	0.88	0.14	-	45,45,45,45	0
54	MG	B8	103	1/1	0.98	0.14	-	51,51,51,51	0
54	MG	DA	3214	1/1	0.86	0.75	-	74,74,74,74	0
54	MG	DA	3238	1/1	0.95	0.61	-	52,52,52,52	0
54	MG	DA	3313	1/1	0.60	0.19	-	64,64,64,64	0
54	MG	BA	3305	1/1	0.97	0.09	-	37,37,37,37	0
54	MG	DA	3388	1/1	0.71	0.12	-	72,72,72,72	0
54	MG	BA	3611	1/1	0.93	0.07	-	70,70,70,70	0
54	MG	DA	3160	1/1	0.96	0.50	-	48,48,48,48	0
54	MG	BA	3334	1/1	0.86	0.16	-	43,43,43,43	0
54	MG	BA	3289	1/1	0.91	0.67	-	50,50,50,50	0
54	MG	BA	3259	1/1	0.89	0.31	-	51,51,51,51	0
54	MG	BA	3499	1/1	0.65	0.23	-	107,107,107,107	0
54	MG	BA	3227	1/1	0.93	0.19	-	42,42,42,42	0
54	MG	DA	3046	1/1	0.92	0.70	-	43,43,43,43	0
54	MG	B8	101	1/1	0.92	0.40	-	64,64,64,64	0
54	MG	BA	3040	1/1	0.90	0.23	-	33,33,33,33	0
54	MG	BA	3370	1/1	0.98	0.10	-	66,66,66,66	0
54	MG	BA	3208	1/1	0.93	0.29	-	54,54,54,54	0
54	MG	CA	1614	1/1	0.96	0.26	-	69,69,69,69	0
54	MG	DA	3061	1/1	0.93	0.38	-	52,52,52,52	0
54	MG	BA	3420	1/1	0.88	0.28	-	41,41,41,41	0
54	MG	DA	3283	1/1	0.97	0.14	-	48,48,48,48	0
54	MG	DA	3393	1/1	0.73	0.11	-	81,81,81,81	0
54	MG	BA	3067	1/1	0.89	0.36	-	35,35,35,35	0
54	MG	B3	102	1/1	0.94	0.28	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3087	1/1	0.94	0.31	-	58,58,58,58	0
54	MG	DA	3350	1/1	0.95	0.14	-	50,50,50,50	0
54	MG	DA	3186	1/1	0.90	0.24	-	42,42,42,42	0
54	MG	BA	3480	1/1	0.91	0.13	-	70,70,70,70	0
54	MG	AA	1647	1/1	0.96	0.33	-	61,61,61,61	0
54	MG	DA	3122	1/1	0.95	0.52	-	47,47,47,47	0
54	MG	DA	3154	1/1	0.97	0.83	-	62,62,62,62	0
54	MG	BA	3060	1/1	0.98	0.30	-	45,45,45,45	0
54	MG	DA	3373	1/1	0.99	0.27	-	38,38,38,38	0
54	MG	DA	3055	1/1	0.95	0.45	-	43,43,43,43	0
54	MG	CA	1615	1/1	0.83	0.62	-	76,76,76,76	0
54	MG	BA	3579	1/1	0.98	0.12	-	53,53,53,53	0
54	MG	DA	3174	1/1	0.91	0.46	-	60,60,60,60	0
54	MG	BA	3121	1/1	0.89	0.15	-	38,38,38,38	0
54	MG	BA	3371	1/1	0.88	0.10	-	67,67,67,67	0
54	MG	AA	1654	1/1	0.91	0.06	-	87,87,87,87	0
54	MG	BA	3472	1/1	0.95	0.21	-	29,29,29,29	0
54	MG	AA	1623	1/1	0.87	0.47	-	74,74,74,74	0
54	MG	DA	3383	1/1	0.87	0.25	-	63,63,63,63	0
54	MG	DA	3114	1/1	0.84	0.15	-	51,51,51,51	0
54	MG	CA	1664	1/1	0.91	0.16	-	94,94,94,94	0
54	MG	BA	3594	1/1	0.78	0.15	-	70,70,70,70	0
54	MG	CA	1609	1/1	0.71	0.87	-	70,70,70,70	0
54	MG	BA	3123	1/1	0.95	0.20	-	43,43,43,43	0
54	MG	DA	3237	1/1	0.94	0.51	-	39,39,39,39	0
54	MG	BA	3151	1/1	0.92	0.21	-	62,62,62,62	0
54	MG	BA	3112	1/1	0.95	0.40	-	47,47,47,47	0
54	MG	B0	102	1/1	0.89	0.17	-	56,56,56,56	0
54	MG	AA	1625	1/1	0.82	0.25	-	102,102,102,102	0
54	MG	BA	3326	1/1	0.96	0.14	-	30,30,30,30	0
54	MG	DA	3246	1/1	0.87	0.45	-	41,41,41,41	0
54	MG	CA	1658	1/1	0.89	0.17	-	83,83,83,83	0
54	MG	DA	3196	1/1	0.96	0.48	-	63,63,63,63	0
54	MG	AA	1669	1/1	0.90	0.37	-	96,96,96,96	0
54	MG	AA	1695	1/1	0.91	0.12	-	93,93,93,93	0
54	MG	BA	3268	1/1	0.97	0.29	-	44,44,44,44	0
54	MG	DA	3245	1/1	0.83	0.34	-	47,47,47,47	0
54	MG	DA	3409	1/1	0.91	0.06	-	79,79,79,79	0
54	MG	BA	3300	1/1	0.93	0.15	-	37,37,37,37	0
54	MG	BA	3501	1/1	0.91	0.11	-	61,61,61,61	0
54	MG	BA	3200	1/1	0.83	0.23	-	51,51,51,51	0
54	MG	AA	1624	1/1	0.91	0.87	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3033	1/1	0.78	0.30	-	68,68,68,68	0
54	MG	DA	3203	1/1	0.91	0.75	-	48,48,48,48	0
54	MG	AA	1653	1/1	0.82	0.61	-	80,80,80,80	0
54	MG	CA	1635	1/1	0.81	0.18	-	68,68,68,68	0
54	MG	BA	3483	1/1	0.97	0.16	-	57,57,57,57	0
54	MG	DA	3327	1/1	0.77	0.45	-	94,94,94,94	0
54	MG	BA	3525	1/1	0.92	0.07	-	112,112,112,112	0
54	MG	BA	3028	1/1	0.93	0.23	-	46,46,46,46	0
54	MG	AA	1670	1/1	0.89	0.16	-	115,115,115,115	0
54	MG	BA	3139	1/1	0.79	0.28	-	53,53,53,53	0
54	MG	BA	3394	1/1	0.94	0.10	-	29,29,29,29	0
54	MG	CA	1637	1/1	0.90	0.65	-	67,67,67,67	0
54	MG	BA	3548	1/1	0.96	0.20	-	41,41,41,41	0
54	MG	DA	3001	1/1	0.69	0.21	-	62,62,62,62	0
54	MG	DA	3264	1/1	0.98	0.20	-	46,46,46,46	0
54	MG	BB	208	1/1	0.86	0.31	-	70,70,70,70	0
54	MG	BA	3081	1/1	0.90	0.19	-	66,66,66,66	0
54	MG	DF	302	1/1	0.87	0.24	-	64,64,64,64	0
54	MG	BA	3587	1/1	0.78	0.08	-	66,66,66,66	0
54	MG	CA	1639	1/1	0.94	0.64	-	61,61,61,61	0
54	MG	CA	1647	1/1	0.98	0.14	-	78,78,78,78	0
54	MG	DA	3134	1/1	0.90	0.22	-	64,64,64,64	0
54	MG	BA	3274	1/1	0.79	0.14	-	81,81,81,81	0
54	MG	BA	3095	1/1	0.92	0.37	-	45,45,45,45	0
54	MG	AA	1705	1/1	0.96	0.14	-	68,68,68,68	0
54	MG	DA	3334	1/1	0.93	0.16	-	56,56,56,56	0
54	MG	BA	3267	1/1	0.79	0.55	-	53,53,53,53	0
54	MG	DA	3067	1/1	0.95	0.33	-	32,32,32,32	0
54	MG	BA	3447	1/1	0.94	0.28	-	37,37,37,37	0
54	MG	BA	3241	1/1	0.81	0.74	-	62,62,62,62	0
54	MG	DA	3277	1/1	0.96	0.12	-	42,42,42,42	0
54	MG	CA	1640	1/1	0.89	0.28	-	62,62,62,62	0
54	MG	DA	3420	1/1	0.87	0.09	-	97,97,97,97	0
54	MG	DA	3344	1/1	0.98	0.09	-	51,51,51,51	0
54	MG	BA	3468	1/1	0.93	0.15	-	38,38,38,38	0
54	MG	AA	1655	1/1	0.79	0.19	-	90,90,90,90	0
54	MG	BA	3303	1/1	0.98	0.20	-	36,36,36,36	0
54	MG	BA	3554	1/1	0.86	0.21	-	58,58,58,58	0
54	MG	BA	3152	1/1	0.69	0.24	-	73,73,73,73	0
54	MG	AA	1619	1/1	0.92	0.34	-	68,68,68,68	0
54	MG	BA	3097	1/1	0.86	0.38	-	58,58,58,58	0
54	MG	BA	3544	1/1	0.96	0.19	-	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3301	1/1	0.92	0.17	-	55,55,55,55	0
54	MG	DA	3078	1/1	0.93	0.43	-	53,53,53,53	0
54	MG	BA	3210	1/1	0.93	0.24	-	57,57,57,57	0
54	MG	AA	1702	1/1	0.66	0.21	-	97,97,97,97	0
54	MG	BA	3090	1/1	0.93	0.15	-	45,45,45,45	0
54	MG	DA	3132	1/1	0.97	0.40	-	49,49,49,49	0
54	MG	BA	3170	1/1	0.82	0.57	-	52,52,52,52	0
54	MG	DA	3284	1/1	0.95	0.16	-	61,61,61,61	0
54	MG	BA	3045	1/1	0.93	0.21	-	62,62,62,62	0
54	MG	DA	3416	1/1	0.95	0.13	-	32,32,32,32	0
54	MG	BA	3237	1/1	0.82	0.40	-	56,56,56,56	0
54	MG	AA	1682	1/1	0.73	0.18	-	111,111,111,111	0
54	MG	BA	3014	1/1	0.89	0.19	-	57,57,57,57	0
54	MG	BA	3486	1/1	0.88	0.10	-	48,48,48,48	0
54	MG	CA	1648	1/1	0.79	0.13	-	100,100,100,100	0
54	MG	BA	3575	1/1	0.98	0.07	-	54,54,54,54	0
54	MG	DA	3053	1/1	0.89	0.36	-	54,54,54,54	0
54	MG	BQ	201	1/1	0.93	0.20	-	49,49,49,49	0
54	MG	AA	1699	1/1	0.76	0.16	-	69,69,69,69	0
54	MG	AA	1609	1/1	0.59	0.32	-	91,91,91,91	0
54	MG	BA	3509	1/1	0.78	0.23	-	85,85,85,85	0
54	MG	B1	101	1/1	0.84	0.28	-	50,50,50,50	0
54	MG	BA	3137	1/1	0.91	0.17	-	38,38,38,38	0
54	MG	BA	3372	1/1	0.98	0.13	-	50,50,50,50	0
54	MG	DA	3123	1/1	0.83	0.20	-	56,56,56,56	0
54	MG	DA	3052	1/1	0.94	0.29	-	71,71,71,71	0
54	MG	DA	3112	1/1	0.78	0.34	-	60,60,60,60	0
54	MG	BA	3148	1/1	0.91	0.28	-	54,54,54,54	0
54	MG	DA	3125	1/1	0.89	0.43	-	66,66,66,66	0
54	MG	BA	3159	1/1	0.57	0.22	-	66,66,66,66	0
54	MG	DA	3425	1/1	0.94	0.07	-	60,60,60,60	0
54	MG	BA	3437	1/1	0.95	0.20	-	28,28,28,28	0
54	MG	BA	3522	1/1	0.90	0.56	-	68,68,68,68	0
54	MG	BA	3471	1/1	0.99	0.21	-	38,38,38,38	0
54	MG	BA	3520	1/1	0.93	0.23	-	67,67,67,67	0
54	MG	BA	3460	1/1	0.94	0.09	-	58,58,58,58	0
54	MG	DA	3259	1/1	0.91	0.59	-	64,64,64,64	0
54	MG	BA	3070	1/1	0.91	0.18	-	61,61,61,61	0
54	MG	BA	3474	1/1	0.87	0.20	-	66,66,66,66	0
54	MG	BA	3556	1/1	0.86	0.21	-	58,58,58,58	0
54	MG	CA	1616	1/1	0.92	0.42	-	72,72,72,72	0
54	MG	BA	3395	1/1	0.98	0.14	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3007	1/1	0.93	0.18	-	36,36,36,36	0
54	MG	BA	3301	1/1	0.94	0.05	-	62,62,62,62	0
54	MG	DA	3205	1/1	0.89	0.07	-	82,82,82,82	0
54	MG	BA	3262	1/1	0.97	0.38	-	32,32,32,32	0
54	MG	DA	3305	1/1	0.96	0.09	-	55,55,55,55	0
54	MG	BA	3052	1/1	0.92	0.26	-	61,61,61,61	0
54	MG	BA	3271	1/1	0.92	0.15	-	60,60,60,60	0
54	MG	BA	3493	1/1	0.95	0.19	-	52,52,52,52	0
54	MG	BA	3240	1/1	0.79	0.38	-	64,64,64,64	0
54	MG	BA	3323	1/1	0.99	0.09	-	40,40,40,40	0
54	MG	DA	3268	1/1	0.98	0.16	-	43,43,43,43	0
54	MG	BA	3249	1/1	0.89	0.30	-	70,70,70,70	0
54	MG	BA	3243	1/1	0.57	0.11	-	117,117,117,117	0
54	MG	DA	3113	1/1	0.93	0.37	-	42,42,42,42	0
54	MG	BA	3454	1/1	0.97	0.17	-	34,34,34,34	0
54	MG	DA	3163	1/1	0.95	0.38	-	56,56,56,56	0
54	MG	DA	3054	1/1	0.95	0.72	-	75,75,75,75	0
54	MG	BA	3292	1/1	0.97	0.20	-	44,44,44,44	0
54	MG	BA	3607	1/1	0.95	0.13	-	38,38,38,38	0
54	MG	AA	1622	1/1	0.77	0.72	-	67,67,67,67	0
54	MG	BA	3059	1/1	0.94	0.30	-	49,49,49,49	0
54	MG	DA	3002	1/1	0.92	0.70	-	67,67,67,67	0
54	MG	BA	3111	1/1	0.90	0.30	-	57,57,57,57	0
54	MG	DA	3397	1/1	0.92	0.05	-	65,65,65,65	0
54	MG	DA	3127	1/1	0.84	0.29	-	63,63,63,63	0
54	MG	BA	3010	1/1	0.95	0.20	-	48,48,48,48	0
54	MG	BA	3405	1/1	0.94	0.19	-	38,38,38,38	0
54	MG	DA	3366	1/1	0.97	0.14	-	35,35,35,35	0
54	MG	BA	3329	1/1	0.86	0.17	-	45,45,45,45	0
54	MG	BA	3392	1/1	0.84	0.12	-	55,55,55,55	0
54	MG	BA	3348	1/1	0.98	0.22	-	37,37,37,37	0
54	MG	AA	1673	1/1	0.80	0.30	-	67,67,67,67	0
54	MG	AA	1700	1/1	0.82	0.34	-	114,114,114,114	0
54	MG	BA	3104	1/1	0.98	0.21	-	48,48,48,48	0
54	MG	BA	3201	1/1	0.80	0.58	-	79,79,79,79	0
54	MG	BA	3332	1/1	0.88	0.28	-	60,60,60,60	0
54	MG	BA	3016	1/1	0.89	0.43	-	57,57,57,57	0
54	MG	BA	3173	1/1	0.89	0.29	-	65,65,65,65	0
54	MG	BA	3207	1/1	0.80	0.16	-	59,59,59,59	0
54	MG	DA	3181	1/1	0.86	0.67	-	51,51,51,51	0
54	MG	DA	3328	1/1	0.91	0.09	-	34,34,34,34	0
54	MG	BA	3283	1/1	0.86	0.55	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	DA	3030	1/1	0.85	0.17	-	52,52,52,52	0
54	MG	BA	3281	1/1	0.95	0.28	-	56,56,56,56	0
54	MG	BA	3132	1/1	0.93	0.31	-	31,31,31,31	0
54	MG	BA	3457	1/1	0.86	0.15	-	91,91,91,91	0
54	MG	CA	1624	1/1	0.75	0.42	-	82,82,82,82	0
54	MG	DA	3162	1/1	0.78	0.38	-	55,55,55,55	0
54	MG	DA	3319	1/1	0.97	0.10	-	59,59,59,59	0
54	MG	BA	3288	1/1	0.96	0.51	-	33,33,33,33	0
54	MG	BA	3555	1/1	0.91	0.31	-	49,49,49,49	0
54	MG	CA	1663	1/1	0.89	0.18	-	91,91,91,91	0
54	MG	BA	3122	1/1	0.83	0.33	-	56,56,56,56	0
54	MG	DA	3199	1/1	0.90	0.06	-	74,74,74,74	0
54	MG	BA	3350	1/1	0.93	0.18	-	60,60,60,60	0
54	MG	BA	3498	1/1	0.91	0.14	-	69,69,69,69	0
54	MG	BA	3580	1/1	0.94	0.08	-	61,61,61,61	0
54	MG	DA	3282	1/1	0.94	0.08	-	42,42,42,42	0
54	MG	BA	3130	1/1	0.89	0.38	-	32,32,32,32	0
54	MG	DA	3043	1/1	0.86	0.18	-	63,63,63,63	0
54	MG	AA	1618	1/1	0.91	0.12	-	69,69,69,69	0
54	MG	DB	204	1/1	0.98	0.14	-	74,74,74,74	0
54	MG	AA	1666	1/1	0.91	0.53	-	62,62,62,62	0
54	MG	B0	101	1/1	0.77	0.16	-	75,75,75,75	0
54	MG	BA	3017	1/1	0.93	0.14	-	47,47,47,47	0
54	MG	BA	3091	1/1	0.91	0.35	-	47,47,47,47	0
54	MG	DA	3398	1/1	0.98	0.12	-	52,52,52,52	0
54	MG	BA	3559	1/1	0.84	0.27	-	39,39,39,39	0
54	MG	BA	3106	1/1	0.87	0.41	-	48,48,48,48	0
54	MG	BB	211	1/1	0.96	0.09	-	51,51,51,51	0
54	MG	DA	3036	1/1	0.86	0.18	-	65,65,65,65	0
54	MG	BA	3169	1/1	0.73	0.48	-	60,60,60,60	0
54	MG	CA	1646	1/1	0.89	0.49	-	92,92,92,92	0
54	MG	DA	3365	1/1	0.95	0.08	-	50,50,50,50	0
54	MG	DA	3209	1/1	0.92	0.24	-	79,79,79,79	0
54	MG	BA	3153	1/1	0.89	0.32	-	53,53,53,53	0
54	MG	AA	1684	1/1	0.96	0.05	-	76,76,76,76	0
54	MG	AA	1602	1/1	0.86	0.28	-	111,111,111,111	0
54	MG	DA	3029	1/1	0.94	0.15	-	72,72,72,72	0
54	MG	BA	3565	1/1	0.75	0.28	-	90,90,90,90	0
54	MG	BA	3043	1/1	0.94	0.34	-	54,54,54,54	0
54	MG	BA	3258	1/1	0.95	0.44	-	56,56,56,56	0
54	MG	BA	3086	1/1	0.92	0.26	-	57,57,57,57	0
54	MG	BA	3083	1/1	0.95	0.47	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	BA	3497	1/1	0.94	0.16	-	55,55,55,55	0
54	MG	DA	3017	1/1	0.92	0.29	-	61,61,61,61	0
54	MG	DA	3243	1/1	0.96	0.36	-	53,53,53,53	0
54	MG	BA	3366	1/1	0.99	0.08	-	50,50,50,50	0
54	MG	DA	3178	1/1	0.96	0.47	-	58,58,58,58	0
54	MG	DA	3421	1/1	0.86	0.09	-	69,69,69,69	0
54	MG	BA	3175	1/1	0.90	0.35	-	70,70,70,70	0
54	MG	BA	3411	1/1	0.98	0.28	-	43,43,43,43	0
54	MG	AA	1686	1/1	0.91	0.19	-	115,115,115,115	0
54	MG	BA	3276	1/1	0.89	0.62	-	56,56,56,56	0
54	MG	BA	3226	1/1	0.88	0.31	-	62,62,62,62	0
54	MG	BA	3256	1/1	0.96	0.68	-	69,69,69,69	0
54	MG	CA	1633	1/1	0.96	0.25	-	71,71,71,71	0
54	MG	BA	3583	1/1	0.95	0.05	-	50,50,50,50	0
54	MG	BA	3546	1/1	0.90	0.09	-	57,57,57,57	0
54	MG	BA	3209	1/1	0.93	0.37	-	67,67,67,67	0
54	MG	DB	205	1/1	0.96	0.15	-	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.